



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:35 am GMT

PDB ID : 5J91  
Title : Structure of the Wild-type 70S E coli ribosome bound to Tigecycline  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-08  
Resolution : 2.96 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

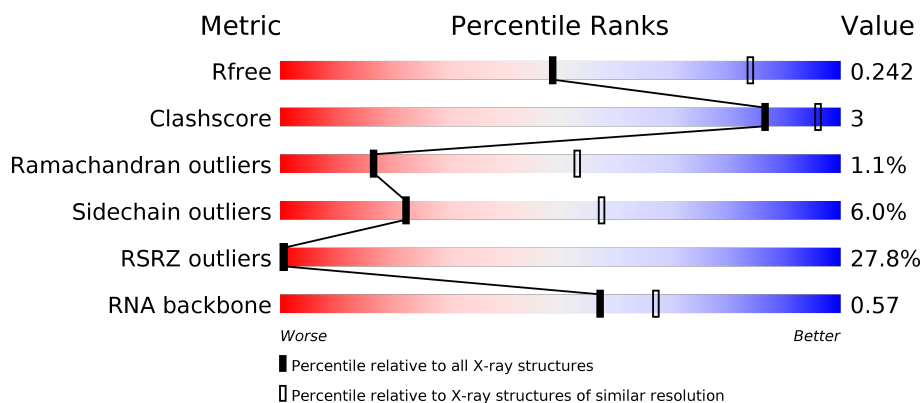
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 2395 (3.00-2.92)                                      |
| Clashscore            | 112137                      | 2773 (3.00-2.92)                                      |
| Ramachandran outliers | 110173                      | 2680 (3.00-2.92)                                      |
| Sidechain outliers    | 110143                      | 2683 (3.00-2.92)                                      |
| RSRZ outliers         | 101464                      | 2421 (3.00-2.92)                                      |
| RNA backbone          | 2435                        | 1008 (3.30-2.62)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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   | AA    | 1534   |                  |
| 1   | BA    | 1534   |                  |
| 2   | AB    | 224    |                  |
| 2   | BB    | 224    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AC    | 206    |                  |
| 3   | BC    | 206    |                  |
| 4   | AD    | 205    |                  |
| 4   | BD    | 205    |                  |
| 5   | AE    | 155    |                  |
| 5   | BE    | 155    |                  |
| 6   | AF    | 106    |                  |
| 6   | BF    | 106    |                  |
| 7   | AG    | 151    |                  |
| 7   | BG    | 151    |                  |
| 8   | AH    | 129    |                  |
| 8   | BH    | 129    |                  |
| 9   | AI    | 127    |                  |
| 9   | BI    | 127    |                  |
| 10  | AJ    | 99     |                  |
| 10  | BJ    | 99     |                  |
| 11  | AK    | 117    |                  |
| 11  | BK    | 117    |                  |
| 12  | AL    | 123    |                  |
| 12  | BL    | 123    |                  |
| 13  | AM    | 114    |                  |
| 13  | BM    | 114    |                  |
| 14  | AN    | 100    |                  |
| 14  | BN    | 100    |                  |
| 15  | AO    | 88     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | BO    | 88     |                  |
| 16  | AP    | 82     |                  |
| 16  | BP    | 82     |                  |
| 17  | AQ    | 80     |                  |
| 17  | BQ    | 80     |                  |
| 18  | AR    | 55     |                  |
| 18  | BR    | 55     |                  |
| 19  | AS    | 79     |                  |
| 19  | BS    | 79     |                  |
| 20  | AT    | 86     |                  |
| 20  | BT    | 86     |                  |
| 21  | AU    | 56     |                  |
| 21  | BU    | 56     |                  |
| 22  | C1    | 56     |                  |
| 22  | D1    | 56     |                  |
| 23  | C2    | 51     |                  |
| 23  | D2    | 51     |                  |
| 24  | C3    | 46     |                  |
| 24  | D3    | 46     |                  |
| 25  | C4    | 64     |                  |
| 25  | D4    | 64     |                  |
| 26  | C5    | 38     |                  |
| 26  | D5    | 38     |                  |
| 27  | C0    | 58     |                  |
| 27  | D0    | 58     |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 28  | CB    | 120    | <div> <div>38%</div> <div>86%</div> <div>11%</div> <div>..</div> </div> |
| 28  | DB    | 120    | <div> <div>91%</div> <div>8%</div> <div>.</div> </div>                  |
| 29  | CC    | 272    | <div> <div>32%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>  |
| 29  | DC    | 272    | <div> <div>2%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>    |
| 30  | CD    | 209    | <div> <div>62%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>  |
| 31  | CA    | 2904   | <div> <div>35%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>  |
| 32  | DD    | 209    | <div> <div>89%</div> <div>11%</div> </div>                              |
| 33  | CE    | 201    | <div> <div>70%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>  |
| 33  | DE    | 201    | <div> <div>%</div> <div>91%</div> <div>9%</div> </div>                  |
| 34  | CF    | 178    | <div> <div>86%</div> <div>80%</div> <div>17%</div> <div>..</div> </div> |
| 34  | DF    | 178    | <div> <div>9%</div> <div>82%</div> <div>17%</div> <div>..</div> </div>  |
| 35  | CG    | 176    | <div> <div>82%</div> <div>88%</div> <div>12%</div> </div>               |
| 35  | DG    | 176    | <div> <div>5%</div> <div>88%</div> <div>12%</div> </div>                |
| 36  | CH    | 149    | <div> <div>54%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>  |
| 36  | DH    | 149    | <div> <div>42%</div> <div>83%</div> <div>17%</div> <div>.</div> </div>  |
| 37  | CJ    | 134    | <div> <div>95%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>   |
| 37  | DJ    | 134    | <div> <div>82%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>  |
| 38  | CK    | 142    | <div> <div>50%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>   |
| 38  | DK    | 142    | <div> <div>94%</div> <div>6%</div> <div>.</div> </div>                  |
| 39  | CL    | 123    | <div> <div>33%</div> <div>88%</div> <div>10%</div> <div>..</div> </div> |
| 39  | DL    | 123    | <div> <div>90%</div> <div>8%</div> <div>.</div> </div>                  |
| 40  | CM    | 144    | <div> <div>81%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>  |
| 40  | DM    | 144    | <div> <div>2%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>   |
| 41  | CN    | 136    | <div> <div>26%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>   |
| 41  | DN    | 136    | <div> <div>92%</div> <div>7%</div> <div>.</div> </div>                  |


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 42  | CO    | 125    |                  |
| 42  | DO    | 125    |                  |
| 43  | CP    | 117    |                  |
| 43  | DP    | 117    |                  |
| 44  | CQ    | 114    |                  |
| 44  | DQ    | 114    |                  |
| 45  | CR    | 117    |                  |
| 45  | DR    | 117    |                  |
| 46  | CS    | 103    |                  |
| 46  | DS    | 103    |                  |
| 47  | CT    | 110    |                  |
| 47  | DT    | 110    |                  |
| 48  | CU    | 93     |                  |
| 48  | DU    | 93     |                  |
| 49  | CV    | 103    |                  |
| 49  | DV    | 103    |                  |
| 50  | CW    | 94     |                  |
| 50  | DW    | 94     |                  |
| 51  | CX    | 76     |                  |
| 51  | DX    | 76     |                  |
| 52  | CY    | 77     |                  |
| 52  | DY    | 77     |                  |
| 53  | CZ    | 62     |                  |
| 53  | DZ    | 62     |                  |
| 54  | DI    | 135    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 55  | DA    | 2904   |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | AA    | 1607 | -         | -        | -       | X                |
| 56  | MG   | AA    | 1612 | -         | -        | -       | X                |
| 56  | MG   | AA    | 1633 | -         | -        | -       | X                |
| 56  | MG   | AA    | 1642 | -         | -        | -       | X                |
| 56  | MG   | AA    | 1657 | -         | -        | -       | X                |
| 56  | MG   | AA    | 1661 | -         | -        | -       | X                |
| 56  | MG   | BA    | 1612 | -         | -        | -       | X                |
| 56  | MG   | BA    | 1626 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3003 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3022 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3026 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3032 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3037 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3100 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3105 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3110 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3131 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3133 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3137 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3147 | -         | -        | -       | X                |
| 56  | MG   | CA    | 3151 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3038 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3123 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3125 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3127 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3128 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3133 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3148 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3163 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3172 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3182 | -         | -        | -       | X                |
| 57  | PG4  | AA    | 1670 | -         | -        | -       | X                |
| 57  | PG4  | BA    | 1642 | -         | -        | -       | X                |
| 57  | PG4  | DA    | 3193 | -         | -        | -       | X                |
| 57  | PG4  | DA    | 3215 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | PG4  | DS    | 202  | -         | -        | -       | X                |
| 58  | MPD  | AA    | 1671 | -         | -        | -       | X                |
| 58  | MPD  | AA    | 1676 | -         | -        | -       | X                |
| 58  | MPD  | DA    | 3192 | -         | -        | -       | X                |
| 58  | MPD  | DA    | 3203 | -         | -        | -       | X                |
| 58  | MPD  | DA    | 3206 | -         | -        | -       | X                |
| 58  | MPD  | DE    | 301  | -         | -        | -       | X                |
| 58  | MPD  | DE    | 302  | -         | -        | -       | X                |
| 59  | PUT  | AA    | 1672 | -         | -        | -       | X                |
| 59  | PUT  | AA    | 1673 | -         | -        | -       | X                |
| 59  | PUT  | AA    | 1674 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3189 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3195 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3204 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3211 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3212 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3218 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3220 | -         | -        | -       | X                |
| 59  | PUT  | DA    | 3221 | -         | -        | -       | X                |
| 62  | PEG  | AL    | 201  | -         | -        | -       | X                |
| 62  | PEG  | D1    | 103  | -         | -        | -       | X                |
| 62  | PEG  | D3    | 102  | -         | -        | -       | X                |
| 62  | PEG  | DA    | 3200 | -         | -        | -       | X                |
| 62  | PEG  | DA    | 3217 | -         | -        | -       | X                |
| 62  | PEG  | DL    | 201  | -         | -        | -       | X                |
| 62  | PEG  | DQ    | 201  | -         | -        | -       | X                |
| 63  | EDO  | D1    | 101  | -         | -        | -       | X                |
| 63  | EDO  | DA    | 3001 | -         | -        | -       | X                |
| 63  | EDO  | DA    | 3197 | -         | -        | -       | X                |
| 63  | EDO  | DA    | 3198 | -         | -        | -       | X                |
| 64  | PGE  | D1    | 102  | -         | -        | -       | X                |
| 64  | PGE  | D3    | 101  | -         | -        | -       | X                |
| 64  | PGE  | DA    | 3213 | -         | -        | -       | X                |
| 64  | PGE  | DA    | 3224 | -         | -        | -       | X                |
| 64  | PGE  | DD    | 301  | -         | -        | -       | X                |
| 64  | PGE  | DU    | 101  | -         | -        | -       | X                |
| 65  | SPD  | DA    | 3183 | -         | -        | -       | X                |
| 65  | SPD  | DA    | 3187 | -         | -        | -       | X                |
| 65  | SPD  | DA    | 3205 | -         | -        | -       | X                |
| 65  | SPD  | DA    | 3223 | -         | -        | -       | X                |
| 66  | 1PE  | DA    | 3185 | -         | -        | -       | X                |
| 66  | 1PE  | DA    | 3202 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 67  | ACY  | DA    | 3201 | -         | -        | -       | X                |
| 68  | GUN  | DA    | 3210 | -         | -        | -       | X                |

## 2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295202 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   | AA    | 1534     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32930 | 14694 | 6041 | 10661 | 1534 |         |         |       |
| 1   | BA    | 1533     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32908 | 14684 | 6036 | 10655 | 1533 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1753  | 1109 | 315 | 321 | 8 |         |         |       |
| 2   | BB    | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1753  | 1109 | 315 | 321 | 8 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |
| 3   | BC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 4   | BD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1144  | 711 | 216 | 211 | 6 |         |         |       |
| 5   | BE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 862   | 545 | 156 | 154 | 7 |         |         |       |
| 6   | BF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |         |       |
| 7   | BG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |
| 8   | BH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |
| 9   | BI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 796   | 498 | 152 | 145 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | BJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |
| 11  | BK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |         |       |
| 12  | BL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |         |       |
| 13  | BM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AN    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |         |       |
| 14  | BN    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |
| 15  | BO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |
| 16  | BP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |         |       |
| 17  | BQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18  | AR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |         |         |       |
| 18  | BR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |         |       |
| 19  | BS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |         |       |
| 20  | BT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21  | AU    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 465   | 290 | 96 | 78 | 1 |         |         |       |
| 21  | BU    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 465   | 290 | 96 | 78 | 1 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 22  | C1    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |
| 22  | D1    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 23  | C2    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |         |       |
| 23  | D2    | 51       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 414   | 266 | 76 | 72 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 24  | C3    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |
| 24  | D3    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 25  | C4    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 25  | D4    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | C5    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | D5    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | C0    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |
| 27  | D0    | 58       | Total | C   | N  | O  | S | 0       | 2       | 0     |
|     |       |          | 463   | 290 | 90 | 81 | 2 |         |         |       |

- Molecule 28 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 28  | CB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2529  | 1126 | 464 | 821 | 118 |         |         |       |
| 28  | DB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2569  | 1144 | 468 | 837 | 120 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | CC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |         |       |
| 29  | DC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | CD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

- Molecule 31 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 31  | CA    | 2898     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62229 | 27768 | 11448 | 20115 | 2898 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | DD    | 209      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1576  | 986 | 290 | 296 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | CE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |
| 33  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | CF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |         |       |
| 34  | DF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | CG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 35  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | CH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |
| 36  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | CJ    | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 619 | 169 | 185 | 6 |         |         |       |
| 37  | DJ    | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 619 | 169 | 185 | 6 |         |         |       |



- Molecule 38 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | CK    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |
| 38  | DK    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | CL    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |         |       |
| 39  | DL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | CM    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |         |       |
| 40  | DM    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | CN    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1075  | 686 | 205 | 178 | 6 |         |         |       |
| 41  | DN    | 136      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1092  | 696 | 211 | 179 | 6 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CN    | 81      | 4D4      | ARG    | conflict | UNP P0ADY7 |
| DN    | 81      | 4D4      | ARG    | conflict | UNP P0ADY7 |

- Molecule 42 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | CO    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | DO    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 993   | 613 | 202 | 173 | 5 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | CP    | 116      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |   |         |         |       |
| 43  | DP    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 557 | 179 | 163 | 1 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | CQ    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 44  | DQ    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 45  | CR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |         |       |
| 45  | DR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | CS    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |
| 46  | DS    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | CT    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |
| 47  | DT    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | CU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |
| 48  | DU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 49  | CV    | 102      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |         |       |
| 49  | DV    | 102      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | CW    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |
| 50  | DW    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | CX    | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 569   | 353 | 113 | 102 | 1 |         |         |       |
| 51  | DX    | 76       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 591   | 365 | 121 | 104 | 1 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | CY    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |
| 52  | DY    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | CZ    | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |         |       |
| 53  | DZ    | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | DI    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1023  | 649 | 179 | 192 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DI    | 85      | VAL      | SER    | conflict | UNP P0A7J3 |
| DI    | 86      | THR      | MET    | conflict | UNP P0A7J3 |

- Molecule 55 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 55  | DA    | 2897     | Total | C     | N     | O     | P    | 0       | 11      | 0     |
|     |       |          | 62423 | 27855 | 11485 | 20176 | 2907 |         |         |       |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

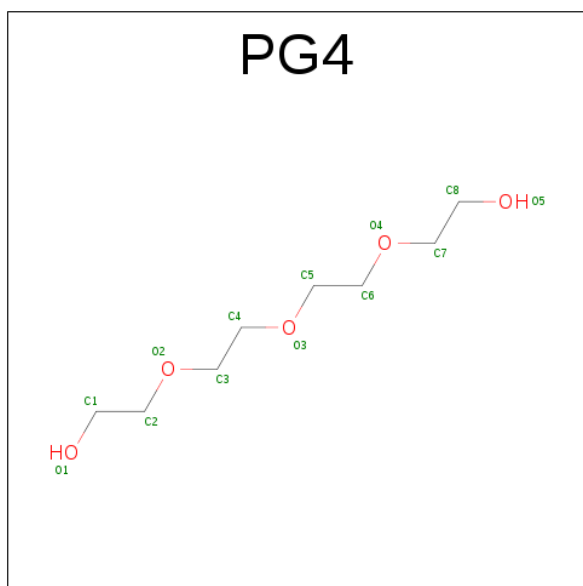
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56  | BA    | 43       | Total | Mg  | 0       | 0       |
|     |       |          | 43    | 43  |         |         |
| 56  | CA    | 156      | Total | Mg  | 0       | 0       |
|     |       |          | 156   | 156 |         |         |
| 56  | CB    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 56  | DM    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | DR    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 56  | AA    | 71       | Total | Mg  | 0       | 0       |
|     |       |          | 71    | 71  |         |         |
| 56  | DA    | 182      | Total | Mg  | 0       | 0       |
|     |       |          | 182   | 182 |         |         |
| 56  | DB    | 9        | Total | Mg  | 0       | 0       |
|     |       |          | 9     | 9   |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | DD    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



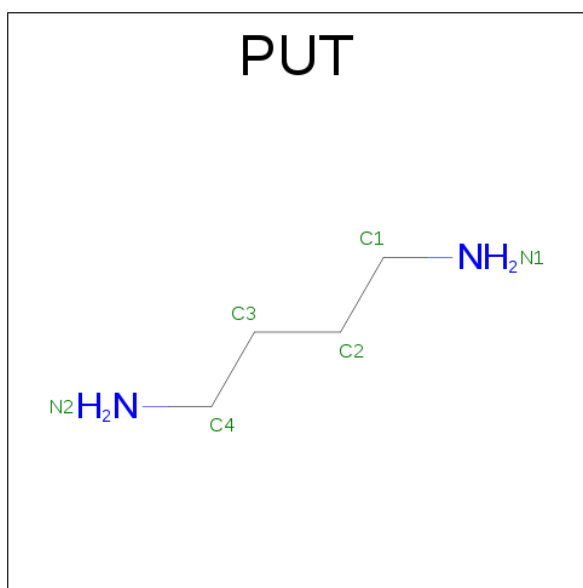
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 57  | AA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 57  | BA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 57  | DQ    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 57  | DR    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 57  | DS    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 57  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 57  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 58  | AA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | AA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DE    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DE    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DK    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DN    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DS    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DT    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DT    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 58  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



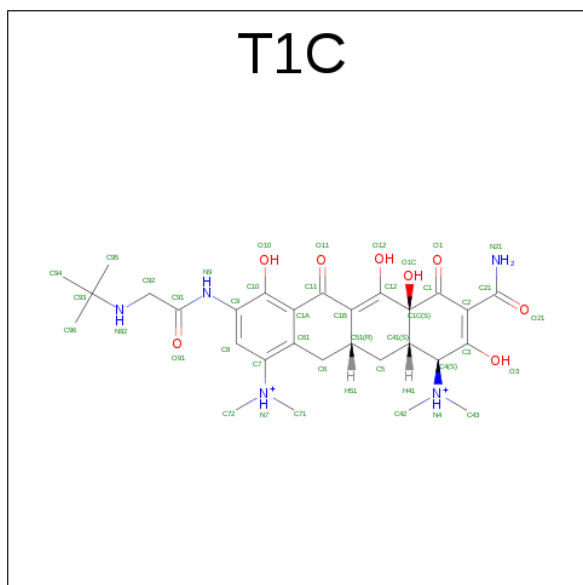
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 59  | AA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | AA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | AA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | AA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 59  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |

- Molecule 60 is TIGECYCLINE (three-letter code: T1C) (formula: C<sub>29</sub>H<sub>41</sub>N<sub>5</sub>O<sub>8</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 60  | AA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |         |
| 60  | BA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 29 | 5 | 8 |         |         |

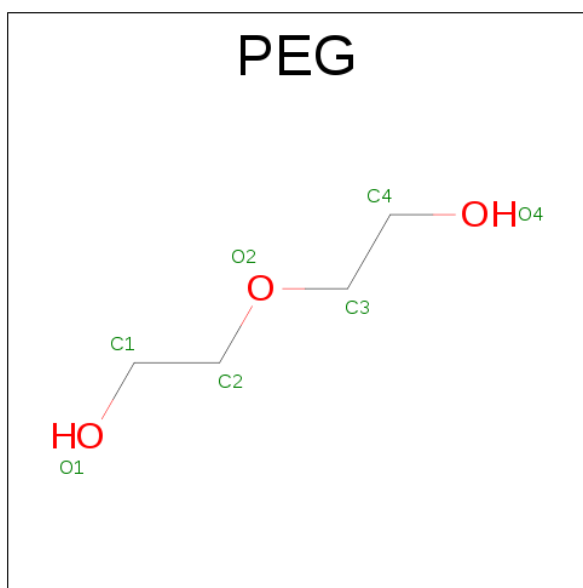
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 61  | C5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | AB    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | D5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 62 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

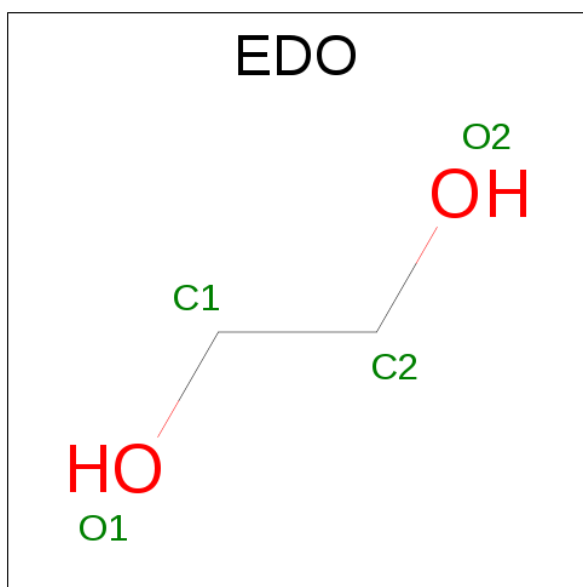


C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



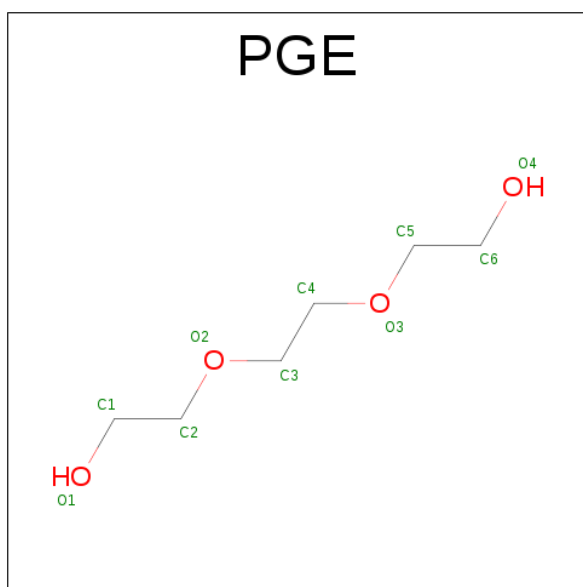
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 62  | AL    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | D1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | D3    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DL    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DP    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DQ    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 62  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |

- Molecule 63 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



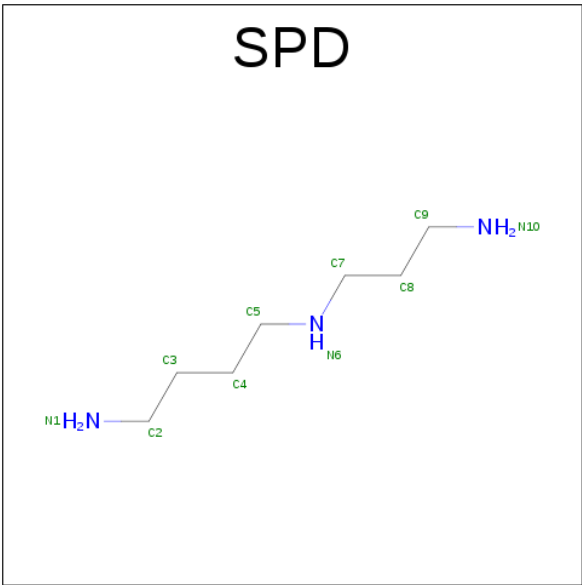
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 63  | D1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DB    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DB    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 63  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



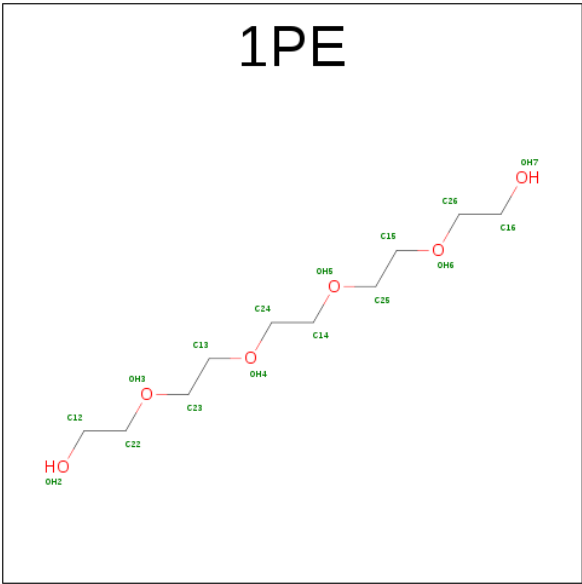
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 64  | D1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | D3    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | DD    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | DS    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | DU    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 64  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



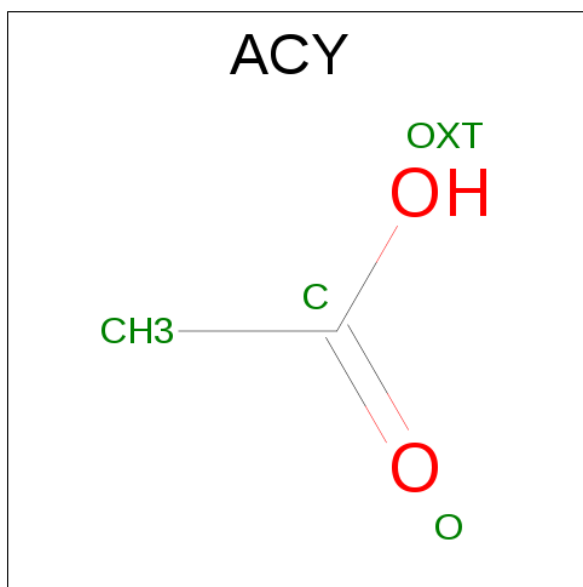
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 65  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 65  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 65  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 65  | DA    | 1        | Total | C | N | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |

- Molecule 66 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



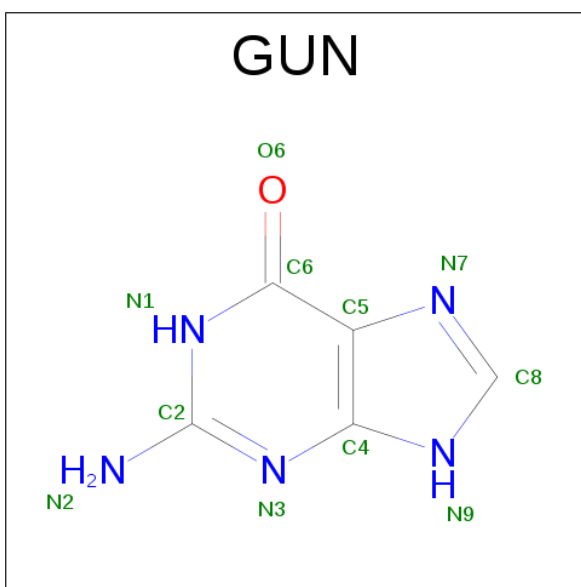
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 66  | DA    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 66  | DA    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |

- Molecule 67 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



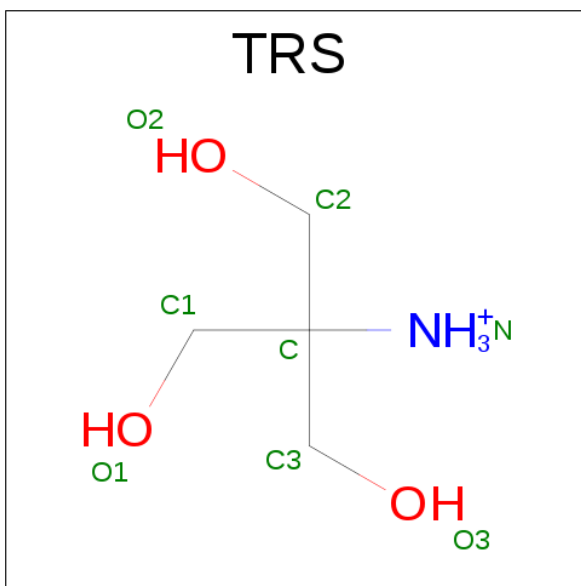
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 67  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 67  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 67  | DA    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 68 is GUANINE (three-letter code: GUN) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 68  | DA    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 5 | 5 | 1 |         |         |

- Molecule 69 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 69  | DA    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |

- Molecule 70 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 70  | AA    | 507      | Total O<br>507 507 | 0       | 0       |
| 70  | AC    | 4        | Total O<br>4 4     | 0       | 0       |
| 70  | AD    | 2        | Total O<br>2 2     | 0       | 0       |
| 70  | AE    | 4        | Total O<br>4 4     | 0       | 0       |
| 70  | AF    | 1        | Total O<br>1 1     | 0       | 0       |
| 70  | AG    | 1        | Total O<br>1 1     | 0       | 0       |
| 70  | AH    | 1        | Total O<br>1 1     | 0       | 0       |
| 70  | AJ    | 2        | Total O<br>2 2     | 0       | 0       |
| 70  | AK    | 5        | Total O<br>5 5     | 0       | 0       |
| 70  | AL    | 8        | Total O<br>8 8     | 0       | 0       |
| 70  | AM    | 4        | Total O<br>4 4     | 0       | 0       |
| 70  | AN    | 5        | Total O<br>5 5     | 0       | 0       |
| 70  | AO    | 2        | Total O<br>2 2     | 0       | 0       |
| 70  | AP    | 2        | Total O<br>2 2     | 0       | 0       |
| 70  | AR    | 1        | Total O<br>1 1     | 0       | 0       |
| 70  | AS    | 1        | Total O<br>1 1     | 0       | 0       |
| 70  | AT    | 2        | Total O<br>2 2     | 0       | 0       |
| 70  | AU    | 3        | Total O<br>3 3     | 0       | 0       |
| 70  | C3    | 3        | Total O<br>3 3     | 0       | 0       |
| 70  | C4    | 1        | Total O<br>1 1     | 0       | 0       |
| 70  | BA    | 287      | Total O<br>287 287 | 0       | 0       |
| 70  | BD    | 13       | Total O<br>13 13   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 70  | BE    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | BF    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | BK    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | BL    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 70  | BN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 70  | BO    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | BP    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 70  | BR    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | BT    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 70  | BU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 70  | D1    | 42       | Total<br>42  | O<br>42  | 0       | 0       |
| 70  | D2    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 70  | D3    | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 70  | D4    | 32       | Total<br>32  | O<br>32  | 0       | 0       |
| 70  | D5    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 70  | D0    | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 70  | CB    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 70  | CC    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 70  | CD    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 70  | CA    | 694      | Total<br>694 | O<br>694 | 0       | 0       |
| 70  | DC    | 102      | Total<br>102 | O<br>102 | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 70  | DD    | 105      | Total<br>105 | O<br>105 | 0       | 0       |
| 70  | CE    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 70  | CL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | CM    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 70  | CO    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | CU    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 70  | CV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | CW    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | CY    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 70  | DE    | 63       | Total<br>63  | O<br>63  | 0       | 0       |
| 70  | DF    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 70  | DG    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 70  | DH    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 70  | DK    | 58       | Total<br>58  | O<br>58  | 0       | 0       |
| 70  | DL    | 51       | Total<br>51  | O<br>51  | 0       | 0       |
| 70  | DM    | 60       | Total<br>60  | O<br>60  | 0       | 0       |
| 70  | DN    | 71       | Total<br>71  | O<br>71  | 0       | 0       |
| 70  | DO    | 44       | Total<br>44  | O<br>44  | 0       | 0       |
| 70  | DP    | 35       | Total<br>35  | O<br>35  | 0       | 0       |
| 70  | DQ    | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 70  | DR    | 64       | Total<br>64  | O<br>64  | 0       | 0       |

*Continued on next page...*

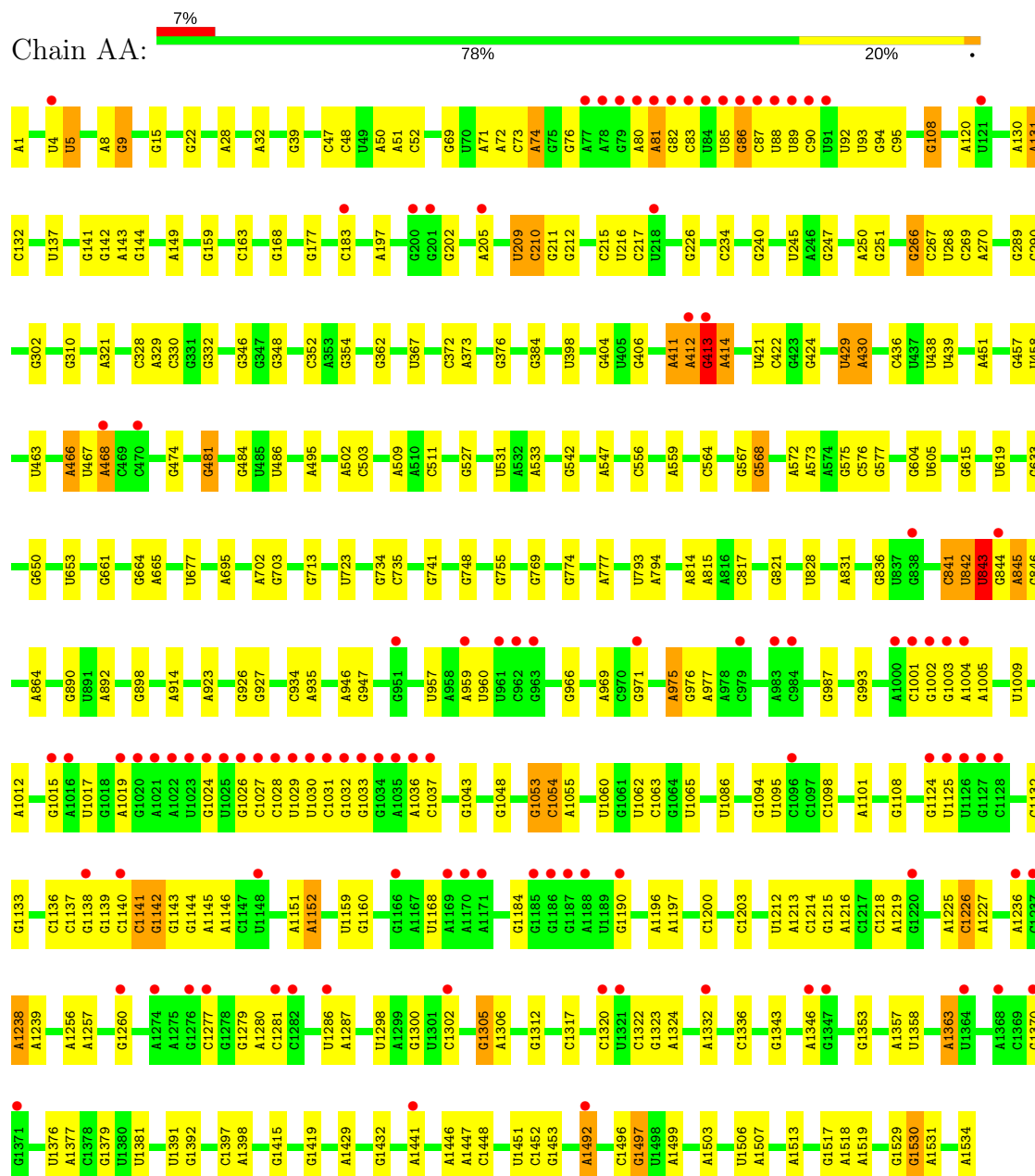
*Continued from previous page...*

| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 70  | DS    | 51       | Total<br>51   | O<br>51   | 0       | 0       |
| 70  | DT    | 70       | Total<br>70   | O<br>70   | 0       | 0       |
| 70  | DU    | 17       | Total<br>17   | O<br>17   | 0       | 0       |
| 70  | DV    | 19       | Total<br>19   | O<br>19   | 0       | 0       |
| 70  | DW    | 31       | Total<br>31   | O<br>31   | 0       | 0       |
| 70  | DX    | 30       | Total<br>30   | O<br>30   | 0       | 0       |
| 70  | DY    | 9        | Total<br>9    | O<br>9    | 0       | 0       |
| 70  | DZ    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 70  | DB    | 213      | Total<br>213  | O<br>213  | 0       | 0       |
| 70  | DA    | 4836     | Total<br>4836 | O<br>4836 | 0       | 0       |

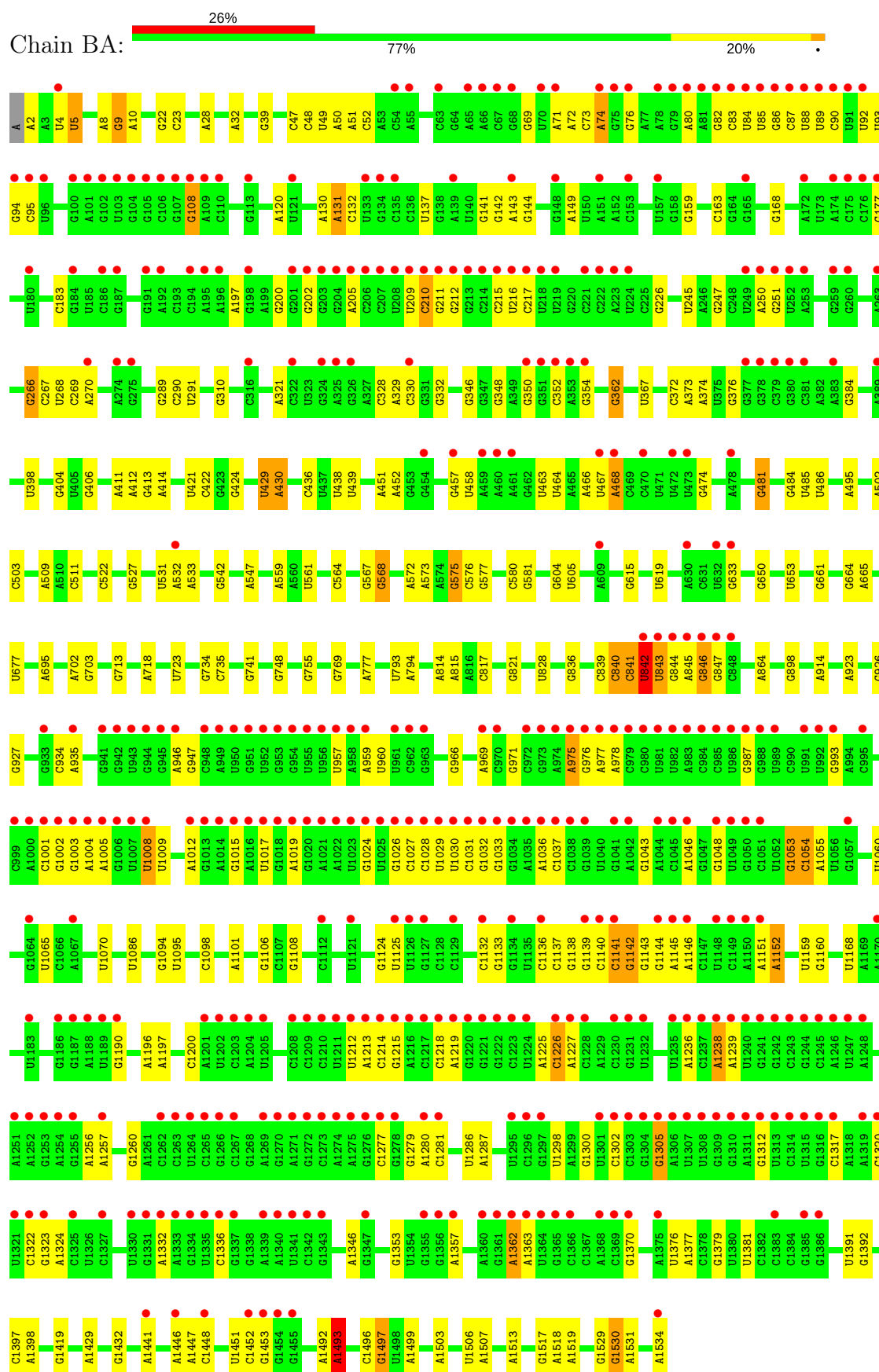
### 3 Residue-property plots

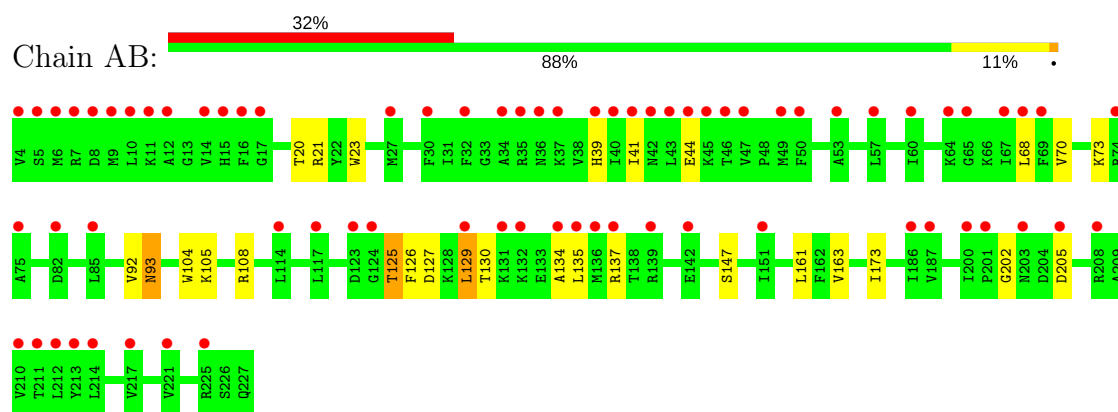
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S rRNA

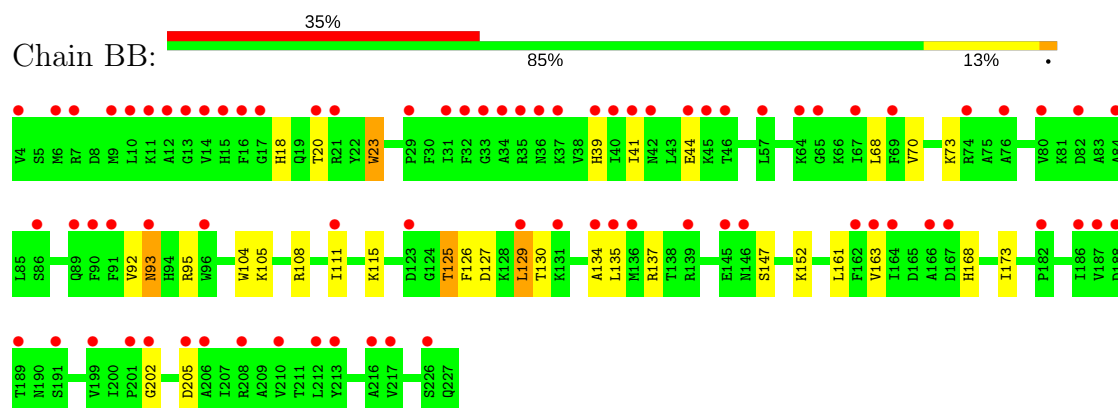


#### • Molecule 1: 16S rRNA

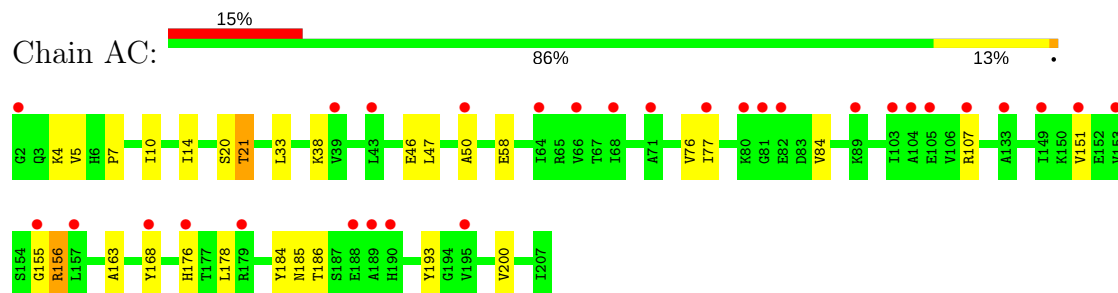




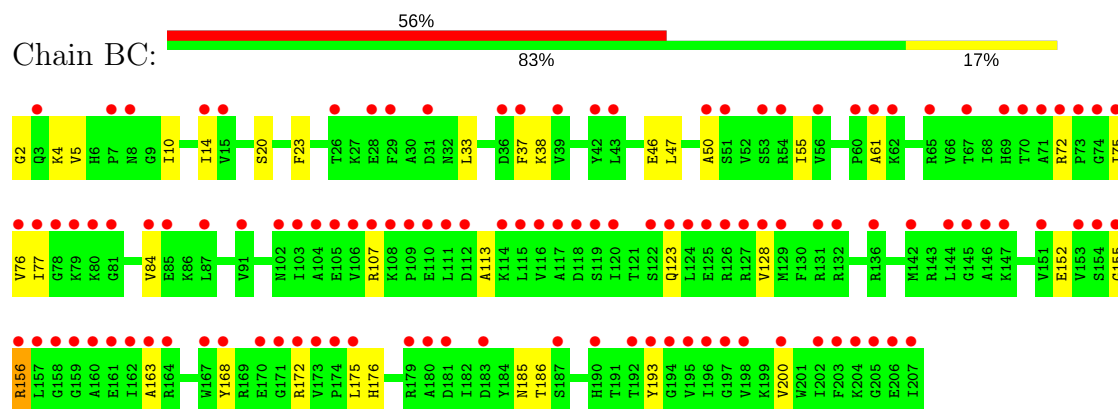
• Molecule 2: 30S ribosomal protein S2



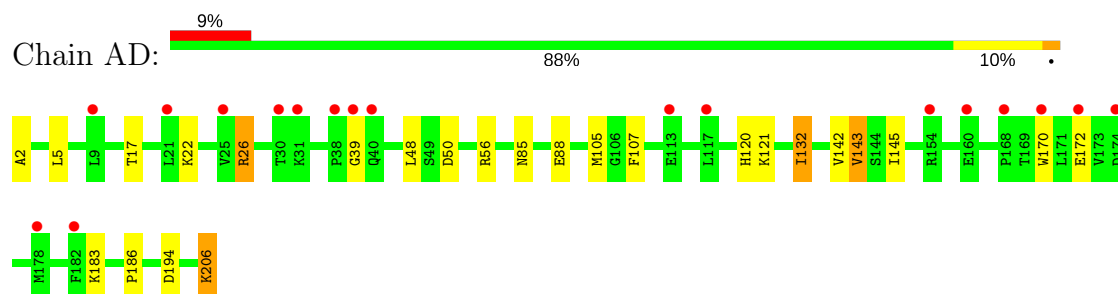
• Molecule 3: 30S ribosomal protein S3



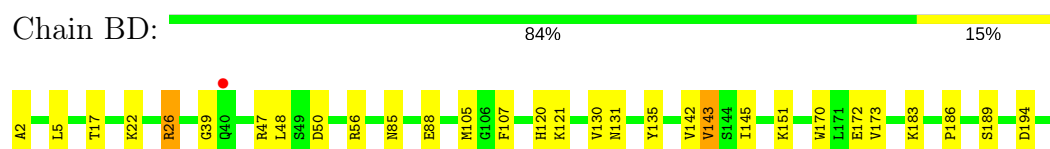
• Molecule 3: 30S ribosomal protein S3



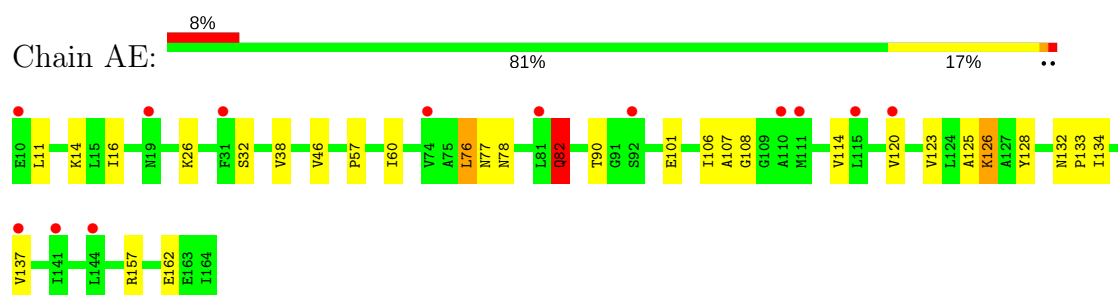
- Molecule 4: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S4



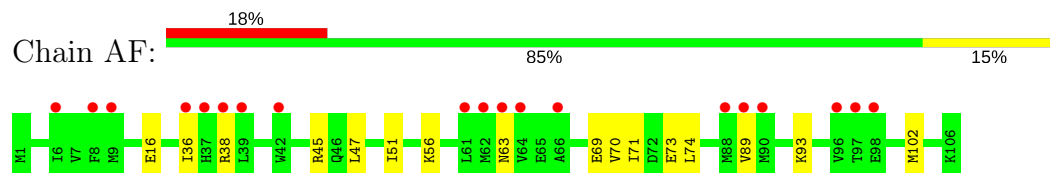
- Molecule 5: 30S ribosomal protein S5



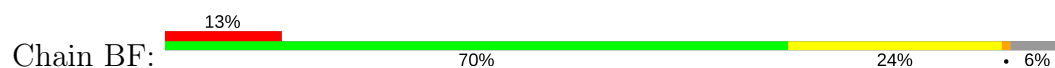
- Molecule 5: 30S ribosomal protein S5

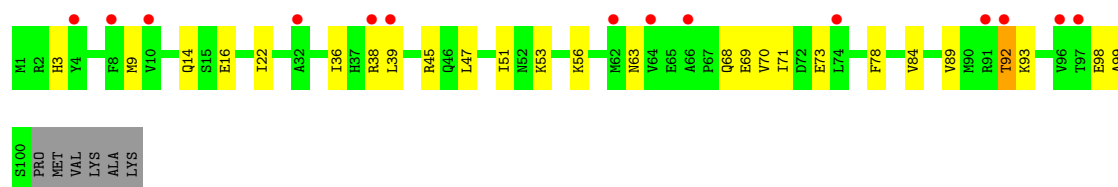


- Molecule 6: 30S ribosomal protein S6

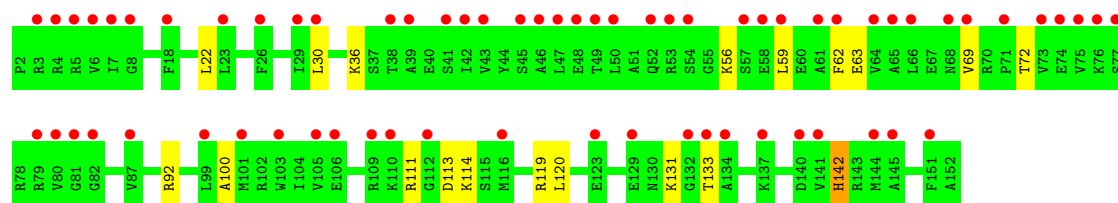
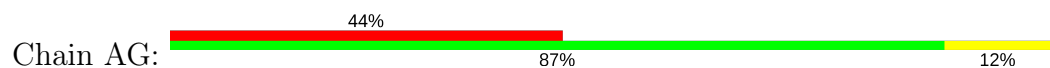


- Molecule 6: 30S ribosomal protein S6

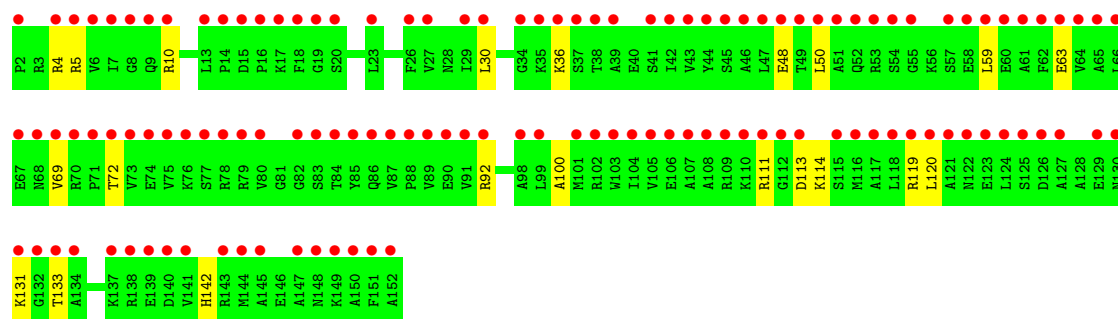
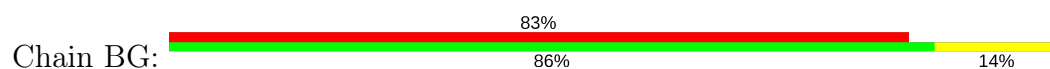




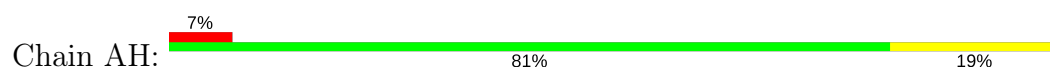
• Molecule 7: 30S ribosomal protein S7



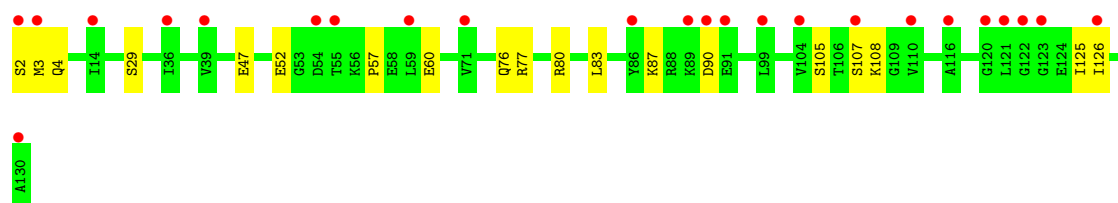
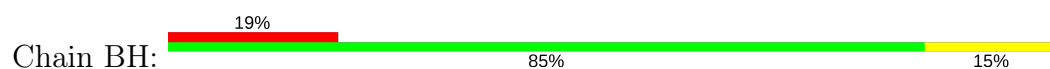
• Molecule 7: 30S ribosomal protein S7



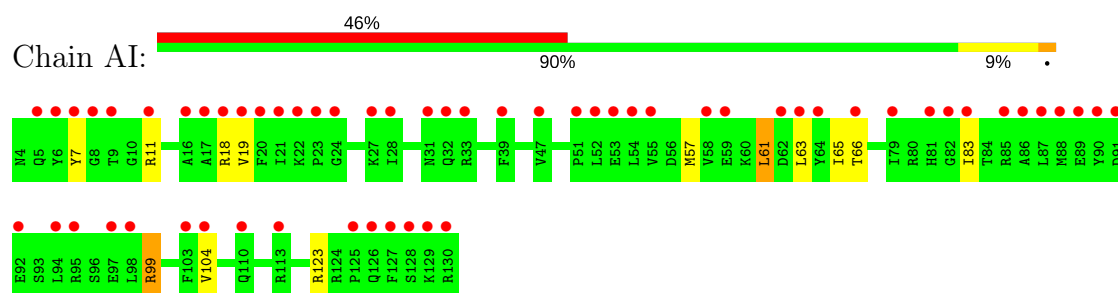
• Molecule 8: 30S ribosomal protein S8



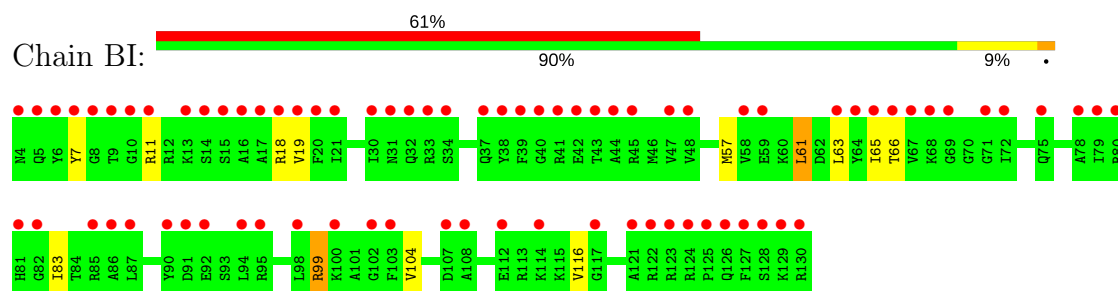
• Molecule 8: 30S ribosomal protein S8



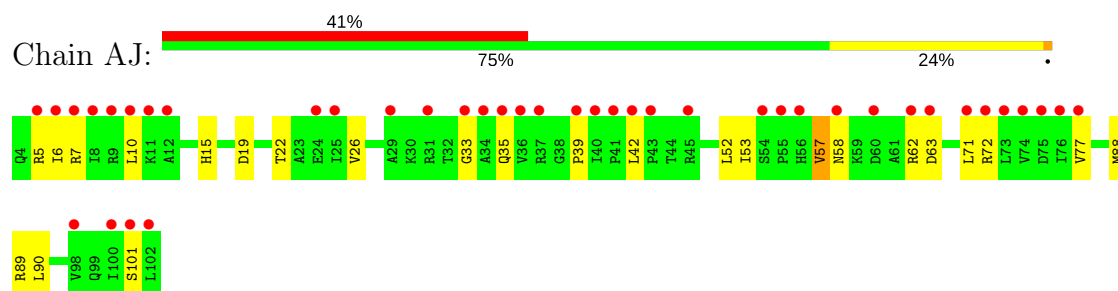
• Molecule 9: 30S ribosomal protein S9



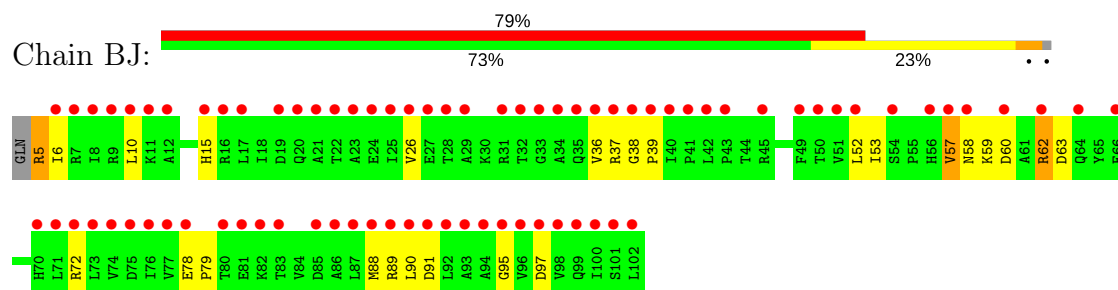
- Molecule 9: 30S ribosomal protein S9



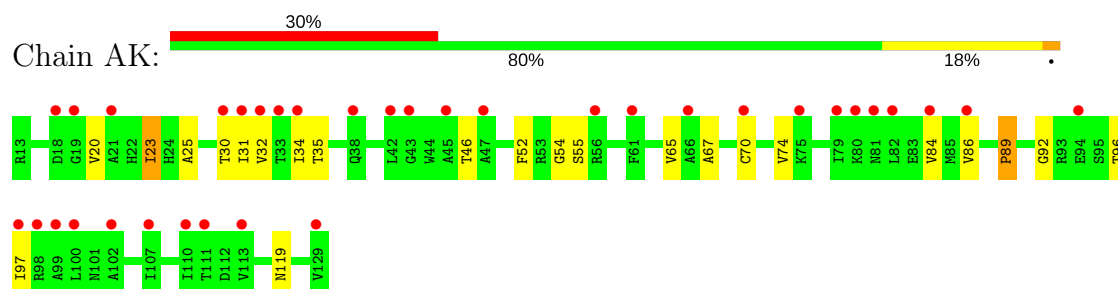
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

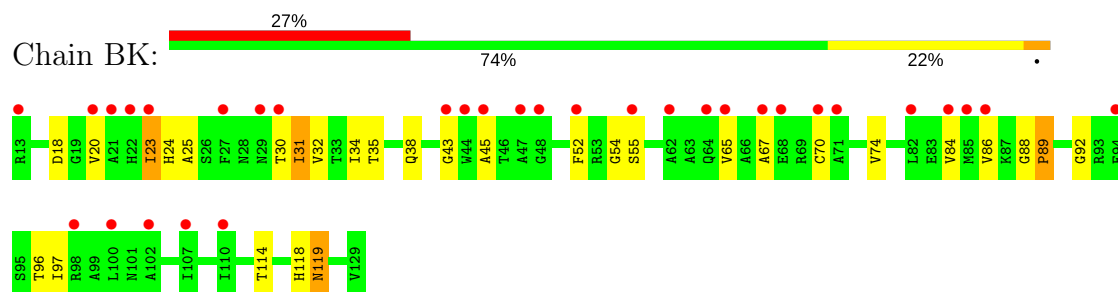


- Molecule 11: 30S ribosomal protein S11

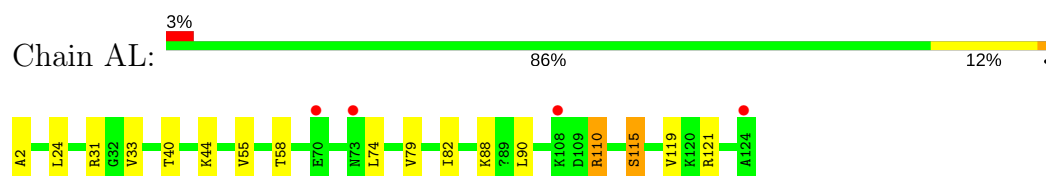




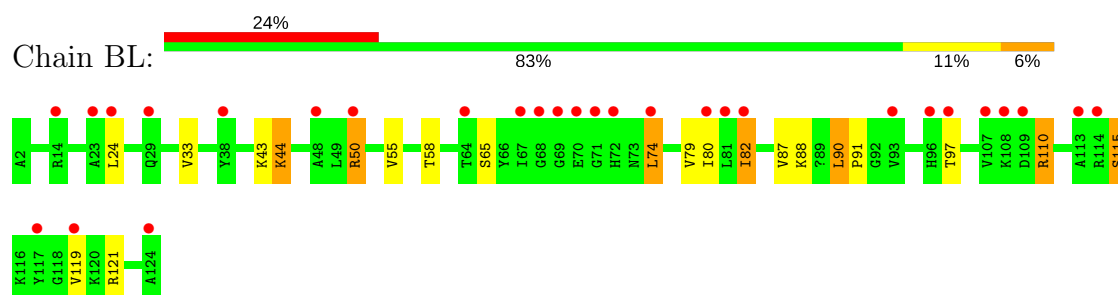
- Molecule 11: 30S ribosomal protein S11



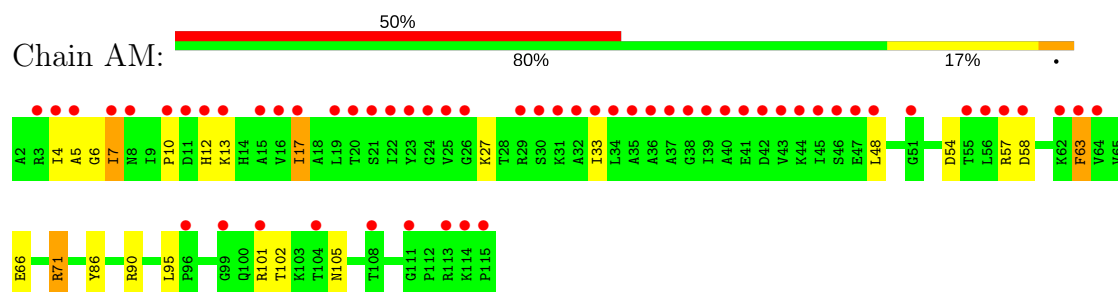
- Molecule 12: 30S ribosomal protein S12



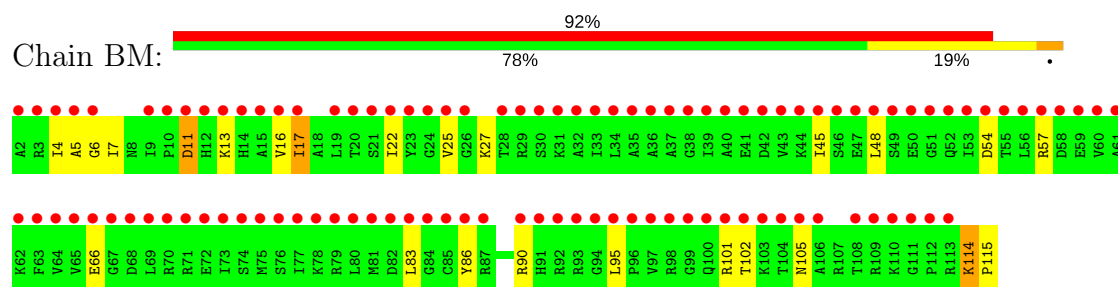
- Molecule 12: 30S ribosomal protein S12



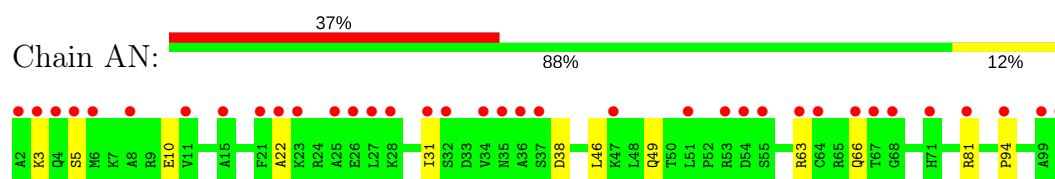
- Molecule 13: 30S ribosomal protein S13



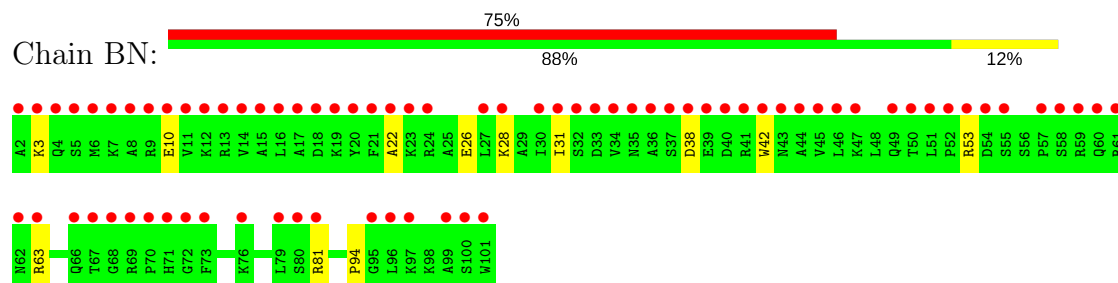
- Molecule 13: 30S ribosomal protein S13



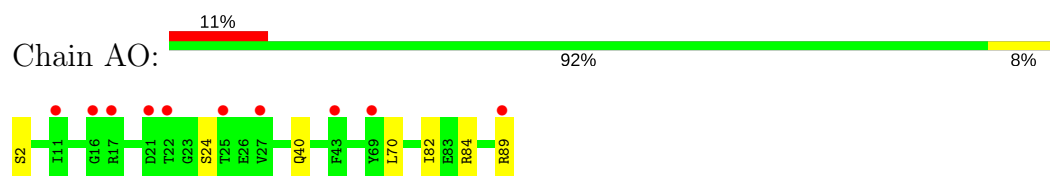
- Molecule 14: 30S ribosomal protein S14



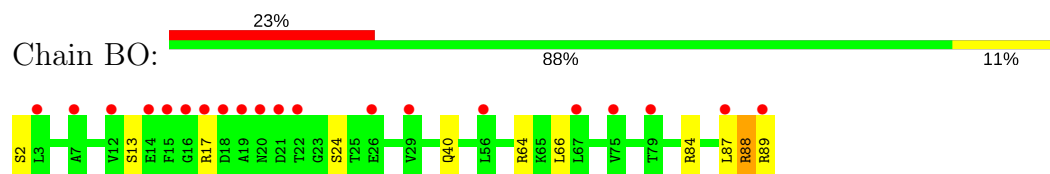
- Molecule 14: 30S ribosomal protein S14



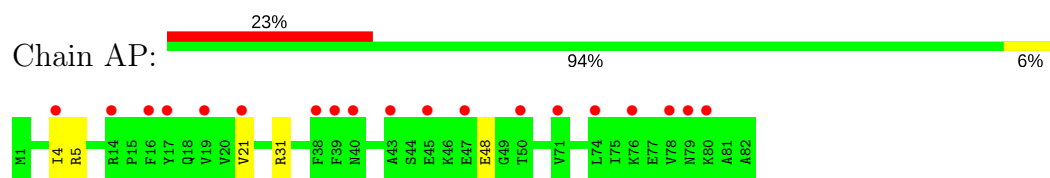
- Molecule 15: 30S ribosomal protein S15



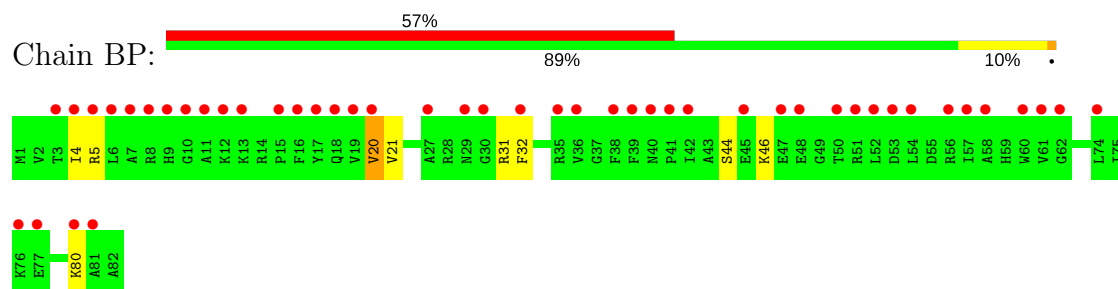
- Molecule 15: 30S ribosomal protein S15



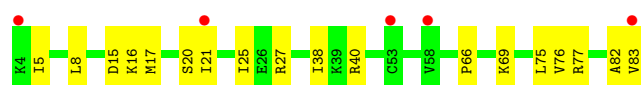
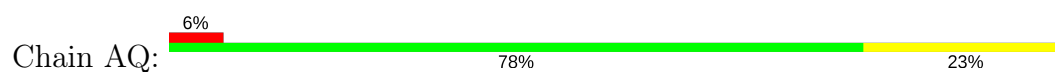
- Molecule 16: 30S ribosomal protein S16



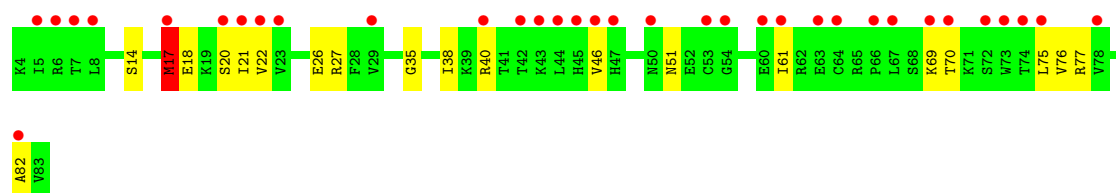
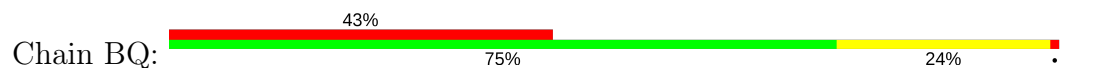
- Molecule 16: 30S ribosomal protein S16



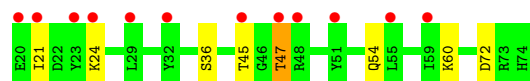
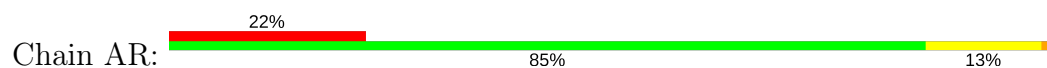
- Molecule 17: 30S ribosomal protein S17



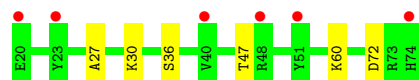
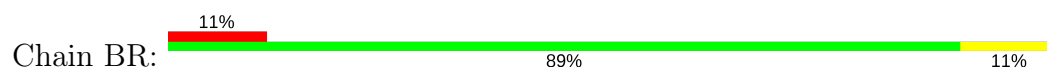
- Molecule 17: 30S ribosomal protein S17



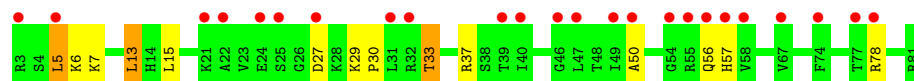
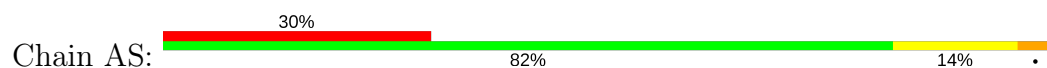
- Molecule 18: 30S ribosomal protein S18



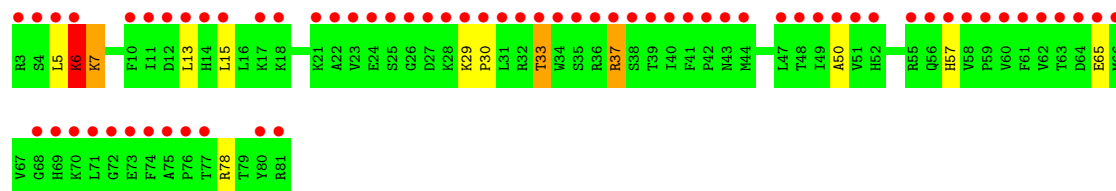
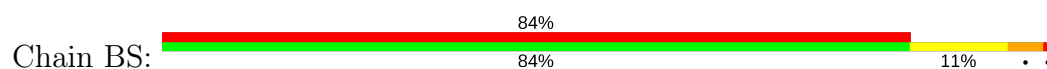
- Molecule 18: 30S ribosomal protein S18



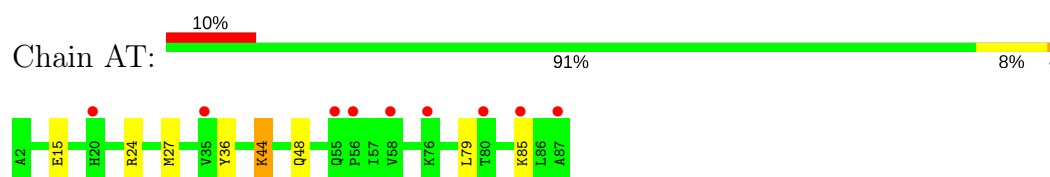
- Molecule 19: 30S ribosomal protein S19



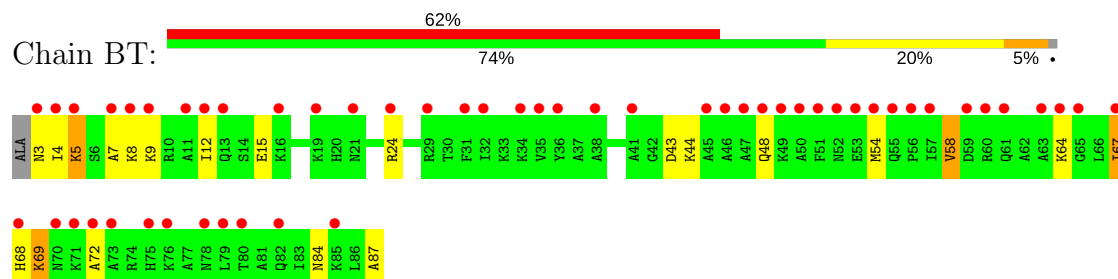
- Molecule 19: 30S ribosomal protein S19



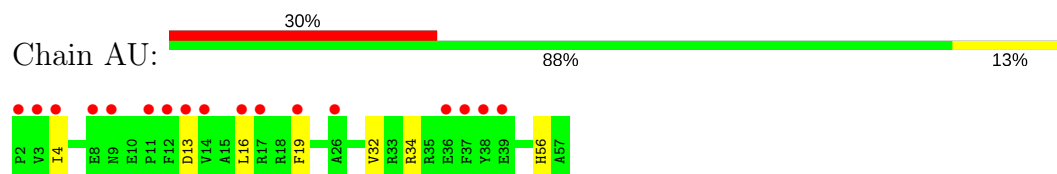
- Molecule 20: 30S ribosomal protein S20



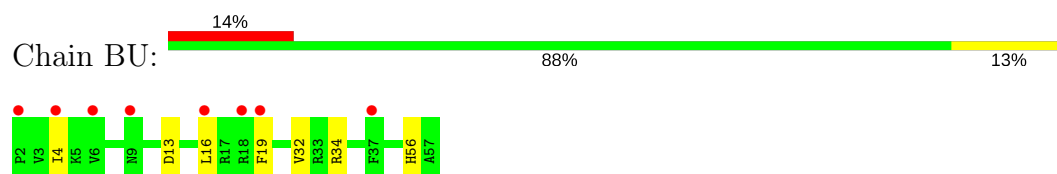
- Molecule 20: 30S ribosomal protein S20



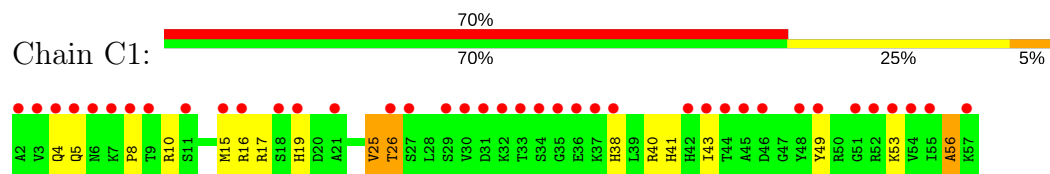
- Molecule 21: 30S ribosomal protein S21



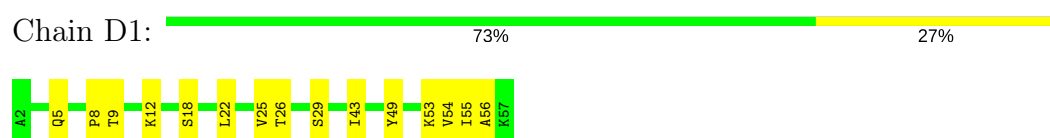
- Molecule 21: 30S ribosomal protein S21



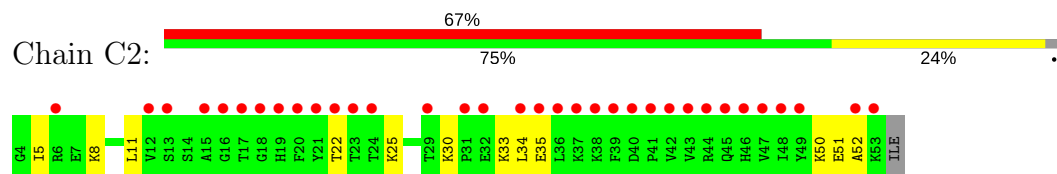
- Molecule 22: 50S ribosomal protein L32



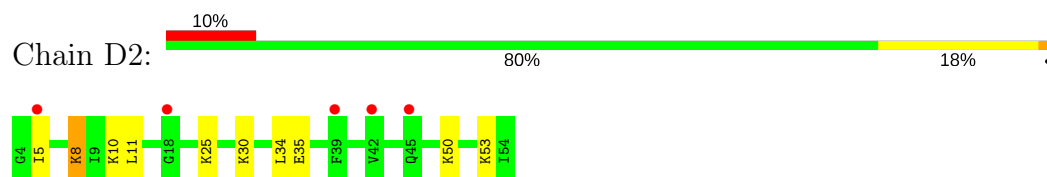
- Molecule 22: 50S ribosomal protein L32



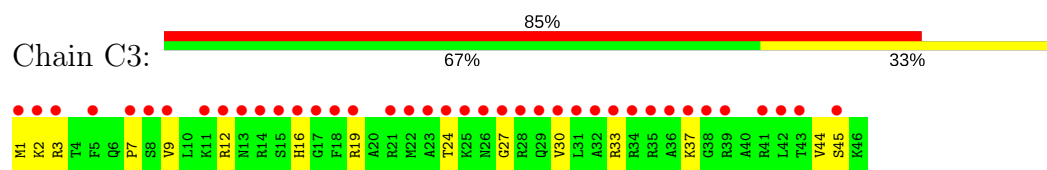
- Molecule 23: 50S ribosomal protein L33



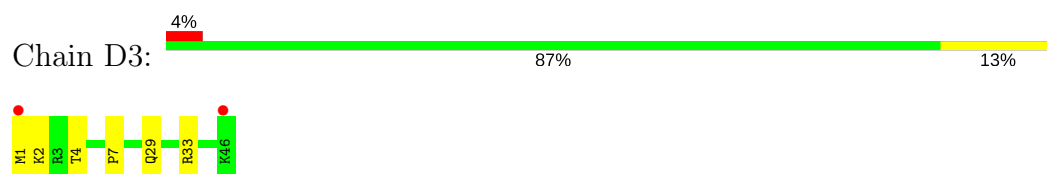
- Molecule 23: 50S ribosomal protein L33



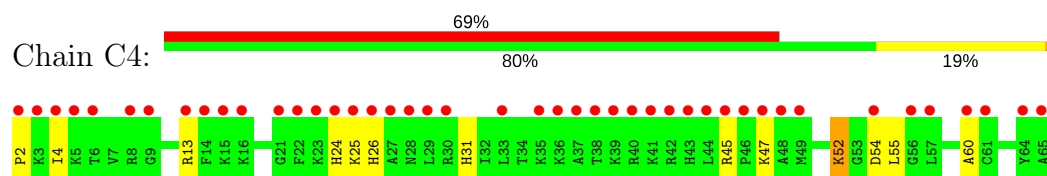
- Molecule 24: 50S ribosomal protein L34



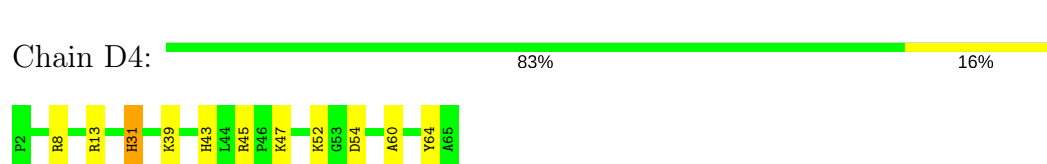
- Molecule 24: 50S ribosomal protein L34



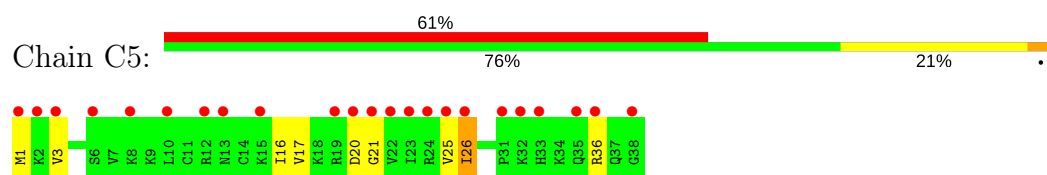
- Molecule 25: 50S ribosomal protein L35



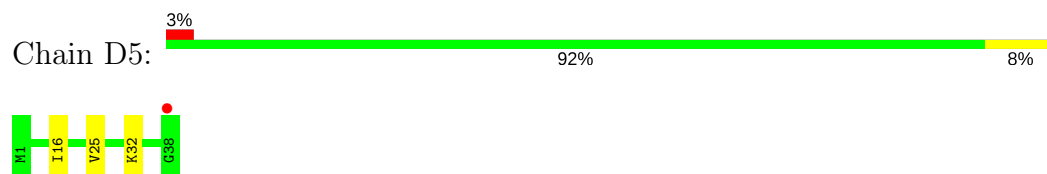
- Molecule 25: 50S ribosomal protein L35



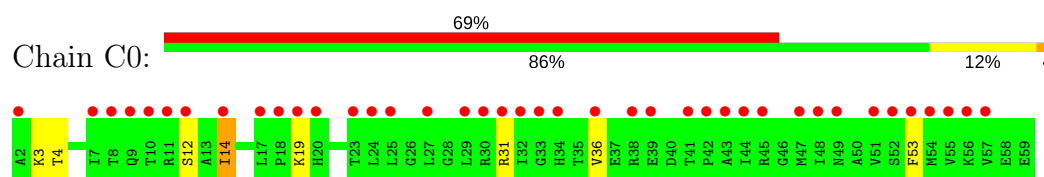
- Molecule 26: 50S ribosomal protein L36



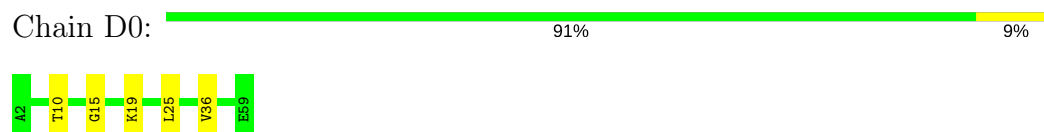
- Molecule 26: 50S ribosomal protein L36



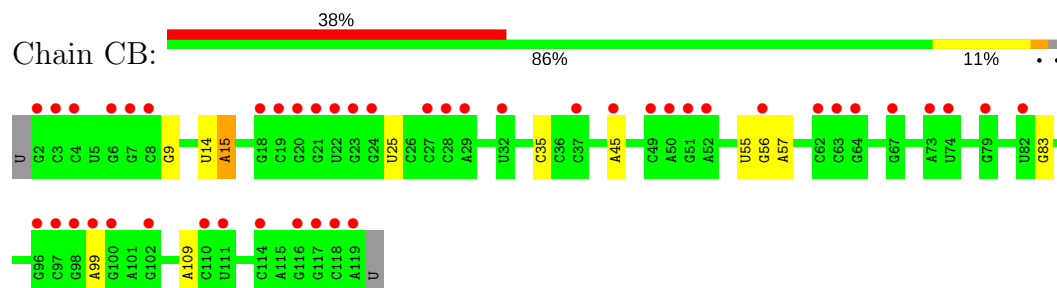
- Molecule 27: 50S ribosomal protein L30



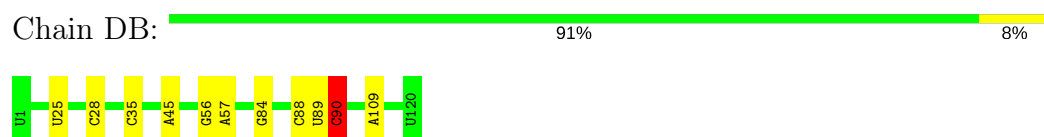
- Molecule 27: 50S ribosomal protein L30



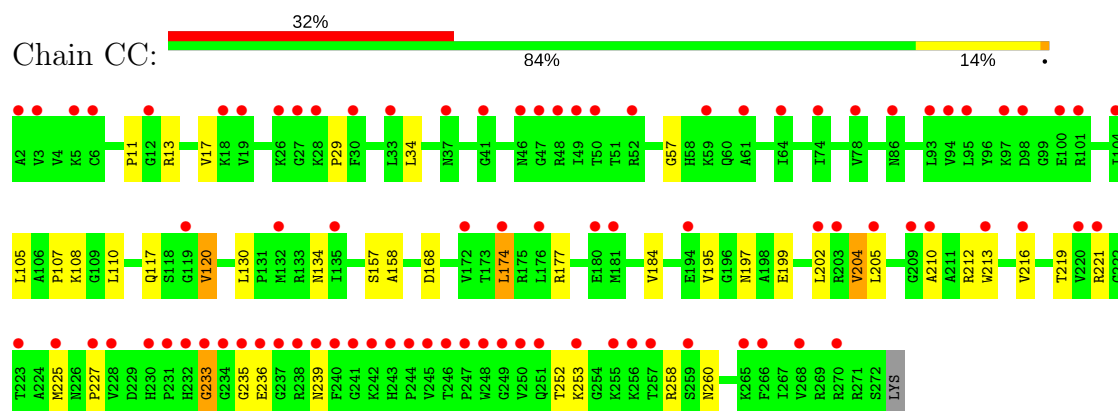
- Molecule 28: 5S rRNA



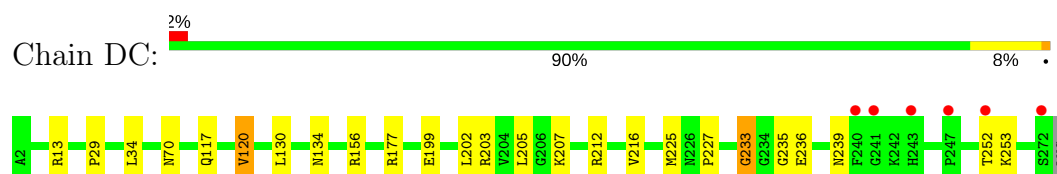
- Molecule 28: 5S rRNA



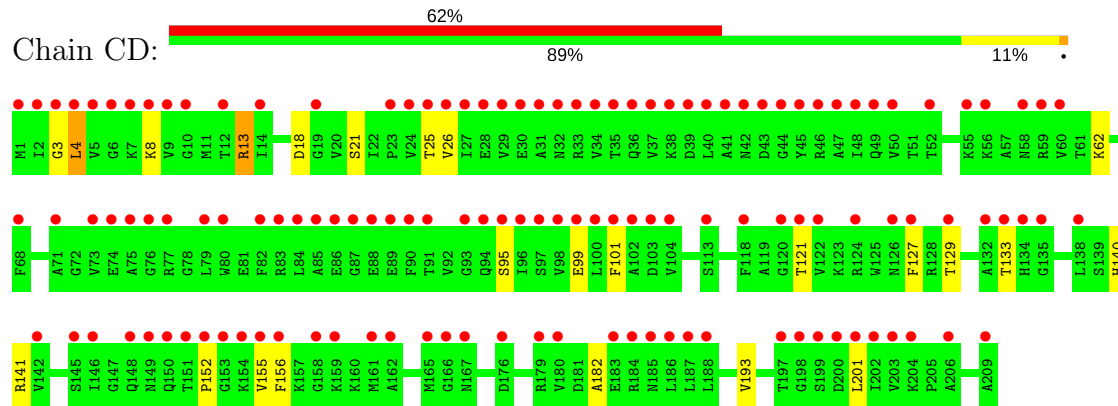
- Molecule 29: 50S ribosomal protein L2



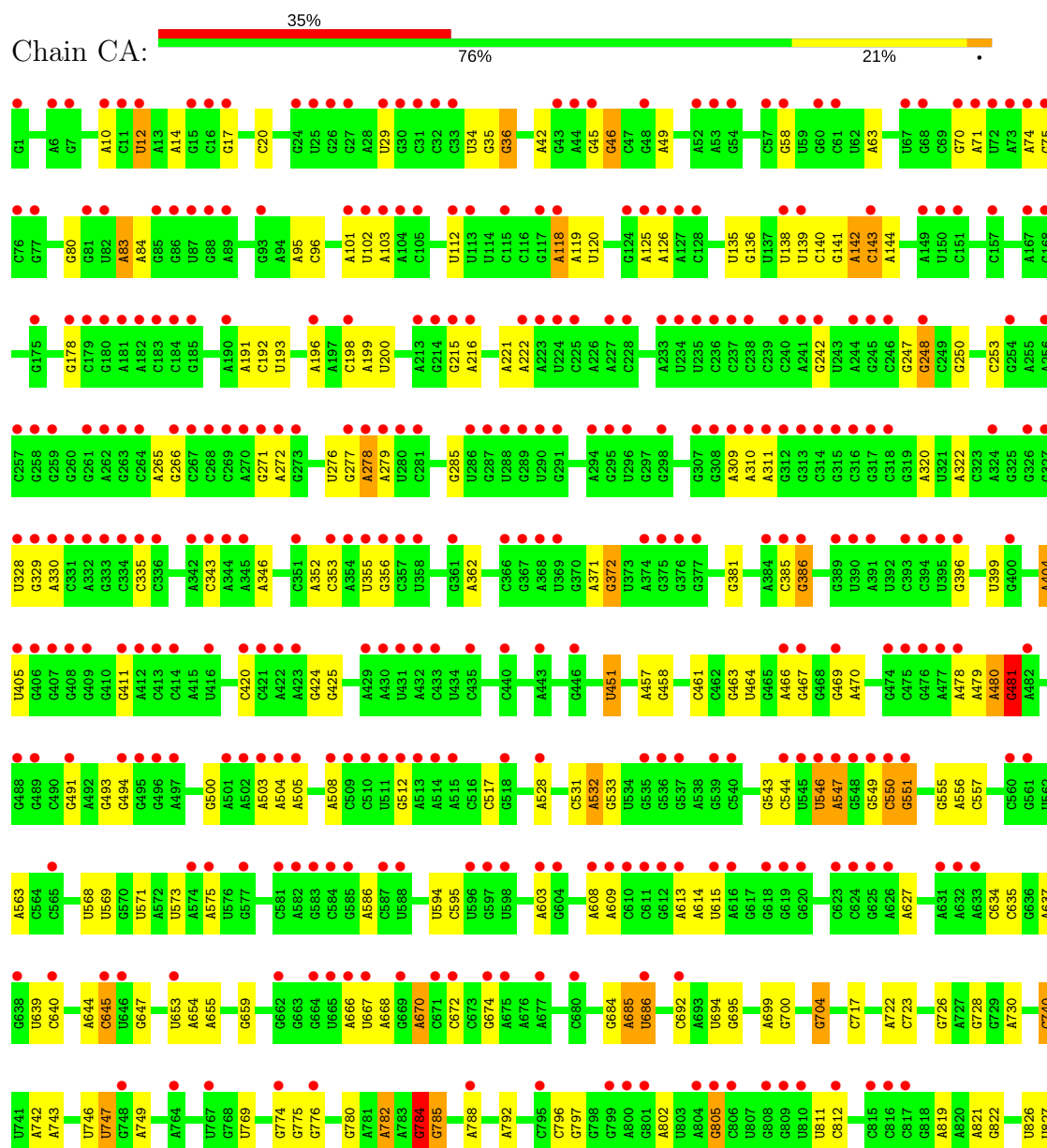
- Molecule 29: 50S ribosomal protein L2

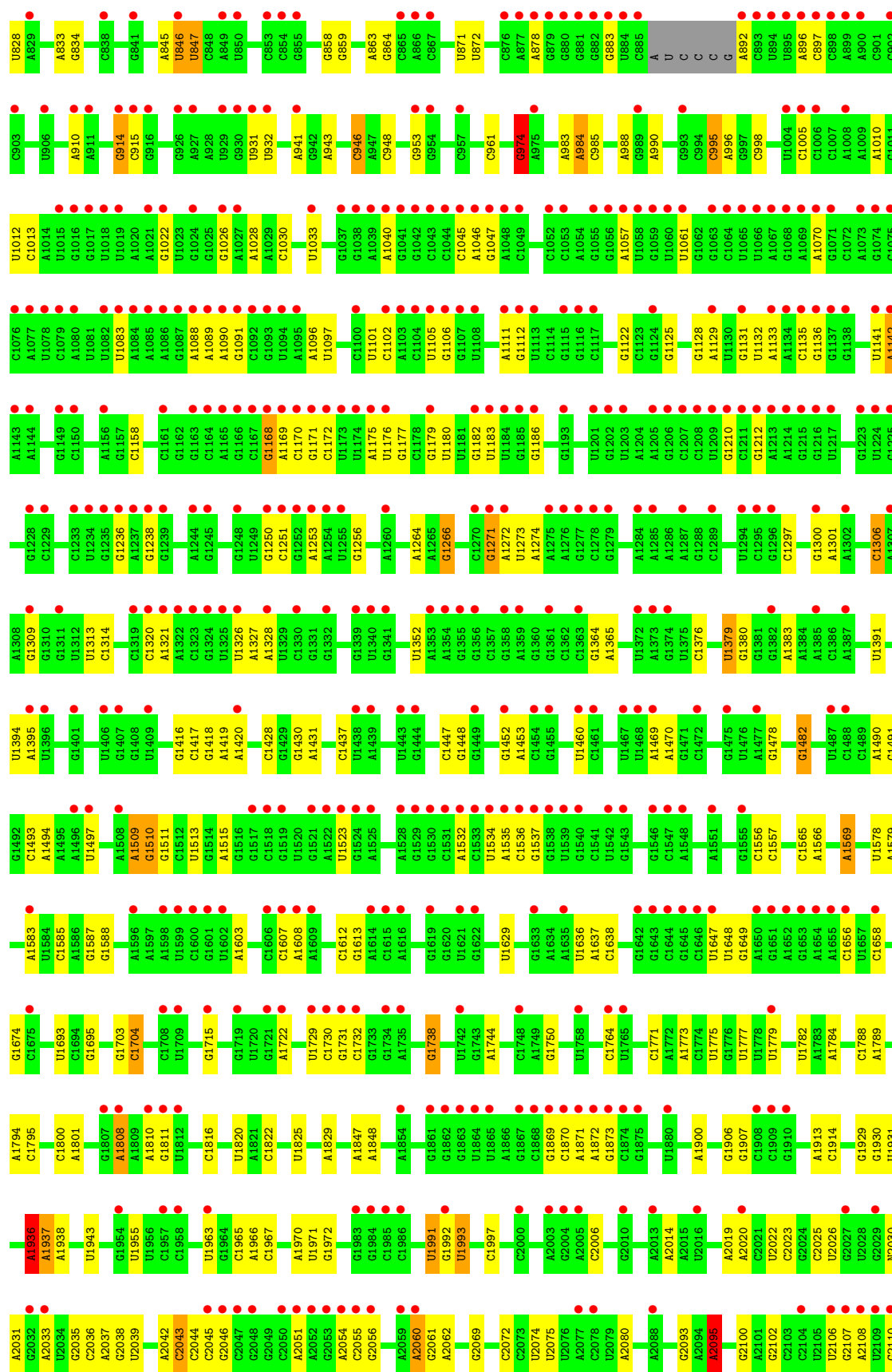


• Molecule 30: 50S ribosomal protein L3

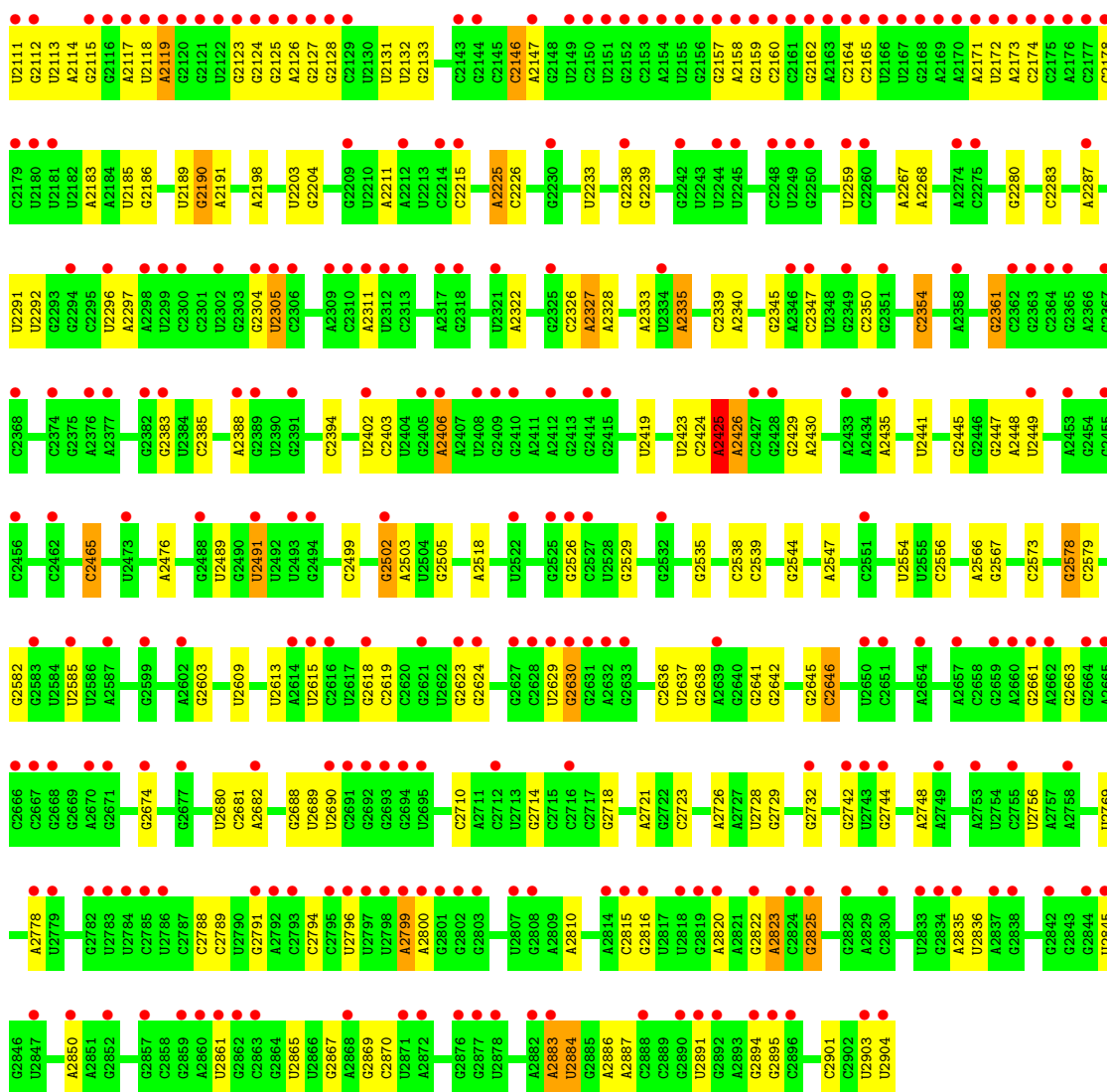


• Molecule 31: 23S rRNA









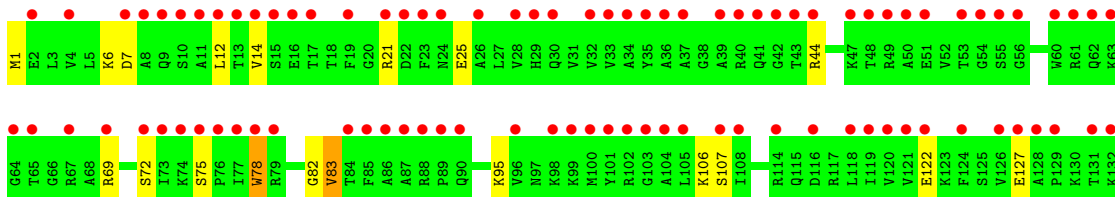
• Molecule 32: 50S ribosomal protein L3

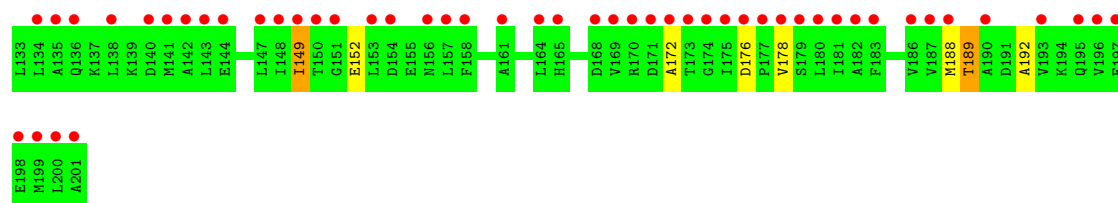
Chain DD: 89% 11%



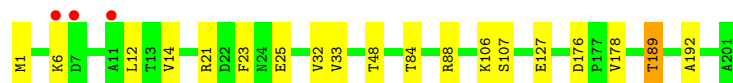
• Molecule 33: 50S ribosomal protein L4

Chain CE: 70% 87% 11%

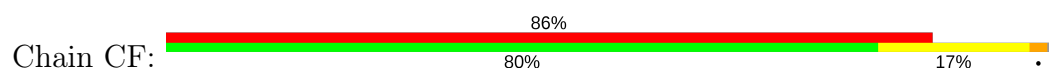




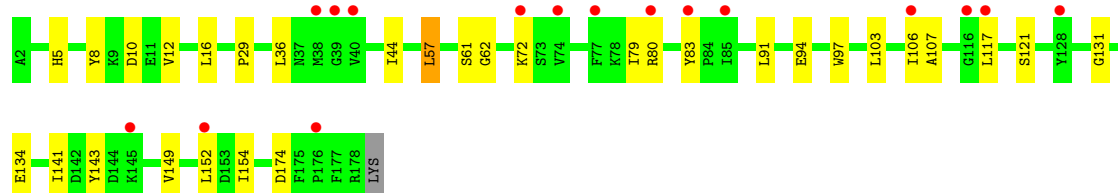
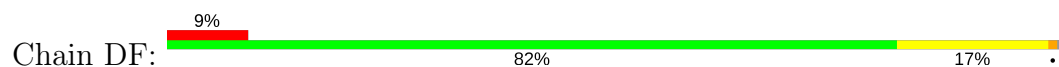
• Molecule 33: 50S ribosomal protein L4



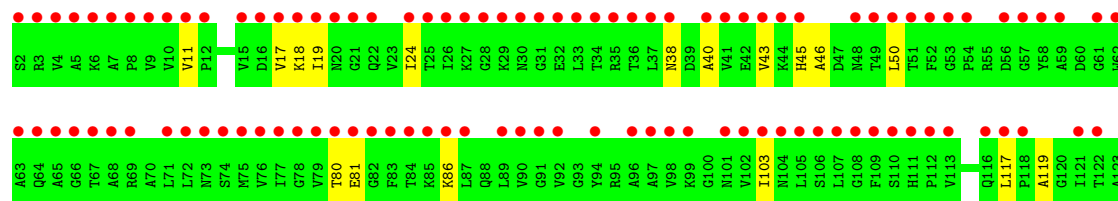
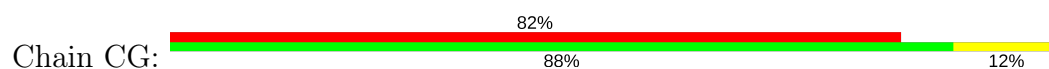
• Molecule 34: 50S ribosomal protein L5

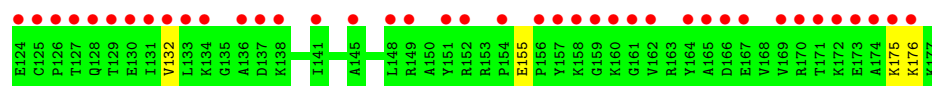


• Molecule 34: 50S ribosomal protein L5

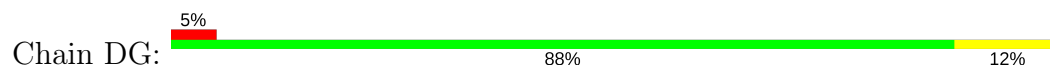


• Molecule 35: 50S ribosomal protein L6

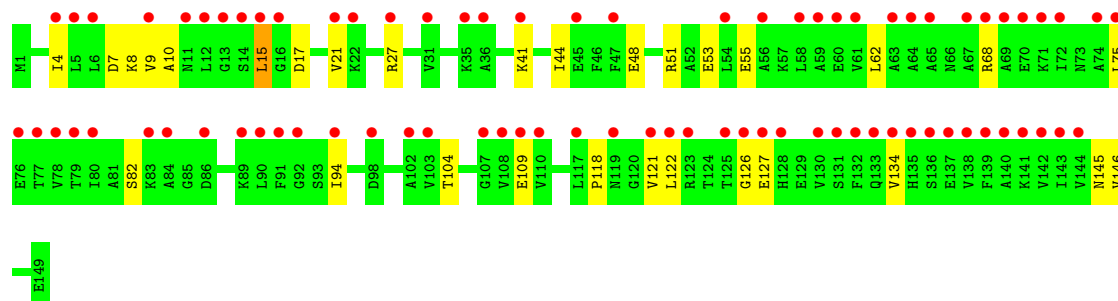
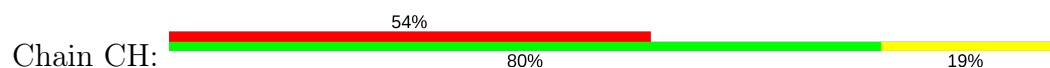




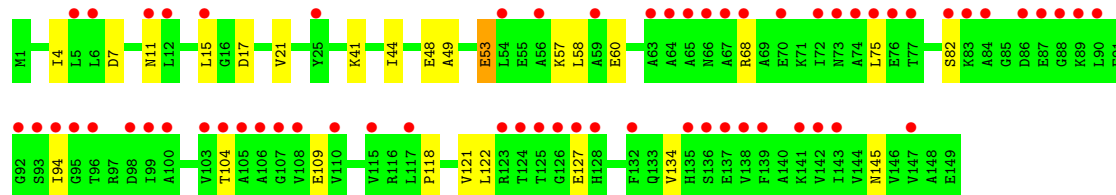
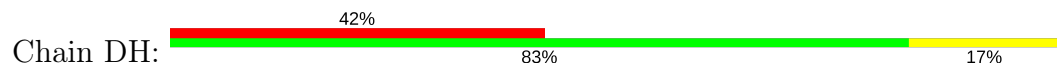
• Molecule 35: 50S ribosomal protein L6



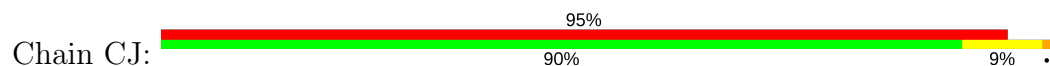
• Molecule 36: 50S ribosomal protein L9



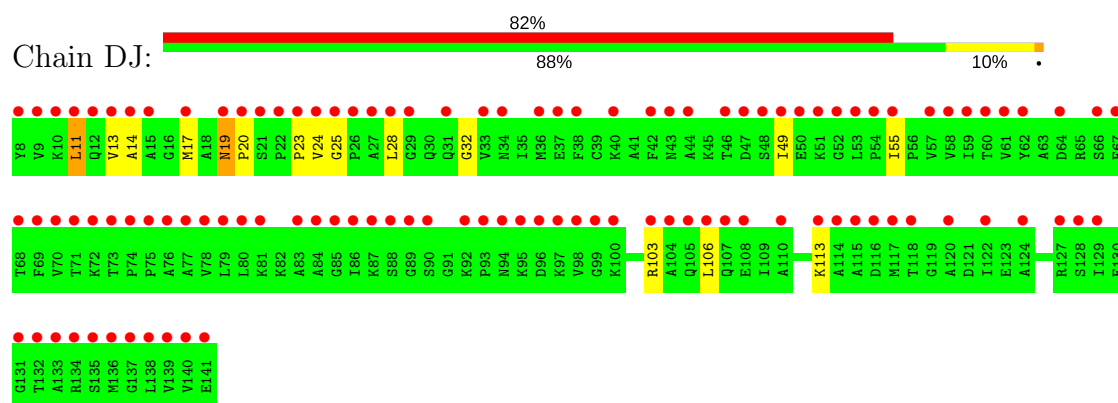
• Molecule 36: 50S ribosomal protein L9



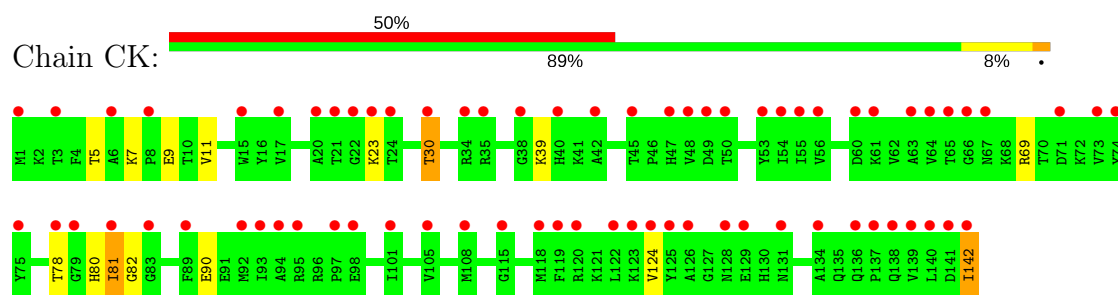
• Molecule 37: 50S ribosomal protein L11



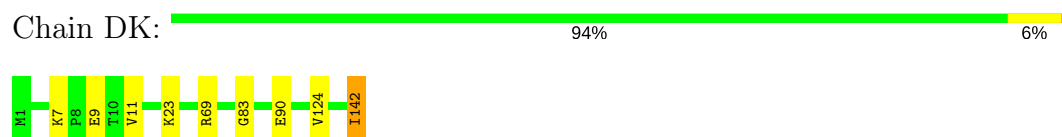
• Molecule 37: 50S ribosomal protein L11



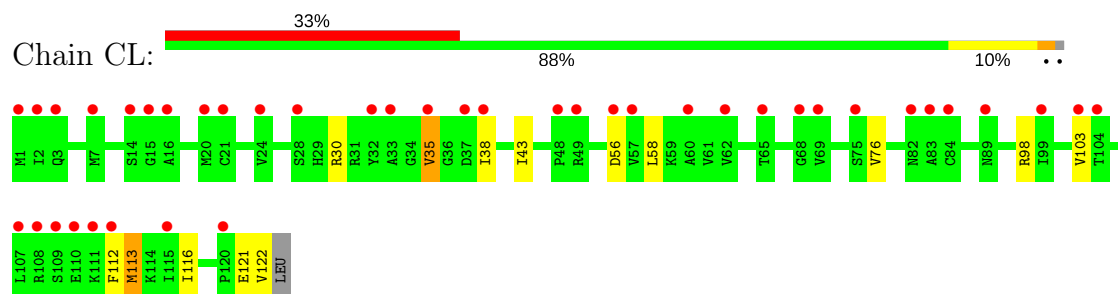
- Molecule 38: 50S ribosomal protein L13



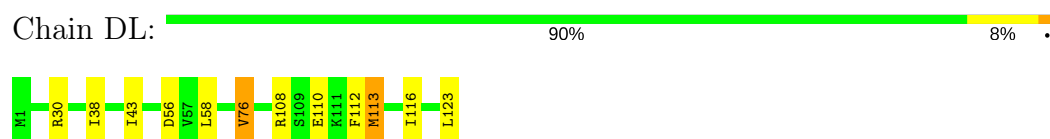
- Molecule 38: 50S ribosomal protein L13



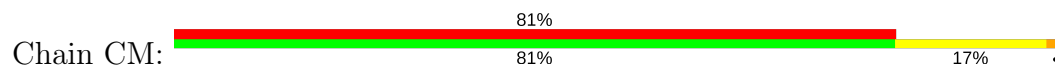
- Molecule 39: 50S ribosomal protein L14

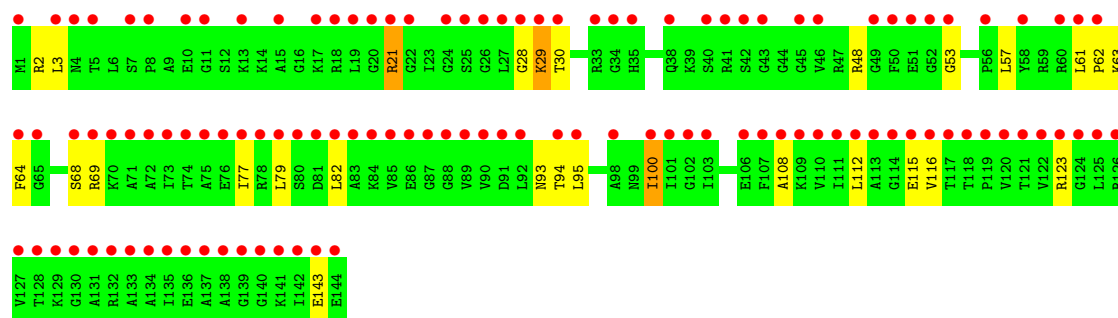


- Molecule 39: 50S ribosomal protein L14

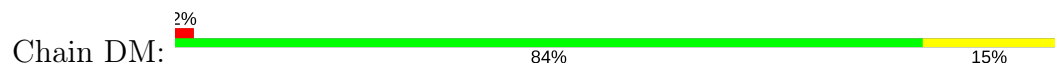


- Molecule 40: 50S ribosomal protein L15

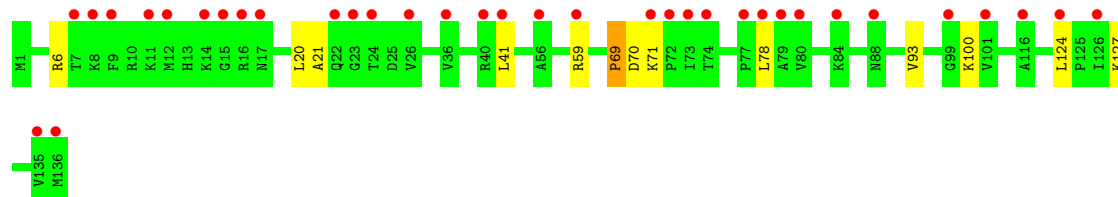
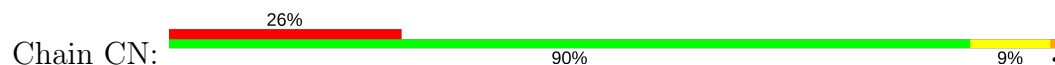




- Molecule 40: 50S ribosomal protein L15



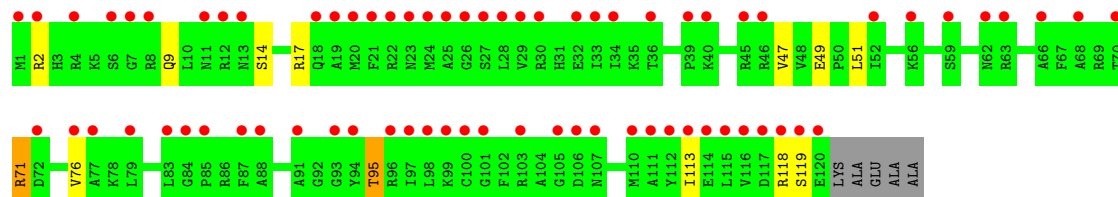
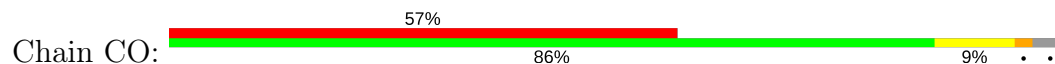
- Molecule 41: 50S ribosomal protein L16



- Molecule 41: 50S ribosomal protein L16



- Molecule 42: 50S ribosomal protein L17



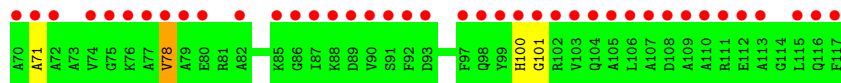
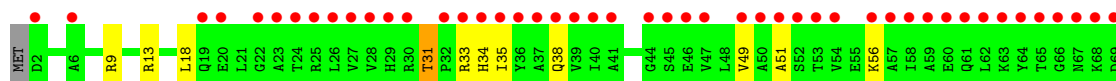
- Molecule 42: 50S ribosomal protein L17





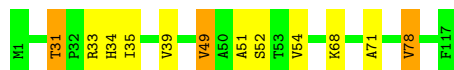
- Molecule 43: 50S ribosomal protein L18

Chain CP: 74% 86% 11% ..



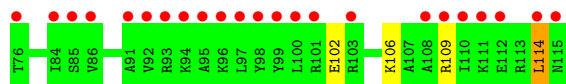
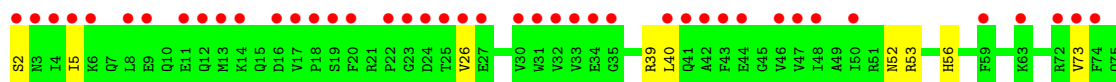
- Molecule 43: 50S ribosomal protein L18

Chain DP: 90% 8% .



- Molecule 44: 50S ribosomal protein L19

Chain CQ: 57% 89% 11% .



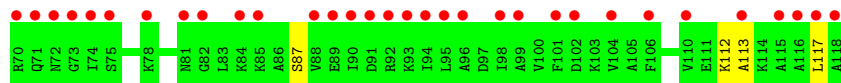
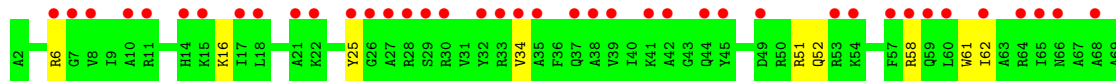
- Molecule 44: 50S ribosomal protein L19

Chain DQ: 3% 90% 10%

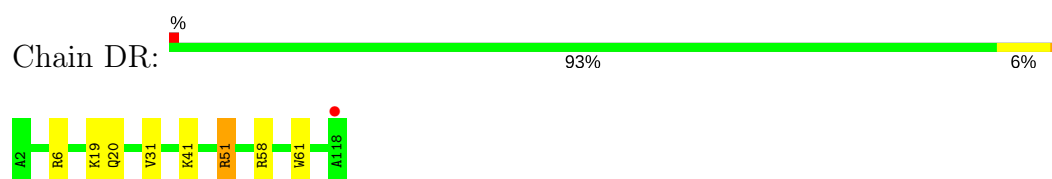


- Molecule 45: 50S ribosomal protein L20

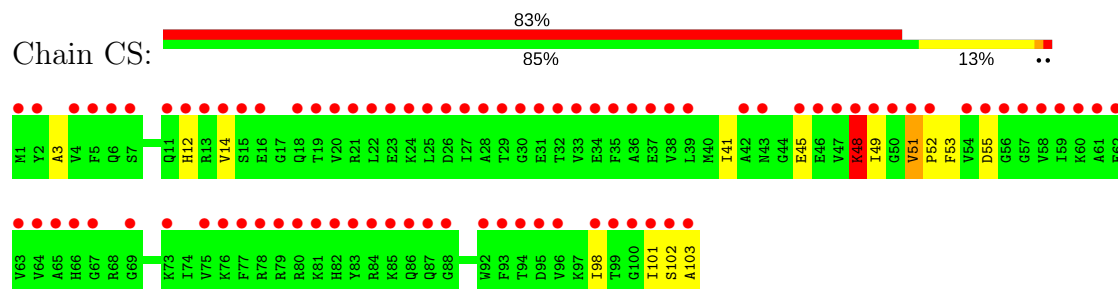
Chain CR: 62% 89% 11%



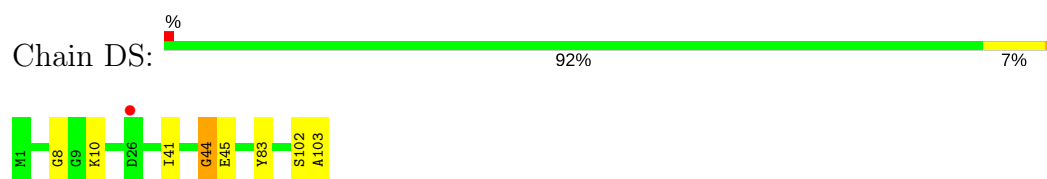
- Molecule 45: 50S ribosomal protein L20



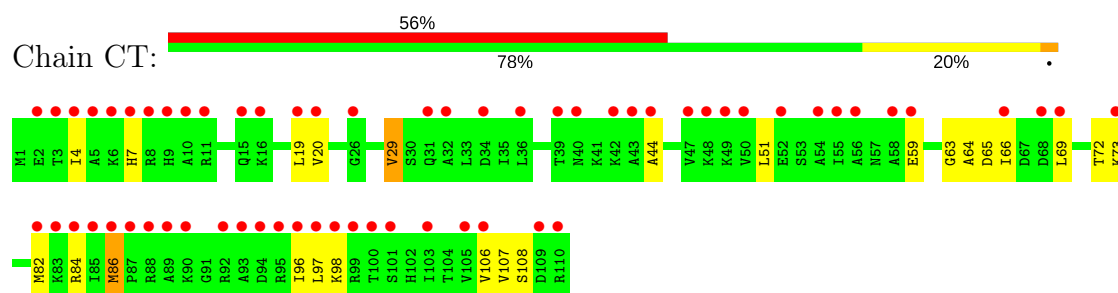
- Molecule 46: 50S ribosomal protein L21



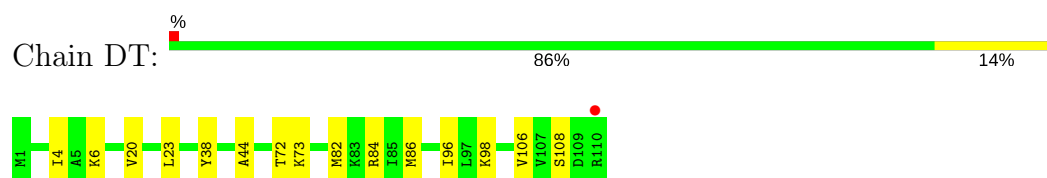
- Molecule 46: 50S ribosomal protein L21



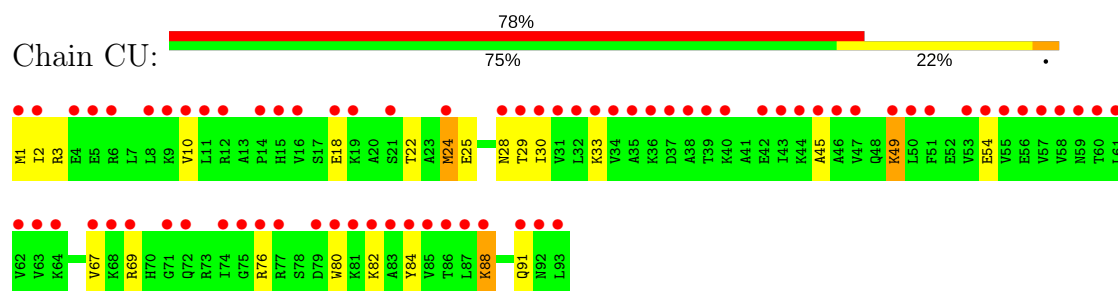
- Molecule 47: 50S ribosomal protein L22



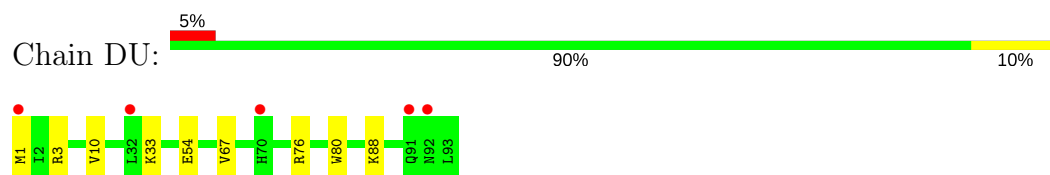
- Molecule 47: 50S ribosomal protein L22



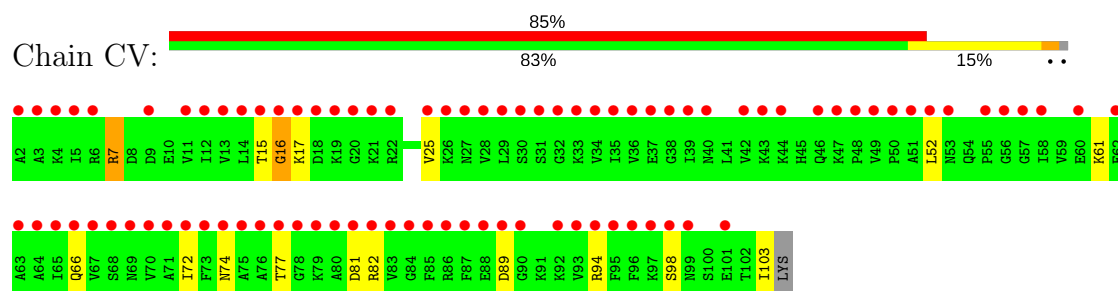
- Molecule 48: 50S ribosomal protein L23



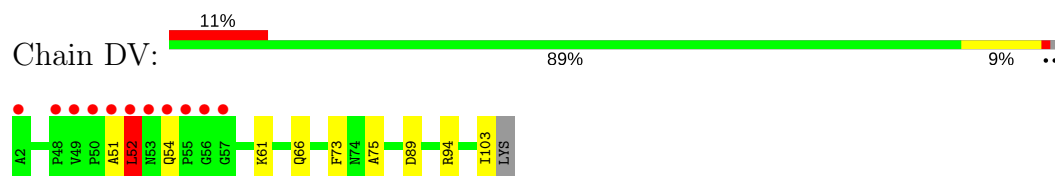
- Molecule 48: 50S ribosomal protein L23



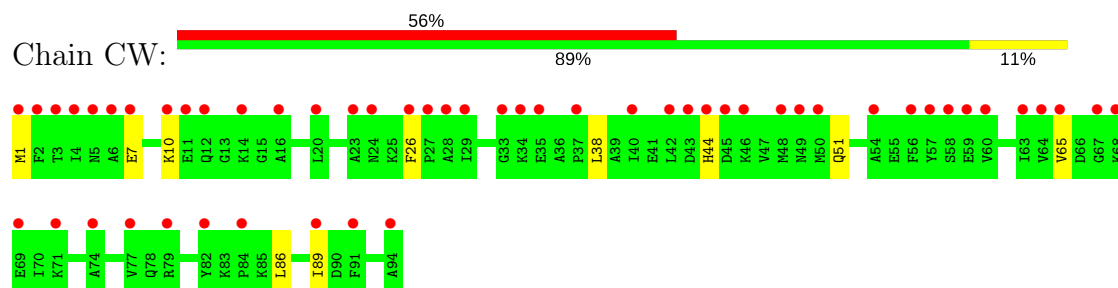
- Molecule 49: 50S ribosomal protein L24



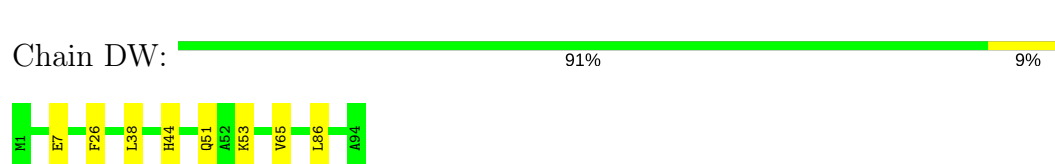
- Molecule 49: 50S ribosomal protein L24



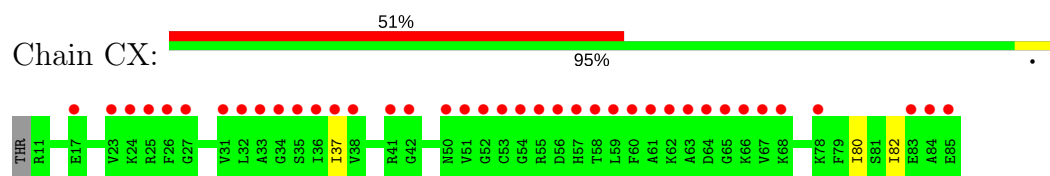
- Molecule 50: 50S ribosomal protein L25



- Molecule 50: 50S ribosomal protein L25

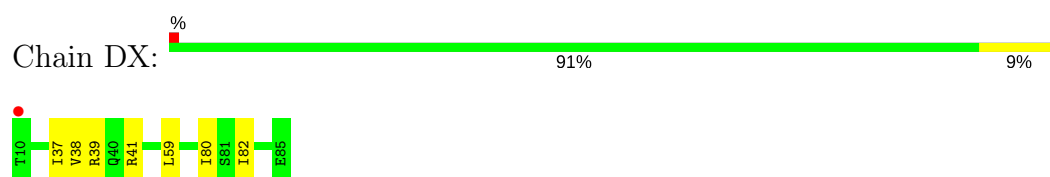


- Molecule 51: 50S ribosomal protein L27

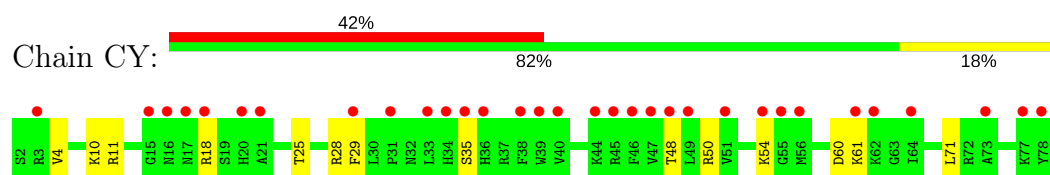


- Molecule 51: 50S ribosomal protein L27

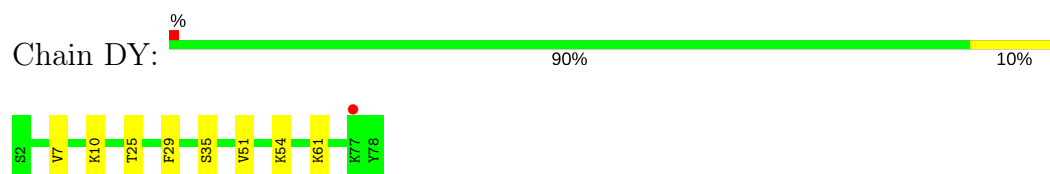




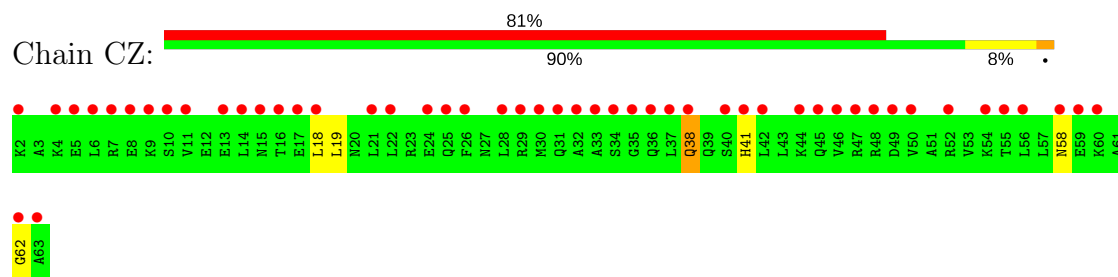
- Molecule 52: 50S ribosomal protein L28



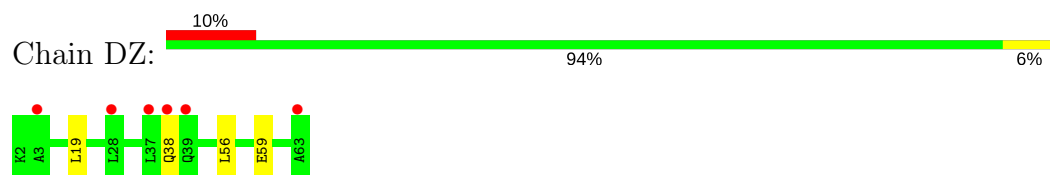
- Molecule 52: 50S ribosomal protein L28



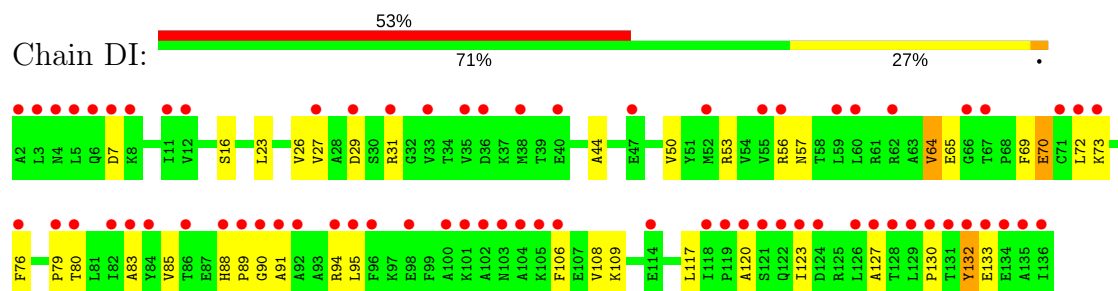
- Molecule 53: 50S ribosomal protein L29



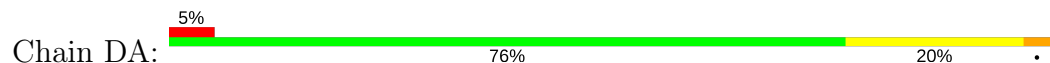
- Molecule 53: 50S ribosomal protein L29

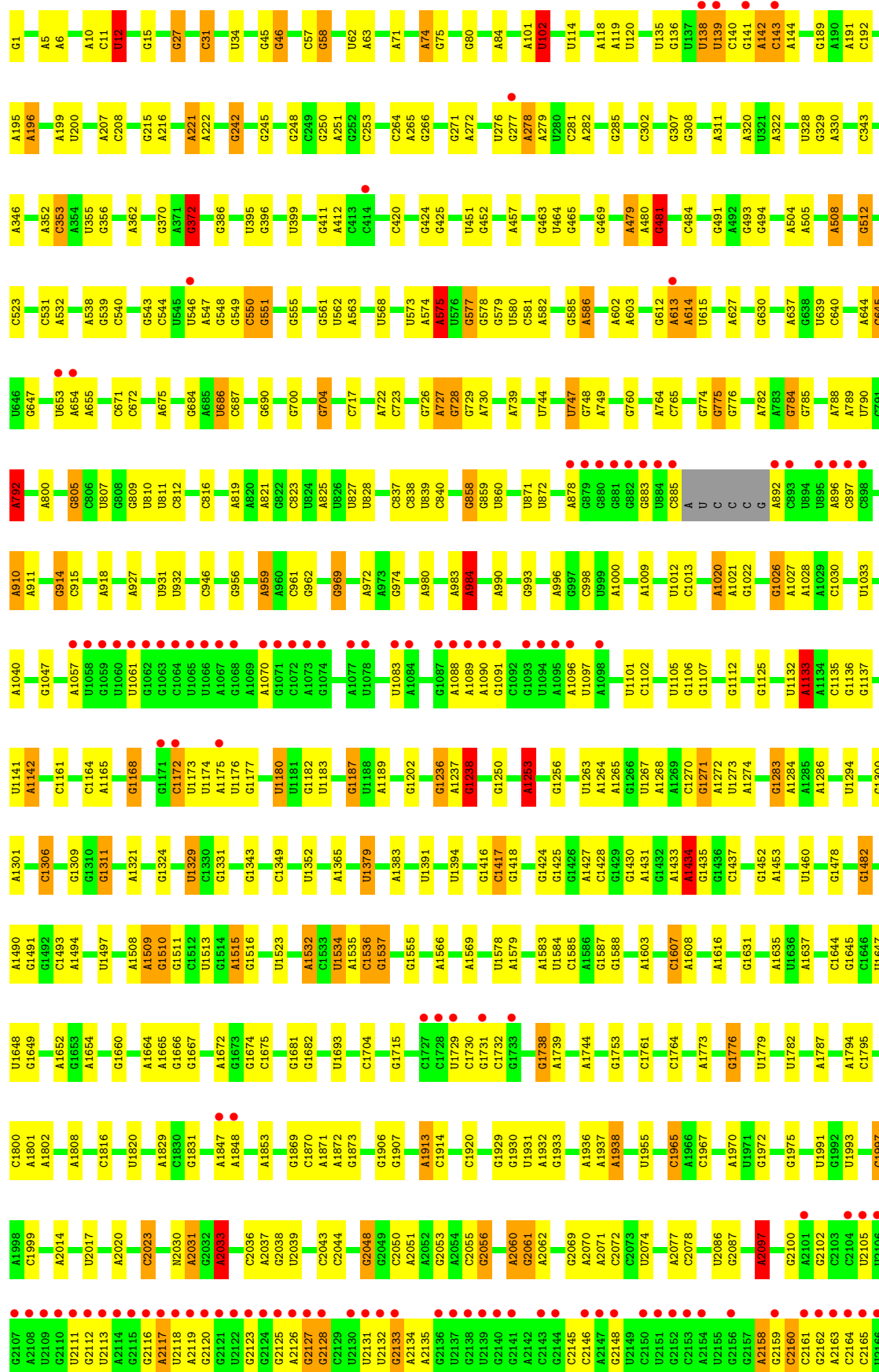


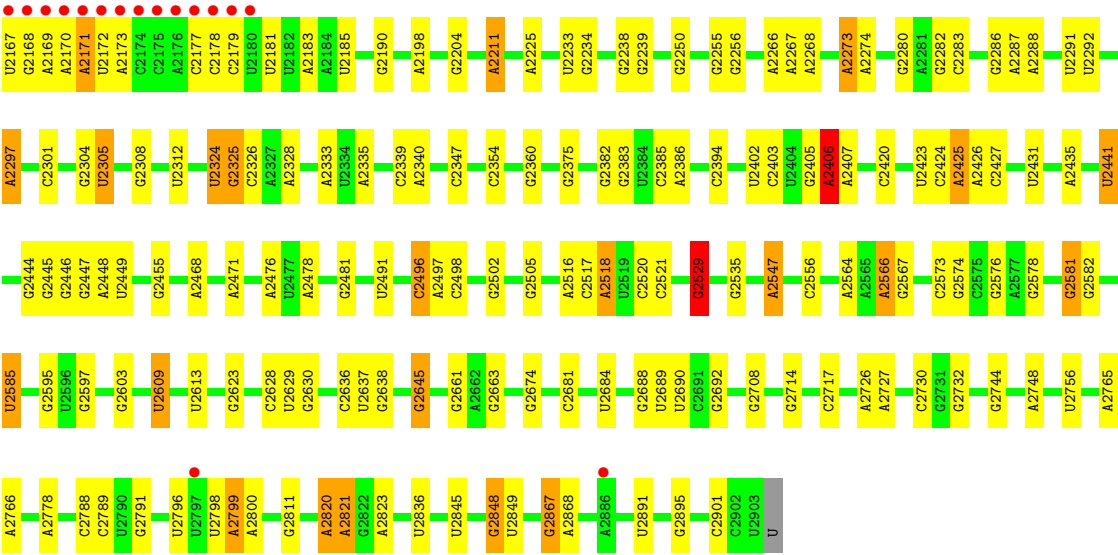
- Molecule 54: 50S ribosomal protein L10



- Molecule 55: 23S rRNA







## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 212.18Å 434.82Å 624.26Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 48.51 – 2.96<br>48.28 – 2.96                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.6 (48.51-2.96)<br>88.6 (48.28-2.96)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 21.17 (at 2.96Å)  | Xtriage          |
| Refinement program  | BUSTER-TNT  | Depositor        |
| R, $R_{free}$   | 0.208 , 0.221<br>0.226 , 0.242                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4163 reflections (0.40%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.6  | Xtriage          |
| Anisotropy  | 0.403   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 89.4   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 295202  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 123.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% 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: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, G7M, D2T, UR3, SPD, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, T1C, H2U, EDO, MEQ, OMU, PUT, 4OC, PSU

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

| Mol | Chain | Bond lengths |                 | Bond angles |                |
|-----|-------|--------------|-----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5        |
| 1   | AA    | 1.04         | 9/36593 (0.0%)  | 0.86        | 5/57081 (0.0%) |
| 1   | BA    | 1.05         | 10/36568 (0.0%) | 0.86        | 5/57042 (0.0%) |
| 2   | AB    | 0.48         | 0/1784          | 0.65        | 0/2403         |
| 2   | BB    | 0.48         | 0/1784          | 0.65        | 0/2403         |
| 3   | AC    | 0.48         | 0/1652          | 0.67        | 0/2225         |
| 3   | BC    | 0.47         | 0/1652          | 0.67        | 0/2225         |
| 4   | AD    | 0.44         | 0/1665          | 0.69        | 0/2227         |
| 4   | BD    | 0.43         | 0/1665          | 0.70        | 0/2227         |
| 5   | AE    | 0.48         | 0/1157          | 0.77        | 0/1557         |
| 5   | BE    | 0.51         | 0/1118          | 0.81        | 0/1504         |
| 6   | AF    | 0.46         | 0/881           | 0.69        | 0/1189         |
| 6   | BF    | 0.47         | 0/835           | 0.77        | 0/1128         |
| 7   | AG    | 0.45         | 0/1196          | 0.61        | 0/1602         |
| 7   | BG    | 0.46         | 0/1196          | 0.62        | 0/1602         |
| 8   | AH    | 0.46         | 0/989           | 0.71        | 0/1326         |
| 8   | BH    | 0.46         | 0/989           | 0.69        | 0/1326         |
| 9   | AI    | 0.44         | 0/1034          | 0.66        | 0/1375         |
| 9   | BI    | 0.44         | 0/1034          | 0.65        | 0/1375         |
| 10  | AJ    | 0.44         | 0/806           | 0.68        | 0/1089         |
| 10  | BJ    | 0.48         | 0/797           | 0.71        | 0/1077         |
| 11  | AK    | 0.46         | 0/893           | 0.65        | 0/1205         |
| 11  | BK    | 0.45         | 0/893           | 0.68        | 0/1205         |
| 12  | AL    | 0.44         | 0/960           | 0.74        | 0/1286         |
| 12  | BL    | 0.47         | 0/960           | 0.74        | 0/1286         |
| 13  | AM    | 0.51         | 0/893           | 0.72        | 0/1193         |
| 13  | BM    | 0.49         | 0/893           | 0.72        | 0/1193         |
| 14  | AN    | 0.46         | 0/817           | 0.63        | 0/1088         |
| 14  | BN    | 0.44         | 0/817           | 0.63        | 0/1088         |
| 15  | AO    | 0.48         | 0/722           | 0.60        | 0/964          |
| 15  | BO    | 0.47         | 0/722           | 0.63        | 0/964          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 16  | AP    | 0.48         | 0/659           | 0.70        | 0/884            |
| 16  | BP    | 0.50         | 0/659           | 0.76        | 0/884            |
| 17  | AQ    | 0.48         | 0/658           | 0.73        | 0/881            |
| 17  | BQ    | 0.51         | 0/658           | 0.78        | 0/881            |
| 18  | AR    | 0.53         | 0/463           | 0.65        | 0/621            |
| 18  | BR    | 0.50         | 0/463           | 0.64        | 0/621            |
| 19  | AS    | 0.46         | 0/653           | 0.59        | 0/877            |
| 19  | BS    | 0.45         | 0/653           | 0.60        | 0/877            |
| 20  | AT    | 0.48         | 0/676           | 0.66        | 0/895            |
| 20  | BT    | 0.52         | 0/671           | 0.68        | 0/888            |
| 21  | AU    | 0.45         | 0/472           | 0.61        | 0/627            |
| 21  | BU    | 0.43         | 0/472           | 0.63        | 0/627            |
| 22  | C1    | 0.49         | 0/450           | 0.71        | 0/599            |
| 22  | D1    | 0.61         | 0/450           | 0.79        | 0/599            |
| 23  | C2    | 0.46         | 0/416           | 0.73        | 0/554            |
| 23  | D2    | 0.51         | 0/421           | 0.73        | 0/561            |
| 24  | C3    | 0.46         | 0/380           | 0.69        | 0/498            |
| 24  | D3    | 0.55         | 0/380           | 0.76        | 0/498            |
| 25  | C4    | 0.46         | 0/513           | 0.67        | 0/676            |
| 25  | D4    | 0.56         | 0/513           | 0.71        | 0/676            |
| 26  | C5    | 0.43         | 0/303           | 0.77        | 0/397            |
| 26  | D5    | 0.53         | 0/303           | 0.76        | 0/397            |
| 27  | C0    | 0.52         | 0/453           | 0.77        | 0/605            |
| 27  | D0    | 0.62         | 0/467           | 0.81        | 0/623            |
| 28  | CB    | 0.98         | 0/2828          | 0.88        | 2/4410 (0.0%)    |
| 28  | DB    | 1.13         | 1/2872 (0.0%)   | 0.90        | 0/4478           |
| 29  | CC    | 0.45         | 0/2121          | 0.76        | 0/2852           |
| 29  | DC    | 0.50         | 0/2121          | 0.76        | 1/2852 (0.0%)    |
| 30  | CD    | 0.43         | 0/1586          | 0.70        | 0/2134           |
| 31  | CA    | 1.07         | 44/69165 (0.1%) | 0.87        | 17/107896 (0.0%) |
| 32  | DD    | 0.54         | 0/1576          | 0.73        | 0/2119           |
| 33  | CE    | 0.45         | 0/1571          | 0.72        | 0/2113           |
| 33  | DE    | 0.52         | 0/1571          | 0.72        | 0/2113           |
| 34  | CF    | 0.43         | 0/1434          | 0.68        | 0/1926           |
| 34  | DF    | 0.46         | 0/1434          | 0.70        | 0/1926           |
| 35  | CG    | 0.42         | 0/1343          | 0.66        | 0/1816           |
| 35  | DG    | 0.44         | 0/1343          | 0.64        | 0/1816           |
| 36  | CH    | 0.48         | 0/1121          | 0.68        | 0/1515           |
| 36  | DH    | 0.48         | 0/1121          | 0.68        | 0/1515           |
| 37  | CJ    | 0.48         | 0/993           | 0.62        | 0/1341           |
| 37  | DJ    | 0.48         | 0/993           | 0.61        | 0/1341           |
| 38  | CK    | 0.43         | 0/1152          | 0.70        | 0/1551           |
| 38  | DK    | 0.56         | 0/1152          | 0.74        | 0/1551           |

| Mol | Chain | Bond lengths |                   | Bond angles |                  |
|-----|-------|--------------|-------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5          |
| 39  | CL    | 0.47         | 0/947             | 0.74        | 0/1268           |
| 39  | DL    | 0.54         | 0/955             | 0.75        | 0/1279           |
| 40  | CM    | 0.46         | 0/1062            | 0.74        | 1/1413 (0.1%)    |
| 40  | DM    | 0.50         | 0/1062            | 0.75        | 1/1413 (0.1%)    |
| 41  | CN    | 0.45         | 0/1081            | 0.75        | 1/1443 (0.1%)    |
| 41  | DN    | 0.59         | 0/1092            | 0.81        | 0/1457           |
| 42  | CO    | 0.46         | 0/973             | 0.72        | 0/1301           |
| 42  | DO    | 0.58         | 0/1006            | 0.80        | 0/1345           |
| 43  | CP    | 0.43         | 0/902             | 0.73        | 0/1209           |
| 43  | DP    | 0.47         | 0/910             | 0.73        | 0/1219           |
| 44  | CQ    | 0.41         | 0/929             | 0.71        | 0/1242           |
| 44  | DQ    | 0.48         | 0/929             | 0.72        | 0/1242           |
| 45  | CR    | 0.48         | 0/960             | 0.69        | 0/1278           |
| 45  | DR    | 0.62         | 0/960             | 0.76        | 0/1278           |
| 46  | CS    | 0.44         | 0/829             | 0.74        | 0/1107           |
| 46  | DS    | 0.55         | 0/829             | 0.78        | 0/1107           |
| 47  | CT    | 0.43         | 0/864             | 0.74        | 0/1156           |
| 47  | DT    | 0.55         | 0/864             | 0.75        | 0/1156           |
| 48  | CU    | 0.44         | 0/745             | 0.72        | 0/994            |
| 48  | DU    | 0.48         | 0/745             | 0.72        | 0/994            |
| 49  | CV    | 0.44         | 0/787             | 0.76        | 0/1051           |
| 49  | DV    | 0.49         | 0/787             | 0.77        | 0/1051           |
| 50  | CW    | 0.40         | 0/766             | 0.65        | 0/1025           |
| 50  | DW    | 0.50         | 0/766             | 0.69        | 0/1025           |
| 51  | CX    | 0.39         | 0/576             | 0.65        | 0/762            |
| 51  | DX    | 0.53         | 0/598             | 0.73        | 0/790            |
| 52  | CY    | 0.43         | 0/635             | 0.73        | 0/848            |
| 52  | DY    | 0.46         | 0/635             | 0.72        | 0/848            |
| 53  | CZ    | 0.42         | 0/502             | 0.61        | 0/667            |
| 53  | DZ    | 0.43         | 0/502             | 0.60        | 0/667            |
| 54  | DI    | 0.51         | 0/1037            | 0.74        | 1/1402 (0.1%)    |
| 55  | DA    | 1.27         | 148/69364 (0.2%)  | 0.97        | 26/108207 (0.0%) |
| All | All   | 0.98         | 212/309267 (0.1%) | 0.85        | 60/462210 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 3                   |
| 1   | BA    | 0                   | 4                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | AE    | 0                   | 1                   |
| 10  | BJ    | 0                   | 1                   |
| 31  | CA    | 0                   | 12                  |
| 55  | DA    | 0                   | 87                  |
| All | All   | 0                   | 108                 |

All (212) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | DA    | 1020 | A    | N3-C4   | 9.93  | 1.40        | 1.34     |
| 31  | CA    | 1936 | A    | N9-C4   | -9.29 | 1.32        | 1.37     |
| 31  | CA    | 2095 | A    | O5'-C5' | -9.00 | 1.28        | 1.42     |
| 55  | DA    | 539  | G    | N7-C5   | 7.77  | 1.44        | 1.39     |
| 55  | DA    | 12   | U    | C1'-N1  | 7.58  | 1.60        | 1.48     |
| 55  | DA    | 195  | A    | N9-C4   | 7.54  | 1.42        | 1.37     |
| 55  | DA    | 2097 | A    | O5'-C5' | -7.36 | 1.31        | 1.42     |
| 55  | DA    | 2050 | C    | N1-C6   | 7.35  | 1.41        | 1.37     |
| 31  | CA    | 769  | U    | C1'-N1  | 7.22  | 1.59        | 1.48     |
| 31  | CA    | 12   | U    | C1'-N1  | 7.06  | 1.59        | 1.48     |
| 55  | DA    | 2585 | U    | C1'-N1  | 7.03  | 1.59        | 1.48     |
| 55  | DA    | 1286 | A    | N3-C4   | 7.01  | 1.39        | 1.34     |
| 31  | CA    | 2425 | A    | C3'-O3' | 6.97  | 1.51        | 1.42     |
| 55  | DA    | 2060 | A    | N3-C4   | 6.87  | 1.39        | 1.34     |
| 55  | DA    | 2520 | C    | N1-C6   | 6.87  | 1.41        | 1.37     |
| 1   | BA    | 1493 | A    | C3'-O3' | 6.83  | 1.51        | 1.42     |
| 31  | CA    | 546  | U    | C1'-N1  | 6.76  | 1.58        | 1.48     |
| 55  | DA    | 484  | C    | C1'-N1  | 6.76  | 1.58        | 1.48     |
| 55  | DA    | 1665 | A    | N7-C5   | 6.69  | 1.43        | 1.39     |
| 1   | BA    | 1397 | C    | N1-C2   | 6.62  | 1.46        | 1.40     |
| 55  | DA    | 1787 | A    | N9-C4   | 6.58  | 1.41        | 1.37     |
| 1   | BA    | 5    | U    | C1'-N1  | 6.53  | 1.58        | 1.48     |
| 1   | BA    | 28   | A    | O5'-C5' | -6.51 | 1.32        | 1.42     |
| 55  | DA    | 2053 | G    | C6-N1   | 6.37  | 1.44        | 1.39     |
| 55  | DA    | 582  | A    | N9-C4   | 6.37  | 1.41        | 1.37     |
| 55  | DA    | 671  | C    | C1'-N1  | 6.33  | 1.58        | 1.48     |
| 55  | DA    | 1306 | C    | C1'-N1  | 6.29  | 1.58        | 1.48     |
| 31  | CA    | 2225 | A    | C3'-O3' | 6.25  | 1.50        | 1.42     |
| 55  | DA    | 2547 | A    | O5'-C5' | -6.23 | 1.32        | 1.42     |
| 55  | DA    | 998  | C    | C1'-N1  | 6.23  | 1.58        | 1.48     |
| 55  | DA    | 727  | A    | N3-C4   | 6.19  | 1.38        | 1.34     |
| 55  | DA    | 959  | A    | N3-C4   | 6.13  | 1.38        | 1.34     |
| 28  | DB    | 90   | C    | O5'-C5' | -6.12 | 1.33        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 28   | A    | O5'-C5' | -6.11 | 1.33        | 1.42     |
| 55  | DA    | 2867 | G    | C3'-O3' | 6.10  | 1.50        | 1.42     |
| 55  | DA    | 372  | G    | C3'-O3' | 6.08  | 1.50        | 1.42     |
| 55  | DA    | 31   | C    | N1-C6   | 6.07  | 1.40        | 1.37     |
| 55  | DA    | 2547 | A    | P-O5'   | -6.06 | 1.53        | 1.59     |
| 55  | DA    | 2023 | C    | N1-C6   | 6.03  | 1.40        | 1.37     |
| 55  | DA    | 2521 | C    | N1-C6   | 6.01  | 1.40        | 1.37     |
| 55  | DA    | 1000 | A    | N3-C4   | 6.00  | 1.38        | 1.34     |
| 1   | BA    | 1008 | U    | O5'-C5' | -6.00 | 1.33        | 1.42     |
| 55  | DA    | 578  | G    | N3-C4   | 5.98  | 1.39        | 1.35     |
| 55  | DA    | 102  | U    | N1-C2   | 5.97  | 1.44        | 1.38     |
| 55  | DA    | 579  | G    | C2'-C1' | -5.97 | 1.46        | 1.53     |
| 55  | DA    | 2717 | C    | N1-C6   | 5.96  | 1.40        | 1.37     |
| 55  | DA    | 1137 | G    | N3-C4   | 5.95  | 1.39        | 1.35     |
| 55  | DA    | 1294 | U    | O5'-C5' | -5.94 | 1.33        | 1.42     |
| 55  | DA    | 2297 | A    | O5'-C5' | -5.93 | 1.33        | 1.42     |
| 1   | AA    | 1397 | C    | N1-C6   | 5.93  | 1.40        | 1.37     |
| 55  | DA    | 1965 | C    | C1'-N1  | 5.92  | 1.57        | 1.48     |
| 55  | DA    | 972  | A    | C6-N6   | 5.90  | 1.38        | 1.33     |
| 31  | CA    | 253  | C    | C1'-N1  | 5.88  | 1.57        | 1.48     |
| 55  | DA    | 2044 | C    | N1-C6   | 5.88  | 1.40        | 1.37     |
| 55  | DA    | 575  | A    | N9-C4   | 5.87  | 1.41        | 1.37     |
| 1   | AA    | 5    | U    | C1'-N1  | 5.86  | 1.57        | 1.48     |
| 55  | DA    | 969  | G    | C8-N7   | -5.84 | 1.27        | 1.30     |
| 55  | DA    | 2756 | U    | C3'-O3' | 5.83  | 1.50        | 1.42     |
| 55  | DA    | 2036 | C    | N1-C6   | 5.81  | 1.40        | 1.37     |
| 55  | DA    | 2518 | A    | N9-C4   | 5.80  | 1.41        | 1.37     |
| 31  | CA    | 1306 | C    | C1'-N1  | 5.79  | 1.57        | 1.48     |
| 55  | DA    | 2447 | G    | N3-C4   | 5.79  | 1.39        | 1.35     |
| 55  | DA    | 2127 | G    | C3'-O3' | 5.79  | 1.50        | 1.42     |
| 31  | CA    | 2619 | C    | C1'-N1  | 5.78  | 1.57        | 1.48     |
| 55  | DA    | 1635 | A    | N3-C4   | 5.77  | 1.38        | 1.34     |
| 55  | DA    | 1164 | C    | N1-C6   | 5.76  | 1.40        | 1.37     |
| 55  | DA    | 2446 | G    | N3-C4   | 5.76  | 1.39        | 1.35     |
| 31  | CA    | 2579 | C    | C1'-N1  | 5.76  | 1.57        | 1.48     |
| 31  | CA    | 1788 | C    | C1'-N1  | 5.74  | 1.57        | 1.48     |
| 55  | DA    | 984  | A    | N3-C4   | 5.70  | 1.38        | 1.34     |
| 55  | DA    | 2766 | A    | N9-C4   | 5.69  | 1.41        | 1.37     |
| 55  | DA    | 457  | A    | N3-C4   | 5.69  | 1.38        | 1.34     |
| 55  | DA    | 838  | C    | N1-C6   | 5.68  | 1.40        | 1.37     |
| 1   | BA    | 485  | U    | N1-C2   | 5.66  | 1.43        | 1.38     |
| 1   | BA    | 290  | C    | C1'-N1  | 5.65  | 1.57        | 1.48     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | DA    | 821  | A    | N3-C4   | 5.65  | 1.38        | 1.34     |
| 55  | DA    | 1534 | U    | C1'-N1  | 5.65  | 1.57        | 1.48     |
| 55  | DA    | 1311 | G    | C6-N1   | 5.63  | 1.43        | 1.39     |
| 31  | CA    | 1314 | C    | C1'-N1  | 5.63  | 1.57        | 1.48     |
| 55  | DA    | 12   | U    | N1-C2   | 5.63  | 1.43        | 1.38     |
| 55  | DA    | 1267 | U    | C2-N3   | 5.63  | 1.41        | 1.37     |
| 55  | DA    | 744  | U    | N1-C6   | 5.60  | 1.43        | 1.38     |
| 55  | DA    | 2056 | G    | C6-N1   | 5.58  | 1.43        | 1.39     |
| 55  | DA    | 816  | C    | N1-C6   | 5.57  | 1.40        | 1.37     |
| 55  | DA    | 1660 | G    | O5'-C5' | -5.57 | 1.33        | 1.42     |
| 55  | DA    | 2426 | A    | N3-C4   | 5.57  | 1.38        | 1.34     |
| 55  | DA    | 823  | C    | N1-C6   | 5.56  | 1.40        | 1.37     |
| 55  | DA    | 990  | A    | N7-C5   | 5.55  | 1.42        | 1.39     |
| 31  | CA    | 1658 | C    | C1'-N1  | 5.54  | 1.57        | 1.48     |
| 55  | DA    | 1920 | C    | C1'-N1  | 5.54  | 1.57        | 1.48     |
| 55  | DA    | 959  | A    | N9-C4   | 5.52  | 1.41        | 1.37     |
| 55  | DA    | 508  | A    | N3-C4   | 5.52  | 1.38        | 1.34     |
| 55  | DA    | 1965 | C    | C3'-O3' | -5.52 | 1.34        | 1.42     |
| 55  | DA    | 2425 | A    | C3'-O3' | 5.52  | 1.49        | 1.42     |
| 55  | DA    | 2576 | G    | O3'-P   | -5.51 | 1.54        | 1.61     |
| 55  | DA    | 1021 | A    | N9-C4   | 5.51  | 1.41        | 1.37     |
| 55  | DA    | 2821 | A    | N3-C4   | 5.51  | 1.38        | 1.34     |
| 55  | DA    | 2444 | G    | N7-C5   | 5.50  | 1.42        | 1.39     |
| 55  | DA    | 739  | A    | N3-C4   | 5.50  | 1.38        | 1.34     |
| 55  | DA    | 613  | A    | N9-C4   | 5.50  | 1.41        | 1.37     |
| 31  | CA    | 2006 | C    | C1'-N1  | 5.49  | 1.56        | 1.48     |
| 55  | DA    | 196  | A    | N9-C4   | 5.48  | 1.41        | 1.37     |
| 55  | DA    | 809  | G    | N7-C5   | 5.48  | 1.42        | 1.39     |
| 1   | BA    | 575  | G    | C3'-O3' | 5.47  | 1.49        | 1.42     |
| 55  | DA    | 1265 | A    | N9-C4   | 5.46  | 1.41        | 1.37     |
| 31  | CA    | 2680 | U    | C3'-O3' | 5.46  | 1.49        | 1.42     |
| 55  | DA    | 2692 | G    | N3-C4   | 5.44  | 1.39        | 1.35     |
| 55  | DA    | 1133 | A    | O5'-C5' | -5.42 | 1.34        | 1.42     |
| 31  | CA    | 995  | C    | O5'-C5' | -5.42 | 1.34        | 1.42     |
| 31  | CA    | 2146 | C    | C3'-O3' | 5.42  | 1.49        | 1.42     |
| 55  | DA    | 1189 | A    | N9-C4   | 5.42  | 1.41        | 1.37     |
| 55  | DA    | 12   | U    | P-O5'   | 5.41  | 1.65        | 1.59     |
| 55  | DA    | 561  | G    | N3-C4   | 5.41  | 1.39        | 1.35     |
| 1   | AA    | 1203 | C    | C1'-N1  | 5.39  | 1.56        | 1.48     |
| 31  | CA    | 946  | C    | C1'-N1  | 5.39  | 1.56        | 1.48     |
| 55  | DA    | 810  | U    | N1-C2   | 5.39  | 1.43        | 1.38     |
| 31  | CA    | 2233 | U    | C1'-N1  | 5.39  | 1.56        | 1.48     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31  | CA    | 2823 | A    | C3'-O3' | 5.38  | 1.49        | 1.42     |
| 31  | CA    | 480  | A    | N9-C4   | 5.36  | 1.41        | 1.37     |
| 55  | DA    | 469  | G    | N3-C4   | 5.36  | 1.39        | 1.35     |
| 31  | CA    | 404  | A    | C3'-O3' | 5.35  | 1.49        | 1.42     |
| 31  | CA    | 1825 | U    | C1'-N1  | 5.34  | 1.56        | 1.48     |
| 31  | CA    | 451  | U    | C1'-N1  | 5.34  | 1.56        | 1.48     |
| 31  | CA    | 461  | C    | C1'-N1  | 5.34  | 1.56        | 1.48     |
| 55  | DA    | 819  | A    | N3-C4   | 5.34  | 1.38        | 1.34     |
| 55  | DA    | 2036 | C    | C1'-N1  | 5.31  | 1.56        | 1.48     |
| 55  | DA    | 613  | A    | C3'-O3' | 5.31  | 1.49        | 1.42     |
| 1   | BA    | 842  | U    | C3'-O3' | 5.30  | 1.49        | 1.42     |
| 55  | DA    | 2077 | A    | N3-C4   | 5.30  | 1.38        | 1.34     |
| 55  | DA    | 653  | U    | C1'-N1  | 5.30  | 1.56        | 1.48     |
| 31  | CA    | 557  | C    | C1'-N1  | 5.30  | 1.56        | 1.48     |
| 55  | DA    | 1030 | C    | N1-C6   | 5.29  | 1.40        | 1.37     |
| 55  | DA    | 962  | G    | N3-C4   | 5.29  | 1.39        | 1.35     |
| 31  | CA    | 1629 | U    | C1'-N1  | 5.29  | 1.56        | 1.48     |
| 55  | DA    | 271  | G    | C3'-O3' | 5.28  | 1.49        | 1.42     |
| 31  | CA    | 2723 | C    | C1'-N1  | 5.28  | 1.56        | 1.48     |
| 55  | DA    | 1274 | A    | N7-C5   | -5.26 | 1.36        | 1.39     |
| 31  | CA    | 653  | U    | C1'-N1  | 5.26  | 1.56        | 1.48     |
| 55  | DA    | 2585 | U    | N1-C2   | 5.25  | 1.43        | 1.38     |
| 55  | DA    | 2730 | C    | N1-C6   | 5.24  | 1.40        | 1.37     |
| 31  | CA    | 198  | C    | C1'-N1  | 5.24  | 1.56        | 1.48     |
| 31  | CA    | 1771 | C    | C1'-N1  | 5.22  | 1.56        | 1.48     |
| 31  | CA    | 2646 | C    | C1'-N1  | 5.22  | 1.56        | 1.48     |
| 55  | DA    | 918  | A    | N3-C4   | 5.22  | 1.38        | 1.34     |
| 55  | DA    | 577  | G    | N3-C4   | 5.22  | 1.39        | 1.35     |
| 1   | AA    | 575  | G    | C3'-O3' | 5.22  | 1.49        | 1.42     |
| 55  | DA    | 1268 | A    | N3-C4   | 5.22  | 1.38        | 1.34     |
| 55  | DA    | 2288 | A    | N3-C4   | 5.22  | 1.38        | 1.34     |
| 55  | DA    | 195  | A    | N3-C4   | 5.21  | 1.38        | 1.34     |
| 55  | DA    | 1584 | U    | C1'-N1  | 5.21  | 1.56        | 1.48     |
| 55  | DA    | 264  | C    | N1-C2   | 5.21  | 1.45        | 1.40     |
| 55  | DA    | 27   | G    | C6-N1   | 5.21  | 1.43        | 1.39     |
| 1   | BA    | 291  | U    | C1'-N1  | 5.21  | 1.56        | 1.48     |
| 55  | DA    | 2521 | C    | C1'-N1  | 5.20  | 1.56        | 1.48     |
| 55  | DA    | 911  | A    | N3-C4   | 5.20  | 1.38        | 1.34     |
| 55  | DA    | 2901 | C    | C1'-N1  | 5.20  | 1.56        | 1.48     |
| 55  | DA    | 1664 | A    | N9-C4   | 5.19  | 1.41        | 1.37     |
| 55  | DA    | 2211 | A    | C3'-O3' | 5.18  | 1.49        | 1.42     |
| 55  | DA    | 512  | G    | N9-C4   | 5.17  | 1.42        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | DA    | 581  | C    | C1'-N1  | 5.17  | 1.56        | 1.48     |
| 1   | AA    | 15   | G    | N3-C4   | 5.17  | 1.39        | 1.35     |
| 31  | CA    | 1971 | U    | C1'-N1  | 5.16  | 1.56        | 1.48     |
| 55  | DA    | 1675 | C    | N1-C6   | 5.16  | 1.40        | 1.37     |
| 55  | DA    | 1776 | G    | O5'-C5' | -5.16 | 1.34        | 1.42     |
| 55  | DA    | 1270 | C    | N1-C6   | 5.15  | 1.40        | 1.37     |
| 55  | DA    | 2354 | C    | O5'-C5' | -5.15 | 1.34        | 1.42     |
| 55  | DA    | 2033 | A    | P-O5'   | 5.15  | 1.64        | 1.59     |
| 55  | DA    | 353  | C    | C1'-N1  | 5.14  | 1.56        | 1.48     |
| 55  | DA    | 465  | G    | N3-C4   | 5.14  | 1.39        | 1.35     |
| 55  | DA    | 1607 | C    | N1-C6   | 5.13  | 1.40        | 1.37     |
| 55  | DA    | 2273 | A    | N3-C4   | 5.13  | 1.38        | 1.34     |
| 31  | CA    | 2465 | C    | C1'-N1  | 5.13  | 1.56        | 1.48     |
| 31  | CA    | 2756 | U    | C3'-O3' | 5.13  | 1.49        | 1.42     |
| 55  | DA    | 672  | C    | N1-C6   | 5.12  | 1.40        | 1.37     |
| 55  | DA    | 2581 | G    | C3'-O3' | 5.12  | 1.49        | 1.42     |
| 55  | DA    | 562  | U    | N1-C6   | 5.12  | 1.42        | 1.38     |
| 55  | DA    | 792  | A    | N3-C4   | 5.12  | 1.38        | 1.34     |
| 55  | DA    | 1704 | C    | C1'-N1  | 5.12  | 1.56        | 1.48     |
| 55  | DA    | 1965 | C    | O5'-C5' | -5.12 | 1.34        | 1.42     |
| 55  | DA    | 1020 | A    | C6-N1   | 5.12  | 1.39        | 1.35     |
| 55  | DA    | 2496 | C    | O5'-C5' | -5.11 | 1.34        | 1.42     |
| 1   | AA    | 290  | C    | C1'-N1  | 5.11  | 1.56        | 1.48     |
| 31  | CA    | 672  | C    | C1'-N1  | 5.11  | 1.56        | 1.48     |
| 55  | DA    | 2406 | A    | P-O5'   | 5.11  | 1.64        | 1.59     |
| 55  | DA    | 2427 | C    | N1-C6   | 5.11  | 1.40        | 1.37     |
| 55  | DA    | 2471 | A    | N3-C4   | 5.10  | 1.38        | 1.34     |
| 55  | DA    | 585  | G    | N9-C4   | 5.09  | 1.42        | 1.38     |
| 31  | CA    | 2044 | C    | C1'-N1  | 5.08  | 1.56        | 1.48     |
| 55  | DA    | 1999 | C    | N1-C6   | 5.08  | 1.40        | 1.37     |
| 55  | DA    | 2455 | G    | C3'-O3' | -5.08 | 1.35        | 1.42     |
| 31  | CA    | 2354 | C    | C1'-N1  | 5.08  | 1.56        | 1.48     |
| 31  | CA    | 2901 | C    | C1'-N1  | 5.07  | 1.56        | 1.48     |
| 31  | CA    | 1704 | C    | C1'-N1  | 5.07  | 1.56        | 1.48     |
| 55  | DA    | 684  | G    | N3-C4   | 5.07  | 1.39        | 1.35     |
| 55  | DA    | 2708 | G    | N3-C4   | 5.06  | 1.39        | 1.35     |
| 55  | DA    | 2301 | C    | C1'-N1  | 5.06  | 1.56        | 1.48     |
| 55  | DA    | 1437 | C    | O5'-C5' | -5.05 | 1.34        | 1.42     |
| 1   | AA    | 209  | U    | C3'-O3' | 5.04  | 1.49        | 1.42     |
| 55  | DA    | 1253 | A    | O5'-C5' | -5.04 | 1.34        | 1.42     |
| 55  | DA    | 114  | U    | C1'-N1  | 5.04  | 1.56        | 1.48     |
| 55  | DA    | 1284 | A    | N3-C4   | 5.04  | 1.37        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31  | CA    | 692  | C    | C1'-N1  | 5.04  | 1.56        | 1.48     |
| 55  | DA    | 251  | A    | N3-C4   | 5.04  | 1.37        | 1.34     |
| 1   | AA    | 843  | U    | C1'-N1  | 5.03  | 1.56        | 1.48     |
| 55  | DA    | 2585 | U    | C3'-O3' | 5.03  | 1.49        | 1.42     |
| 55  | DA    | 574  | A    | O5'-C5' | -5.02 | 1.34        | 1.42     |
| 55  | DA    | 2061 | G    | N3-C4   | 5.02  | 1.39        | 1.35     |
| 31  | CA    | 20   | C    | C1'-N1  | 5.01  | 1.56        | 1.48     |
| 55  | DA    | 1644 | C    | C1'-N1  | 5.01  | 1.56        | 1.48     |
| 55  | DA    | 1331 | G    | N3-C4   | 5.01  | 1.39        | 1.35     |
| 55  | DA    | 1637 | A    | N7-C5   | 5.01  | 1.42        | 1.39     |
| 31  | CA    | 2215 | C    | C1'-N1  | 5.00  | 1.56        | 1.48     |

All (60) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | CB    | 15   | A    | O4'-C1'-N9  | 10.06 | 116.25      | 108.20   |
| 55  | DA    | 512  | G    | O4'-C1'-N9  | 8.55  | 115.04      | 108.20   |
| 1   | AA    | 413  | G    | C1'-O4'-C4' | -8.26 | 103.29      | 109.90   |
| 55  | DA    | 784  | G    | P-O3'-C3'   | 7.86  | 129.13      | 119.70   |
| 41  | CN    | 69   | PRO  | C-N-CA      | 7.39  | 140.18      | 121.70   |
| 55  | DA    | 1936 | A    | O4'-C1'-N9  | 7.18  | 113.94      | 108.20   |
| 1   | AA    | 1    | A    | OP1-P-OP2   | -7.13 | 108.90      | 119.60   |
| 55  | DA    | 2820 | A    | P-O3'-C3'   | 7.09  | 128.21      | 119.70   |
| 55  | DA    | 892  | A    | OP1-P-OP2   | -7.05 | 109.03      | 119.60   |
| 54  | DI    | 132  | TYR  | C-N-CA      | 7.01  | 139.24      | 121.70   |
| 31  | CA    | 892  | A    | OP1-P-OP2   | -6.96 | 109.17      | 119.60   |
| 55  | DA    | 1    | G    | OP1-P-OP2   | -6.87 | 109.29      | 119.60   |
| 1   | BA    | 1362 | A    | C1'-O4'-C4' | -6.87 | 104.40      | 109.90   |
| 31  | CA    | 974  | G    | N9-C1'-C2'  | 6.74  | 122.76      | 114.00   |
| 1   | BA    | 2    | A    | OP1-P-OP2   | -6.72 | 109.52      | 119.60   |
| 31  | CA    | 271  | G    | P-O3'-C3'   | 6.49  | 127.49      | 119.70   |
| 55  | DA    | 271  | G    | P-O3'-C3'   | 6.46  | 127.45      | 119.70   |
| 1   | AA    | 413  | G    | O4'-C1'-N9  | 6.44  | 113.35      | 108.20   |
| 55  | DA    | 2848 | G    | O4'-C1'-N9  | 6.20  | 113.16      | 108.20   |
| 55  | DA    | 1311 | G    | O4'-C1'-N9  | 6.05  | 113.04      | 108.20   |
| 31  | CA    | 2425 | A    | P-O3'-C3'   | 5.92  | 126.80      | 119.70   |
| 31  | CA    | 451  | U    | C1'-O4'-C4' | -5.89 | 105.19      | 109.90   |
| 1   | BA    | 842  | U    | P-O3'-C3'   | 5.84  | 126.71      | 119.70   |
| 31  | CA    | 512  | G    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 55  | DA    | 1379 | U    | P-O3'-C3'   | 5.81  | 126.67      | 119.70   |
| 31  | CA    | 784  | G    | P-O3'-C3'   | 5.76  | 126.61      | 119.70   |
| 1   | BA    | 485  | U    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 40  | DM    | 60   | ARG  | CG-CD-NE    | 5.73  | 123.84      | 111.80   |
| 31  | CA    | 1379 | U    | P-O3'-C3'   | 5.71  | 126.55      | 119.70   |
| 55  | DA    | 704  | G    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 55  | DA    | 242  | G    | C3'-C2'-C1' | -5.56 | 97.05       | 101.50   |
| 55  | DA    | 2406 | A    | C5'-C4'-O4' | -5.56 | 102.42      | 109.10   |
| 55  | DA    | 1434 | A    | O4'-C1'-N9  | 5.42  | 112.53      | 108.20   |
| 55  | DA    | 1165 | A    | O4'-C1'-N9  | 5.40  | 112.52      | 108.20   |
| 1   | BA    | 1397 | C    | C2-N1-C1'   | 5.39  | 124.72      | 118.80   |
| 55  | DA    | 27   | G    | O4'-C1'-N9  | 5.36  | 112.49      | 108.20   |
| 29  | DC    | 156  | ARG  | CB-CG-CD    | -5.34 | 97.71       | 111.60   |
| 31  | CA    | 2225 | A    | P-O3'-C3'   | 5.31  | 126.08      | 119.70   |
| 31  | CA    | 2095 | A    | C5'-C4'-C3' | -5.28 | 107.55      | 116.00   |
| 55  | DA    | 2280 | G    | C4'-C3'-C2' | -5.27 | 97.33       | 102.60   |
| 31  | CA    | 2035 | G    | C1'-O4'-C4' | -5.26 | 105.69      | 109.90   |
| 55  | DA    | 2645 | G    | O4'-C1'-N9  | 5.23  | 112.39      | 108.20   |
| 31  | CA    | 704  | G    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 31  | CA    | 2825 | G    | O4'-C1'-N9  | 5.19  | 112.35      | 108.20   |
| 31  | CA    | 242  | G    | C3'-C2'-C1' | -5.18 | 97.35       | 101.50   |
| 40  | CM    | 68   | SER  | C-N-CA      | 5.18  | 134.66      | 121.70   |
| 31  | CA    | 2406 | A    | C5'-C4'-O4' | 5.18  | 115.31      | 109.10   |
| 55  | DA    | 512  | G    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |
| 55  | DA    | 479  | A    | C3'-C2'-C1' | -5.17 | 97.36       | 101.50   |
| 55  | DA    | 807  | U    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 55  | DA    | 2048 | G    | C8-N9-C4    | -5.15 | 104.34      | 106.40   |
| 28  | CB    | 89   | U    | O4'-C1'-N1  | 5.13  | 112.31      | 108.20   |
| 55  | DA    | 1238 | G    | C4'-C3'-C2' | -5.13 | 97.47       | 102.60   |
| 1   | AA    | 841  | C    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 1   | AA    | 890  | G    | C3'-C2'-C1' | -5.08 | 97.44       | 101.50   |
| 55  | DA    | 1997 | C    | C4'-C3'-C2' | -5.08 | 97.52       | 102.60   |
| 31  | CA    | 2447 | G    | C3'-C2'-C1' | -5.04 | 97.46       | 101.50   |
| 55  | DA    | 1936 | A    | C1'-O4'-C4' | -5.03 | 105.88      | 109.90   |
| 55  | DA    | 2447 | G    | C3'-C2'-C1' | -5.02 | 97.48       | 101.50   |
| 31  | CA    | 974  | G    | C3'-C2'-C1' | -5.01 | 97.49       | 101.50   |

There are no chirality outliers.

All (108) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1432 | G    | Sidechain |
| 1   | AA    | 362  | G    | Sidechain |
| 1   | AA    | 898  | G    | Sidechain |
| 5   | AE    | 82   | GLN  | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | BA    | 1432 | G    | Sidechain |
| 1   | BA    | 362  | G    | Sidechain |
| 1   | BA    | 575  | G    | Sidechain |
| 1   | BA    | 898  | G    | Sidechain |
| 10  | BJ    | 37   | ARG  | Mainchain |
| 31  | CA    | 1693 | U    | Sidechain |
| 31  | CA    | 1777 | U    | Sidechain |
| 31  | CA    | 1936 | A    | Sidechain |
| 31  | CA    | 1937 | A    | Sidechain |
| 31  | CA    | 2267 | A    | Sidechain |
| 31  | CA    | 2638 | G    | Sidechain |
| 31  | CA    | 2732 | G    | Sidechain |
| 31  | CA    | 463  | G    | Sidechain |
| 31  | CA    | 481  | G    | Sidechain |
| 31  | CA    | 704  | G    | Sidechain |
| 31  | CA    | 726  | G    | Sidechain |
| 31  | CA    | 805  | G    | Sidechain |
| 55  | DA    | 1009 | A    | Sidechain |
| 55  | DA    | 1142 | A    | Sidechain |
| 55  | DA    | 1236 | G    | Sidechain |
| 55  | DA    | 1253 | A    | Sidechain |
| 55  | DA    | 1283 | G    | Sidechain |
| 55  | DA    | 1311 | G    | Sidechain |
| 55  | DA    | 1324 | G    | Sidechain |
| 55  | DA    | 1343 | G    | Sidechain |
| 55  | DA    | 1425 | G    | Sidechain |
| 55  | DA    | 15   | G    | Sidechain |
| 55  | DA    | 1631 | G    | Sidechain |
| 55  | DA    | 1645 | G    | Sidechain |
| 55  | DA    | 1666 | G    | Sidechain |
| 55  | DA    | 1667 | G    | Sidechain |
| 55  | DA    | 1672 | A    | Sidechain |
| 55  | DA    | 1681 | G    | Sidechain |
| 55  | DA    | 1682 | G    | Sidechain |
| 55  | DA    | 1693 | U    | Sidechain |
| 55  | DA    | 1753 | G    | Sidechain |
| 55  | DA    | 1761 | C    | Sidechain |
| 55  | DA    | 1779 | U    | Sidechain |
| 55  | DA    | 1802 | A    | Sidechain |
| 55  | DA    | 1938 | A    | Sidechain |
| 55  | DA    | 2037 | A    | Sidechain |
| 55  | DA    | 2048 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 55  | DA    | 2074 | U    | Sidechain |
| 55  | DA    | 2078 | C    | Sidechain |
| 55  | DA    | 221  | A    | Sidechain |
| 55  | DA    | 2250 | G    | Sidechain |
| 55  | DA    | 2266 | A    | Sidechain |
| 55  | DA    | 2267 | A    | Sidechain |
| 55  | DA    | 2282 | G    | Sidechain |
| 55  | DA    | 2328 | A    | Sidechain |
| 55  | DA    | 2375 | G    | Sidechain |
| 55  | DA    | 2382 | G    | Sidechain |
| 55  | DA    | 2405 | G    | Sidechain |
| 55  | DA    | 2468 | A    | Sidechain |
| 55  | DA    | 2481 | G    | Sidechain |
| 55  | DA    | 2497 | A    | Sidechain |
| 55  | DA    | 250  | G    | Sidechain |
| 55  | DA    | 2516 | A    | Sidechain |
| 55  | DA    | 2517 | C    | Sidechain |
| 55  | DA    | 2529 | G    | Sidechain |
| 55  | DA    | 2564 | A    | Sidechain |
| 55  | DA    | 2566 | A    | Sidechain |
| 55  | DA    | 2581 | G    | Sidechain |
| 55  | DA    | 2582 | G    | Sidechain |
| 55  | DA    | 2595 | G    | Sidechain |
| 55  | DA    | 2597 | G    | Sidechain |
| 55  | DA    | 2638 | G    | Sidechain |
| 55  | DA    | 2645 | G    | Sidechain |
| 55  | DA    | 2688 | G    | Sidechain |
| 55  | DA    | 27   | G    | Sidechain |
| 55  | DA    | 2727 | A    | Sidechain |
| 55  | DA    | 2732 | G    | Sidechain |
| 55  | DA    | 2848 | G    | Sidechain |
| 55  | DA    | 307  | G    | Sidechain |
| 55  | DA    | 308  | G    | Sidechain |
| 55  | DA    | 395  | U    | Sidechain |
| 55  | DA    | 452  | G    | Sidechain |
| 55  | DA    | 463  | G    | Sidechain |
| 55  | DA    | 464  | U    | Sidechain |
| 55  | DA    | 481  | G    | Sidechain |
| 55  | DA    | 512  | G    | Sidechain |
| 55  | DA    | 555  | G    | Sidechain |
| 55  | DA    | 575  | A    | Sidechain |
| 55  | DA    | 577  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 55  | DA    | 58  | G    | Sidechain |
| 55  | DA    | 630 | G    | Sidechain |
| 55  | DA    | 675 | A    | Sidechain |
| 55  | DA    | 690 | G    | Sidechain |
| 55  | DA    | 700 | G    | Sidechain |
| 55  | DA    | 704 | G    | Sidechain |
| 55  | DA    | 726 | G    | Sidechain |
| 55  | DA    | 727 | A    | Sidechain |
| 55  | DA    | 728 | G    | Sidechain |
| 55  | DA    | 748 | G    | Sidechain |
| 55  | DA    | 774 | G    | Sidechain |
| 55  | DA    | 775 | G    | Sidechain |
| 55  | DA    | 800 | A    | Sidechain |
| 55  | DA    | 805 | G    | Sidechain |
| 55  | DA    | 858 | G    | Sidechain |
| 55  | DA    | 910 | A    | Sidechain |
| 55  | DA    | 956 | G    | Sidechain |
| 55  | DA    | 959 | A    | Sidechain |
| 55  | DA    | 980 | A    | Sidechain |
| 55  | DA    | 984 | A    | Sidechain |

## 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   | AA    | 32930 | 0        | 16591    | 90      | 0            |
| 1   | BA    | 32908 | 0        | 16580    | 97      | 0            |
| 2   | AB    | 1753  | 0        | 1780     | 10      | 0            |
| 2   | BB    | 1753  | 0        | 1780     | 15      | 0            |
| 3   | AC    | 1625  | 0        | 1696     | 14      | 0            |
| 3   | BC    | 1625  | 0        | 1696     | 18      | 0            |
| 4   | AD    | 1643  | 0        | 1707     | 13      | 0            |
| 4   | BD    | 1643  | 0        | 1707     | 17      | 0            |
| 5   | AE    | 1144  | 0        | 1185     | 15      | 0            |
| 5   | BE    | 1105  | 0        | 1148     | 30      | 0            |
| 6   | AF    | 862   | 0        | 864      | 7       | 0            |
| 6   | BF    | 817   | 0        | 808      | 9       | 0            |
| 7   | AG    | 1182  | 0        | 1238     | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | BG    | 1182  | 0        | 1238     | 4       | 0            |
| 8   | AH    | 979   | 0        | 1031     | 8       | 0            |
| 8   | BH    | 979   | 0        | 1031     | 4       | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 6       | 0            |
| 9   | BI    | 1022  | 0        | 1070     | 6       | 0            |
| 10  | AJ    | 796   | 0        | 836      | 11      | 0            |
| 10  | BJ    | 787   | 0        | 828      | 10      | 0            |
| 11  | AK    | 877   | 0        | 887      | 14      | 0            |
| 11  | BK    | 877   | 0        | 887      | 17      | 0            |
| 12  | AL    | 957   | 0        | 1017     | 7       | 0            |
| 12  | BL    | 957   | 0        | 1017     | 9       | 0            |
| 13  | AM    | 884   | 0        | 941      | 11      | 0            |
| 13  | BM    | 884   | 0        | 941      | 11      | 0            |
| 14  | AN    | 805   | 0        | 844      | 8       | 0            |
| 14  | BN    | 805   | 0        | 844      | 8       | 0            |
| 15  | AO    | 714   | 0        | 734      | 1       | 0            |
| 15  | BO    | 714   | 0        | 734      | 0       | 0            |
| 16  | AP    | 649   | 0        | 666      | 3       | 0            |
| 16  | BP    | 649   | 0        | 666      | 5       | 0            |
| 17  | AQ    | 649   | 0        | 691      | 6       | 0            |
| 17  | BQ    | 649   | 0        | 691      | 5       | 0            |
| 18  | AR    | 456   | 0        | 478      | 5       | 0            |
| 18  | BR    | 456   | 0        | 478      | 3       | 0            |
| 19  | AS    | 638   | 0        | 665      | 7       | 0            |
| 19  | BS    | 638   | 0        | 665      | 8       | 0            |
| 20  | AT    | 670   | 0        | 719      | 2       | 0            |
| 20  | BT    | 665   | 0        | 714      | 8       | 0            |
| 21  | AU    | 465   | 0        | 491      | 2       | 0            |
| 21  | BU    | 465   | 0        | 491      | 2       | 0            |
| 22  | C1    | 444   | 0        | 458      | 18      | 0            |
| 22  | D1    | 444   | 0        | 458      | 13      | 0            |
| 23  | C2    | 409   | 0        | 440      | 5       | 0            |
| 23  | D2    | 414   | 0        | 442      | 5       | 0            |
| 24  | C3    | 377   | 0        | 418      | 17      | 0            |
| 24  | D3    | 377   | 0        | 418      | 6       | 0            |
| 25  | C4    | 504   | 0        | 572      | 13      | 0            |
| 25  | D4    | 504   | 0        | 572      | 12      | 0            |
| 26  | C5    | 302   | 0        | 340      | 9       | 0            |
| 26  | D5    | 302   | 0        | 340      | 2       | 0            |
| 27  | C0    | 449   | 0        | 488      | 4       | 0            |
| 27  | D0    | 463   | 0        | 504      | 1       | 0            |
| 28  | CB    | 2529  | 0        | 1281     | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | DB    | 2569  | 0        | 1301     | 5       | 0            |
| 29  | CC    | 2082  | 0        | 2154     | 17      | 0            |
| 29  | DC    | 2082  | 0        | 2154     | 11      | 0            |
| 30  | CD    | 1565  | 0        | 1616     | 16      | 0            |
| 31  | CA    | 62229 | 0        | 31318    | 236     | 0            |
| 32  | DD    | 1576  | 0        | 1627     | 16      | 0            |
| 33  | CE    | 1552  | 0        | 1619     | 14      | 0            |
| 33  | DE    | 1552  | 0        | 1619     | 11      | 0            |
| 34  | CF    | 1410  | 0        | 1444     | 16      | 0            |
| 34  | DF    | 1410  | 0        | 1444     | 12      | 0            |
| 35  | CG    | 1323  | 0        | 1371     | 9       | 0            |
| 35  | DG    | 1323  | 0        | 1371     | 9       | 0            |
| 36  | CH    | 1110  | 0        | 1148     | 8       | 0            |
| 36  | DH    | 1110  | 0        | 1148     | 6       | 0            |
| 37  | CJ    | 979   | 0        | 1028     | 4       | 0            |
| 37  | DJ    | 979   | 0        | 1028     | 5       | 0            |
| 38  | CK    | 1129  | 0        | 1162     | 9       | 0            |
| 38  | DK    | 1129  | 0        | 1162     | 5       | 0            |
| 39  | CL    | 938   | 0        | 1012     | 8       | 0            |
| 39  | DL    | 946   | 0        | 1023     | 6       | 0            |
| 40  | CM    | 1053  | 0        | 1129     | 19      | 0            |
| 40  | DM    | 1053  | 0        | 1129     | 15      | 0            |
| 41  | CN    | 1075  | 0        | 1154     | 5       | 0            |
| 41  | DN    | 1092  | 0        | 1177     | 7       | 0            |
| 42  | CO    | 960   | 0        | 1000     | 5       | 0            |
| 42  | DO    | 993   | 0        | 1034     | 5       | 0            |
| 43  | CP    | 892   | 0        | 923      | 7       | 0            |
| 43  | DP    | 900   | 0        | 935      | 9       | 0            |
| 44  | CQ    | 917   | 0        | 962      | 7       | 0            |
| 44  | DQ    | 917   | 0        | 962      | 7       | 0            |
| 45  | CR    | 947   | 0        | 1019     | 13      | 0            |
| 45  | DR    | 947   | 0        | 1019     | 9       | 0            |
| 46  | CS    | 816   | 0        | 839      | 8       | 0            |
| 46  | DS    | 816   | 0        | 839      | 5       | 0            |
| 47  | CT    | 857   | 0        | 922      | 12      | 0            |
| 47  | DT    | 857   | 0        | 922      | 10      | 0            |
| 48  | CU    | 739   | 0        | 807      | 10      | 0            |
| 48  | DU    | 739   | 0        | 807      | 4       | 0            |
| 49  | CV    | 779   | 0        | 831      | 8       | 0            |
| 49  | DV    | 779   | 0        | 831      | 5       | 0            |
| 50  | CW    | 753   | 0        | 780      | 5       | 0            |
| 50  | DW    | 753   | 0        | 780      | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 51  | CX    | 569   | 0        | 581      | 1       | 0            |
| 51  | DX    | 591   | 0        | 606      | 5       | 0            |
| 52  | CY    | 625   | 0        | 652      | 8       | 0            |
| 52  | DY    | 625   | 0        | 652      | 4       | 0            |
| 53  | CZ    | 501   | 0        | 531      | 2       | 0            |
| 53  | DZ    | 501   | 0        | 531      | 1       | 0            |
| 54  | DI    | 1023  | 0        | 1052     | 19      | 0            |
| 55  | DA    | 62423 | 0        | 31411    | 173     | 0            |
| 56  | AA    | 71    | 0        | 0        | 0       | 0            |
| 56  | BA    | 43    | 0        | 0        | 0       | 0            |
| 56  | CA    | 156   | 0        | 0        | 0       | 0            |
| 56  | CB    | 3     | 0        | 0        | 0       | 0            |
| 56  | DA    | 182   | 0        | 0        | 0       | 0            |
| 56  | DB    | 9     | 0        | 0        | 0       | 0            |
| 56  | DD    | 2     | 0        | 0        | 0       | 0            |
| 56  | DM    | 1     | 0        | 0        | 0       | 0            |
| 56  | DR    | 2     | 0        | 0        | 0       | 0            |
| 57  | AA    | 13    | 0        | 18       | 1       | 0            |
| 57  | BA    | 13    | 0        | 18       | 0       | 0            |
| 57  | DA    | 26    | 0        | 36       | 2       | 0            |
| 57  | DQ    | 13    | 0        | 18       | 0       | 0            |
| 57  | DR    | 13    | 0        | 18       | 5       | 0            |
| 57  | DS    | 13    | 0        | 18       | 1       | 0            |
| 58  | AA    | 16    | 0        | 28       | 0       | 0            |
| 58  | DA    | 40    | 0        | 70       | 5       | 0            |
| 58  | DE    | 16    | 0        | 28       | 0       | 0            |
| 58  | DK    | 8     | 0        | 14       | 0       | 0            |
| 58  | DN    | 8     | 0        | 14       | 1       | 0            |
| 58  | DS    | 8     | 0        | 14       | 0       | 0            |
| 58  | DT    | 16    | 0        | 28       | 0       | 0            |
| 59  | AA    | 24    | 0        | 48       | 0       | 0            |
| 59  | DA    | 72    | 0        | 144      | 10      | 0            |
| 60  | AA    | 42    | 0        | 38       | 0       | 0            |
| 60  | BA    | 42    | 0        | 38       | 0       | 0            |
| 61  | AB    | 1     | 0        | 0        | 0       | 0            |
| 61  | C5    | 1     | 0        | 0        | 0       | 0            |
| 61  | D5    | 1     | 0        | 0        | 0       | 0            |
| 62  | AL    | 7     | 0        | 10       | 0       | 0            |
| 62  | D1    | 7     | 0        | 10       | 1       | 0            |
| 62  | D3    | 7     | 0        | 10       | 2       | 0            |
| 62  | DA    | 35    | 0        | 50       | 1       | 0            |
| 62  | DL    | 7     | 0        | 10       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 62  | DP    | 7     | 0        | 10       | 1       | 0            |
| 62  | DQ    | 7     | 0        | 10       | 0       | 0            |
| 63  | D1    | 4     | 0        | 6        | 0       | 0            |
| 63  | DA    | 36    | 0        | 54       | 2       | 0            |
| 63  | DB    | 8     | 0        | 12       | 1       | 0            |
| 64  | D1    | 10    | 0        | 14       | 2       | 0            |
| 64  | D3    | 10    | 0        | 14       | 0       | 0            |
| 64  | DA    | 40    | 0        | 56       | 5       | 0            |
| 64  | DD    | 10    | 0        | 14       | 2       | 0            |
| 64  | DS    | 10    | 0        | 14       | 0       | 0            |
| 64  | DU    | 10    | 0        | 14       | 1       | 0            |
| 65  | DA    | 40    | 0        | 76       | 4       | 0            |
| 66  | DA    | 32    | 0        | 44       | 0       | 0            |
| 67  | DA    | 12    | 0        | 12       | 0       | 0            |
| 68  | DA    | 11    | 0        | 5        | 0       | 0            |
| 69  | DA    | 8     | 0        | 12       | 1       | 0            |
| 70  | AA    | 507   | 0        | 0        | 0       | 0            |
| 70  | AC    | 4     | 0        | 0        | 0       | 0            |
| 70  | AD    | 2     | 0        | 0        | 0       | 0            |
| 70  | AE    | 4     | 0        | 0        | 0       | 0            |
| 70  | AF    | 1     | 0        | 0        | 0       | 0            |
| 70  | AG    | 1     | 0        | 0        | 0       | 0            |
| 70  | AH    | 1     | 0        | 0        | 0       | 0            |
| 70  | AJ    | 2     | 0        | 0        | 0       | 0            |
| 70  | AK    | 5     | 0        | 0        | 0       | 0            |
| 70  | AL    | 8     | 0        | 0        | 0       | 0            |
| 70  | AM    | 4     | 0        | 0        | 1       | 0            |
| 70  | AN    | 5     | 0        | 0        | 1       | 0            |
| 70  | AO    | 2     | 0        | 0        | 0       | 0            |
| 70  | AP    | 2     | 0        | 0        | 0       | 0            |
| 70  | AR    | 1     | 0        | 0        | 0       | 0            |
| 70  | AS    | 1     | 0        | 0        | 0       | 0            |
| 70  | AT    | 2     | 0        | 0        | 0       | 0            |
| 70  | AU    | 3     | 0        | 0        | 0       | 0            |
| 70  | BA    | 287   | 0        | 0        | 1       | 0            |
| 70  | BD    | 13    | 0        | 0        | 0       | 0            |
| 70  | BE    | 1     | 0        | 0        | 0       | 0            |
| 70  | BF    | 1     | 0        | 0        | 0       | 0            |
| 70  | BK    | 1     | 0        | 0        | 0       | 0            |
| 70  | BL    | 3     | 0        | 0        | 0       | 0            |
| 70  | BN    | 2     | 0        | 0        | 0       | 0            |
| 70  | BO    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 70  | BP    | 3     | 0        | 0        | 0       | 0            |
| 70  | BR    | 1     | 0        | 0        | 0       | 0            |
| 70  | BT    | 4     | 0        | 0        | 0       | 0            |
| 70  | BU    | 2     | 0        | 0        | 0       | 0            |
| 70  | C3    | 3     | 0        | 0        | 1       | 0            |
| 70  | C4    | 1     | 0        | 0        | 0       | 0            |
| 70  | CA    | 694   | 0        | 0        | 1       | 0            |
| 70  | CB    | 13    | 0        | 0        | 0       | 0            |
| 70  | CC    | 10    | 0        | 0        | 0       | 0            |
| 70  | CD    | 5     | 0        | 0        | 0       | 0            |
| 70  | CE    | 6     | 0        | 0        | 0       | 0            |
| 70  | CL    | 1     | 0        | 0        | 0       | 0            |
| 70  | CM    | 3     | 0        | 0        | 0       | 0            |
| 70  | CO    | 1     | 0        | 0        | 0       | 0            |
| 70  | CU    | 3     | 0        | 0        | 0       | 0            |
| 70  | CV    | 1     | 0        | 0        | 0       | 0            |
| 70  | CW    | 1     | 0        | 0        | 0       | 0            |
| 70  | CY    | 1     | 0        | 0        | 0       | 0            |
| 70  | D0    | 25    | 0        | 0        | 0       | 0            |
| 70  | D1    | 42    | 0        | 0        | 0       | 0            |
| 70  | D2    | 7     | 0        | 0        | 0       | 0            |
| 70  | D3    | 25    | 0        | 0        | 0       | 0            |
| 70  | D4    | 32    | 0        | 0        | 1       | 0            |
| 70  | D5    | 13    | 0        | 0        | 0       | 0            |
| 70  | DA    | 4836  | 0        | 0        | 8       | 0            |
| 70  | DB    | 213   | 0        | 0        | 0       | 0            |
| 70  | DC    | 102   | 0        | 0        | 0       | 0            |
| 70  | DD    | 105   | 0        | 0        | 1       | 0            |
| 70  | DE    | 63    | 0        | 0        | 0       | 0            |
| 70  | DF    | 14    | 0        | 0        | 0       | 0            |
| 70  | DG    | 6     | 0        | 0        | 0       | 0            |
| 70  | DH    | 2     | 0        | 0        | 0       | 0            |
| 70  | DK    | 58    | 0        | 0        | 0       | 0            |
| 70  | DL    | 51    | 0        | 0        | 0       | 0            |
| 70  | DM    | 60    | 0        | 0        | 0       | 0            |
| 70  | DN    | 71    | 0        | 0        | 0       | 0            |
| 70  | DO    | 44    | 0        | 0        | 0       | 0            |
| 70  | DP    | 35    | 0        | 0        | 0       | 0            |
| 70  | DQ    | 27    | 0        | 0        | 1       | 0            |
| 70  | DR    | 64    | 0        | 0        | 0       | 0            |
| 70  | DS    | 51    | 0        | 0        | 0       | 0            |
| 70  | DT    | 70    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 70  | DU    | 17     | 0        | 0        | 0       | 0            |
| 70  | DV    | 19     | 0        | 0        | 0       | 0            |
| 70  | DW    | 31     | 0        | 0        | 0       | 0            |
| 70  | DX    | 30     | 0        | 0        | 1       | 0            |
| 70  | DY    | 9      | 0        | 0        | 0       | 0            |
| 70  | DZ    | 7      | 0        | 0        | 0       | 0            |
| All | All   | 295202 | 0        | 194489   | 1207    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1207) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:C5:3:VAL:HG11   | 31:CA:2539:C:H5'   | 1.32                     | 1.05              |
| 46:CS:14:VAL:HG21  | 46:CS:98:ILE:HG13  | 1.32                     | 1.05              |
| 4:BD:85:ASN:HA     | 5:BE:102:GLY:HA2   | 1.43                     | 0.99              |
| 31:CA:1936:A:H2    | 31:CA:1943:U:H3    | 1.01                     | 0.98              |
| 48:CU:28:ASN:HD21  | 48:CU:91:GLN:HB3   | 1.29                     | 0.96              |
| 14:AN:66:GLN:HB2   | 70:AN:205:HOH:O    | 1.67                     | 0.95              |
| 40:CM:82:LEU:HD11  | 40:CM:116:VAL:HG23 | 1.52                     | 0.92              |
| 24:C3:7:PRO:HB2    | 31:CA:1309:G:H4'   | 1.52                     | 0.91              |
| 46:CS:14:VAL:CG2   | 46:CS:98:ILE:HG13  | 2.00                     | 0.90              |
| 5:AE:77:ASN:HB2    | 5:AE:82:GLN:NE2    | 1.86                     | 0.90              |
| 40:CM:77:ILE:HD11  | 40:CM:108:ALA:HB1  | 1.55                     | 0.89              |
| 8:BH:87:LYS:HB2    | 8:BH:125:ILE:HD11  | 1.55                     | 0.87              |
| 22:C1:4:GLN:HA     | 31:CA:2615:U:C2    | 2.10                     | 0.86              |
| 5:BE:77:ASN:HB2    | 5:BE:82:GLN:NE2    | 1.91                     | 0.86              |
| 8:AH:87:LYS:HB2    | 8:AH:125:ILE:HD11  | 1.58                     | 0.85              |
| 31:CA:2796:U:H3    | 31:CA:2799:A:H61   | 1.23                     | 0.85              |
| 31:CA:1779:U:H5    | 31:CA:1784:A:N7    | 1.74                     | 0.85              |
| 31:CA:1005:C:O2'   | 38:CK:30:THR:HG21  | 1.78                     | 0.84              |
| 55:DA:2796:U:H3    | 55:DA:2799:A:H61   | 1.21                     | 0.83              |
| 1:BA:1305:G:H21    | 1:BA:1332:A:H2     | 1.24                     | 0.83              |
| 11:BK:88:GLY:H     | 11:BK:114:THR:HG22 | 1.43                     | 0.82              |
| 2:BB:23:TRP:HB3    | 2:BB:39:HIS:CE1    | 2.14                     | 0.82              |
| 1:AA:1305:G:H21    | 1:AA:1332:A:H2     | 1.23                     | 0.81              |
| 18:AR:21:ILE:HG21  | 18:AR:54:GLN:HB3   | 1.61                     | 0.81              |
| 31:CA:740:C:H5'    | 31:CA:1784:A:H3'   | 1.62                     | 0.81              |
| 33:CE:149:ILE:HG12 | 33:CE:188:MET:HG2  | 1.62                     | 0.81              |
| 12:BL:65:SER:HB2   | 12:BL:82:ILE:HD11  | 1.62                     | 0.80              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:BM:114:LYS:HB3   | 13:BM:115:PRO:HD3   | 1.62                     | 0.80              |
| 55:DA:2033:A:H5'    | 70:DA:4099:HOH:O    | 1.81                     | 0.80              |
| 22:C1:38:HIS:HE1    | 31:CA:2884:U:O4     | 1.64                     | 0.80              |
| 2:BB:20:THR:HA      | 2:BB:39:HIS:CE1     | 2.18                     | 0.79              |
| 46:CS:14:VAL:HG21   | 46:CS:98:ILE:CG1    | 2.11                     | 0.79              |
| 45:DR:20:GLN:CG     | 57:DR:202:PG4:H42   | 2.12                     | 0.79              |
| 1:BA:9:G:H5'        | 5:BE:108:GLY:HA3    | 1.63                     | 0.79              |
| 25:C4:60:ALA:O      | 40:CM:48:ARG:HD2    | 1.83                     | 0.78              |
| 45:DR:20:GLN:HG3    | 57:DR:202:PG4:H42   | 1.65                     | 0.78              |
| 55:DA:135:U:H3      | 55:DA:144:A:H61     | 1.32                     | 0.78              |
| 35:CG:24:ILE:HD11   | 35:CG:43:VAL:HG11   | 1.66                     | 0.77              |
| 41:DN:18[A]:ARG:HG2 | 28:DB:90:C:H5'      | 1.65                     | 0.77              |
| 35:DG:24:ILE:HD11   | 35:DG:43:VAL:HG11   | 1.66                     | 0.77              |
| 31:CA:135:U:H3      | 31:CA:144:A:H61     | 1.33                     | 0.77              |
| 13:BM:22:ILE:HB     | 13:BM:25:VAL:CG1    | 2.15                     | 0.77              |
| 55:DA:568:U:H1'     | 55:DA:2030:6MZ:H9C1 | 1.66                     | 0.77              |
| 1:BA:664:G:H22      | 1:BA:741:G:H1       | 1.34                     | 0.76              |
| 31:CA:568:U:H1'     | 31:CA:2030:6MZ:H9C1 | 1.67                     | 0.76              |
| 39:CL:38:ILE:HD11   | 39:CL:112:PHE:HZ    | 1.49                     | 0.76              |
| 13:AM:6:GLY:HA3     | 13:AM:66:GLU:HG3    | 1.68                     | 0.75              |
| 1:AA:664:G:H22      | 1:AA:741:G:H1       | 1.34                     | 0.74              |
| 10:AJ:7:ARG:HB3     | 10:AJ:101:SER:HB2   | 1.69                     | 0.74              |
| 4:AD:107:PHE:HB3    | 4:AD:145:ILE:HD11   | 1.70                     | 0.74              |
| 4:BD:107:PHE:HB3    | 4:BD:145:ILE:HD11   | 1.70                     | 0.74              |
| 13:BM:83:LEU:HD21   | 19:BS:65:GLU:HB2    | 1.70                     | 0.74              |
| 31:CA:528:A:C2      | 31:CA:2043:C:H4'    | 2.23                     | 0.73              |
| 3:BC:123:GLN:HB3    | 3:BC:128:VAL:HG21   | 1.69                     | 0.73              |
| 1:AA:842:U:H4'      | 1:AA:843:U:OP1      | 1.88                     | 0.73              |
| 25:D4:54:ASP:HB3    | 40:DM:57:LEU:HD22   | 1.70                     | 0.73              |
| 1:BA:522:C:H5       | 12:BL:50:ARG:HH12   | 1.37                     | 0.73              |
| 13:BM:6:GLY:HA3     | 13:BM:66:GLU:HG3    | 1.69                     | 0.73              |
| 1:BA:1060:U:C5      | 3:BC:2:GLY:HA3      | 2.23                     | 0.73              |
| 55:DA:2127:G:H4'    | 55:DA:2128:G:OP1    | 1.90                     | 0.72              |
| 1:AA:1492:A:H5''    | 12:AL:44:LYS:HG2    | 1.72                     | 0.71              |
| 24:C3:30:VAL:HG13   | 31:CA:466:A:H5''    | 1.72                     | 0.71              |
| 39:DL:38:ILE:HD11   | 39:DL:112:PHE:HZ    | 1.53                     | 0.71              |
| 1:AA:73:C:HO2'      | 1:AA:74:A:H8        | 1.38                     | 0.70              |
| 1:BA:202:G:HO2'     | 1:BA:468:A:H8       | 1.39                     | 0.70              |
| 47:CT:86:MET:HB2    | 47:CT:96:ILE:HD11   | 1.74                     | 0.70              |
| 31:CA:1936:A:H2     | 31:CA:1943:U:N3     | 1.83                     | 0.70              |
| 55:DA:1913:A:H4'    | 55:DA:1913:A:OP1    | 1.90                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:DA:2255:G:H21   | 69:DA:3219:TRS:H12 | 1.56                     | 0.70              |
| 31:CA:846:U:H1'    | 31:CA:847:U:H5     | 1.56                     | 0.70              |
| 55:DA:2628:C:H5'   | 59:DA:3195:PUT:H12 | 1.73                     | 0.69              |
| 31:CA:1478:G:H1    | 31:CA:1513:U:H3    | 1.39                     | 0.69              |
| 54:DI:64:VAL:HG22  | 54:DI:69:PHE:HB2   | 1.75                     | 0.69              |
| 39:DL:30:ARG:HD2   | 55:DA:2674:G:H4'   | 1.74                     | 0.69              |
| 24:C3:19:ARG:HG3   | 31:CA:126:A:O5'    | 1.94                     | 0.68              |
| 55:DA:1478:G:H1    | 55:DA:1513:U:H3    | 1.38                     | 0.68              |
| 2:BB:23:TRP:HB3    | 2:BB:39:HIS:HE1    | 1.56                     | 0.68              |
| 34:CF:36:LEU:HD21  | 34:CF:91:LEU:HD11  | 1.76                     | 0.68              |
| 59:DA:3195:PUT:H11 | 70:DA:5703:HOH:O   | 1.94                     | 0.68              |
| 4:BD:201:VAL:HG11  | 5:BE:103:THR:HB    | 1.76                     | 0.67              |
| 11:BK:88:GLY:N     | 11:BK:114:THR:HG22 | 2.09                     | 0.67              |
| 22:D1:55:ILE:HD12  | 42:DO:33:ILE:HD11  | 1.76                     | 0.67              |
| 52:CY:4:VAL:HG22   | 52:CY:11:ARG:HG3   | 1.75                     | 0.67              |
| 49:DV:52:LEU:HB3   | 49:DV:54:GLN:HB2   | 1.76                     | 0.67              |
| 31:CA:45:G:H5''    | 31:CA:46:G:H5'     | 1.76                     | 0.67              |
| 31:CA:1250:G:H5''  | 45:CR:6:ARG:HD3    | 1.77                     | 0.67              |
| 43:DP:39:VAL:HB    | 43:DP:49:VAL:HG23  | 1.76                     | 0.67              |
| 1:BA:73:C:HO2'     | 1:BA:74:A:H8       | 1.42                     | 0.66              |
| 27:C0:12:SER:HB3   | 31:CA:988:A:P      | 2.35                     | 0.66              |
| 1:BA:502:A:OP1     | 12:BL:115:SER:HB2  | 1.95                     | 0.66              |
| 1:BA:451:A:H2'     | 70:BA:1701:HOH:O   | 1.94                     | 0.66              |
| 1:AA:202:G:HO2'    | 1:AA:468:A:H8      | 1.44                     | 0.66              |
| 40:CM:79:LEU:HD11  | 40:CM:112:LEU:HD12 | 1.77                     | 0.66              |
| 55:DA:45:G:H5''    | 55:DA:46:G:H5'     | 1.77                     | 0.65              |
| 43:DP:31:THR:HG21  | 28:DB:28:C:OP1     | 1.97                     | 0.65              |
| 35:CG:80:THR:HG23  | 35:CG:81:GLU:H     | 1.60                     | 0.65              |
| 30:CD:133:THR:HG22 | 31:CA:1993:U:H4'   | 1.78                     | 0.65              |
| 26:C5:3:VAL:HG11   | 31:CA:2539:C:C5'   | 2.19                     | 0.64              |
| 31:CA:974:G:H8     | 31:CA:990:A:H62    | 1.46                     | 0.64              |
| 1:AA:502:A:OP1     | 12:AL:115:SER:HB2  | 1.97                     | 0.64              |
| 12:BL:110:ARG:HB2  | 12:BL:119:VAL:HG21 | 1.78                     | 0.64              |
| 1:AA:412:A:H3'     | 1:AA:413:G:H5'     | 1.79                     | 0.64              |
| 1:BA:841:C:H3'     | 1:BA:842:U:C5'     | 2.27                     | 0.64              |
| 31:CA:372:G:H5''   | 52:CY:61:LYS:HD3   | 1.78                     | 0.64              |
| 34:DF:61:SER:HB2   | 34:DF:91:LEU:HD21  | 1.79                     | 0.64              |
| 12:BL:43:LYS:HD2   | 12:BL:91:PRO:HG3   | 1.79                     | 0.64              |
| 24:C3:12:ARG:HD2   | 24:C3:44:VAL:HG11  | 1.80                     | 0.64              |
| 31:CA:2394:C:H5''  | 40:CM:63:LYS:HE2   | 1.80                     | 0.64              |
| 22:C1:43:ILE:HG22  | 22:C1:49:TYR:HB2   | 1.81                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:CF:61:SER:HB2  | 34:CF:91:LEU:HD21  | 1.80                     | 0.63              |
| 29:CC:29:PRO:HG2  | 29:CC:34:LEU:HD11  | 1.80                     | 0.63              |
| 31:CA:17:G:H4'    | 45:CR:25:TYR:HE2   | 1.62                     | 0.63              |
| 31:CA:1105:U:H2'  | 31:CA:1106:G:C8    | 2.33                     | 0.63              |
| 17:BQ:14:SER:HB3  | 17:BQ:22:VAL:HG12  | 1.80                     | 0.63              |
| 39:CL:76:VAL:HG12 | 44:CQ:73:VAL:HB    | 1.81                     | 0.63              |
| 55:DA:1105:U:H2'  | 55:DA:1106:G:C8    | 2.34                     | 0.63              |
| 55:DA:31:C:O3'    | 55:DA:1238:G:H5''  | 1.98                     | 0.63              |
| 24:D3:7:PRO:HB2   | 55:DA:1309:G:H4'   | 1.80                     | 0.63              |
| 40:DM:77:ILE:HD11 | 40:DM:101:ILE:CG2  | 2.29                     | 0.63              |
| 22:C1:15:MET:HB3  | 31:CA:2045:C:O3'   | 1.98                     | 0.63              |
| 47:CT:82:MET:HB2  | 47:CT:98:LYS:HB2   | 1.79                     | 0.63              |
| 55:DA:2256:G:H21  | 57:DA:3193:PG4:H31 | 1.63                     | 0.63              |
| 20:BT:9:LYS:O     | 20:BT:12:ILE:HG13  | 1.98                     | 0.62              |
| 24:C3:30:VAL:CG1  | 31:CA:466:A:H5''   | 2.29                     | 0.62              |
| 45:DR:20:GLN:HG2  | 57:DR:202:PG4:H51  | 1.81                     | 0.62              |
| 55:DA:1482:G:H1'  | 55:DA:1509:A:H61   | 1.65                     | 0.62              |
| 26:C5:3:VAL:CG1   | 31:CA:2539:C:H5'   | 2.20                     | 0.62              |
| 31:CA:2728:U:HO2' | 31:CA:2729:G:H8    | 1.47                     | 0.62              |
| 29:DC:29:PRO:HG2  | 29:DC:34:LEU:HD11  | 1.82                     | 0.62              |
| 17:AQ:17:MET:HG2  | 17:AQ:20:SER:HB2   | 1.82                     | 0.62              |
| 5:BE:72:ILE:HG12  | 5:BE:145:GLU:HG3   | 1.80                     | 0.62              |
| 22:C1:8:PRO:HG2   | 31:CA:1264:A:H5'   | 1.80                     | 0.62              |
| 31:CA:328:U:O3'   | 49:CV:66:GLN:HG3   | 2.00                     | 0.62              |
| 6:BF:38:ARG:HB3   | 6:BF:63:ASN:HB2    | 1.80                     | 0.62              |
| 1:BA:209:U:H4'    | 1:BA:210:C:OP2     | 2.00                     | 0.61              |
| 55:DA:788:A:H3'   | 59:DA:3221:PUT:H41 | 1.82                     | 0.61              |
| 5:AE:77:ASN:HB2   | 5:AE:82:GLN:HE22   | 1.62                     | 0.61              |
| 6:AF:38:ARG:HB3   | 6:AF:63:ASN:HB2    | 1.82                     | 0.61              |
| 16:BP:20:VAL:HG13 | 16:BP:32:PHE:HB2   | 1.82                     | 0.61              |
| 55:DA:1847:A:HO2' | 55:DA:1848:A:H8    | 1.48                     | 0.61              |
| 19:BS:6:LYS:HD2   | 19:BS:7:LYS:H      | 1.65                     | 0.61              |
| 22:D1:43:ILE:HG22 | 22:D1:49:TYR:HB2   | 1.83                     | 0.61              |
| 64:DD:301:PGE:H12 | 55:DA:2623:G:OP1   | 2.01                     | 0.61              |
| 2:BB:41:ILE:HD13  | 2:BB:202:GLY:HA2   | 1.83                     | 0.61              |
| 36:CH:15:LEU:HD22 | 36:CH:15:LEU:H     | 1.66                     | 0.61              |
| 31:CA:674:G:H1'   | 33:CE:69:ARG:HD2   | 1.83                     | 0.61              |
| 45:DR:20:GLN:HG2  | 57:DR:202:PG4:H42  | 1.81                     | 0.60              |
| 12:AL:110:ARG:HB2 | 12:AL:119:VAL:HG21 | 1.81                     | 0.60              |
| 25:C4:13:ARG:NH1  | 31:CA:250:G:OP2    | 2.33                     | 0.60              |
| 34:CF:31:VAL:CG1  | 34:CF:97:TRP:CH2   | 2.84                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DE:48:THR:HG23 | 33:DE:88:ARG:NH1   | 2.16                     | 0.60              |
| 47:DT:82:MET:HB2  | 47:DT:98:LYS:HB2   | 1.82                     | 0.60              |
| 29:CC:17:VAL:HB   | 29:CC:204:VAL:HG13 | 1.83                     | 0.60              |
| 48:DU:80:TRP:HB3  | 64:DU:101:PGE:H32  | 1.83                     | 0.60              |
| 1:AA:1151:A:HO2'  | 1:AA:1152:A:H8     | 1.49                     | 0.60              |
| 13:AM:33:ILE:HD11 | 13:AM:63:PHE:HE1   | 1.66                     | 0.60              |
| 1:BA:1323:G:H2'   | 1:BA:1324:A:C8     | 2.36                     | 0.60              |
| 22:C1:25:VAL:HG13 | 22:C1:26:THR:H     | 1.67                     | 0.60              |
| 31:CA:1482:G:H1'  | 31:CA:1509:A:H61   | 1.66                     | 0.60              |
| 47:CT:59:GLU:HA   | 47:CT:64:ALA:HA    | 1.82                     | 0.60              |
| 1:BA:843:U:H5''   | 1:BA:843:U:H6      | 1.67                     | 0.59              |
| 31:CA:528:A:H3'   | 31:CA:528:A:H8     | 1.67                     | 0.59              |
| 6:AF:16:GLU:HB3   | 4:BD:189:SER:HA    | 1.83                     | 0.59              |
| 1:BA:978:A:HO2'   | 1:BA:1322:C:H5     | 1.51                     | 0.59              |
| 1:BA:9:G:H4'      | 5:BE:109:GLY:H     | 1.66                     | 0.59              |
| 31:CA:1779:U:C5   | 31:CA:1784:A:N7    | 2.64                     | 0.59              |
| 1:AA:1238:A:H5'   | 1:AA:1336:C:H41    | 1.68                     | 0.59              |
| 2:AB:41:ILE:HD13  | 2:AB:202:GLY:HA2   | 1.83                     | 0.59              |
| 1:BA:1141:C:HO2'  | 1:BA:1142:G:H8     | 1.51                     | 0.59              |
| 5:BE:104:GLY:HA3  | 5:BE:122:ASN:HA    | 1.83                     | 0.59              |
| 1:AA:1323:G:H2'   | 1:AA:1324:A:C8     | 2.38                     | 0.59              |
| 31:CA:528:A:H3'   | 31:CA:528:A:C8     | 2.38                     | 0.59              |
| 22:C1:15:MET:SD   | 31:CA:2045:C:H5''  | 2.43                     | 0.59              |
| 45:DR:19:LYS:HB3  | 57:DR:202:PG4:H41  | 1.85                     | 0.59              |
| 1:AA:202:G:H21    | 1:AA:466:A:H61     | 1.51                     | 0.59              |
| 1:AA:451:A:H61    | 1:AA:481:G:H5'     | 1.67                     | 0.59              |
| 26:C5:16:ILE:HD13 | 26:C5:25:VAL:HG22  | 1.85                     | 0.59              |
| 33:DE:33:VAL:HG22 | 58:DA:3192:MPD:H12 | 1.84                     | 0.59              |
| 31:CA:1847:A:HO2' | 31:CA:1848:A:H8    | 1.48                     | 0.58              |
| 31:CA:2728:U:O2'  | 31:CA:2729:G:H5''  | 2.04                     | 0.58              |
| 13:BM:22:ILE:HB   | 13:BM:25:VAL:HG12  | 1.86                     | 0.58              |
| 11:AK:34:ILE:HG12 | 11:AK:70:CYS:SG    | 2.43                     | 0.58              |
| 1:BA:841:C:H3'    | 1:BA:842:U:H5''    | 1.86                     | 0.58              |
| 55:DA:2128:G:H1   | 55:DA:2160:C:H42   | 1.52                     | 0.58              |
| 1:BA:946:A:H2'    | 1:BA:947:G:C8      | 2.38                     | 0.58              |
| 5:BE:133:PRO:O    | 5:BE:137:VAL:HG12  | 2.02                     | 0.58              |
| 42:CO:49:GLU:OE2  | 42:CO:95:THR:HG22  | 2.04                     | 0.58              |
| 55:DA:12:U:O2     | 55:DA:12:U:H2'     | 2.04                     | 0.58              |
| 45:DR:31:VAL:HG13 | 55:DA:580:U:O3'    | 2.03                     | 0.58              |
| 1:AA:946:A:H2'    | 1:AA:947:G:C8      | 2.39                     | 0.58              |
| 32:DD:114:LYS:HE2 | 55:DA:2681:C:OP2   | 2.03                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:CH:41:LYS:HA    | 36:CH:44:ILE:HG12  | 1.86                     | 0.58              |
| 55:DA:1105:U:H2'   | 55:DA:1106:G:H8    | 1.68                     | 0.58              |
| 23:C2:35:GLU:HG2   | 23:C2:50:LYS:HG2   | 1.86                     | 0.57              |
| 19:AS:50:ALA:HB1   | 19:AS:57:HIS:HB3   | 1.86                     | 0.57              |
| 29:CC:120:VAL:HG12 | 29:CC:134:ASN:ND2  | 2.19                     | 0.57              |
| 1:BA:209:U:O2      | 1:BA:209:U:H2'     | 2.03                     | 0.57              |
| 26:D5:16:ILE:HD13  | 26:D5:25:VAL:HG22  | 1.86                     | 0.57              |
| 18:AR:36:SER:HA    | 18:AR:72:ASP:HB3   | 1.87                     | 0.57              |
| 7:BG:113:ASP:HB2   | 7:BG:119:ARG:HG3   | 1.86                     | 0.57              |
| 24:D3:4:THR:HG22   | 55:DA:687:C:H1'    | 1.87                     | 0.57              |
| 33:DE:189:THR:HG22 | 33:DE:192:ALA:H    | 1.69                     | 0.57              |
| 31:CA:1105:U:H2'   | 31:CA:1106:G:H8    | 1.68                     | 0.57              |
| 31:CA:550:C:H2'    | 31:CA:551:G:H5''   | 1.86                     | 0.57              |
| 1:AA:1492:A:C5'    | 12:AL:44:LYS:HG2   | 2.34                     | 0.57              |
| 31:CA:1703:G:H2'   | 31:CA:1704:C:C6    | 2.40                     | 0.57              |
| 36:CH:27:ARG:HH11  | 52:CY:60:ASP:HA    | 1.70                     | 0.57              |
| 31:CA:310:A:H5''   | 49:CV:15:THR:HG23  | 1.86                     | 0.57              |
| 1:AA:769:G:H4'     | 1:AA:1513:A:H4'    | 1.87                     | 0.57              |
| 1:BA:1238:A:H5'    | 1:BA:1336:C:H41    | 1.68                     | 0.57              |
| 34:CF:36:LEU:HD21  | 34:CF:91:LEU:CD1   | 2.34                     | 0.57              |
| 40:CM:82:LEU:HD11  | 40:CM:116:VAL:CG2  | 2.32                     | 0.57              |
| 48:CU:24:MET:HG2   | 48:CU:29:THR:O     | 2.05                     | 0.57              |
| 40:CM:28:GLY:O     | 40:CM:29:LYS:O     | 2.21                     | 0.57              |
| 7:AG:113:ASP:HB2   | 7:AG:119:ARG:HG3   | 1.86                     | 0.57              |
| 47:CT:66:ILE:HA    | 47:CT:69:LEU:HD22  | 1.87                     | 0.57              |
| 35:DG:42:GLU:HG2   | 35:DG:55:ARG:HH21  | 1.68                     | 0.57              |
| 36:DH:41:LYS:HA    | 36:DH:44:ILE:HG12  | 1.86                     | 0.57              |
| 1:AA:1141:C:HO2'   | 1:AA:1142:G:H8     | 1.52                     | 0.57              |
| 1:AA:81:A:H61      | 1:AA:86:G:H1       | 1.53                     | 0.57              |
| 29:DC:120:VAL:HG12 | 29:DC:134:ASN:ND2  | 2.20                     | 0.57              |
| 3:AC:77:ILE:HA     | 3:AC:84:VAL:HG23   | 1.87                     | 0.56              |
| 7:AG:22:LEU:HD12   | 7:AG:62:PHE:HE2    | 1.69                     | 0.56              |
| 22:C1:5:GLN:HG3    | 31:CA:2054:A:C2    | 2.39                     | 0.56              |
| 1:BA:451:A:H61     | 1:BA:481:G:H5'     | 1.69                     | 0.56              |
| 33:CE:189:THR:HG22 | 33:CE:192:ALA:H    | 1.70                     | 0.56              |
| 5:BE:77:ASN:HB2    | 5:BE:82:GLN:HE22   | 1.68                     | 0.56              |
| 31:CA:2095:A:H8    | 31:CA:2095:A:H5''  | 1.69                     | 0.56              |
| 40:DM:77:ILE:HD11  | 40:DM:101:ILE:HG21 | 1.87                     | 0.56              |
| 55:DA:62:U:O4'     | 58:DA:3203:MPD:H31 | 2.05                     | 0.56              |
| 1:AA:8:A:C6        | 4:AD:206:LYS:HB3   | 2.40                     | 0.56              |
| 1:BA:1012:A:H61    | 1:BA:1017:U:H3     | 1.54                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 32:DD:146:ILE:HD12  | 32:DD:155:VAL:HG21 | 1.88                     | 0.56              |
| 44:DQ:96:LYS:HE3    | 70:DQ:306:HOH:O    | 2.04                     | 0.56              |
| 55:DA:550:C:H2'     | 55:DA:551:G:H5''   | 1.87                     | 0.56              |
| 1:AA:1277:C:HO2'    | 1:AA:1279:G:H8     | 1.53                     | 0.56              |
| 3:AC:77:ILE:HA      | 3:AC:84:VAL:CG2    | 2.36                     | 0.56              |
| 31:CA:2304:G:H5'    | 34:CF:121:SER:HB2  | 1.87                     | 0.56              |
| 11:AK:67:ALA:HB2    | 11:AK:96:THR:HG23  | 1.88                     | 0.56              |
| 23:D2:35:GLU:HG2    | 23:D2:50:LYS:HG2   | 1.86                     | 0.56              |
| 3:BC:77:ILE:HA      | 3:BC:84:VAL:CG2    | 2.36                     | 0.55              |
| 22:C1:17:ARG:NH2    | 31:CA:1266:G:OP2   | 2.39                     | 0.55              |
| 31:CA:2019:A:H4'    | 45:CR:34:VAL:HG21  | 1.87                     | 0.55              |
| 41:DN:18[B]:ARG:HG3 | 28:DB:90:C:H5'     | 1.89                     | 0.55              |
| 1:AA:1012:A:H61     | 1:AA:1017:U:H3     | 1.55                     | 0.55              |
| 10:AJ:5:ARG:HE      | 10:AJ:77:VAL:HG22  | 1.70                     | 0.55              |
| 1:BA:1106:G:H5''    | 3:BC:172:ARG:HG3   | 1.87                     | 0.55              |
| 13:BM:86:TYR:CZ     | 13:BM:90:ARG:HD2   | 2.41                     | 0.55              |
| 31:CA:457:A:N1      | 31:CA:470:A:H5''   | 2.21                     | 0.55              |
| 1:BA:619:U:H3       | 4:BD:131:ASN:HB3   | 1.71                     | 0.55              |
| 19:BS:50:ALA:HB1    | 19:BS:57:HIS:HB3   | 1.89                     | 0.55              |
| 24:C3:9:VAL:N       | 31:CA:1309:G:OP1   | 2.33                     | 0.55              |
| 22:D1:8:PRO:HG2     | 55:DA:1264:A:H5'   | 1.88                     | 0.55              |
| 55:DA:31:C:O2'      | 55:DA:1238:G:H5'   | 2.06                     | 0.55              |
| 35:DG:175:LYS:HG3   | 55:DA:2529:G:H4'   | 1.88                     | 0.55              |
| 8:AH:29:SER:HB3     | 8:AH:57:PRO:HB2    | 1.88                     | 0.55              |
| 5:BE:72:ILE:HG13    | 5:BE:73:ASN:H      | 1.72                     | 0.55              |
| 1:AA:412:A:H3'      | 1:AA:413:G:C5'     | 2.37                     | 0.55              |
| 10:AJ:35:GLN:HB2    | 10:AJ:77:VAL:HB    | 1.88                     | 0.55              |
| 1:BA:1151:A:HO2'    | 1:BA:1152:A:H8     | 1.53                     | 0.55              |
| 3:BC:77:ILE:HA      | 3:BC:84:VAL:HG23   | 1.88                     | 0.55              |
| 26:C5:1:MET:HB2     | 31:CA:2526:G:O2'   | 2.06                     | 0.55              |
| 26:C5:36:ARG:HD3    | 31:CA:2742:G:OP1   | 2.07                     | 0.55              |
| 4:BD:85:ASN:HB3     | 4:BD:88:GLU:HB2    | 1.89                     | 0.55              |
| 48:CU:22:THR:HA     | 48:CU:25:GLU:HG2   | 1.87                     | 0.55              |
| 3:AC:155:GLY:HA2    | 3:AC:163:ALA:HB1   | 1.89                     | 0.55              |
| 31:CA:2822:G:H2'    | 31:CA:2823:A:H5''  | 1.88                     | 0.55              |
| 55:DA:2297:A:H5''   | 55:DA:2297:A:C8    | 2.42                     | 0.55              |
| 25:D4:64:TYR:CE2    | 55:DA:242:G:H5''   | 2.42                     | 0.55              |
| 13:AM:86:TYR:CZ     | 13:AM:90:ARG:HD2   | 2.41                     | 0.54              |
| 11:BK:67:ALA:HB2    | 11:BK:96:THR:HG23  | 1.88                     | 0.54              |
| 11:BK:89:PRO:HG3    | 21:BU:32:VAL:HG11  | 1.88                     | 0.54              |
| 31:CA:2845:U:H5''   | 44:CQ:52:ASN:O     | 2.07                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:D4:8:ARG:HD3    | 55:DA:245:G:O6      | 2.08                     | 0.54              |
| 64:D1:102:PGE:H42  | 47:DT:23:LEU:HD23   | 1.89                     | 0.54              |
| 16:AP:4:ILE:HG12   | 16:AP:21:VAL:HG22   | 1.89                     | 0.54              |
| 31:CA:2502:G:H5''  | 31:CA:2503:2MA:H5'' | 1.90                     | 0.54              |
| 1:BA:108:G:N3      | 1:BA:108:G:H5''     | 2.23                     | 0.54              |
| 65:DA:3223:SPD:H92 | 65:DA:3223:SPD:H52  | 1.90                     | 0.54              |
| 44:DQ:106:LYS:HA   | 44:DQ:109:ARG:HD3   | 1.90                     | 0.54              |
| 11:AK:31:ILE:HG12  | 11:AK:46:THR:HG22   | 1.88                     | 0.54              |
| 16:BP:4:ILE:HG12   | 16:BP:21:VAL:HG22   | 1.90                     | 0.54              |
| 45:CR:87:SER:HB3   | 46:CS:52:PRO:HD3    | 1.90                     | 0.54              |
| 5:AE:76:LEU:HD11   | 5:AE:120:VAL:HG22   | 1.90                     | 0.54              |
| 26:C5:17:VAL:CG1   | 26:C5:26:ILE:HD12   | 2.38                     | 0.54              |
| 39:DL:76:VAL:CG2   | 55:DA:2684:U:H4'    | 2.37                     | 0.54              |
| 1:AA:404:G:N7      | 4:AD:2:ALA:HB3      | 2.23                     | 0.54              |
| 5:BE:72:ILE:HG13   | 5:BE:73:ASN:N       | 2.22                     | 0.54              |
| 23:D2:8:LYS:HE3    | 55:DA:2420:C:H5''   | 1.89                     | 0.54              |
| 13:AM:33:ILE:HD11  | 13:AM:63:PHE:CE1    | 2.42                     | 0.54              |
| 10:BJ:5:ARG:HG2    | 10:BJ:79:PRO:HG3    | 1.90                     | 0.54              |
| 11:BK:52:PHE:HE2   | 11:BK:65:VAL:HG21   | 1.73                     | 0.54              |
| 22:C1:4:GLN:HB3    | 31:CA:2615:U:H1'    | 1.90                     | 0.54              |
| 1:AA:108:G:H5''    | 1:AA:108:G:N3       | 2.22                     | 0.54              |
| 5:BE:35:ALA:O      | 5:BE:50:TYR:O       | 2.26                     | 0.54              |
| 31:CA:1394:U:H4'   | 31:CA:1603:A:H4'    | 1.90                     | 0.54              |
| 48:DU:67:VAL:HG22  | 48:DU:76:ARG:HG3    | 1.90                     | 0.54              |
| 1:BA:769:G:H4'     | 1:BA:1513:A:H4'     | 1.88                     | 0.53              |
| 1:BA:374:A:OP1     | 1:BA:452:A:N1       | 2.41                     | 0.53              |
| 5:BE:126:LYS:HG2   | 5:BE:128:TYR:CZ     | 2.44                     | 0.53              |
| 33:CE:149:ILE:HD12 | 33:CE:172:ALA:HA    | 1.89                     | 0.53              |
| 44:CQ:106:LYS:HA   | 44:CQ:109:ARG:HD3   | 1.90                     | 0.53              |
| 1:AA:1144:G:H21    | 1:AA:1146:A:H62     | 1.56                     | 0.53              |
| 4:AD:85:ASN:HB3    | 4:AD:88:GLU:HB2     | 1.90                     | 0.53              |
| 34:CF:31:VAL:HG11  | 34:CF:97:TRP:CH2    | 2.43                     | 0.53              |
| 1:AA:209:U:H4'     | 1:AA:210:C:OP2      | 2.08                     | 0.53              |
| 31:CA:1251:C:OP2   | 45:CR:6:ARG:HD2     | 2.09                     | 0.53              |
| 1:BA:1144:G:H21    | 1:BA:1146:A:H62     | 1.56                     | 0.53              |
| 6:BF:45:ARG:O      | 6:BF:56:LYS:HA      | 2.08                     | 0.53              |
| 12:BL:33:VAL:HG22  | 12:BL:79:VAL:HG22   | 1.90                     | 0.53              |
| 36:CH:4:ILE:HD11   | 36:CH:44:ILE:HG22   | 1.90                     | 0.53              |
| 3:BC:5:VAL:HG21    | 3:BC:10:ILE:HD13    | 1.91                     | 0.53              |
| 2:BB:129:LEU:HD13  | 2:BB:134:ALA:HB2    | 1.91                     | 0.53              |
| 8:BH:29:SER:HB3    | 8:BH:57:PRO:HB2     | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:52:PHE:HE2   | 11:AK:65:VAL:HG21  | 1.73                     | 0.53              |
| 55:DA:2796:U:H3    | 55:DA:2799:A:N6    | 1.97                     | 0.53              |
| 54:DI:69:PHE:HB3   | 54:DI:72:LEU:HD12  | 1.91                     | 0.53              |
| 10:AJ:42:LEU:HB2   | 10:AJ:71:LEU:HB3   | 1.91                     | 0.53              |
| 11:AK:89:PRO:HG3   | 21:AU:32:VAL:HG11  | 1.90                     | 0.53              |
| 1:AA:735:C:H5'     | 18:AR:60:LYS:HD3   | 1.91                     | 0.53              |
| 6:BF:38:ARG:HH12   | 6:BF:99:ALA:HB3    | 1.74                     | 0.53              |
| 44:DQ:52:ASN:O     | 55:DA:2845:U:H5''  | 2.09                     | 0.53              |
| 2:AB:129:LEU:HD13  | 2:AB:134:ALA:HB2   | 1.91                     | 0.53              |
| 19:AS:29:LYS:HB3   | 19:AS:30:PRO:HD2   | 1.91                     | 0.53              |
| 10:BJ:26:VAL:HG21  | 10:BJ:39:PRO:HD3   | 1.91                     | 0.53              |
| 31:CA:1936:A:C2    | 31:CA:1943:U:N3    | 2.59                     | 0.53              |
| 25:C4:2:PRO:HD2    | 31:CA:667:U:O2     | 2.09                     | 0.52              |
| 25:C4:47:LYS:NZ    | 40:CM:64:PHE:CE1   | 2.77                     | 0.52              |
| 3:AC:5:VAL:HG21    | 3:AC:10:ILE:HD13   | 1.92                     | 0.52              |
| 31:CA:1847:A:O2'   | 31:CA:1848:A:H8    | 1.92                     | 0.52              |
| 6:AF:45:ARG:O      | 6:AF:56:LYS:HA     | 2.08                     | 0.52              |
| 3:BC:155:GLY:HA2   | 3:BC:163:ALA:HB1   | 1.91                     | 0.52              |
| 6:BF:3:HIS:H       | 6:BF:92:THR:HG23   | 1.73                     | 0.52              |
| 31:CA:2037:A:H2'   | 31:CA:2038:G:C8    | 2.44                     | 0.52              |
| 22:C1:38:HIS:CE1   | 31:CA:2884:U:O4    | 2.54                     | 0.52              |
| 31:CA:2796:U:H3    | 31:CA:2799:A:N6    | 1.99                     | 0.52              |
| 32:DD:128:ARG:HG3  | 70:DA:7412:HOH:O   | 2.09                     | 0.52              |
| 8:AH:2:SER:HB2     | 8:AH:4:GLN:HE21    | 1.75                     | 0.52              |
| 26:C5:3:VAL:HG12   | 31:CA:2538:C:O2'   | 2.10                     | 0.52              |
| 31:CA:118:A:N3     | 31:CA:178:G:H1'    | 2.25                     | 0.52              |
| 43:CP:100:HIS:CD2  | 43:CP:101:GLY:H    | 2.28                     | 0.52              |
| 13:AM:71:ARG:HH21  | 34:DF:143:TYR:HB2  | 1.74                     | 0.52              |
| 35:DG:86:LYS:HG2   | 35:DG:132:VAL:HG22 | 1.91                     | 0.52              |
| 23:C2:11:LEU:HD21  | 23:C2:34:LEU:HD23  | 1.91                     | 0.52              |
| 31:CA:2297:A:C8    | 31:CA:2297:A:H5''  | 2.45                     | 0.52              |
| 24:C3:33:ARG:NE    | 31:CA:467:G:OP1    | 2.36                     | 0.52              |
| 31:CA:668:A:H2'    | 31:CA:670:A:H62    | 1.75                     | 0.52              |
| 65:DA:3223:SPD:H92 | 65:DA:3223:SPD:C5  | 2.40                     | 0.52              |
| 55:DA:74:A:N3      | 55:DA:74:A:H5''    | 2.25                     | 0.52              |
| 48:DU:54:GLU:HB3   | 48:DU:88:LYS:HD2   | 1.92                     | 0.52              |
| 1:AA:86:G:H21      | 1:AA:87:C:H41      | 1.58                     | 0.52              |
| 1:BA:404:G:N7      | 4:BD:2:ALA:HB3     | 2.24                     | 0.52              |
| 6:BF:38:ARG:NH1    | 6:BF:99:ALA:HB3    | 2.24                     | 0.52              |
| 22:C1:41:HIS:HE2   | 31:CA:2884:U:P     | 2.32                     | 0.52              |
| 35:CG:86:LYS:HG2   | 35:CG:132:VAL:HG22 | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1277:C:O2'    | 1:AA:1279:G:H8     | 1.93                     | 0.52              |
| 1:AA:845:A:O4'     | 1:AA:845:A:P       | 2.68                     | 0.52              |
| 10:BJ:57:VAL:HG22  | 10:BJ:58:ASN:H     | 1.75                     | 0.52              |
| 22:C1:19:HIS:CE1   | 31:CA:2624:G:H1'   | 2.45                     | 0.52              |
| 33:CE:21:ARG:HD3   | 33:CE:106:LYS:HB3  | 1.92                     | 0.52              |
| 40:DM:79:LEU:HD11  | 40:DM:112:LEU:HD12 | 1.92                     | 0.52              |
| 41:DN:81[B]:4D4:H9 | 55:DA:2496:C:OP2   | 2.10                     | 0.52              |
| 1:AA:1218:C:H2'    | 1:AA:1219:A:C8     | 2.45                     | 0.51              |
| 10:AJ:26:VAL:HG21  | 10:AJ:39:PRO:HD3   | 1.91                     | 0.51              |
| 10:AJ:57:VAL:HG22  | 10:AJ:58:ASN:H     | 1.76                     | 0.51              |
| 11:AK:23:ILE:HD11  | 11:AK:86:VAL:HG13  | 1.92                     | 0.51              |
| 1:BA:1518:MA6:H103 | 1:BA:1519:MA6:H102 | 1.92                     | 0.51              |
| 19:BS:29:LYS:HB3   | 19:BS:30:PRO:HD2   | 1.93                     | 0.51              |
| 31:CA:699:A:H2'    | 31:CA:700:G:O4'    | 2.10                     | 0.51              |
| 33:DE:21:ARG:HD3   | 33:DE:106:LYS:HB3  | 1.91                     | 0.51              |
| 29:CC:13:ARG:HD3   | 31:CA:728:G:H4'    | 1.92                     | 0.51              |
| 43:CP:51:ALA:HB3   | 43:CP:78:VAL:HG13  | 1.92                     | 0.51              |
| 1:BA:350:G:H5''    | 20:BT:3:ASN:HD22   | 1.76                     | 0.51              |
| 1:BA:374:A:H5''    | 1:BA:452:A:N1      | 2.25                     | 0.51              |
| 4:BD:48:LEU:HD21   | 4:BD:56:ARG:HG3    | 1.93                     | 0.51              |
| 31:CA:17:G:H4'     | 45:CR:25:TYR:CE2   | 2.43                     | 0.51              |
| 48:CU:54:GLU:HB3   | 48:CU:88:LYS:HD2   | 1.92                     | 0.51              |
| 32:DD:25:THR:HG21  | 32:DD:193:VAL:HG22 | 1.92                     | 0.51              |
| 54:DI:44:ALA:HB1   | 54:DI:95:LEU:HD11  | 1.91                     | 0.51              |
| 11:BK:23:ILE:HD11  | 11:BK:86:VAL:HG13  | 1.91                     | 0.51              |
| 31:CA:569:U:H5''   | 31:CA:821:A:C2     | 2.46                     | 0.51              |
| 25:D4:8:ARG:CD     | 55:DA:245:G:O6     | 2.59                     | 0.51              |
| 55:DA:1853:A:N1    | 55:DA:2087:G:H1'   | 2.25                     | 0.51              |
| 7:BG:111:ARG:HB3   | 7:BG:119:ARG:HG2   | 1.93                     | 0.51              |
| 31:CA:1447:C:H2'   | 31:CA:1448:G:C8    | 2.46                     | 0.51              |
| 31:CA:532:A:N1     | 31:CA:2020:A:H1'   | 2.25                     | 0.51              |
| 1:AA:1518:MA6:H103 | 1:AA:1519:MA6:H102 | 1.92                     | 0.51              |
| 1:BA:1218:C:H2'    | 1:BA:1219:A:C8     | 2.46                     | 0.51              |
| 1:BA:1277:C:O2'    | 1:BA:1279:G:H8     | 1.93                     | 0.51              |
| 31:CA:12:U:H2'     | 31:CA:12:U:O2      | 2.11                     | 0.51              |
| 30:CD:25:THR:HG21  | 30:CD:193:VAL:HG22 | 1.93                     | 0.51              |
| 47:CT:69:LEU:HG    | 47:CT:107:VAL:HG22 | 1.92                     | 0.51              |
| 22:D1:22:LEU:HD23  | 62:D1:103:PEG:H31  | 1.91                     | 0.51              |
| 39:DL:38:ILE:HD11  | 39:DL:112:PHE:CZ   | 2.42                     | 0.51              |
| 11:AK:23:ILE:HG22  | 11:AK:32:VAL:HG13  | 1.92                     | 0.51              |
| 30:CD:4:LEU:HD22   | 30:CD:101:PHE:CE2  | 2.45                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:D4:31:HIS:HB2   | 70:D4:103:HOH:O    | 2.10                     | 0.51              |
| 43:DP:51:ALA:HB3   | 43:DP:78:VAL:HG13  | 1.93                     | 0.51              |
| 5:AE:126:LYS:HG2   | 5:AE:128:TYR:CZ    | 2.46                     | 0.51              |
| 31:CA:998:C:OP2    | 45:CR:58:ARG:NH2   | 2.44                     | 0.51              |
| 31:CA:2025:C:H2'   | 31:CA:2026:U:C6    | 2.46                     | 0.51              |
| 31:CA:2189:U:H2'   | 31:CA:2190:G:H8    | 1.76                     | 0.51              |
| 30:CD:129:THR:HG23 | 30:CD:140:HIS:O    | 2.11                     | 0.51              |
| 25:D4:60:ALA:O     | 40:DM:48:ARG:HD2   | 2.10                     | 0.51              |
| 55:DA:1847:A:O2'   | 55:DA:1848:A:H8    | 1.93                     | 0.51              |
| 47:CT:73:LYS:HB2   | 47:CT:106:VAL:HB   | 1.92                     | 0.50              |
| 36:DH:4:ILE:HD11   | 36:DH:44:ILE:HG22  | 1.93                     | 0.50              |
| 12:AL:33:VAL:HG22  | 12:AL:79:VAL:HG22  | 1.92                     | 0.50              |
| 31:CA:784:G:H5'    | 31:CA:785:G:OP1    | 2.10                     | 0.50              |
| 38:CK:81:ILE:HG23  | 38:CK:82:GLY:H     | 1.76                     | 0.50              |
| 1:AA:774:G:H21     | 57:AA:1670:PG4:H51 | 1.75                     | 0.50              |
| 5:BE:106:ILE:HD11  | 5:BE:124:LEU:HD23  | 1.93                     | 0.50              |
| 11:BK:23:ILE:HG22  | 11:BK:32:VAL:HG13  | 1.93                     | 0.50              |
| 20:BT:4:ILE:HA     | 20:BT:8:LYS:HE2    | 1.93                     | 0.50              |
| 31:CA:335:C:H5''   | 49:CV:82:ARG:HD3   | 1.93                     | 0.50              |
| 55:DA:1026:G:H2'   | 55:DA:1027:A:C8    | 2.45                     | 0.50              |
| 34:DF:131:GLY:HA3  | 55:DA:2305:U:H5''  | 1.94                     | 0.50              |
| 24:C3:19:ARG:NH2   | 31:CA:125:A:OP2    | 2.41                     | 0.50              |
| 48:CU:18:GLU:H     | 48:CU:18:GLU:CD    | 2.15                     | 0.50              |
| 35:DG:19:ILE:HG12  | 35:DG:24:ILE:HG12  | 1.93                     | 0.50              |
| 9:BI:19:VAL:HG22   | 9:BI:65:ILE:HG22   | 1.92                     | 0.50              |
| 1:AA:1358:U:H3     | 1:AA:1363:A:H62    | 1.59                     | 0.50              |
| 19:AS:15:LEU:HD13  | 19:AS:33:THR:HG21  | 1.93                     | 0.50              |
| 54:DI:57:ASN:HB3   | 54:DI:76:PHE:HB3   | 1.93                     | 0.50              |
| 1:BA:1003:G:H21    | 1:BA:1005:A:H5'    | 1.77                     | 0.50              |
| 17:BQ:17:MET:HB3   | 17:BQ:20:SER:HB3   | 1.93                     | 0.50              |
| 23:D2:25:LYS:HE2   | 23:D2:30:LYS:O     | 2.12                     | 0.50              |
| 43:DP:31:THR:HG21  | 28:DB:28:C:P       | 2.51                     | 0.50              |
| 3:AC:20:SER:HB3    | 14:AN:94:PRO:HG3   | 1.92                     | 0.50              |
| 18:AR:45:THR:OG1   | 18:AR:47:THR:HG22  | 2.12                     | 0.50              |
| 8:BH:2:SER:HB2     | 8:BH:4:GLN:HE21    | 1.76                     | 0.50              |
| 31:CA:1638:C:H5''  | 31:CA:2710:C:O2'   | 2.12                     | 0.50              |
| 55:DA:1536:C:H4'   | 55:DA:1537:G:H5''  | 1.93                     | 0.50              |
| 7:AG:111:ARG:HB3   | 7:AG:119:ARG:HG2   | 1.93                     | 0.50              |
| 11:BK:43:GLY:HA3   | 11:BK:74:VAL:HG12  | 1.93                     | 0.50              |
| 31:CA:70:G:H5''    | 31:CA:112:U:O2     | 2.12                     | 0.50              |
| 55:DA:914:G:H8     | 55:DA:914:G:H5''   | 1.77                     | 0.50              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 9:AI:19:VAL:HG22    | 9:AI:65:ILE:HG22   | 1.93                     | 0.49              |
| 1:BA:374:A:H5''     | 1:BA:452:A:C2      | 2.47                     | 0.49              |
| 9:BI:57:MET:HG3     | 9:BI:61:LEU:HG     | 1.93                     | 0.49              |
| 1:BA:735:C:H5'      | 18:BR:60:LYS:HD3   | 1.93                     | 0.49              |
| 31:CA:532:A:H2'     | 31:CA:532:A:N3     | 2.26                     | 0.49              |
| 30:CD:99:GLU:HG2    | 30:CD:182:ALA:HB2  | 1.94                     | 0.49              |
| 43:DP:68:LYS:HB3    | 62:DP:201:PEG:H22  | 1.93                     | 0.49              |
| 7:AG:69:VAL:HG23    | 7:AG:100:ALA:HB1   | 1.94                     | 0.49              |
| 24:C3:24:THR:HG23   | 24:C3:27:GLY:H     | 1.77                     | 0.49              |
| 34:CF:44:ILE:HG21   | 34:CF:79:ILE:HG22  | 1.94                     | 0.49              |
| 55:DA:479:A:N3      | 55:DA:481:G:H5''   | 2.26                     | 0.49              |
| 3:AC:47:LEU:HB3     | 3:AC:50:ALA:HB3    | 1.94                     | 0.49              |
| 7:BG:69:VAL:HG23    | 7:BG:100:ALA:HB1   | 1.94                     | 0.49              |
| 18:BR:36:SER:HA     | 18:BR:72:ASP:HB3   | 1.93                     | 0.49              |
| 31:CA:2185:U:H2'    | 31:CA:2186:G:C8    | 2.46                     | 0.49              |
| 31:CA:2445:2MG:HM21 | 31:CA:2449:U:O4    | 2.11                     | 0.49              |
| 29:CC:210:ALA:HA    | 29:CC:213:TRP:CE2  | 2.47                     | 0.49              |
| 22:D1:9:THR:HG21    | 55:DA:2020:A:H5'   | 1.94                     | 0.49              |
| 41:CN:21:ALA:HB1    | 41:CN:100:LYS:HG2  | 1.94                     | 0.49              |
| 55:DA:1433:A:O2'    | 55:DA:1434:A:H5'   | 2.12                     | 0.49              |
| 29:DC:227:PRO:HA    | 29:DC:233:GLY:HA2  | 1.95                     | 0.49              |
| 54:DI:31:ARG:HB2    | 54:DI:79:PRO:HG2   | 1.93                     | 0.49              |
| 29:CC:227:PRO:HA    | 29:CC:233:GLY:HA2  | 1.95                     | 0.49              |
| 35:CG:19:ILE:HG12   | 35:CG:24:ILE:HG12  | 1.93                     | 0.49              |
| 55:DA:2441:U:O2'    | 65:DA:3223:SPD:H91 | 2.13                     | 0.49              |
| 1:AA:411:A:P        | 4:AD:26:ARG:HH12   | 2.36                     | 0.49              |
| 11:AK:84:VAL:HG21   | 11:AK:97:ILE:HG23  | 1.95                     | 0.49              |
| 1:BA:202:G:H1       | 1:BA:215:C:H42     | 1.59                     | 0.49              |
| 55:DA:789:A:OP1     | 59:DA:3221:PUT:H12 | 2.12                     | 0.49              |
| 1:BA:76:G:H1        | 1:BA:93:U:H3       | 1.61                     | 0.49              |
| 3:BC:113:ALA:O      | 3:BC:200:VAL:HG11  | 2.12                     | 0.49              |
| 31:CA:1587:G:H2'    | 31:CA:1588:G:H8    | 1.78                     | 0.49              |
| 28:CB:14:U:H2'      | 28:CB:15:A:H2      | 1.76                     | 0.49              |
| 1:AA:202:G:O2'      | 1:AA:468:A:H8      | 1.95                     | 0.49              |
| 1:BA:202:G:O2'      | 1:BA:468:A:H8      | 1.95                     | 0.49              |
| 1:AA:1003:G:H21     | 1:AA:1005:A:H5'    | 1.77                     | 0.49              |
| 1:BA:840:C:H2'      | 1:BA:841:C:O4'     | 2.13                     | 0.49              |
| 47:CT:4:ILE:HG12    | 47:CT:106:VAL:HG22 | 1.94                     | 0.49              |
| 5:AE:107:ALA:HB2    | 5:AE:125:ALA:HB3   | 1.94                     | 0.48              |
| 11:AK:34:ILE:HB     | 11:AK:74:VAL:HG11  | 1.95                     | 0.48              |
| 3:BC:47:LEU:HB3     | 3:BC:50:ALA:HB3    | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:BC:20:SER:HB3   | 14:BN:94:PRO:HG3   | 1.93                     | 0.48              |
| 31:CA:1182:G:H2'  | 31:CA:1183:U:O4'   | 2.13                     | 0.48              |
| 31:CA:479:A:N3    | 31:CA:481:G:H5''   | 2.28                     | 0.48              |
| 33:CE:75:SER:O    | 33:CE:78:TRP:HB2   | 2.13                     | 0.48              |
| 39:CL:43:ILE:HD12 | 39:CL:56:ASP:HB2   | 1.94                     | 0.48              |
| 55:DA:837:C:H5    | 70:DA:6720:HOH:O   | 1.95                     | 0.48              |
| 28:DB:84:G:H21    | 63:DB:211:EDO:H11  | 1.78                     | 0.48              |
| 32:DD:99:GLU:HG2  | 32:DD:182:ALA:HB2  | 1.94                     | 0.48              |
| 15:AO:82:ILE:HG21 | 15:AO:89:ARG:OXT   | 2.13                     | 0.48              |
| 31:CA:2630:G:O4'  | 31:CA:2894:G:H1'   | 2.13                     | 0.48              |
| 32:DD:13:ARG:NH1  | 70:DD:401:HOH:O    | 2.44                     | 0.48              |
| 4:AD:48:LEU:HD21  | 4:AD:56:ARG:HG3    | 1.94                     | 0.48              |
| 2:BB:73:LYS:HD2   | 2:BB:168:HIS:HD2   | 1.77                     | 0.48              |
| 3:BC:72:ARG:HB3   | 3:BC:75:ILE:HG22   | 1.94                     | 0.48              |
| 31:CA:2060:A:N6   | 33:CE:69:ARG:NH2   | 2.60                     | 0.48              |
| 29:CC:177:ARG:HG2 | 31:CA:1820:U:OP1   | 2.14                     | 0.48              |
| 31:CA:2623:G:H4'  | 31:CA:2825:G:H8    | 1.78                     | 0.48              |
| 31:CA:914:G:H8    | 31:CA:914:G:H5''   | 1.79                     | 0.48              |
| 1:BA:975:A:H8     | 1:BA:1357:A:HO2'   | 1.61                     | 0.48              |
| 35:CG:80:THR:HG23 | 35:CG:81:GLU:N     | 2.24                     | 0.48              |
| 9:AI:57:MET:HG3   | 9:AI:61:LEU:HG     | 1.94                     | 0.48              |
| 1:BA:677:U:H3     | 1:BA:713:G:H22     | 1.61                     | 0.48              |
| 11:BK:30:THR:HG21 | 11:BK:92:GLY:HA3   | 1.96                     | 0.48              |
| 25:C4:24:HIS:CG   | 40:CM:61:LEU:HD13  | 2.49                     | 0.48              |
| 31:CA:634:C:H2'   | 31:CA:635:C:C6     | 2.49                     | 0.48              |
| 28:CB:14:U:H2'    | 28:CB:15:A:C2      | 2.49                     | 0.48              |
| 54:DI:50:VAL:HG13 | 54:DI:85:VAL:HG22  | 1.95                     | 0.48              |
| 43:DP:31:THR:HG22 | 43:DP:33:ARG:H     | 1.79                     | 0.48              |
| 1:AA:413:G:H5''   | 1:AA:414:A:H5'     | 1.96                     | 0.48              |
| 24:C3:37:LYS:O    | 31:CA:458:G:H2'    | 2.13                     | 0.48              |
| 25:D4:64:TYR:CZ   | 55:DA:242:G:H5''   | 2.49                     | 0.48              |
| 1:AA:975:A:H8     | 1:AA:1357:A:HO2'   | 1.59                     | 0.48              |
| 2:AB:20:THR:HG22  | 2:AB:39:HIS:CE1    | 2.48                     | 0.48              |
| 11:AK:30:THR:HG21 | 11:AK:92:GLY:HA3   | 1.95                     | 0.48              |
| 31:CA:247:G:H4'   | 31:CA:386:G:C5     | 2.49                     | 0.48              |
| 39:CL:38:ILE:HD11 | 39:CL:112:PHE:CZ   | 2.38                     | 0.48              |
| 25:C4:54:ASP:HB3  | 40:CM:57:LEU:HD22  | 1.95                     | 0.48              |
| 47:DT:4:ILE:HG12  | 47:DT:106:VAL:HG22 | 1.94                     | 0.48              |
| 47:DT:72:THR:HG21 | 47:DT:108:SER:HB3  | 1.95                     | 0.48              |
| 5:AE:38:VAL:HG11  | 5:AE:114:VAL:HG22  | 1.96                     | 0.48              |
| 23:D2:11:LEU:HD21 | 23:D2:34:LEU:HD23  | 1.94                     | 0.48              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 40:DM:21:ARG:HA      | 55:DA:811:U:H2'    | 1.95                     | 0.48              |
| 41:DN:41:LEU:HG      | 41:DN:96:ILE:HG13  | 1.96                     | 0.48              |
| 7:AG:22:LEU:HD12     | 7:AG:62:PHE:CE2    | 2.48                     | 0.48              |
| 5:BE:36:LEU:HD21     | 5:BE:137:VAL:HG11  | 1.95                     | 0.48              |
| 22:D1:55:ILE:HD12    | 42:DO:33:ILE:CD1   | 2.44                     | 0.48              |
| 55:DA:11:C:H2'       | 55:DA:12:U:H5'     | 1.95                     | 0.48              |
| 32:DD:150[B]:MEQ:HE2 | 55:DA:2033:A:O5'   | 2.14                     | 0.48              |
| 51:DX:41[A]:ARG:HG3  | 55:DA:2386:A:N3    | 2.28                     | 0.48              |
| 34:DF:44:ILE:HG21    | 34:DF:79:ILE:HG22  | 1.95                     | 0.48              |
| 47:DT:73:LYS:HB2     | 47:DT:106:VAL:HB   | 1.95                     | 0.48              |
| 1:AA:542:G:H5'       | 4:AD:39:GLY:HA3    | 1.96                     | 0.47              |
| 24:C3:16:HIS:CD2     | 31:CA:464:U:HO2'   | 2.32                     | 0.47              |
| 34:CF:36:LEU:HB2     | 34:CF:57:LEU:HD21  | 1.96                     | 0.47              |
| 55:DA:1172:C:C5      | 55:DA:1173:U:H1'   | 2.49                     | 0.47              |
| 45:DR:6:ARG:HD3      | 55:DA:1250:G:H5''  | 1.95                     | 0.47              |
| 55:DA:1587:G:H2'     | 55:DA:1588:G:H8    | 1.79                     | 0.47              |
| 22:D1:25:VAL:HG11    | 47:DT:38:TYR:HB2   | 1.96                     | 0.47              |
| 5:AE:133:PRO:O       | 5:AE:137:VAL:HG13  | 2.14                     | 0.47              |
| 1:BA:542:G:H5'       | 4:BD:39:GLY:HA3    | 1.96                     | 0.47              |
| 17:BQ:76:VAL:HG12    | 17:BQ:77:ARG:HG3   | 1.97                     | 0.47              |
| 23:C2:25:LYS:HE2     | 23:C2:30:LYS:O     | 2.14                     | 0.47              |
| 37:CJ:19:ASN:H       | 37:CJ:20:PRO:HD2   | 1.80                     | 0.47              |
| 31:CA:1364:G:P       | 52:CY:50:ARG:HH22  | 2.36                     | 0.47              |
| 55:DA:1975:G:H21     | 64:DA:3224:PGE:C2  | 2.27                     | 0.47              |
| 1:AA:1055:A:H2'      | 3:AC:156:ARG:HD2   | 1.96                     | 0.47              |
| 6:AF:38:ARG:HE       | 6:AF:63:ASN:ND2    | 2.12                     | 0.47              |
| 1:BA:1391:U:H2'      | 1:BA:1392:G:C8     | 2.49                     | 0.47              |
| 32:DD:8:LYS:HB2      | 32:DD:201:LEU:HD11 | 1.96                     | 0.47              |
| 39:DL:43:ILE:HD12    | 39:DL:56:ASP:HB2   | 1.96                     | 0.47              |
| 1:BA:1190:G:H5'      | 3:BC:176:HIS:NE2   | 2.29                     | 0.47              |
| 55:DA:2291:U:H2'     | 55:DA:2292:U:C6    | 2.49                     | 0.47              |
| 32:DD:105:LYS:NZ     | 32:DD:106:LYS:HE3  | 2.30                     | 0.47              |
| 37:DJ:103:ARG:HA     | 37:DJ:106:LEU:HD12 | 1.96                     | 0.47              |
| 11:BK:84:VAL:HG21    | 11:BK:97:ILE:HG23  | 1.97                     | 0.47              |
| 31:CA:2185:U:H2'     | 31:CA:2186:G:H8    | 1.79                     | 0.47              |
| 34:CF:8:TYR:HA       | 34:CF:12:VAL:HB    | 1.97                     | 0.47              |
| 13:AM:4:ILE:HD12     | 13:AM:10:PRO:HG2   | 1.95                     | 0.47              |
| 31:CA:1141:U:H4'     | 31:CA:1142:A:O4'   | 2.15                     | 0.47              |
| 25:C4:25:LYS:HD3     | 40:CM:62:PRO:HG2   | 1.97                     | 0.47              |
| 52:CY:10:LYS:HE3     | 52:CY:54:LYS:HG2   | 1.97                     | 0.47              |
| 55:DA:789:A:OP1      | 59:DA:3221:PUT:C1  | 2.63                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:269:C:H2'     | 1:AA:270:A:C8      | 2.50                     | 0.47              |
| 55:DA:1975:G:H21   | 64:DA:3224:PGE:H2  | 1.79                     | 0.47              |
| 55:DA:644:A:H2'    | 55:DA:645:C:O4'    | 2.14                     | 0.47              |
| 43:DP:52:SER:OG    | 43:DP:54:VAL:HG22  | 2.14                     | 0.47              |
| 49:DV:73:PHE:CE2   | 49:DV:75:ALA:HA    | 2.49                     | 0.47              |
| 31:CA:2030:6MZ:C2  | 31:CA:2499:C:H5''  | 2.45                     | 0.47              |
| 30:CD:26:VAL:HG21  | 44:CQ:5:ILE:HG12   | 1.97                     | 0.47              |
| 22:D1:5:GLN:O      | 55:DA:2017:U:H4'   | 2.15                     | 0.47              |
| 34:DF:36:LEU:HB2   | 34:DF:57:LEU:HD21  | 1.96                     | 0.47              |
| 34:DF:8:TYR:HA     | 34:DF:12:VAL:HB    | 1.97                     | 0.47              |
| 36:DH:49:ALA:O     | 36:DH:53:GLU:HB3   | 2.15                     | 0.47              |
| 37:DJ:19:ASN:H     | 37:DJ:20:PRO:HD2   | 1.80                     | 0.47              |
| 52:DY:10:LYS:HE3   | 52:DY:54:LYS:HG2   | 1.97                     | 0.47              |
| 1:BA:269:C:H2'     | 1:BA:270:A:C8      | 2.50                     | 0.47              |
| 1:BA:846:G:H2'     | 1:BA:847:G:H8      | 1.79                     | 0.47              |
| 24:C3:3:ARG:HD3    | 31:CA:1613:G:O2'   | 2.15                     | 0.47              |
| 31:CA:2291:U:H2'   | 31:CA:2292:U:C6    | 2.50                     | 0.47              |
| 30:CD:155:VAL:HG21 | 31:CA:2618:G:H21   | 1.79                     | 0.47              |
| 31:CA:608:A:H2'    | 31:CA:609:A:C8     | 2.50                     | 0.47              |
| 31:CA:2060:A:N6    | 33:CE:69:ARG:HH21  | 2.13                     | 0.47              |
| 49:CV:74:ASN:HD22  | 49:CV:77:THR:H     | 1.63                     | 0.47              |
| 32:DD:186:LEU:HD21 | 44:DQ:4:ILE:HG21   | 1.95                     | 0.47              |
| 1:AA:677:U:H3      | 1:AA:713:G:H22     | 1.63                     | 0.47              |
| 24:C3:7:PRO:CB     | 31:CA:1309:G:H4'   | 2.37                     | 0.47              |
| 55:DA:1236:G:N7    | 59:DA:3189:PUT:H41 | 2.30                     | 0.47              |
| 31:CA:193:U:H5     | 70:CA:3372:HOH:O   | 1.98                     | 0.47              |
| 31:CA:1936:A:H62   | 31:CA:1963:U:H3    | 1.60                     | 0.47              |
| 33:CE:1:MET:HG2    | 33:CE:14:VAL:HG23  | 1.97                     | 0.47              |
| 25:C4:25:LYS:O     | 40:CM:62:PRO:HD2   | 2.15                     | 0.47              |
| 55:DA:1182:G:H2'   | 55:DA:1183:U:O4'   | 2.15                     | 0.47              |
| 38:DK:69:ARG:O     | 38:DK:90:GLU:HB2   | 2.16                     | 0.47              |
| 1:AA:310:G:H5''    | 16:AP:31:ARG:HB2   | 1.97                     | 0.46              |
| 5:BE:57:PRO:O      | 5:BE:60:ILE:HG13   | 2.15                     | 0.46              |
| 55:DA:749:A:H4'    | 55:DA:1271:G:N3    | 2.29                     | 0.46              |
| 33:DE:176:ASP:OD2  | 33:DE:178:VAL:HG12 | 2.15                     | 0.46              |
| 1:AA:73:C:O2'      | 1:AA:74:A:H8       | 1.97                     | 0.46              |
| 1:BA:1055:A:H2'    | 3:BC:156:ARG:HD2   | 1.97                     | 0.46              |
| 1:BA:23:C:H5       | 1:BA:561:U:O4      | 1.98                     | 0.46              |
| 2:BB:73:LYS:HD2    | 2:BB:168:HIS:CD2   | 2.51                     | 0.46              |
| 42:CO:47:VAL:O     | 42:CO:51:LEU:HD23  | 2.15                     | 0.46              |
| 43:CP:31:THR:HG22  | 43:CP:33:ARG:H     | 1.79                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DF:121:SER:HB2 | 55:DA:2304:G:H5'   | 1.96                     | 0.46              |
| 6:AF:47:LEU:HD13  | 6:AF:51:ILE:HG12   | 1.97                     | 0.46              |
| 31:CA:309:A:H4'   | 49:CV:16:GLY:HA2   | 1.97                     | 0.46              |
| 31:CA:846:U:H1'   | 31:CA:847:U:C5     | 2.44                     | 0.46              |
| 34:CF:103:LEU:HA  | 34:CF:107:ALA:HB3  | 1.97                     | 0.46              |
| 49:CV:7:ARG:O     | 49:CV:25:VAL:HB    | 2.15                     | 0.46              |
| 55:DA:1180:U:H5'' | 55:DA:1180:U:H6    | 1.80                     | 0.46              |
| 34:DF:103:LEU:HA  | 34:DF:107:ALA:HB3  | 1.97                     | 0.46              |
| 21:AU:4:ILE:HG13  | 21:AU:19:PHE:HA    | 1.97                     | 0.46              |
| 1:BA:202:G:H21    | 1:BA:466:A:H61     | 1.62                     | 0.46              |
| 19:BS:15:LEU:HD13 | 19:BS:33:THR:HG21  | 1.95                     | 0.46              |
| 30:CD:152:PRO:HG3 | 30:CD:156:PHE:CZ   | 2.51                     | 0.46              |
| 51:DX:39:ARG:NH1  | 70:DX:101:HOH:O    | 2.48                     | 0.46              |
| 1:AA:76:G:H1      | 1:AA:93:U:H3       | 1.62                     | 0.46              |
| 30:CD:133:THR:CG2 | 31:CA:1993:U:H4'   | 2.45                     | 0.46              |
| 31:CA:740:C:H5'   | 31:CA:1784:A:C3'   | 2.38                     | 0.46              |
| 30:CD:3:GLY:O     | 30:CD:4:LEU:HD13   | 2.15                     | 0.46              |
| 30:CD:62:LYS:HE2  | 31:CA:2810:A:H5''  | 1.98                     | 0.46              |
| 40:CM:77:ILE:CD1  | 40:CM:108:ALA:HB1  | 2.36                     | 0.46              |
| 64:D1:102:PGE:H4  | 70:DT:313:HOH:O    | 2.15                     | 0.46              |
| 55:DA:57:C:H2'    | 55:DA:58:G:O4'     | 2.16                     | 0.46              |
| 1:AA:1391:U:H2'   | 1:AA:1392:G:C8     | 2.50                     | 0.46              |
| 1:AA:1190:G:H5'   | 3:AC:176:HIS:NE2   | 2.31                     | 0.46              |
| 1:BA:1001:C:H2'   | 1:BA:1002:G:H8     | 1.81                     | 0.46              |
| 21:BU:4:ILE:HG13  | 21:BU:19:PHE:HA    | 1.97                     | 0.46              |
| 31:CA:1010:A:H5'  | 45:CR:62:ILE:CG2   | 2.46                     | 0.46              |
| 29:CC:219:THR:O   | 31:CA:1789:A:H5''  | 2.15                     | 0.46              |
| 31:CA:749:A:H4'   | 31:CA:1271:G:N3    | 2.29                     | 0.46              |
| 44:CQ:114:LEU:H   | 44:CQ:114:LEU:HD23 | 1.81                     | 0.46              |
| 31:CA:1250:G:C5'  | 45:CR:6:ARG:HD3    | 2.44                     | 0.46              |
| 55:DA:102:U:H2'   | 55:DA:102:U:O2     | 2.15                     | 0.46              |
| 45:CR:58:ARG:HA   | 45:CR:61:TRP:CE3   | 2.50                     | 0.46              |
| 48:CU:45:ALA:O    | 48:CU:49:LYS:HG2   | 2.14                     | 0.46              |
| 29:DC:207:LYS:HB2 | 55:DA:729:G:C6     | 2.51                     | 0.46              |
| 52:DY:61:LYS:HD3  | 55:DA:372:G:H5''   | 1.98                     | 0.46              |
| 17:AQ:76:VAL:HG12 | 17:AQ:77:ARG:HG3   | 1.97                     | 0.46              |
| 1:BA:310:G:H5''   | 16:BP:31:ARG:HB2   | 1.97                     | 0.46              |
| 1:BA:438:U:H5'    | 4:BD:120:HIS:HB3   | 1.97                     | 0.46              |
| 1:BA:376:G:H5''   | 16:BP:5:ARG:HB2    | 1.97                     | 0.46              |
| 23:C2:22:THR:HG21 | 31:CA:2419:U:H5''  | 1.98                     | 0.46              |
| 31:CA:948:C:H1'   | 31:CA:984:A:C8     | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CC:235:GLY:HA3  | 29:CC:239:ASN:HB2  | 1.97                     | 0.46              |
| 35:CG:80:THR:CG2   | 35:CG:81:GLU:H     | 2.27                     | 0.46              |
| 40:DM:60:ARG:HD2   | 55:DA:2360:G:H1'   | 1.98                     | 0.46              |
| 24:D3:4:THR:HA     | 55:DA:687:C:O4'    | 2.14                     | 0.46              |
| 1:AA:216:U:H2'     | 1:AA:217:C:C6      | 2.50                     | 0.46              |
| 1:BA:1496:C:H2'    | 1:BA:1497:G:O4'    | 2.16                     | 0.46              |
| 48:CU:67:VAL:HG22  | 48:CU:76:ARG:HG3   | 1.98                     | 0.46              |
| 23:D2:10:LYS:HE3   | 23:D2:53:LYS:O     | 2.16                     | 0.46              |
| 1:AA:1054:C:H5''   | 1:AA:1054:C:H6     | 1.80                     | 0.46              |
| 1:AA:438:U:H5'     | 4:AD:120:HIS:HB3   | 1.98                     | 0.46              |
| 5:AE:57:PRO:O      | 5:AE:60:ILE:HG13   | 2.15                     | 0.46              |
| 18:BR:27:ALA:O     | 18:BR:30:LYS:HG2   | 2.16                     | 0.46              |
| 31:CA:694:U:OP1    | 31:CA:1569:A:H1'   | 2.15                     | 0.46              |
| 31:CA:833:A:H2'    | 31:CA:834:G:C8     | 2.51                     | 0.46              |
| 55:DA:2070:A:H2'   | 55:DA:2071:A:O4'   | 2.16                     | 0.46              |
| 55:DA:2800:A:C2    | 55:DA:2895:G:H1'   | 2.51                     | 0.46              |
| 55:DA:722:A:H2'    | 55:DA:723:C:O4'    | 2.16                     | 0.46              |
| 55:DA:871:U:H2'    | 55:DA:872:U:C6     | 2.51                     | 0.46              |
| 5:AE:16:ILE:HD13   | 5:AE:137:VAL:HG11  | 1.97                     | 0.45              |
| 1:BA:846:G:H2'     | 1:BA:847:G:C8      | 2.51                     | 0.45              |
| 9:BI:7:TYR:HE1     | 9:BI:18:ARG:HB2    | 1.80                     | 0.45              |
| 31:CA:594:U:H2'    | 31:CA:595:C:C6     | 2.51                     | 0.45              |
| 22:D1:9:THR:CG2    | 55:DA:2020:A:H5'   | 2.46                     | 0.45              |
| 36:DH:104:THR:HG22 | 36:DH:109:GLU:HA   | 1.97                     | 0.45              |
| 30:CD:8:LYS:HB2    | 30:CD:201:LEU:HD11 | 1.97                     | 0.45              |
| 41:CN:69:PRO:O     | 41:CN:93:VAL:O     | 2.34                     | 0.45              |
| 55:DA:2086:U:H2'   | 55:DA:2087:G:C8    | 2.51                     | 0.45              |
| 55:DA:2117:A:H61   | 55:DA:2171:A:H61   | 1.63                     | 0.45              |
| 65:DA:3223:SPD:H82 | 70:DA:4260:HOH:O   | 2.16                     | 0.45              |
| 29:DC:177:ARG:HG2  | 55:DA:1820:U:OP1   | 2.16                     | 0.45              |
| 29:DC:235:GLY:HA3  | 29:DC:239:ASN:HB2  | 1.98                     | 0.45              |
| 10:AJ:52:LEU:HB2   | 14:AN:81:ARG:HD2   | 1.99                     | 0.45              |
| 1:BA:1108:G:H5''   | 3:BC:176:HIS:CE1   | 2.52                     | 0.45              |
| 1:BA:216:U:H2'     | 1:BA:217:C:C6      | 2.51                     | 0.45              |
| 1:BA:411:A:P       | 4:BD:26:ARG:HH12   | 2.39                     | 0.45              |
| 31:CA:1326:U:H2'   | 31:CA:1327:A:H8    | 1.81                     | 0.45              |
| 37:CJ:103:ARG:HA   | 37:CJ:106:LEU:HD12 | 1.96                     | 0.45              |
| 43:CP:31:THR:HG22  | 43:CP:34:HIS:H     | 1.81                     | 0.45              |
| 55:DA:2628:C:C5'   | 59:DA:3195:PUT:H12 | 2.42                     | 0.45              |
| 33:DE:1:MET:HG2    | 33:DE:14:VAL:HG23  | 1.97                     | 0.45              |
| 42:DO:9:GLN:O      | 42:DO:17:ARG:HD3   | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:DX:37:ILE:HG21  | 51:DX:80:ILE:HG21  | 1.98                     | 0.45              |
| 52:DY:7:VAL:HG23   | 52:DY:51:VAL:HG12  | 1.98                     | 0.45              |
| 1:AA:845:A:H2'     | 1:AA:846:G:O4'     | 2.17                     | 0.45              |
| 1:AA:923:A:OP1     | 5:AE:26:LYS:HG2    | 2.16                     | 0.45              |
| 1:BA:1053:G:N7     | 1:BA:1200:C:H5''   | 2.32                     | 0.45              |
| 2:BB:163:VAL:HG11  | 2:BB:173:ILE:HD11  | 1.99                     | 0.45              |
| 31:CA:871:U:H2'    | 31:CA:872:U:C6     | 2.51                     | 0.45              |
| 38:CK:69:ARG:O     | 38:CK:90:GLU:HB3   | 2.16                     | 0.45              |
| 55:DA:1133:A:N3    | 59:DA:3212:PUT:H22 | 2.32                     | 0.45              |
| 32:DD:152:PRO:HG3  | 32:DD:156:PHE:CZ   | 2.52                     | 0.45              |
| 45:DR:58:ARG:HA    | 45:DR:61:TRP:CE3   | 2.51                     | 0.45              |
| 1:AA:266:G:H3'     | 17:AQ:69:LYS:HB2   | 1.97                     | 0.45              |
| 1:AA:376:G:H5''    | 16:AP:5:ARG:HB2    | 1.98                     | 0.45              |
| 31:CA:2296:U:H5    | 43:CP:9:ARG:NH2    | 2.14                     | 0.45              |
| 55:DA:1509:A:HO2'  | 55:DA:1510:G:H8    | 1.64                     | 0.45              |
| 27:D0:15:GLY:HA2   | 55:DA:969:G:O3'    | 2.16                     | 0.45              |
| 33:DE:32:VAL:HG21  | 40:DM:6:LEU:HD13   | 1.99                     | 0.45              |
| 2:AB:93:ASN:H      | 2:AB:93:ASN:HD22   | 1.65                     | 0.45              |
| 1:BA:8:A:H1'       | 5:BE:108:GLY:HA2   | 1.97                     | 0.45              |
| 31:CA:191:A:H2'    | 31:CA:192:C:C6     | 2.51                     | 0.45              |
| 31:CA:722:A:H2'    | 31:CA:723:C:O4'    | 2.16                     | 0.45              |
| 47:CT:84:ARG:HB2   | 47:CT:96:ILE:HB    | 1.99                     | 0.45              |
| 48:CU:28:ASN:ND2   | 48:CU:91:GLN:HB3   | 2.14                     | 0.45              |
| 35:DG:103:ILE:HD11 | 35:DG:117:LEU:HD21 | 1.99                     | 0.45              |
| 1:BA:923:A:OP1     | 5:BE:26:LYS:HG2    | 2.17                     | 0.45              |
| 31:CA:248:G:H5'    | 31:CA:250:G:N7     | 2.31                     | 0.45              |
| 31:CA:2544:G:H5'   | 31:CA:2645:G:C2    | 2.51                     | 0.45              |
| 31:CA:381:G:OP1    | 52:CY:18:ARG:HD3   | 2.16                     | 0.45              |
| 31:CA:674:G:H1'    | 33:CE:69:ARG:HH11  | 1.82                     | 0.45              |
| 45:CR:112:LYS:HD3  | 46:CS:48:LYS:HG3   | 1.99                     | 0.45              |
| 55:DA:1168:G:H5''  | 55:DA:1168:G:H8    | 1.81                     | 0.45              |
| 55:DA:136:G:H1     | 55:DA:143:C:H42    | 1.65                     | 0.45              |
| 43:DP:35:ILE:HG21  | 43:DP:71:ALA:HA    | 1.98                     | 0.45              |
| 44:DQ:52:ASN:O     | 44:DQ:53:ARG:HD3   | 2.16                     | 0.45              |
| 4:AD:172:GLU:HG2   | 4:AD:183:LYS:HD2   | 1.99                     | 0.45              |
| 8:AH:105:SER:HB2   | 8:AH:126:ILE:HD11  | 1.98                     | 0.45              |
| 2:BB:93:ASN:H      | 2:BB:93:ASN:HD22   | 1.65                     | 0.45              |
| 31:CA:1810:A:H2'   | 31:CA:1811:G:O4'   | 2.17                     | 0.45              |
| 31:CA:1965:C:H5''  | 31:CA:1966:A:H2'   | 1.99                     | 0.45              |
| 33:CE:176:ASP:OD2  | 33:CE:178:VAL:HG12 | 2.16                     | 0.45              |
| 46:CS:49:ILE:HB    | 46:CS:51:VAL:O     | 2.17                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:DA:2609:U:C5   | 63:DA:3194:EDO:H12 | 2.52                     | 0.45              |
| 1:AA:202:G:H1     | 1:AA:215:C:H42     | 1.64                     | 0.45              |
| 47:CT:72:THR:HG21 | 47:CT:108:SER:HB3  | 1.98                     | 0.45              |
| 54:DI:70:GLU:HG2  | 54:DI:73:LYS:HE3   | 1.98                     | 0.45              |
| 1:AA:1001:C:H2'   | 1:AA:1002:G:H8     | 1.82                     | 0.45              |
| 31:CA:1775:U:O4   | 31:CA:1789:A:H2    | 2.00                     | 0.45              |
| 31:CA:278:A:N3    | 31:CA:278:A:H2'    | 2.32                     | 0.45              |
| 31:CA:826:U:O2'   | 40:CM:53:GLY:HA3   | 2.17                     | 0.45              |
| 25:C4:47:LYS:NZ   | 40:CM:64:PHE:CD1   | 2.75                     | 0.45              |
| 24:D3:33:ARG:HG3  | 62:D3:102:PEG:H31  | 1.99                     | 0.45              |
| 55:DA:355:U:H2'   | 55:DA:356:G:H8     | 1.82                     | 0.45              |
| 38:DK:7:LYS:O     | 38:DK:11:VAL:HG23  | 2.17                     | 0.45              |
| 46:DS:8:GLY:HA2   | 55:DA:1161:C:O2'   | 2.17                     | 0.45              |
| 50:DW:38:LEU:HD21 | 50:DW:65:VAL:HG11  | 1.99                     | 0.45              |
| 4:BD:172:GLU:HG2  | 4:BD:183:LYS:HD2   | 1.99                     | 0.44              |
| 31:CA:320:A:H4'   | 31:CA:322:A:N7     | 2.32                     | 0.44              |
| 31:CA:478:A:H61   | 31:CA:500:G:H4'    | 1.81                     | 0.44              |
| 55:DA:1283:G:H1'  | 55:DA:1329:U:O2    | 2.17                     | 0.44              |
| 55:DA:278:A:H2'   | 55:DA:278:A:N3     | 2.32                     | 0.44              |
| 55:DA:1349:C:O2'  | 57:DA:3215:PG4:H82 | 2.16                     | 0.44              |
| 55:DA:612:G:H2'   | 55:DA:614:A:C8     | 2.52                     | 0.44              |
| 29:DC:199:GLU:O   | 29:DC:202:LEU:HB2  | 2.17                     | 0.44              |
| 9:AI:7:TYR:HE1    | 9:AI:18:ARG:HB2    | 1.81                     | 0.44              |
| 1:BA:1493:A:H1'   | 31:CA:1913:A:H61   | 1.82                     | 0.44              |
| 1:BA:957:U:O2     | 1:BA:959:A:H8      | 2.01                     | 0.44              |
| 2:BB:68:LEU:HD11  | 2:BB:92:VAL:HG23   | 2.00                     | 0.44              |
| 22:C1:16:ARG:HA   | 31:CA:2046:G:C5'   | 2.47                     | 0.44              |
| 55:DA:760:G:H4'   | 55:DA:1776:G:OP1   | 2.18                     | 0.44              |
| 54:DI:132:TYR:H   | 54:DI:133:GLU:HB2  | 1.81                     | 0.44              |
| 1:AA:957:U:O2     | 1:AA:959:A:H8      | 2.01                     | 0.44              |
| 1:BA:1054:C:H6    | 1:BA:1054:C:H5''   | 1.83                     | 0.44              |
| 6:BF:47:LEU:HD13  | 6:BF:51:ILE:HG12   | 1.99                     | 0.44              |
| 31:CA:1556:C:H2'  | 31:CA:1557:C:C6    | 2.52                     | 0.44              |
| 31:CA:639:U:H2'   | 31:CA:640:C:C6     | 2.52                     | 0.44              |
| 31:CA:2641:G:H5'' | 38:CK:78:THR:HB    | 1.99                     | 0.44              |
| 29:DC:212:ARG:HD2 | 29:DC:216:VAL:O    | 2.18                     | 0.44              |
| 34:DF:16:LEU:HD13 | 34:DF:29:PRO:HD2   | 1.99                     | 0.44              |
| 43:DP:31:THR:HG22 | 43:DP:34:HIS:H     | 1.80                     | 0.44              |
| 1:AA:1053:G:N7    | 1:AA:1200:C:H5''   | 2.33                     | 0.44              |
| 2:AB:68:LEU:HD11  | 2:AB:92:VAL:HG23   | 1.99                     | 0.44              |
| 1:BA:73:C:O2'     | 1:BA:74:A:H8       | 1.97                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:BA:1226:C:H2'    | 13:BM:102:THR:HB   | 1.99                     | 0.44              |
| 24:C3:2:LYS:NZ     | 70:C3:101:HOH:O    | 2.49                     | 0.44              |
| 31:CA:811:U:H2'    | 40:CM:21:ARG:HA    | 1.99                     | 0.44              |
| 51:CX:37:ILE:HG21  | 51:CX:80:ILE:HG21  | 1.98                     | 0.44              |
| 55:DA:1738:G:HO2'  | 55:DA:1739:A:H8    | 1.62                     | 0.44              |
| 1:AA:864:A:H4'     | 5:AE:90:THR:HG23   | 2.00                     | 0.44              |
| 1:AA:9:G:H5'       | 5:AE:108:GLY:HA3   | 1.99                     | 0.44              |
| 9:AI:99:ARG:HG2    | 9:AI:104:VAL:HG21  | 1.99                     | 0.44              |
| 13:AM:12:HIS:HB3   | 70:AM:302:HOH:O    | 2.17                     | 0.44              |
| 11:BK:84:VAL:HG11  | 11:BK:97:ILE:HG12  | 2.00                     | 0.44              |
| 14:BN:31:ILE:HG23  | 14:BN:42:TRP:CZ2   | 2.53                     | 0.44              |
| 20:BT:58:VAL:HG13  | 20:BT:72:ALA:HB1   | 1.99                     | 0.44              |
| 22:C1:53:LYS:HE3   | 22:C1:56:ALA:HA    | 1.99                     | 0.44              |
| 31:CA:2489:U:HO2'  | 31:CA:2491:U:H5    | 1.64                     | 0.44              |
| 31:CA:2674:G:H4'   | 39:CL:30:ARG:HD2   | 2.00                     | 0.44              |
| 25:C4:4:ILE:HG23   | 31:CA:666:A:O2'    | 2.17                     | 0.44              |
| 31:CA:747:5MU:O2   | 31:CA:2014:A:H1'   | 2.18                     | 0.44              |
| 31:CA:863:A:H2'    | 31:CA:864:G:C8     | 2.53                     | 0.44              |
| 34:CF:16:LEU:HD13  | 34:CF:29:PRO:HD2   | 1.98                     | 0.44              |
| 50:CW:38:LEU:HD21  | 50:CW:65:VAL:HG11  | 1.98                     | 0.44              |
| 55:DA:1321:A:C2    | 64:DA:3216:PGE:H12 | 2.53                     | 0.44              |
| 29:DC:203:ARG:HH21 | 29:DC:205:LEU:HD21 | 1.82                     | 0.44              |
| 33:DE:84:THR:HG21  | 55:DA:586:A:H5'    | 1.98                     | 0.44              |
| 2:AB:129:LEU:H     | 2:AB:129:LEU:HG    | 1.51                     | 0.44              |
| 43:CP:35:ILE:HG21  | 43:CP:71:ALA:HA    | 1.98                     | 0.44              |
| 55:DA:639:U:H2'    | 55:DA:640:C:C6     | 2.53                     | 0.44              |
| 29:DC:13:ARG:HD3   | 55:DA:728:G:H4'    | 2.00                     | 0.44              |
| 8:AH:87:LYS:HB2    | 8:AH:125:ILE:CD1   | 2.41                     | 0.44              |
| 13:AM:17:ILE:H     | 13:AM:17:ILE:HD12  | 1.83                     | 0.44              |
| 1:BA:266:G:H3'     | 17:BQ:69:LYS:HB2   | 2.00                     | 0.44              |
| 25:C4:13:ARG:NH1   | 31:CA:250:G:P      | 2.91                     | 0.44              |
| 31:CA:659:G:H4'    | 33:CE:95:LYS:HD3   | 1.99                     | 0.44              |
| 36:CH:104:THR:HG22 | 36:CH:109:GLU:HA   | 1.98                     | 0.44              |
| 55:DA:1831:G:H1'   | 64:DA:3224:PGE:H22 | 1.98                     | 0.44              |
| 55:DA:62:U:H5'     | 58:DA:3203:MPD:H53 | 2.00                     | 0.44              |
| 55:DA:493:G:H2'    | 55:DA:494:G:O4'    | 2.18                     | 0.44              |
| 54:DI:85:VAL:HG21  | 54:DI:90:GLY:O     | 2.17                     | 0.44              |
| 1:AA:1496:C:H2'    | 1:AA:1497:G:O4'    | 2.18                     | 0.44              |
| 3:AC:21:THR:HG23   | 3:AC:58:GLU:HB3    | 1.99                     | 0.44              |
| 11:AK:84:VAL:HG11  | 11:AK:97:ILE:HG12  | 1.99                     | 0.44              |
| 1:BA:1060:U:H5     | 3:BC:2:GLY:HA3     | 1.81                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:C2:33:LYS:HA   | 23:C2:52:ALA:HB3   | 2.00                     | 0.44              |
| 31:CA:2051:A:H5'  | 31:CA:2578:G:O4'   | 2.18                     | 0.44              |
| 29:CC:199:GLU:O   | 29:CC:202:LEU:HB2  | 2.18                     | 0.44              |
| 38:CK:7:LYS:O     | 38:CK:11:VAL:HG23  | 2.17                     | 0.44              |
| 37:DJ:11:LEU:HD22 | 37:DJ:24:VAL:HG23  | 2.00                     | 0.44              |
| 20:BT:5:LYS:HB3   | 20:BT:7:ALA:H      | 1.82                     | 0.44              |
| 31:CA:1469:A:H2'  | 31:CA:1470:A:C8    | 2.53                     | 0.44              |
| 24:C3:7:PRO:HG3   | 31:CA:1612:C:H5'   | 2.00                     | 0.44              |
| 31:CA:528:A:C8    | 31:CA:528:A:C3'    | 3.00                     | 0.44              |
| 31:CA:95:A:H4'    | 53:CZ:38:GLN:O     | 2.18                     | 0.44              |
| 29:CC:212:ARG:HD2 | 29:CC:216:VAL:O    | 2.18                     | 0.44              |
| 31:CA:1808:A:N1   | 52:CY:28:ARG:HD2   | 2.33                     | 0.44              |
| 46:DS:41:ILE:HD13 | 46:DS:103:ALA:HA   | 1.99                     | 0.44              |
| 49:DV:94:ARG:HB3  | 49:DV:103:ILE:HD12 | 1.99                     | 0.44              |
| 17:AQ:8:LEU:HD13  | 17:AQ:25:ILE:HG13  | 1.99                     | 0.43              |
| 4:BD:85:ASN:HA    | 5:BE:102:GLY:CA    | 2.31                     | 0.43              |
| 14:BN:10:GLU:HG3  | 14:BN:63:ARG:HD2   | 2.00                     | 0.43              |
| 31:CA:1274:A:N3   | 31:CA:1297:C:H1'   | 2.33                     | 0.43              |
| 31:CA:1991:U:H2'  | 31:CA:1992:G:H5''  | 2.00                     | 0.43              |
| 30:CD:13:ARG:HD3  | 30:CD:21:SER:OG    | 2.18                     | 0.43              |
| 45:CR:113:ALA:O   | 45:CR:117:LEU:HD12 | 2.18                     | 0.43              |
| 50:CW:51:GLN:HG2  | 50:CW:86:LEU:HD11  | 2.00                     | 0.43              |
| 41:DN:42:THR:HG22 | 41:DN:93:VAL:HG12  | 1.99                     | 0.43              |
| 1:AA:1060:U:H4'   | 10:AJ:53:ILE:HG23  | 2.00                     | 0.43              |
| 14:AN:10:GLU:HG3  | 14:AN:63:ARG:HD2   | 2.00                     | 0.43              |
| 14:AN:46:LEU:HA   | 14:AN:49:GLN:HE21  | 1.83                     | 0.43              |
| 16:BP:20:VAL:CG1  | 16:BP:32:PHE:HB2   | 2.47                     | 0.43              |
| 31:CA:355:U:H2'   | 31:CA:356:G:H8     | 1.83                     | 0.43              |
| 34:CF:5:HIS:HB2   | 34:CF:97:TRP:CD1   | 2.53                     | 0.43              |
| 55:DA:1394:U:H4'  | 55:DA:1603:A:H4'   | 2.00                     | 0.43              |
| 2:AB:163:VAL:HG11 | 2:AB:173:ILE:HD11  | 2.00                     | 0.43              |
| 2:AB:70:VAL:HB    | 2:AB:163:VAL:HG22  | 2.00                     | 0.43              |
| 1:BA:1060:U:H4'   | 10:BJ:53:ILE:HG23  | 2.00                     | 0.43              |
| 1:BA:10:A:OP2     | 5:BE:131:THR:HG21  | 2.18                     | 0.43              |
| 6:BF:70:VAL:HA    | 6:BF:73:GLU:HG2    | 2.00                     | 0.43              |
| 10:BJ:52:LEU:HB2  | 14:BN:81:ARG:HD2   | 2.00                     | 0.43              |
| 31:CA:2688:G:H1'  | 31:CA:2721:A:N6    | 2.34                     | 0.43              |
| 31:CA:2623:G:H4'  | 31:CA:2825:G:C8    | 2.53                     | 0.43              |
| 31:CA:532:A:H4'   | 31:CA:533:G:C8     | 2.54                     | 0.43              |
| 35:CG:17:VAL:HG11 | 35:CG:50:LEU:HD21  | 2.00                     | 0.43              |
| 1:AA:604:G:H2'    | 1:AA:605:U:O4'     | 2.19                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AL:31:ARG:O    | 12:AL:58:THR:HG23  | 2.18                     | 0.43              |
| 1:AA:1226:C:H2'   | 13:AM:102:THR:HB   | 2.00                     | 0.43              |
| 1:BA:1277:C:HO2'  | 1:BA:1279:G:H8     | 1.62                     | 0.43              |
| 22:D1:53:LYS:HE3  | 22:D1:56:ALA:HA    | 2.00                     | 0.43              |
| 55:DA:1424:G:H21  | 64:DA:3213:PGE:H32 | 1.84                     | 0.43              |
| 55:DA:142:A:H2'   | 55:DA:143:C:C6     | 2.53                     | 0.43              |
| 55:DA:2031:A:C6   | 55:DA:2498:OMC:H1' | 2.53                     | 0.43              |
| 34:DF:80:ARG:HB3  | 34:DF:83:TYR:CE1   | 2.53                     | 0.43              |
| 34:DF:5:HIS:HB2   | 34:DF:97:TRP:CD1   | 2.54                     | 0.43              |
| 17:AQ:15:ASP:HA   | 17:AQ:21:ILE:HG22  | 1.99                     | 0.43              |
| 20:AT:44:LYS:H    | 20:AT:44:LYS:HG3   | 1.61                     | 0.43              |
| 11:BK:24:HIS:HB3  | 11:BK:31:ILE:HG23  | 2.00                     | 0.43              |
| 13:BM:54:ASP:HA   | 13:BM:57:ARG:HD2   | 2.00                     | 0.43              |
| 17:BQ:46:VAL:HG11 | 17:BQ:61:ILE:CG2   | 2.48                     | 0.43              |
| 30:CD:121:THR:HB  | 30:CD:127:PHE:CD2  | 2.54                     | 0.43              |
| 37:CJ:11:LEU:HD22 | 37:CJ:24:VAL:HG23  | 2.00                     | 0.43              |
| 39:CL:103:VAL:O   | 39:CL:122:VAL:HB   | 2.18                     | 0.43              |
| 31:CA:1030:C:OP2  | 41:CN:127:LYS:HE3  | 2.19                     | 0.43              |
| 42:CO:71:ARG:HG3  | 42:CO:71:ARG:O     | 2.19                     | 0.43              |
| 49:CV:94:ARG:HB3  | 49:CV:103:ILE:HD12 | 1.99                     | 0.43              |
| 31:CA:96:C:H4'    | 53:CZ:41:HIS:CG    | 2.53                     | 0.43              |
| 54:DI:56:ARG:HA   | 55:DA:1107:G:OP1   | 2.19                     | 0.43              |
| 10:AJ:10:LEU:HB2  | 10:AJ:72:ARG:HB2   | 2.00                     | 0.43              |
| 8:BH:105:SER:HB2  | 8:BH:126:ILE:HD11  | 1.99                     | 0.43              |
| 3:BC:23:PHE:CD2   | 10:BJ:97:ASP:HB2   | 2.54                     | 0.43              |
| 31:CA:142:A:H2'   | 31:CA:143:C:C6     | 2.53                     | 0.43              |
| 29:CC:225:MET:O   | 29:CC:233:GLY:O    | 2.36                     | 0.43              |
| 39:CL:113:MET:O   | 39:CL:116:ILE:HG13 | 2.18                     | 0.43              |
| 31:CA:309:A:O3'   | 49:CV:16:GLY:HA2   | 2.18                     | 0.43              |
| 25:D4:13:ARG:HH11 | 55:DA:2394:C:H5'   | 1.82                     | 0.43              |
| 55:DA:1028:A:N6   | 55:DA:1125:G:H2'   | 2.33                     | 0.43              |
| 55:DA:191:A:H2'   | 55:DA:192:C:C6     | 2.53                     | 0.43              |
| 55:DA:2849:U:H4'  | 55:DA:2868:A:C2    | 2.54                     | 0.43              |
| 55:DA:5:A:H2'     | 55:DA:6:A:C8       | 2.53                     | 0.43              |
| 54:DI:50:VAL:HG22 | 54:DI:85:VAL:HG13  | 2.00                     | 0.43              |
| 46:DS:44:GLY:O    | 46:DS:45:GLU:HG2   | 2.17                     | 0.43              |
| 1:BA:502:A:H2'    | 1:BA:503:C:O4'     | 2.19                     | 0.43              |
| 31:CA:2728:U:O2'  | 31:CA:2729:G:H8    | 2.01                     | 0.43              |
| 31:CA:493:G:H2'   | 31:CA:494:G:O4'    | 2.18                     | 0.43              |
| 31:CA:528:A:C2    | 31:CA:2042:A:H2'   | 2.54                     | 0.43              |
| 55:DA:523:C:H4'   | 55:DA:540:C:O2     | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:DI:27:VAL:HG13  | 54:DI:80:THR:HG23  | 2.00                     | 0.43              |
| 45:DR:51:ARG:HH22  | 55:DA:993:G:P      | 2.41                     | 0.43              |
| 48:DU:33:LYS:HG3   | 48:DU:80:TRP:CE3   | 2.53                     | 0.43              |
| 3:AC:7:PRO:HD2     | 3:AC:184:TYR:CD1   | 2.54                     | 0.43              |
| 1:BA:1493:A:H8     | 1:BA:1493:A:OP2    | 2.01                     | 0.43              |
| 4:BD:105:MET:SD    | 4:BD:143:VAL:HG22  | 2.59                     | 0.43              |
| 26:C5:17:VAL:HG12  | 26:C5:26:ILE:HD12  | 2.01                     | 0.43              |
| 31:CA:2636:C:H2'   | 31:CA:2637:U:C6    | 2.54                     | 0.43              |
| 31:CA:685:A:H5''   | 31:CA:774:G:O6     | 2.19                     | 0.43              |
| 40:CM:95:LEU:HD22  | 40:CM:100:ILE:HG12 | 2.00                     | 0.43              |
| 42:CO:9:GLN:O      | 42:CO:17:ARG:HD3   | 2.17                     | 0.43              |
| 46:CS:3:ALA:HB3    | 46:CS:101:ILE:HD12 | 2.01                     | 0.43              |
| 55:DA:1654:A:H1'   | 55:DA:2823:A:H5'   | 2.00                     | 0.43              |
| 34:DF:36:LEU:HD22  | 34:DF:154:ILE:HG12 | 2.01                     | 0.43              |
| 38:DK:23:LYS:HE2   | 38:DK:142:ILE:OXT  | 2.19                     | 0.43              |
| 6:AF:70:VAL:HA     | 6:AF:73:GLU:HG2    | 2.00                     | 0.43              |
| 8:AH:66:PHE:CD2    | 8:AH:67:GLN:HG2    | 2.54                     | 0.43              |
| 1:BA:1152:A:H5'    | 10:BJ:15:HIS:HB2   | 2.01                     | 0.43              |
| 5:BE:40:GLY:HA2    | 5:BE:45:ARG:O      | 2.19                     | 0.43              |
| 5:BE:88:VAL:HG12   | 5:BE:93:ARG:HG2    | 2.00                     | 0.43              |
| 13:BM:90:ARG:HH21  | 13:BM:95:LEU:HB3   | 1.84                     | 0.43              |
| 27:C0:53:PHE:CG    | 28:CB:83:G:H4'     | 2.54                     | 0.43              |
| 31:CA:1168:G:H5''  | 31:CA:1168:G:H8    | 1.83                     | 0.43              |
| 31:CA:83:A:H2      | 31:CA:103:A:N7     | 2.17                     | 0.43              |
| 46:DS:83:TYR:CE1   | 55:DA:1187:G:H5''  | 2.54                     | 0.43              |
| 55:DA:2233:U:H2'   | 55:DA:2234:G:C8    | 2.54                     | 0.43              |
| 1:AA:1062:U:H2'    | 1:AA:1063:C:C6     | 2.54                     | 0.43              |
| 1:AA:1376:U:H2'    | 1:AA:1377:A:C8     | 2.54                     | 0.43              |
| 1:AA:892:A:O2'     | 1:AA:1415:G:H4'    | 2.19                     | 0.43              |
| 31:CA:1936:A:N6    | 31:CA:1963:U:H3    | 2.16                     | 0.43              |
| 31:CA:35:G:H2'     | 31:CA:36:G:O4'     | 2.19                     | 0.43              |
| 30:CD:13:ARG:HH11  | 44:CQ:56:HIS:HA    | 1.84                     | 0.43              |
| 31:CA:2642:G:H5'   | 38:CK:80:HIS:CG    | 2.53                     | 0.43              |
| 62:DA:3200:PEG:H32 | 70:DA:3804:HOH:O   | 2.18                     | 0.43              |
| 32:DD:121:THR:HB   | 32:DD:127:PHE:CD2  | 2.54                     | 0.43              |
| 35:DG:17:VAL:HG11  | 35:DG:50:LEU:HD21  | 2.00                     | 0.43              |
| 54:DI:26:VAL:HB    | 54:DI:83:ALA:HB3   | 2.01                     | 0.43              |
| 41:DN:21:ALA:HB1   | 41:DN:100:LYS:HG2  | 2.00                     | 0.43              |
| 46:DS:10:LYS:HE3   | 57:DS:202:PG4:H21  | 2.00                     | 0.43              |
| 50:DW:51:GLN:HG2   | 50:DW:86:LEU:HD11  | 2.01                     | 0.43              |
| 3:AC:151:VAL:HG12  | 3:AC:200:VAL:HG22  | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:BB:104:TRP:O     | 2:BB:108:ARG:HB2   | 2.19                     | 0.42              |
| 9:BI:99:ARG:HG2    | 9:BI:104:VAL:HG21  | 2.00                     | 0.42              |
| 31:CA:2106:U:H2'   | 31:CA:2107:G:H8    | 1.84                     | 0.42              |
| 29:CC:105:LEU:H    | 29:CC:105:LEU:HD12 | 1.84                     | 0.42              |
| 35:CG:103:ILE:HD11 | 35:CG:117:LEU:HD21 | 2.01                     | 0.42              |
| 24:D3:29:GLN:HG2   | 62:D3:102:PEG:H21  | 2.01                     | 0.42              |
| 55:DA:1101:U:H2'   | 55:DA:1102:C:C6    | 2.54                     | 0.42              |
| 55:DA:2326:C:H3'   | 70:DA:7772:HOH:O   | 2.18                     | 0.42              |
| 1:AA:619:U:C2      | 4:AD:132:ILE:HD11  | 2.54                     | 0.42              |
| 1:BA:978:A:O2'     | 1:BA:1322:C:H5     | 2.00                     | 0.42              |
| 5:BE:81:LEU:HB3    | 5:BE:147:MET:SD    | 2.58                     | 0.42              |
| 12:BL:80:ILE:HD12  | 12:BL:97:THR:HG22  | 2.01                     | 0.42              |
| 22:C1:4:GLN:CB     | 31:CA:2615:U:H1'   | 2.50                     | 0.42              |
| 31:CA:136:G:H1     | 31:CA:143:C:H42    | 1.65                     | 0.42              |
| 31:CA:2815:C:H2'   | 31:CA:2816:G:O4'   | 2.19                     | 0.42              |
| 38:CK:23:LYS:HE3   | 38:CK:142:ILE:OXT  | 2.20                     | 0.42              |
| 55:DA:1510:G:H2'   | 55:DA:1511:G:O4'   | 2.18                     | 0.42              |
| 55:DA:2051:A:H5'   | 55:DA:2578:G:O4'   | 2.19                     | 0.42              |
| 55:DA:2636:C:H2'   | 55:DA:2637:U:C6    | 2.53                     | 0.42              |
| 32:DD:13:ARG:HD3   | 32:DD:21:SER:OG    | 2.18                     | 0.42              |
| 50:DW:26:PHE:CE2   | 50:DW:44:HIS:HA    | 2.54                     | 0.42              |
| 8:AH:94:LYS:HB3    | 8:AH:117:ARG:HH22  | 1.84                     | 0.42              |
| 5:BE:74:VAL:HG11   | 5:BE:144:LEU:HB3   | 2.01                     | 0.42              |
| 34:CF:36:LEU:HD12  | 34:CF:154:ILE:HG12 | 2.01                     | 0.42              |
| 48:CU:33:LYS:HG3   | 48:CU:80:TRP:CE3   | 2.55                     | 0.42              |
| 50:CW:26:PHE:CE1   | 50:CW:44:HIS:HA    | 2.54                     | 0.42              |
| 22:D1:54:VAL:HG23  | 22:D1:55:ILE:HG12  | 2.00                     | 0.42              |
| 42:DO:8:ARG:HD3    | 55:DA:1652:A:OP1   | 2.18                     | 0.42              |
| 55:DA:1932:A:H2'   | 55:DA:1933:G:O4'   | 2.19                     | 0.42              |
| 55:DA:1654:A:C1'   | 55:DA:2823:A:H5'   | 2.50                     | 0.42              |
| 33:DE:48:THR:HG23  | 33:DE:88:ARG:HH12  | 1.82                     | 0.42              |
| 2:BB:70:VAL:HB     | 2:BB:163:VAL:HG22  | 2.00                     | 0.42              |
| 3:BC:47:LEU:HD22   | 3:BC:76:VAL:HG22   | 2.00                     | 0.42              |
| 1:BA:864:A:H4'     | 5:BE:90:THR:HG23   | 2.01                     | 0.42              |
| 14:BN:28:LYS:HA    | 14:BN:31:ILE:HG22  | 2.01                     | 0.42              |
| 31:CA:2869:G:H2'   | 31:CA:2870:C:O4'   | 2.19                     | 0.42              |
| 31:CA:822:G:O6     | 31:CA:943:A:H2     | 2.01                     | 0.42              |
| 46:CS:41:ILE:HD13  | 46:CS:103:ALA:HA   | 2.00                     | 0.42              |
| 55:DA:189:G:N7     | 63:DA:3197:EDO:H21 | 2.35                     | 0.42              |
| 32:DD:167:ASN:O    | 64:DD:301:PGE:H52  | 2.20                     | 0.42              |
| 1:BA:49:U:O2       | 1:BA:362:G:H1'     | 2.20                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:BA:604:G:H2'      | 1:BA:605:U:O4'     | 2.20                     | 0.42              |
| 31:CA:1028:A:N6     | 31:CA:1125:G:H2'   | 2.34                     | 0.42              |
| 31:CA:1430:G:H2'    | 31:CA:1431:A:O4'   | 2.19                     | 0.42              |
| 31:CA:2060:A:H62    | 33:CE:69:ARG:NH2   | 2.18                     | 0.42              |
| 39:CL:121:GLU:HG2   | 39:CL:122:VAL:HG23 | 2.02                     | 0.42              |
| 1:AA:1305:G:HO2'    | 1:AA:1306:A:H8     | 1.65                     | 0.42              |
| 3:AC:47:LEU:HD22    | 3:AC:76:VAL:HG22   | 2.01                     | 0.42              |
| 5:AE:132:ASN:OD1    | 5:AE:134:ILE:HG22  | 2.20                     | 0.42              |
| 2:BB:129:LEU:H      | 2:BB:129:LEU:HG    | 1.53                     | 0.42              |
| 10:BJ:10:LEU:HB2    | 10:BJ:72:ARG:HB2   | 2.00                     | 0.42              |
| 11:BK:25:ALA:HA     | 11:BK:30:THR:HG22  | 2.01                     | 0.42              |
| 13:BM:17:ILE:HD12   | 13:BM:17:ILE:H     | 1.84                     | 0.42              |
| 13:BM:11:ASP:HA     | 13:BM:45:ILE:HD13  | 2.01                     | 0.42              |
| 38:CK:81:ILE:HG23   | 38:CK:82:GLY:N     | 2.35                     | 0.42              |
| 25:D4:47:LYS:HE3    | 40:DM:64:PHE:CD1   | 2.55                     | 0.42              |
| 55:DA:2445:2MG:HM21 | 55:DA:2449:H2U:O4  | 2.20                     | 0.42              |
| 42:DO:67:PHE:O      | 42:DO:71:ARG:HD2   | 2.20                     | 0.42              |
| 1:AA:1530:G:H2'     | 1:AA:1531:A:C8     | 2.55                     | 0.42              |
| 22:C1:15:MET:O      | 31:CA:2045:C:O2'   | 2.31                     | 0.42              |
| 27:C0:31:ARG:HD3    | 31:CA:1158:C:H5''  | 2.02                     | 0.42              |
| 31:CA:1510:G:H2'    | 31:CA:1511:G:O4'   | 2.20                     | 0.42              |
| 31:CA:2800:A:C2     | 31:CA:2895:G:H1'   | 2.54                     | 0.42              |
| 31:CA:686:U:H2'     | 31:CA:788:A:N1     | 2.34                     | 0.42              |
| 28:CB:55:U:H1'      | 34:CF:26:MET:HG3   | 2.01                     | 0.42              |
| 29:CC:57:GLY:HA2    | 29:CC:213:TRP:HA   | 2.01                     | 0.42              |
| 34:CF:138:PHE:HE1   | 34:CF:152:LEU:HD21 | 1.85                     | 0.42              |
| 55:DA:355:U:H2'     | 55:DA:356:G:C8     | 2.55                     | 0.42              |
| 29:DC:225:MET:O     | 29:DC:233:GLY:O    | 2.38                     | 0.42              |
| 49:DV:51:ALA:O      | 49:DV:52:LEU:HB2   | 2.19                     | 0.42              |
| 1:AA:502:A:H2'      | 1:AA:503:C:O4'     | 2.19                     | 0.42              |
| 5:AE:77:ASN:HB2     | 5:AE:82:GLN:HE21   | 1.74                     | 0.42              |
| 20:AT:36:TYR:CE2    | 20:AT:79:LEU:HD21  | 2.55                     | 0.42              |
| 1:BA:1322:C:O2      | 1:BA:1322:C:OP1    | 2.37                     | 0.42              |
| 5:BE:157:ARG:HG2    | 5:BE:158:GLY:N     | 2.35                     | 0.42              |
| 31:CA:2305:U:H5''   | 34:CF:131:GLY:HA3  | 2.02                     | 0.42              |
| 36:CH:68:ARG:HB3    | 36:CH:134:VAL:HG21 | 2.02                     | 0.42              |
| 47:CT:20:VAL:HG11   | 47:CT:44:ALA:HA    | 2.02                     | 0.42              |
| 50:CW:86:LEU:HD13   | 50:CW:89:ILE:HD11  | 2.01                     | 0.42              |
| 55:DA:825:A:H5''    | 59:DA:3222:PUT:H12 | 2.02                     | 0.42              |
| 55:DA:984:A:N3      | 55:DA:984:A:H2'    | 2.34                     | 0.42              |
| 2:AB:104:TRP:O      | 2:AB:108:ARG:HB2   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:105:MET:SD    | 4:AD:143:VAL:HG22  | 2.60                     | 0.42              |
| 1:AA:1322:C:P      | 19:AS:78:ARG:HH22  | 2.43                     | 0.42              |
| 1:BA:1530:G:H2'    | 1:BA:1531:A:C8     | 2.55                     | 0.42              |
| 25:C4:26:HIS:HD1   | 31:CA:2361:G:P     | 2.43                     | 0.42              |
| 31:CA:796:C:H2'    | 31:CA:797:G:C8     | 2.54                     | 0.42              |
| 36:CH:82:SER:HB2   | 36:CH:94:ILE:HD11  | 2.02                     | 0.42              |
| 41:CN:41:LEU:HD21  | 41:CN:124:LEU:HD22 | 2.02                     | 0.42              |
| 55:DA:1555:G:OP1   | 59:DA:3218:PUT:H41 | 2.20                     | 0.42              |
| 55:DA:1794:A:H2'   | 55:DA:1795:C:C6    | 2.54                     | 0.42              |
| 47:DT:6:LYS:HB2    | 55:DA:494:G:H4'    | 2.01                     | 0.42              |
| 24:D3:2:LYS:HE2    | 55:DA:687:C:H5''   | 2.02                     | 0.42              |
| 55:DA:747:5MU:O2   | 55:DA:2014:A:H1'   | 2.20                     | 0.42              |
| 40:DM:109:LYS:HG2  | 40:DM:126:ARG:HB2  | 2.02                     | 0.42              |
| 1:AA:1152:A:H5'    | 10:AJ:15:HIS:HB2   | 2.02                     | 0.42              |
| 1:AA:1298:U:H3     | 7:AG:114:LYS:HA    | 1.85                     | 0.42              |
| 11:AK:25:ALA:HA    | 11:AK:30:THR:HG22  | 2.02                     | 0.42              |
| 5:BE:115:LEU:HG    | 5:BE:123:VAL:HG21  | 2.01                     | 0.42              |
| 31:CA:1101:U:H2'   | 31:CA:1102:C:C6    | 2.54                     | 0.42              |
| 33:CE:178:VAL:HG23 | 40:CM:3:LEU:HD21   | 2.02                     | 0.42              |
| 50:CW:26:PHE:HE1   | 50:CW:44:HIS:HA    | 1.85                     | 0.42              |
| 55:DA:2406:A:H5'   | 55:DA:2406:A:C8    | 2.55                     | 0.42              |
| 55:DA:320:A:H4'    | 55:DA:322:A:N7     | 2.35                     | 0.42              |
| 32:DD:13:ARG:HH11  | 44:DQ:56:HIS:HA    | 1.85                     | 0.42              |
| 38:DK:7:LYS:HG2    | 55:DA:538:A:H4'    | 2.02                     | 0.42              |
| 7:AG:72:THR:HG22   | 7:AG:142:HIS:CE1   | 2.55                     | 0.41              |
| 1:BA:1048:G:H4'    | 14:BN:3:LYS:HE2    | 2.02                     | 0.41              |
| 24:C3:16:HIS:CD2   | 31:CA:464:U:O2'    | 2.73                     | 0.41              |
| 31:CA:2074:U:H2'   | 31:CA:2075:U:C6    | 2.55                     | 0.41              |
| 31:CA:2425:A:H4'   | 31:CA:2426:A:O5'   | 2.20                     | 0.41              |
| 25:D4:39:LYS:O     | 25:D4:43:HIS:HD2   | 2.03                     | 0.41              |
| 3:AC:156:ARG:HD3   | 3:AC:193:TYR:O     | 2.20                     | 0.41              |
| 19:AS:30:PRO:HB2   | 19:AS:50:ALA:HB2   | 2.03                     | 0.41              |
| 11:BK:45:ALA:HB3   | 11:BK:70:CYS:HB2   | 2.02                     | 0.41              |
| 44:CQ:52:ASN:O     | 44:CQ:53:ARG:HD3   | 2.20                     | 0.41              |
| 48:CU:82:LYS:HD3   | 48:CU:84:TYR:CE1   | 2.55                     | 0.41              |
| 55:DA:136:G:H1     | 55:DA:143:C:N4     | 2.18                     | 0.41              |
| 25:D4:8:ARG:HG3    | 55:DA:253:C:N4     | 2.36                     | 0.41              |
| 1:AA:1048:G:H4'    | 14:AN:3:LYS:HE2    | 2.01                     | 0.41              |
| 1:AA:1108:G:H5''   | 3:AC:176:HIS:ND1   | 2.36                     | 0.41              |
| 1:AA:131:A:H2'     | 1:AA:132:C:C6      | 2.56                     | 0.41              |
| 1:AA:302:G:O2'     | 1:AA:556:C:H5''    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:BN:31:ILE:HG23 | 14:BN:42:TRP:HZ2   | 1.85                     | 0.41              |
| 20:BT:67:ILE:O    | 20:BT:68:HIS:HB2   | 2.20                     | 0.41              |
| 31:CA:136:G:H1    | 31:CA:143:C:N4     | 2.19                     | 0.41              |
| 31:CA:2339:C:H2'  | 31:CA:2340:A:C8    | 2.56                     | 0.41              |
| 55:DA:1430:G:H2'  | 55:DA:1431:A:O4'   | 2.20                     | 0.41              |
| 55:DA:686:U:H2'   | 55:DA:788:A:N1     | 2.35                     | 0.41              |
| 32:DD:26:VAL:HG21 | 44:DQ:5:ILE:HG12   | 2.02                     | 0.41              |
| 5:BE:23:LYS:HB3   | 5:BE:30:ILE:HG23   | 2.02                     | 0.41              |
| 31:CA:1794:A:H2'  | 31:CA:1795:C:C6    | 2.56                     | 0.41              |
| 31:CA:2043:C:C6   | 31:CA:2043:C:H5''  | 2.55                     | 0.41              |
| 31:CA:2106:U:H2'  | 31:CA:2107:G:C8    | 2.55                     | 0.41              |
| 31:CA:355:U:H2'   | 31:CA:356:G:C8     | 2.56                     | 0.41              |
| 31:CA:742:A:H2'   | 31:CA:743:A:C8     | 2.55                     | 0.41              |
| 29:CC:221:ARG:NH1 | 31:CA:1789:A:OP2   | 2.53                     | 0.41              |
| 40:CM:123:ARG:HG3 | 40:CM:143:GLU:HG3  | 2.03                     | 0.41              |
| 41:CN:71:LYS:HB3  | 41:CN:93:VAL:O     | 2.21                     | 0.41              |
| 55:DA:1202:G:H1'  | 58:DA:3192:MPD:HM1 | 2.02                     | 0.41              |
| 55:DA:1418:G:H2'  | 55:DA:1579:A:N6    | 2.35                     | 0.41              |
| 54:DI:94:ARG:HG2  | 54:DI:127:ALA:HA   | 2.02                     | 0.41              |
| 1:BA:131:A:H2'    | 1:BA:132:C:C6      | 2.56                     | 0.41              |
| 1:BA:429:U:H1'    | 1:BA:430:A:H5''    | 2.03                     | 0.41              |
| 4:BD:130:VAL:HG11 | 4:BD:135:TYR:CG    | 2.55                     | 0.41              |
| 11:BK:20:VAL:HB   | 11:BK:35:THR:HG23  | 2.02                     | 0.41              |
| 31:CA:2114:A:N6   | 31:CA:2119:A:H62   | 2.18                     | 0.41              |
| 27:C0:14:ILE:HG21 | 31:CA:988:A:C6     | 2.56                     | 0.41              |
| 55:DA:1417:C:H5'  | 55:DA:1588:G:H1'   | 2.01                     | 0.41              |
| 55:DA:602:A:C6    | 58:DA:3190:MPD:H31 | 2.56                     | 0.41              |
| 55:DA:792:A:N3    | 55:DA:2072:C:O2'   | 2.48                     | 0.41              |
| 36:DH:82:SER:HB2  | 36:DH:94:ILE:HD11  | 2.02                     | 0.41              |
| 47:DT:20:VAL:HG11 | 47:DT:44:ALA:HA    | 2.03                     | 0.41              |
| 1:AA:1343:G:O2'   | 9:AI:123:ARG:HD2   | 2.20                     | 0.41              |
| 1:AA:429:U:H1'    | 1:AA:430:A:H5''    | 2.02                     | 0.41              |
| 13:AM:54:ASP:HA   | 13:AM:57:ARG:HD2   | 2.02                     | 0.41              |
| 1:BA:1298:U:H3    | 7:BG:114:LYS:HA    | 1.86                     | 0.41              |
| 14:BN:53:ARG:HH21 | 19:BS:37:ARG:HH22  | 1.69                     | 0.41              |
| 31:CA:2788:C:H2'  | 31:CA:2789:C:C6    | 2.55                     | 0.41              |
| 29:CC:174:LEU:CD2 | 29:CC:184:VAL:HB   | 2.50                     | 0.41              |
| 47:CT:29:VAL:HG22 | 47:CT:51:LEU:HD11  | 2.02                     | 0.41              |
| 55:DA:2128:G:H1   | 55:DA:2160:C:N4    | 2.18                     | 0.41              |
| 55:DA:2324:U:H3'  | 55:DA:2325:G:H5''  | 2.03                     | 0.41              |
| 52:DY:29:PHE:HB3  | 55:DA:396:G:H1'    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:439:U:H5''    | 4:AD:121:LYS:HD2    | 2.02                     | 0.41              |
| 4:AD:170:TRP:CD2   | 4:AD:186:PRO:HB3    | 2.56                     | 0.41              |
| 6:AF:102:MET:CE    | 18:AR:24:LYS:HB3    | 2.50                     | 0.41              |
| 12:BL:87:VAL:HG11  | 12:BL:90:LEU:HD22   | 2.02                     | 0.41              |
| 20:BT:44:LYS:HB3   | 20:BT:87:ALA:HB2    | 2.03                     | 0.41              |
| 30:CD:141:ARG:HB2  | 31:CA:1656:C:H5''   | 2.01                     | 0.41              |
| 31:CA:2095:A:H5''  | 31:CA:2095:A:C8     | 2.54                     | 0.41              |
| 42:CO:95:THR:HG21  | 42:CO:113:ILE:HD11  | 2.02                     | 0.41              |
| 47:CT:69:LEU:HG    | 47:CT:107:VAL:CG2   | 2.51                     | 0.41              |
| 55:DA:138:U:H5'    | 55:DA:139:U:H5'     | 2.03                     | 0.41              |
| 55:DA:2038:G:H2'   | 55:DA:2039:U:O4'    | 2.21                     | 0.41              |
| 51:DX:41[B]:ARG:HA | 51:DX:41[B]:ARG:HD3 | 1.94                     | 0.41              |
| 9:AI:19:VAL:HG11   | 9:AI:83:ILE:HA      | 2.03                     | 0.41              |
| 1:BA:1376:U:H2'    | 1:BA:1377:A:C8      | 2.55                     | 0.41              |
| 4:BD:170:TRP:CD2   | 4:BD:186:PRO:HB3    | 2.56                     | 0.41              |
| 5:BE:77:ASN:HB2    | 5:BE:82:GLN:HE21    | 1.79                     | 0.41              |
| 5:BE:82:GLN:HG2    | 5:BE:149:SER:HA     | 2.01                     | 0.41              |
| 19:BS:30:PRO:HB2   | 19:BS:50:ALA:HB2    | 2.02                     | 0.41              |
| 31:CA:1722:A:N6    | 31:CA:1738:G:H1'    | 2.36                     | 0.41              |
| 31:CA:2038:G:H2'   | 31:CA:2039:U:O4'    | 2.21                     | 0.41              |
| 25:D4:13:ARG:NH1   | 55:DA:2394:C:H5'    | 2.36                     | 0.41              |
| 55:DA:1020:A:C2    | 55:DA:1141:U:C2     | 3.08                     | 0.41              |
| 55:DA:1515:A:H2'   | 55:DA:1516:G:O4'    | 2.20                     | 0.41              |
| 55:DA:2097:A:H8    | 55:DA:2097:A:H5''   | 1.85                     | 0.41              |
| 33:DE:23:PHE:HE2   | 33:DE:25:GLU:HG3    | 1.86                     | 0.41              |
| 35:DG:140:VAL:O    | 35:DG:144:VAL:HG23  | 2.20                     | 0.41              |
| 51:DX:38:VAL:HG12  | 51:DX:59:LEU:HB2    | 2.02                     | 0.41              |
| 19:AS:5:LEU:HG     | 19:AS:5:LEU:H       | 1.75                     | 0.41              |
| 1:BA:567:G:H2'     | 1:BA:568:G:O4'      | 2.20                     | 0.41              |
| 9:BI:19:VAL:HG11   | 9:BI:83:ILE:HA      | 2.03                     | 0.41              |
| 31:CA:547:A:H2'    | 31:CA:547:A:N3      | 2.36                     | 0.41              |
| 29:CC:107:PRO:HD2  | 29:CC:110:LEU:HD22  | 2.03                     | 0.41              |
| 33:DE:178:VAL:HG23 | 40:DM:3:LEU:HD21    | 2.01                     | 0.41              |
| 36:DH:68:ARG:HB3   | 36:DH:134:VAL:HG21  | 2.03                     | 0.41              |
| 5:AE:157:ARG:CD    | 8:AH:43:GLU:O       | 2.69                     | 0.41              |
| 11:AK:20:VAL:HB    | 11:AK:35:THR:HG23   | 2.03                     | 0.41              |
| 1:BA:216:U:H4'     | 1:BA:464:U:H4'      | 2.02                     | 0.41              |
| 1:BA:841:C:H3'     | 1:BA:842:U:C4'      | 2.51                     | 0.41              |
| 31:CA:1636:U:H2'   | 31:CA:1637:A:C8     | 2.55                     | 0.41              |
| 31:CA:396:G:H1'    | 52:CY:29:PHE:HB3    | 2.01                     | 0.41              |
| 54:DI:29:ASP:HB3   | 54:DI:106:PHE:HB2   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1141:C:O2'   | 1:AA:1142:G:H8     | 2.03                     | 0.41              |
| 1:AA:1216:A:H5''  | 14:AN:5:SER:HB3    | 2.02                     | 0.41              |
| 1:AA:831:A:H5''   | 2:AB:21:ARG:HD3    | 2.03                     | 0.41              |
| 13:AM:90:ARG:HH21 | 13:AM:95:LEU:HB3   | 1.85                     | 0.41              |
| 1:BA:439:U:H5''   | 4:BD:121:LYS:HD2   | 2.02                     | 0.41              |
| 11:BK:34:ILE:HG12 | 11:BK:70:CYS:SG    | 2.60                     | 0.41              |
| 20:BT:69:LYS:H    | 20:BT:69:LYS:HG3   | 1.60                     | 0.41              |
| 31:CA:29:U:O5'    | 31:CA:29:U:H6      | 2.02                     | 0.41              |
| 37:CJ:49:ILE:HG13 | 37:CJ:55:ILE:HD13  | 2.03                     | 0.41              |
| 31:CA:2335:A:OP1  | 43:CP:13:ARG:HD2   | 2.21                     | 0.41              |
| 55:DA:207:A:H2'   | 55:DA:208:C:O4'    | 2.20                     | 0.41              |
| 55:DA:2133:G:H21  | 55:DA:2158:A:N6    | 2.18                     | 0.41              |
| 55:DA:281:C:H2'   | 55:DA:282:A:C8     | 2.56                     | 0.41              |
| 54:DI:23:LEU:HD13 | 54:DI:89:PRO:HD3   | 2.03                     | 0.41              |
| 38:DK:9:GLU:HG2   | 70:DA:3412:HOH:O   | 2.21                     | 0.41              |
| 40:DM:74:THR:HG23 | 40:DM:107:PHE:HB2  | 2.02                     | 0.41              |
| 40:DM:123:ARG:HG3 | 40:DM:143:GLU:HG3  | 2.02                     | 0.41              |
| 41:DN:89:VAL:CG1  | 58:DN:201:MPD:HM3  | 2.50                     | 0.41              |
| 10:AJ:19:ASP:HA   | 10:AJ:22:THR:HB    | 2.03                     | 0.40              |
| 1:BA:718:A:H5'    | 11:BK:119:ASN:HB2  | 2.03                     | 0.40              |
| 1:BA:1108:G:H5''  | 3:BC:176:HIS:ND1   | 2.36                     | 0.40              |
| 6:BF:22:ILE:HG23  | 6:BF:39:LEU:HD11   | 2.02                     | 0.40              |
| 22:C1:49:TYR:OH   | 31:CA:2883:A:OP1   | 2.34                     | 0.40              |
| 31:CA:780:G:H2'   | 31:CA:782:A:N7     | 2.36                     | 0.40              |
| 35:CG:38:ASN:HD22 | 35:CG:40:ALA:HB3   | 1.86                     | 0.40              |
| 22:D1:8:PRO:HD2   | 55:DA:1263:U:O2'   | 2.22                     | 0.40              |
| 55:DA:1306:C:H5'' | 55:DA:1306:C:H6    | 1.85                     | 0.40              |
| 55:DA:2273:A:H2'  | 55:DA:2274:A:C8    | 2.55                     | 0.40              |
| 55:DA:839:U:H2'   | 55:DA:840:C:C6     | 2.56                     | 0.40              |
| 35:DG:50:LEU:HD13 | 35:DG:72:LEU:HD23  | 2.02                     | 0.40              |
| 54:DI:132:TYR:N   | 54:DI:133:GLU:HB2  | 2.35                     | 0.40              |
| 37:DJ:14:ALA:HB3  | 37:DJ:17:MET:HB2   | 2.03                     | 0.40              |
| 40:DM:77:ILE:CD1  | 40:DM:101:ILE:CG2  | 2.97                     | 0.40              |
| 1:AA:842:U:H5''   | 2:BB:115:LYS:HD3   | 2.03                     | 0.40              |
| 1:AA:568:G:O6     | 12:AL:2:ALA:HB2    | 2.21                     | 0.40              |
| 10:BJ:59:LYS:HD2  | 10:BJ:60:ASP:OD1   | 2.21                     | 0.40              |
| 55:DA:1532:A:H5'' | 55:DA:1532:A:H8    | 1.85                     | 0.40              |
| 54:DI:120:ALA:HA  | 54:DI:123:ILE:HD11 | 2.03                     | 0.40              |
| 54:DI:65:GLU:HA   | 54:DI:70:GLU:HG3   | 2.02                     | 0.40              |
| 47:DT:84:ARG:HB2  | 47:DT:96:ILE:HB    | 2.02                     | 0.40              |
| 1:AA:268:U:H2'    | 1:AA:269:C:C6      | 2.56                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AK:31:ILE:HG12 | 11:AK:46:THR:CG2   | 2.51                     | 0.40              |
| 14:AN:46:LEU:HD22 | 19:AS:13:LEU:HG    | 2.02                     | 0.40              |
| 1:BA:1322:C:P     | 19:BS:78:ARG:HH22  | 2.43                     | 0.40              |
| 9:BI:116:VAL:HG21 | 10:BJ:62:ARG:HD3   | 2.04                     | 0.40              |
| 25:C4:52:LYS:HA   | 25:C4:55:LEU:HD12  | 2.03                     | 0.40              |
| 31:CA:1418:G:H2'  | 31:CA:1579:A:N6    | 2.36                     | 0.40              |
| 31:CA:2190:G:H2'  | 31:CA:2191:A:C8    | 2.57                     | 0.40              |
| 22:D1:12:LYS:HD2  | 22:D1:12:LYS:HA    | 1.86                     | 0.40              |
| 39:DL:113:MET:O   | 39:DL:116:ILE:HG13 | 2.19                     | 0.40              |
| 40:DM:95:LEU:HD11 | 40:DM:125:LEU:HD21 | 2.03                     | 0.40              |
| 47:DT:72:THR:CG2  | 47:DT:108:SER:HB3  | 2.52                     | 0.40              |
| 53:DZ:56:LEU:HA   | 53:DZ:59:GLU:HG2   | 2.04                     | 0.40              |
| 1:AA:234:C:H4'    | 17:AQ:66:PRO:HG3   | 2.03                     | 0.40              |
| 1:AA:567:G:H2'    | 1:AA:568:G:O4'     | 2.21                     | 0.40              |
| 1:BA:268:U:H2'    | 1:BA:269:C:C6      | 2.56                     | 0.40              |
| 2:BB:111:ILE:HD12 | 2:BB:152:LYS:HA    | 2.04                     | 0.40              |
| 31:CA:1306:C:H5'' | 31:CA:1306:C:H6    | 1.86                     | 0.40              |
| 36:CH:126:GLY:H   | 36:CH:146:VAL:HB   | 1.87                     | 0.40              |
| 31:CA:1131:G:OP1  | 38:CK:82:GLY:HA2   | 2.21                     | 0.40              |
| 45:CR:58:ARG:HH11 | 45:CR:62:ILE:HD11  | 1.86                     | 0.40              |
| 26:D5:32:LYS:HG2  | 55:DA:2478:A:H5'   | 2.03                     | 0.40              |
| 55:DA:2788:C:H2'  | 55:DA:2789:C:C6    | 2.57                     | 0.40              |
| 1:BA:580:C:H2'    | 1:BA:581:G:O4'     | 2.21                     | 0.40              |
| 6:BF:78:PHE:HA    | 6:BF:84:VAL:HG11   | 2.04                     | 0.40              |
| 12:BL:74:LEU:HD21 | 12:BL:80:ILE:HG21  | 2.03                     | 0.40              |
| 31:CA:1101:U:H2'  | 31:CA:1102:C:H6    | 1.87                     | 0.40              |
| 31:CA:2327:A:H2'  | 31:CA:2328:A:C8    | 2.57                     | 0.40              |
| 24:C3:37:LYS:NZ   | 31:CA:469:G:O6     | 2.53                     | 0.40              |
| 31:CA:644:A:H2'   | 31:CA:645:C:O4'    | 2.22                     | 0.40              |
| 55:DA:2339:C:H2'  | 55:DA:2340:A:C8    | 2.57                     | 0.40              |
| 37:DJ:49:ILE:HG13 | 37:DJ:55:ILE:HD13  | 2.03                     | 0.40              |
| 49:DV:66:GLN:HG3  | 55:DA:328:U:O3'    | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

of similar resolution.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | AB    | 222/224 (99%) | 210 (95%) | 9 (4%)   | 3 (1%)   | 13          | 46  |
| 2   | BB    | 222/224 (99%) | 211 (95%) | 7 (3%)   | 4 (2%)   | 10          | 39  |
| 3   | AC    | 204/206 (99%) | 192 (94%) | 11 (5%)  | 1 (0%)   | 32          | 71  |
| 3   | BC    | 204/206 (99%) | 194 (95%) | 8 (4%)   | 2 (1%)   | 18          | 55  |
| 4   | AD    | 203/205 (99%) | 198 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 4   | BD    | 203/205 (99%) | 198 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 5   | AE    | 153/155 (99%) | 147 (96%) | 5 (3%)   | 1 (1%)   | 25          | 64  |
| 5   | BE    | 148/155 (96%) | 132 (89%) | 12 (8%)  | 4 (3%)   | 6           | 27  |
| 6   | AF    | 104/106 (98%) | 101 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 6   | BF    | 98/106 (92%)  | 91 (93%)  | 5 (5%)   | 2 (2%)   | 9           | 36  |
| 7   | AG    | 149/151 (99%) | 137 (92%) | 11 (7%)  | 1 (1%)   | 25          | 64  |
| 7   | BG    | 149/151 (99%) | 140 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 8   | AH    | 127/129 (98%) | 120 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 8   | BH    | 127/129 (98%) | 119 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 9   | AI    | 125/127 (98%) | 110 (88%) | 15 (12%) | 0        | 100         | 100 |
| 9   | BI    | 125/127 (98%) | 110 (88%) | 15 (12%) | 0        | 100         | 100 |
| 10  | AJ    | 97/99 (98%)   | 88 (91%)  | 7 (7%)   | 2 (2%)   | 8           | 35  |
| 10  | BJ    | 96/99 (97%)   | 77 (80%)  | 14 (15%) | 5 (5%)   | 2           | 11  |
| 11  | AK    | 115/117 (98%) | 107 (93%) | 6 (5%)   | 2 (2%)   | 11          | 41  |
| 11  | BK    | 115/117 (98%) | 104 (90%) | 9 (8%)   | 2 (2%)   | 11          | 41  |
| 12  | AL    | 120/123 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 12  | BL    | 120/123 (98%) | 114 (95%) | 5 (4%)   | 1 (1%)   | 22          | 61  |
| 13  | AM    | 112/114 (98%) | 103 (92%) | 6 (5%)   | 3 (3%)   | 6           | 27  |
| 13  | BM    | 112/114 (98%) | 102 (91%) | 5 (4%)   | 5 (4%)   | 3           | 14  |
| 14  | AN    | 98/100 (98%)  | 88 (90%)  | 8 (8%)   | 2 (2%)   | 9           | 36  |
| 14  | BN    | 98/100 (98%)  | 90 (92%)  | 6 (6%)   | 2 (2%)   | 9           | 36  |
| 15  | AO    | 86/88 (98%)   | 84 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 15  | BO    | 86/88 (98%)   | 83 (96%)  | 2 (2%)   | 1 (1%)   | 15          | 50  |
| 16  | AP    | 80/82 (98%)   | 74 (92%)  | 6 (8%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 16  | BP    | 80/82 (98%)   | 70 (88%)  | 8 (10%) | 2 (2%)   | 6           | 29  |
| 17  | AQ    | 78/80 (98%)   | 70 (90%)  | 7 (9%)  | 1 (1%)   | 14          | 48  |
| 17  | BQ    | 78/80 (98%)   | 68 (87%)  | 5 (6%)  | 5 (6%)   | 1           | 7   |
| 18  | AR    | 53/55 (96%)   | 53 (100%) | 0       | 0        | 100         | 100 |
| 18  | BR    | 53/55 (96%)   | 50 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 19  | AS    | 77/79 (98%)   | 70 (91%)  | 6 (8%)  | 1 (1%)   | 14          | 48  |
| 19  | BS    | 77/79 (98%)   | 68 (88%)  | 7 (9%)  | 2 (3%)   | 6           | 28  |
| 20  | AT    | 84/86 (98%)   | 83 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 20  | BT    | 83/86 (96%)   | 79 (95%)  | 3 (4%)  | 1 (1%)   | 15          | 50  |
| 21  | AU    | 54/56 (96%)   | 53 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 21  | BU    | 54/56 (96%)   | 53 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 22  | C1    | 54/56 (96%)   | 47 (87%)  | 4 (7%)  | 3 (6%)   | 2           | 10  |
| 22  | D1    | 54/56 (96%)   | 51 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 23  | C2    | 48/51 (94%)   | 44 (92%)  | 2 (4%)  | 2 (4%)   | 3           | 16  |
| 23  | D2    | 49/51 (96%)   | 48 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 24  | C3    | 44/46 (96%)   | 41 (93%)  | 2 (4%)  | 1 (2%)   | 7           | 32  |
| 24  | D3    | 44/46 (96%)   | 43 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 25  | C4    | 62/64 (97%)   | 60 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 25  | D4    | 62/64 (97%)   | 60 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 26  | C5    | 36/38 (95%)   | 34 (94%)  | 1 (3%)  | 1 (3%)   | 6           | 26  |
| 26  | D5    | 36/38 (95%)   | 36 (100%) | 0       | 0        | 100         | 100 |
| 27  | C0    | 56/58 (97%)   | 54 (96%)  | 0       | 2 (4%)   | 4           | 19  |
| 27  | D0    | 57/58 (98%)   | 56 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 29  | CC    | 269/272 (99%) | 252 (94%) | 12 (4%) | 5 (2%)   | 9           | 38  |
| 29  | DC    | 269/272 (99%) | 257 (96%) | 10 (4%) | 2 (1%)   | 25          | 64  |
| 30  | CD    | 207/209 (99%) | 201 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 32  | DD    | 206/209 (99%) | 202 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 33  | CE    | 199/201 (99%) | 191 (96%) | 5 (2%)  | 3 (2%)   | 12          | 45  |
| 33  | DE    | 199/201 (99%) | 194 (98%) | 4 (2%)  | 1 (0%)   | 32          | 71  |
| 34  | CF    | 175/178 (98%) | 168 (96%) | 6 (3%)  | 1 (1%)   | 28          | 67  |
| 34  | DF    | 175/178 (98%) | 169 (97%) | 5 (3%)  | 1 (1%)   | 28          | 67  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 35  | CG    | 174/176 (99%) | 162 (93%) | 7 (4%)  | 5 (3%)   | 5           | 25  |
| 35  | DG    | 174/176 (99%) | 165 (95%) | 8 (5%)  | 1 (1%)   | 28          | 67  |
| 36  | CH    | 147/149 (99%) | 136 (92%) | 6 (4%)  | 5 (3%)   | 4           | 21  |
| 36  | DH    | 147/149 (99%) | 138 (94%) | 6 (4%)  | 3 (2%)   | 9           | 36  |
| 37  | CJ    | 132/134 (98%) | 125 (95%) | 3 (2%)  | 4 (3%)   | 5           | 24  |
| 37  | DJ    | 132/134 (98%) | 125 (95%) | 3 (2%)  | 4 (3%)   | 5           | 24  |
| 38  | CK    | 140/142 (99%) | 135 (96%) | 4 (3%)  | 1 (1%)   | 25          | 64  |
| 38  | DK    | 140/142 (99%) | 137 (98%) | 2 (1%)  | 1 (1%)   | 25          | 64  |
| 39  | CL    | 120/123 (98%) | 112 (93%) | 7 (6%)  | 1 (1%)   | 22          | 61  |
| 39  | DL    | 121/123 (98%) | 117 (97%) | 3 (2%)  | 1 (1%)   | 22          | 61  |
| 40  | CM    | 142/144 (99%) | 132 (93%) | 7 (5%)  | 3 (2%)   | 8           | 35  |
| 40  | DM    | 142/144 (99%) | 136 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 41  | CN    | 133/136 (98%) | 125 (94%) | 7 (5%)  | 1 (1%)   | 22          | 61  |
| 41  | DN    | 134/136 (98%) | 129 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 42  | CO    | 118/125 (94%) | 111 (94%) | 5 (4%)  | 2 (2%)   | 11          | 41  |
| 42  | DO    | 123/125 (98%) | 116 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 43  | CP    | 114/117 (97%) | 110 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 43  | DP    | 115/117 (98%) | 112 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 44  | CQ    | 112/114 (98%) | 107 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 44  | DQ    | 112/114 (98%) | 107 (96%) | 4 (4%)  | 1 (1%)   | 20          | 58  |
| 45  | CR    | 115/117 (98%) | 113 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 45  | DR    | 115/117 (98%) | 114 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 46  | CS    | 101/103 (98%) | 93 (92%)  | 5 (5%)  | 3 (3%)   | 5           | 24  |
| 46  | DS    | 101/103 (98%) | 98 (97%)  | 2 (2%)  | 1 (1%)   | 18          | 55  |
| 47  | CT    | 108/110 (98%) | 101 (94%) | 5 (5%)  | 2 (2%)   | 9           | 38  |
| 47  | DT    | 108/110 (98%) | 106 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 48  | CU    | 91/93 (98%)   | 86 (94%)  | 4 (4%)  | 1 (1%)   | 17          | 53  |
| 48  | DU    | 91/93 (98%)   | 85 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 49  | CV    | 100/103 (97%) | 91 (91%)  | 4 (4%)  | 5 (5%)   | 2           | 12  |
| 49  | DV    | 100/103 (97%) | 96 (96%)  | 2 (2%)  | 2 (2%)   | 9           | 36  |
| 50  | CW    | 92/94 (98%)   | 91 (99%)  | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 50  | DW    | 92/94 (98%)       | 91 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 51  | CX    | 73/76 (96%)       | 72 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 51  | DX    | 75/76 (99%)       | 74 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 52  | CY    | 75/77 (97%)       | 74 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 52  | DY    | 75/77 (97%)       | 74 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 53  | CZ    | 60/62 (97%)       | 58 (97%)    | 1 (2%)   | 1 (2%)   | 11          | 41  |
| 53  | DZ    | 60/62 (97%)       | 59 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 54  | DI    | 133/135 (98%)     | 114 (86%)   | 13 (10%) | 6 (4%)   | 3           | 14  |
| All | All   | 11407/11635 (98%) | 10791 (95%) | 485 (4%) | 131 (1%) | 17          | 53  |

All (131) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 126 | PHE  |
| 3   | AC    | 156 | ARG  |
| 13  | AM    | 5   | ALA  |
| 22  | C1    | 25  | VAL  |
| 2   | BB    | 126 | PHE  |
| 3   | BC    | 156 | ARG  |
| 5   | BE    | 51  | GLY  |
| 10  | BJ    | 38  | GLY  |
| 10  | BJ    | 91  | ASP  |
| 13  | BM    | 7   | ILE  |
| 16  | BP    | 80  | LYS  |
| 20  | BT    | 5   | LYS  |
| 29  | CC    | 158 | ALA  |
| 29  | CC    | 197 | ASN  |
| 33  | CE    | 83  | VAL  |
| 35  | CG    | 119 | ALA  |
| 35  | CG    | 175 | LYS  |
| 35  | CG    | 176 | LYS  |
| 36  | CH    | 10  | ALA  |
| 37  | CJ    | 19  | ASN  |
| 38  | CK    | 81  | ILE  |
| 39  | CL    | 35  | VAL  |
| 40  | CM    | 29  | LYS  |
| 41  | CN    | 70  | ASP  |
| 42  | CO    | 118 | ARG  |
| 48  | CU    | 88  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | CV    | 7   | ARG  |
| 37  | DJ    | 19  | ASN  |
| 49  | DV    | 52  | LEU  |
| 10  | AJ    | 57  | VAL  |
| 13  | AM    | 105 | ASN  |
| 14  | AN    | 38  | ASP  |
| 17  | AQ    | 82  | ALA  |
| 22  | C1    | 56  | ALA  |
| 23  | C2    | 5   | ILE  |
| 23  | C2    | 51  | GLU  |
| 27  | C0    | 4   | THR  |
| 27  | C0    | 14  | ILE  |
| 3   | BC    | 61  | ALA  |
| 5   | BE    | 110 | ALA  |
| 6   | BF    | 92  | THR  |
| 6   | BF    | 98  | GLU  |
| 10  | BJ    | 57  | VAL  |
| 12  | BL    | 44  | LYS  |
| 13  | BM    | 5   | ALA  |
| 13  | BM    | 105 | ASN  |
| 13  | BM    | 114 | LYS  |
| 17  | BQ    | 70  | THR  |
| 17  | BQ    | 82  | ALA  |
| 19  | BS    | 6   | LYS  |
| 29  | CC    | 233 | GLY  |
| 29  | CC    | 253 | LYS  |
| 29  | DC    | 233 | GLY  |
| 29  | DC    | 253 | LYS  |
| 33  | CE    | 82  | GLY  |
| 35  | CG    | 46  | ALA  |
| 37  | CJ    | 25  | GLY  |
| 40  | CM    | 69  | ARG  |
| 49  | CV    | 16  | GLY  |
| 49  | CV    | 17  | LYS  |
| 35  | DG    | 46  | ALA  |
| 37  | DJ    | 25  | GLY  |
| 2   | AB    | 125 | THR  |
| 2   | AB    | 127 | ASP  |
| 7   | AG    | 56  | LYS  |
| 11  | AK    | 54  | GLY  |
| 11  | AK    | 89  | PRO  |
| 13  | AM    | 7   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | C1    | 26  | THR  |
| 24  | C3    | 45  | SER  |
| 2   | BB    | 125 | THR  |
| 2   | BB    | 127 | ASP  |
| 5   | BE    | 103 | THR  |
| 10  | BJ    | 95  | GLY  |
| 11  | BK    | 54  | GLY  |
| 11  | BK    | 89  | PRO  |
| 14  | BN    | 38  | ASP  |
| 15  | BO    | 88  | ARG  |
| 17  | BQ    | 17  | MET  |
| 17  | BQ    | 18  | GLU  |
| 19  | BS    | 5   | LEU  |
| 29  | CC    | 108 | LYS  |
| 33  | CE    | 6   | LYS  |
| 36  | CH    | 118 | PRO  |
| 49  | CV    | 89  | ASP  |
| 33  | DE    | 6   | LYS  |
| 36  | DH    | 118 | PRO  |
| 39  | DL    | 108 | ARG  |
| 46  | DS    | 44  | GLY  |
| 49  | DV    | 89  | ASP  |
| 54  | DI    | 70  | GLU  |
| 54  | DI    | 91  | ALA  |
| 54  | DI    | 109 | LYS  |
| 54  | DI    | 130 | PRO  |
| 5   | AE    | 162 | GLU  |
| 5   | BE    | 105 | ILE  |
| 10  | BJ    | 36  | VAL  |
| 13  | BM    | 4   | ILE  |
| 36  | CH    | 9   | VAL  |
| 40  | CM    | 30  | THR  |
| 42  | CO    | 119 | SER  |
| 46  | CS    | 55  | ASP  |
| 47  | CT    | 63  | GLY  |
| 36  | DH    | 11  | ASN  |
| 54  | DI    | 88  | HIS  |
| 19  | AS    | 6   | LYS  |
| 2   | BB    | 95  | ARG  |
| 14  | BN    | 22  | ALA  |
| 36  | CH    | 8   | LYS  |
| 36  | CH    | 122 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | CJ    | 23  | PRO  |
| 46  | CS    | 48  | LYS  |
| 46  | CS    | 53  | PHE  |
| 36  | DH    | 122 | LEU  |
| 37  | DJ    | 23  | PRO  |
| 44  | DQ    | 105 | GLY  |
| 54  | DI    | 108 | VAL  |
| 14  | AN    | 22  | ALA  |
| 16  | BP    | 44  | SER  |
| 35  | CG    | 45  | HIS  |
| 47  | CT    | 65  | ASP  |
| 49  | CV    | 52  | LEU  |
| 53  | CZ    | 62  | GLY  |
| 38  | DK    | 83  | GLY  |
| 26  | C5    | 21  | GLY  |
| 34  | CF    | 62  | GLY  |
| 37  | CJ    | 32  | GLY  |
| 34  | DF    | 62  | GLY  |
| 37  | DJ    | 32  | GLY  |
| 17  | BQ    | 35  | GLY  |
| 10  | AJ    | 33  | GLY  |

### 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   | AB    | 186/186 (100%) | 173 (93%) | 13 (7%)  | 18          | 50 |
| 2   | BB    | 186/186 (100%) | 173 (93%) | 13 (7%)  | 18          | 50 |
| 3   | AC    | 170/170 (100%) | 159 (94%) | 11 (6%)  | 20          | 53 |
| 3   | BC    | 170/170 (100%) | 156 (92%) | 14 (8%)  | 13          | 41 |
| 4   | AD    | 172/172 (100%) | 162 (94%) | 10 (6%)  | 23          | 59 |
| 4   | BD    | 172/172 (100%) | 160 (93%) | 12 (7%)  | 18          | 50 |
| 5   | AE    | 118/118 (100%) | 107 (91%) | 11 (9%)  | 10          | 35 |
| 5   | BE    | 113/118 (96%)  | 95 (84%)  | 18 (16%) | 3           | 12 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6   | AF    | 92/92 (100%)   | 86 (94%)  | 6 (6%)   | 20          | 53 |
| 6   | BF    | 87/92 (95%)    | 77 (88%)  | 10 (12%) | 6           | 24 |
| 7   | AG    | 124/124 (100%) | 115 (93%) | 9 (7%)   | 16          | 48 |
| 7   | BG    | 124/124 (100%) | 109 (88%) | 15 (12%) | 6           | 22 |
| 8   | AH    | 104/104 (100%) | 93 (89%)  | 11 (11%) | 8           | 28 |
| 8   | BH    | 104/104 (100%) | 93 (89%)  | 11 (11%) | 8           | 28 |
| 9   | AI    | 105/105 (100%) | 100 (95%) | 5 (5%)   | 30          | 66 |
| 9   | BI    | 105/105 (100%) | 100 (95%) | 5 (5%)   | 30          | 66 |
| 10  | AJ    | 87/87 (100%)   | 81 (93%)  | 6 (7%)   | 18          | 51 |
| 10  | BJ    | 86/87 (99%)    | 78 (91%)  | 8 (9%)   | 10          | 35 |
| 11  | AK    | 90/90 (100%)   | 87 (97%)  | 3 (3%)   | 43          | 77 |
| 11  | BK    | 90/90 (100%)   | 83 (92%)  | 7 (8%)   | 15          | 44 |
| 12  | AL    | 102/102 (100%) | 92 (90%)  | 10 (10%) | 9           | 32 |
| 12  | BL    | 102/102 (100%) | 90 (88%)  | 12 (12%) | 6           | 23 |
| 13  | AM    | 92/92 (100%)   | 83 (90%)  | 9 (10%)  | 9           | 32 |
| 13  | BM    | 92/92 (100%)   | 85 (92%)  | 7 (8%)   | 15          | 46 |
| 14  | AN    | 83/83 (100%)   | 82 (99%)  | 1 (1%)   | 75          | 92 |
| 14  | BN    | 83/83 (100%)   | 82 (99%)  | 1 (1%)   | 75          | 92 |
| 15  | AO    | 76/76 (100%)   | 71 (93%)  | 5 (7%)   | 19          | 53 |
| 15  | BO    | 76/76 (100%)   | 65 (86%)  | 11 (14%) | 4           | 15 |
| 16  | AP    | 65/65 (100%)   | 64 (98%)  | 1 (2%)   | 70          | 90 |
| 16  | BP    | 65/65 (100%)   | 63 (97%)  | 2 (3%)   | 45          | 78 |
| 17  | AQ    | 74/74 (100%)   | 67 (90%)  | 7 (10%)  | 10          | 34 |
| 17  | BQ    | 74/74 (100%)   | 66 (89%)  | 8 (11%)  | 7           | 27 |
| 18  | AR    | 48/48 (100%)   | 47 (98%)  | 1 (2%)   | 59          | 85 |
| 18  | BR    | 48/48 (100%)   | 47 (98%)  | 1 (2%)   | 59          | 85 |
| 19  | AS    | 70/70 (100%)   | 63 (90%)  | 7 (10%)  | 9           | 31 |
| 19  | BS    | 70/70 (100%)   | 65 (93%)  | 5 (7%)   | 17          | 49 |
| 20  | AT    | 65/65 (100%)   | 59 (91%)  | 6 (9%)   | 11          | 35 |
| 20  | BT    | 65/65 (100%)   | 55 (85%)  | 10 (15%) | 3           | 13 |
| 21  | AU    | 48/48 (100%)   | 44 (92%)  | 4 (8%)   | 13          | 41 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 21  | BU    | 48/48 (100%)   | 44 (92%)  | 4 (8%)   | 13          | 41  |
| 22  | C1    | 47/47 (100%)   | 45 (96%)  | 2 (4%)   | 33          | 70  |
| 22  | D1    | 47/47 (100%)   | 44 (94%)  | 3 (6%)   | 20          | 54  |
| 23  | C2    | 45/46 (98%)    | 44 (98%)  | 1 (2%)   | 57          | 85  |
| 23  | D2    | 45/46 (98%)    | 43 (96%)  | 2 (4%)   | 33          | 69  |
| 24  | C3    | 38/38 (100%)   | 37 (97%)  | 1 (3%)   | 51          | 82  |
| 24  | D3    | 38/38 (100%)   | 37 (97%)  | 1 (3%)   | 51          | 82  |
| 25  | C4    | 51/51 (100%)   | 48 (94%)  | 3 (6%)   | 23          | 58  |
| 25  | D4    | 51/51 (100%)   | 48 (94%)  | 3 (6%)   | 23          | 58  |
| 26  | C5    | 34/34 (100%)   | 32 (94%)  | 2 (6%)   | 23          | 58  |
| 26  | D5    | 34/34 (100%)   | 34 (100%) | 0        | 100         | 100 |
| 27  | C0    | 48/48 (100%)   | 45 (94%)  | 3 (6%)   | 21          | 55  |
| 27  | D0    | 49/48 (102%)   | 45 (92%)  | 4 (8%)   | 13          | 41  |
| 29  | CC    | 216/217 (100%) | 202 (94%) | 14 (6%)  | 20          | 53  |
| 29  | DC    | 216/217 (100%) | 210 (97%) | 6 (3%)   | 49          | 80  |
| 30  | CD    | 164/164 (100%) | 160 (98%) | 4 (2%)   | 54          | 83  |
| 32  | DD    | 163/163 (100%) | 160 (98%) | 3 (2%)   | 64          | 87  |
| 33  | CE    | 165/165 (100%) | 152 (92%) | 13 (8%)  | 14          | 43  |
| 33  | DE    | 165/165 (100%) | 161 (98%) | 4 (2%)   | 54          | 83  |
| 34  | CF    | 148/149 (99%)  | 133 (90%) | 15 (10%) | 9           | 30  |
| 34  | DF    | 148/149 (99%)  | 137 (93%) | 11 (7%)  | 16          | 47  |
| 35  | CG    | 137/137 (100%) | 134 (98%) | 3 (2%)   | 57          | 85  |
| 35  | DG    | 137/137 (100%) | 132 (96%) | 5 (4%)   | 40          | 75  |
| 36  | CH    | 114/114 (100%) | 101 (89%) | 13 (11%) | 7           | 25  |
| 36  | DH    | 114/114 (100%) | 101 (89%) | 13 (11%) | 7           | 25  |
| 37  | CJ    | 104/104 (100%) | 100 (96%) | 4 (4%)   | 38          | 73  |
| 37  | DJ    | 104/104 (100%) | 100 (96%) | 4 (4%)   | 38          | 73  |
| 38  | CK    | 116/116 (100%) | 110 (95%) | 6 (5%)   | 27          | 63  |
| 38  | DK    | 116/116 (100%) | 114 (98%) | 2 (2%)   | 66          | 88  |
| 39  | CL    | 103/104 (99%)  | 99 (96%)  | 4 (4%)   | 37          | 73  |
| 39  | DL    | 104/104 (100%) | 99 (95%)  | 5 (5%)   | 30          | 66  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 40  | CM    | 103/103 (100%)   | 97 (94%)   | 6 (6%)   | 23          | 59 |
| 40  | DM    | 103/103 (100%)   | 99 (96%)   | 4 (4%)   | 37          | 73 |
| 41  | CN    | 108/108 (100%)   | 104 (96%)  | 4 (4%)   | 39          | 74 |
| 41  | DN    | 109/108 (101%)   | 106 (97%)  | 3 (3%)   | 49          | 80 |
| 42  | CO    | 100/102 (98%)    | 95 (95%)   | 5 (5%)   | 28          | 65 |
| 42  | DO    | 102/102 (100%)   | 99 (97%)   | 3 (3%)   | 48          | 80 |
| 43  | CP    | 86/87 (99%)      | 80 (93%)   | 6 (7%)   | 18          | 50 |
| 43  | DP    | 87/87 (100%)     | 84 (97%)   | 3 (3%)   | 42          | 76 |
| 44  | CQ    | 99/99 (100%)     | 93 (94%)   | 6 (6%)   | 22          | 56 |
| 44  | DQ    | 99/99 (100%)     | 97 (98%)   | 2 (2%)   | 60          | 86 |
| 45  | CR    | 89/89 (100%)     | 86 (97%)   | 3 (3%)   | 42          | 76 |
| 45  | DR    | 89/89 (100%)     | 87 (98%)   | 2 (2%)   | 57          | 85 |
| 46  | CS    | 84/84 (100%)     | 79 (94%)   | 5 (6%)   | 22          | 57 |
| 46  | DS    | 84/84 (100%)     | 83 (99%)   | 1 (1%)   | 75          | 92 |
| 47  | CT    | 93/93 (100%)     | 88 (95%)   | 5 (5%)   | 26          | 61 |
| 47  | DT    | 93/93 (100%)     | 92 (99%)   | 1 (1%)   | 78          | 92 |
| 48  | CU    | 80/80 (100%)     | 72 (90%)   | 8 (10%)  | 9           | 31 |
| 48  | DU    | 80/80 (100%)     | 77 (96%)   | 3 (4%)   | 38          | 73 |
| 49  | CV    | 83/84 (99%)      | 79 (95%)   | 4 (5%)   | 30          | 66 |
| 49  | DV    | 83/84 (99%)      | 81 (98%)   | 2 (2%)   | 54          | 83 |
| 50  | CW    | 78/78 (100%)     | 75 (96%)   | 3 (4%)   | 38          | 73 |
| 50  | DW    | 78/78 (100%)     | 76 (97%)   | 2 (3%)   | 51          | 82 |
| 51  | CX    | 56/58 (97%)      | 55 (98%)   | 1 (2%)   | 64          | 87 |
| 51  | DX    | 58/58 (100%)     | 57 (98%)   | 1 (2%)   | 66          | 88 |
| 52  | CY    | 67/67 (100%)     | 63 (94%)   | 4 (6%)   | 22          | 57 |
| 52  | DY    | 67/67 (100%)     | 65 (97%)   | 2 (3%)   | 46          | 79 |
| 53  | CZ    | 54/54 (100%)     | 50 (93%)   | 4 (7%)   | 16          | 47 |
| 53  | DZ    | 54/54 (100%)     | 52 (96%)   | 2 (4%)   | 39          | 74 |
| 54  | DI    | 103/103 (100%)   | 98 (95%)   | 5 (5%)   | 29          | 65 |
| All | All   | 9461/9484 (100%) | 8897 (94%) | 564 (6%) | 22          | 57 |

All (564) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 23  | TRP  |
| 2   | AB    | 44  | GLU  |
| 2   | AB    | 73  | LYS  |
| 2   | AB    | 93  | ASN  |
| 2   | AB    | 105 | LYS  |
| 2   | AB    | 125 | THR  |
| 2   | AB    | 129 | LEU  |
| 2   | AB    | 130 | THR  |
| 2   | AB    | 135 | LEU  |
| 2   | AB    | 137 | ARG  |
| 2   | AB    | 147 | SER  |
| 2   | AB    | 161 | LEU  |
| 2   | AB    | 205 | ASP  |
| 3   | AC    | 4   | LYS  |
| 3   | AC    | 14  | ILE  |
| 3   | AC    | 21  | THR  |
| 3   | AC    | 33  | LEU  |
| 3   | AC    | 38  | LYS  |
| 3   | AC    | 46  | GLU  |
| 3   | AC    | 107 | ARG  |
| 3   | AC    | 168 | TYR  |
| 3   | AC    | 178 | LEU  |
| 3   | AC    | 185 | ASN  |
| 3   | AC    | 186 | THR  |
| 4   | AD    | 5   | LEU  |
| 4   | AD    | 17  | THR  |
| 4   | AD    | 22  | LYS  |
| 4   | AD    | 26  | ARG  |
| 4   | AD    | 50  | ASP  |
| 4   | AD    | 132 | ILE  |
| 4   | AD    | 142 | VAL  |
| 4   | AD    | 143 | VAL  |
| 4   | AD    | 194 | ASP  |
| 4   | AD    | 206 | LYS  |
| 5   | AE    | 11  | LEU  |
| 5   | AE    | 14  | LYS  |
| 5   | AE    | 32  | SER  |
| 5   | AE    | 46  | VAL  |
| 5   | AE    | 76  | LEU  |
| 5   | AE    | 78  | ASN  |
| 5   | AE    | 82  | GLN  |
| 5   | AE    | 101 | GLU  |
| 5   | AE    | 106 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AE    | 123 | VAL  |
| 5   | AE    | 126 | LYS  |
| 6   | AF    | 36  | ILE  |
| 6   | AF    | 69  | GLU  |
| 6   | AF    | 71  | ILE  |
| 6   | AF    | 74  | LEU  |
| 6   | AF    | 89  | VAL  |
| 6   | AF    | 93  | LYS  |
| 7   | AG    | 30  | LEU  |
| 7   | AG    | 36  | LYS  |
| 7   | AG    | 59  | LEU  |
| 7   | AG    | 63  | GLU  |
| 7   | AG    | 92  | ARG  |
| 7   | AG    | 120 | LEU  |
| 7   | AG    | 131 | LYS  |
| 7   | AG    | 133 | THR  |
| 7   | AG    | 142 | HIS  |
| 8   | AH    | 3   | MET  |
| 8   | AH    | 31  | LYS  |
| 8   | AH    | 47  | GLU  |
| 8   | AH    | 52  | GLU  |
| 8   | AH    | 54  | ASP  |
| 8   | AH    | 60  | GLU  |
| 8   | AH    | 63  | LEU  |
| 8   | AH    | 76  | GLN  |
| 8   | AH    | 90  | ASP  |
| 8   | AH    | 107 | SER  |
| 8   | AH    | 108 | LYS  |
| 9   | AI    | 11  | ARG  |
| 9   | AI    | 61  | LEU  |
| 9   | AI    | 63  | LEU  |
| 9   | AI    | 66  | THR  |
| 9   | AI    | 99  | ARG  |
| 10  | AJ    | 6   | ILE  |
| 10  | AJ    | 62  | ARG  |
| 10  | AJ    | 63  | ASP  |
| 10  | AJ    | 88  | MET  |
| 10  | AJ    | 89  | ARG  |
| 10  | AJ    | 90  | LEU  |
| 11  | AK    | 23  | ILE  |
| 11  | AK    | 55  | SER  |
| 11  | AK    | 119 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AL    | 24  | LEU  |
| 12  | AL    | 40  | THR  |
| 12  | AL    | 55  | VAL  |
| 12  | AL    | 74  | LEU  |
| 12  | AL    | 82  | ILE  |
| 12  | AL    | 88  | LYS  |
| 12  | AL    | 90  | LEU  |
| 12  | AL    | 110 | ARG  |
| 12  | AL    | 115 | SER  |
| 12  | AL    | 121 | ARG  |
| 13  | AM    | 7   | ILE  |
| 13  | AM    | 13  | LYS  |
| 13  | AM    | 17  | ILE  |
| 13  | AM    | 27  | LYS  |
| 13  | AM    | 48  | LEU  |
| 13  | AM    | 58  | ASP  |
| 13  | AM    | 63  | PHE  |
| 13  | AM    | 71  | ARG  |
| 13  | AM    | 101 | ARG  |
| 14  | AN    | 31  | ILE  |
| 15  | AO    | 2   | SER  |
| 15  | AO    | 24  | SER  |
| 15  | AO    | 40  | GLN  |
| 15  | AO    | 70  | LEU  |
| 15  | AO    | 84  | ARG  |
| 16  | AP    | 48  | GLU  |
| 17  | AQ    | 5   | ILE  |
| 17  | AQ    | 16  | LYS  |
| 17  | AQ    | 27  | ARG  |
| 17  | AQ    | 38  | ILE  |
| 17  | AQ    | 40  | ARG  |
| 17  | AQ    | 75  | LEU  |
| 17  | AQ    | 83  | VAL  |
| 18  | AR    | 47  | THR  |
| 19  | AS    | 5   | LEU  |
| 19  | AS    | 7   | LYS  |
| 19  | AS    | 13  | LEU  |
| 19  | AS    | 27  | ASP  |
| 19  | AS    | 33  | THR  |
| 19  | AS    | 37  | ARG  |
| 19  | AS    | 56  | GLN  |
| 20  | AT    | 15  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AT    | 24  | ARG  |
| 20  | AT    | 27  | MET  |
| 20  | AT    | 44  | LYS  |
| 20  | AT    | 48  | GLN  |
| 20  | AT    | 85  | LYS  |
| 21  | AU    | 13  | ASP  |
| 21  | AU    | 16  | LEU  |
| 21  | AU    | 34  | ARG  |
| 21  | AU    | 56  | HIS  |
| 22  | C1    | 10  | ARG  |
| 22  | C1    | 40  | ARG  |
| 23  | C2    | 8   | LYS  |
| 24  | C3    | 1   | MET  |
| 25  | C4    | 31  | HIS  |
| 25  | C4    | 45  | ARG  |
| 25  | C4    | 52  | LYS  |
| 26  | C5    | 20  | ASP  |
| 26  | C5    | 26  | ILE  |
| 27  | C0    | 3   | LYS  |
| 27  | C0    | 19  | LYS  |
| 27  | C0    | 36  | VAL  |
| 2   | BB    | 18  | HIS  |
| 2   | BB    | 23  | TRP  |
| 2   | BB    | 44  | GLU  |
| 2   | BB    | 93  | ASN  |
| 2   | BB    | 105 | LYS  |
| 2   | BB    | 125 | THR  |
| 2   | BB    | 129 | LEU  |
| 2   | BB    | 130 | THR  |
| 2   | BB    | 135 | LEU  |
| 2   | BB    | 137 | ARG  |
| 2   | BB    | 147 | SER  |
| 2   | BB    | 161 | LEU  |
| 2   | BB    | 205 | ASP  |
| 3   | BC    | 4   | LYS  |
| 3   | BC    | 14  | ILE  |
| 3   | BC    | 33  | LEU  |
| 3   | BC    | 37  | PHE  |
| 3   | BC    | 38  | LYS  |
| 3   | BC    | 46  | GLU  |
| 3   | BC    | 55  | ILE  |
| 3   | BC    | 107 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | BC    | 152 | GLU  |
| 3   | BC    | 168 | TYR  |
| 3   | BC    | 175 | LEU  |
| 3   | BC    | 185 | ASN  |
| 3   | BC    | 186 | THR  |
| 3   | BC    | 193 | TYR  |
| 4   | BD    | 5   | LEU  |
| 4   | BD    | 17  | THR  |
| 4   | BD    | 22  | LYS  |
| 4   | BD    | 26  | ARG  |
| 4   | BD    | 47  | ARG  |
| 4   | BD    | 50  | ASP  |
| 4   | BD    | 142 | VAL  |
| 4   | BD    | 143 | VAL  |
| 4   | BD    | 151 | LYS  |
| 4   | BD    | 173 | VAL  |
| 4   | BD    | 194 | ASP  |
| 4   | BD    | 206 | LYS  |
| 5   | BE    | 11  | LEU  |
| 5   | BE    | 14  | LYS  |
| 5   | BE    | 32  | SER  |
| 5   | BE    | 46  | VAL  |
| 5   | BE    | 76  | LEU  |
| 5   | BE    | 81  | LEU  |
| 5   | BE    | 82  | GLN  |
| 5   | BE    | 88  | VAL  |
| 5   | BE    | 101 | GLU  |
| 5   | BE    | 103 | THR  |
| 5   | BE    | 114 | VAL  |
| 5   | BE    | 115 | LEU  |
| 5   | BE    | 123 | VAL  |
| 5   | BE    | 126 | LYS  |
| 5   | BE    | 151 | GLU  |
| 5   | BE    | 152 | MET  |
| 5   | BE    | 157 | ARG  |
| 5   | BE    | 159 | LYS  |
| 6   | BF    | 9   | MET  |
| 6   | BF    | 14  | GLN  |
| 6   | BF    | 16  | GLU  |
| 6   | BF    | 36  | ILE  |
| 6   | BF    | 53  | LYS  |
| 6   | BF    | 68  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | BF    | 69  | GLU  |
| 6   | BF    | 71  | ILE  |
| 6   | BF    | 89  | VAL  |
| 6   | BF    | 93  | LYS  |
| 7   | BG    | 4   | ARG  |
| 7   | BG    | 5   | ARG  |
| 7   | BG    | 10  | ARG  |
| 7   | BG    | 30  | LEU  |
| 7   | BG    | 36  | LYS  |
| 7   | BG    | 48  | GLU  |
| 7   | BG    | 50  | LEU  |
| 7   | BG    | 59  | LEU  |
| 7   | BG    | 63  | GLU  |
| 7   | BG    | 72  | THR  |
| 7   | BG    | 92  | ARG  |
| 7   | BG    | 120 | LEU  |
| 7   | BG    | 131 | LYS  |
| 7   | BG    | 133 | THR  |
| 7   | BG    | 142 | HIS  |
| 8   | BH    | 3   | MET  |
| 8   | BH    | 47  | GLU  |
| 8   | BH    | 52  | GLU  |
| 8   | BH    | 60  | GLU  |
| 8   | BH    | 76  | GLN  |
| 8   | BH    | 77  | ARG  |
| 8   | BH    | 80  | ARG  |
| 8   | BH    | 83  | LEU  |
| 8   | BH    | 90  | ASP  |
| 8   | BH    | 107 | SER  |
| 8   | BH    | 108 | LYS  |
| 9   | BI    | 11  | ARG  |
| 9   | BI    | 61  | LEU  |
| 9   | BI    | 63  | LEU  |
| 9   | BI    | 66  | THR  |
| 9   | BI    | 99  | ARG  |
| 10  | BJ    | 5   | ARG  |
| 10  | BJ    | 6   | ILE  |
| 10  | BJ    | 62  | ARG  |
| 10  | BJ    | 63  | ASP  |
| 10  | BJ    | 78  | GLU  |
| 10  | BJ    | 88  | MET  |
| 10  | BJ    | 89  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | BJ    | 90  | LEU  |
| 11  | BK    | 18  | ASP  |
| 11  | BK    | 23  | ILE  |
| 11  | BK    | 31  | ILE  |
| 11  | BK    | 38  | GLN  |
| 11  | BK    | 55  | SER  |
| 11  | BK    | 118 | HIS  |
| 11  | BK    | 119 | ASN  |
| 12  | BL    | 24  | LEU  |
| 12  | BL    | 44  | LYS  |
| 12  | BL    | 50  | ARG  |
| 12  | BL    | 55  | VAL  |
| 12  | BL    | 58  | THR  |
| 12  | BL    | 74  | LEU  |
| 12  | BL    | 82  | ILE  |
| 12  | BL    | 88  | LYS  |
| 12  | BL    | 90  | LEU  |
| 12  | BL    | 110 | ARG  |
| 12  | BL    | 115 | SER  |
| 12  | BL    | 121 | ARG  |
| 13  | BM    | 11  | ASP  |
| 13  | BM    | 13  | LYS  |
| 13  | BM    | 16  | VAL  |
| 13  | BM    | 17  | ILE  |
| 13  | BM    | 27  | LYS  |
| 13  | BM    | 48  | LEU  |
| 13  | BM    | 101 | ARG  |
| 14  | BN    | 26  | GLU  |
| 15  | BO    | 2   | SER  |
| 15  | BO    | 13  | SER  |
| 15  | BO    | 17  | ARG  |
| 15  | BO    | 24  | SER  |
| 15  | BO    | 40  | GLN  |
| 15  | BO    | 64  | ARG  |
| 15  | BO    | 66  | LEU  |
| 15  | BO    | 84  | ARG  |
| 15  | BO    | 87  | LEU  |
| 15  | BO    | 88  | ARG  |
| 15  | BO    | 89  | ARG  |
| 16  | BP    | 20  | VAL  |
| 16  | BP    | 46  | LYS  |
| 17  | BQ    | 17  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | BQ    | 21  | ILE  |
| 17  | BQ    | 26  | GLU  |
| 17  | BQ    | 27  | ARG  |
| 17  | BQ    | 38  | ILE  |
| 17  | BQ    | 40  | ARG  |
| 17  | BQ    | 51  | ASN  |
| 17  | BQ    | 75  | LEU  |
| 18  | BR    | 47  | THR  |
| 19  | BS    | 6   | LYS  |
| 19  | BS    | 7   | LYS  |
| 19  | BS    | 13  | LEU  |
| 19  | BS    | 33  | THR  |
| 19  | BS    | 37  | ARG  |
| 20  | BT    | 15  | GLU  |
| 20  | BT    | 24  | ARG  |
| 20  | BT    | 43  | ASP  |
| 20  | BT    | 48  | GLN  |
| 20  | BT    | 54  | MET  |
| 20  | BT    | 58  | VAL  |
| 20  | BT    | 64  | LYS  |
| 20  | BT    | 67  | ILE  |
| 20  | BT    | 69  | LYS  |
| 20  | BT    | 84  | ASN  |
| 21  | BU    | 13  | ASP  |
| 21  | BU    | 16  | LEU  |
| 21  | BU    | 34  | ARG  |
| 21  | BU    | 56  | HIS  |
| 22  | D1    | 18  | SER  |
| 22  | D1    | 26  | THR  |
| 22  | D1    | 29  | SER  |
| 23  | D2    | 5   | ILE  |
| 23  | D2    | 8   | LYS  |
| 24  | D3    | 1   | MET  |
| 25  | D4    | 31  | HIS  |
| 25  | D4    | 45  | ARG  |
| 25  | D4    | 52  | LYS  |
| 27  | D0    | 10  | THR  |
| 27  | D0    | 19  | LYS  |
| 27  | D0    | 25  | LEU  |
| 27  | D0    | 36  | VAL  |
| 29  | CC    | 11  | PRO  |
| 29  | CC    | 117 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | CC    | 120 | VAL  |
| 29  | CC    | 130 | LEU  |
| 29  | CC    | 157 | SER  |
| 29  | CC    | 168 | ASP  |
| 29  | CC    | 174 | LEU  |
| 29  | CC    | 195 | VAL  |
| 29  | CC    | 204 | VAL  |
| 29  | CC    | 205 | LEU  |
| 29  | CC    | 236 | GLU  |
| 29  | CC    | 252 | THR  |
| 29  | CC    | 258 | ARG  |
| 29  | CC    | 260 | ASN  |
| 30  | CD    | 4   | LEU  |
| 30  | CD    | 13  | ARG  |
| 30  | CD    | 18  | ASP  |
| 30  | CD    | 95  | SER  |
| 29  | DC    | 70  | ASN  |
| 29  | DC    | 117 | GLN  |
| 29  | DC    | 120 | VAL  |
| 29  | DC    | 130 | LEU  |
| 29  | DC    | 236 | GLU  |
| 29  | DC    | 252 | THR  |
| 32  | DD    | 13  | ARG  |
| 32  | DD    | 18  | ASP  |
| 32  | DD    | 95  | SER  |
| 33  | CE    | 7   | ASP  |
| 33  | CE    | 12  | LEU  |
| 33  | CE    | 25  | GLU  |
| 33  | CE    | 44  | ARG  |
| 33  | CE    | 72  | SER  |
| 33  | CE    | 78  | TRP  |
| 33  | CE    | 83  | VAL  |
| 33  | CE    | 107 | SER  |
| 33  | CE    | 122 | GLU  |
| 33  | CE    | 127 | GLU  |
| 33  | CE    | 149 | ILE  |
| 33  | CE    | 152 | GLU  |
| 33  | CE    | 189 | THR  |
| 34  | CF    | 18  | THR  |
| 34  | CF    | 36  | LEU  |
| 34  | CF    | 57  | LEU  |
| 34  | CF    | 72  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | CF    | 80  | ARG  |
| 34  | CF    | 94  | GLU  |
| 34  | CF    | 106 | ILE  |
| 34  | CF    | 115 | ARG  |
| 34  | CF    | 117 | LEU  |
| 34  | CF    | 123 | ASP  |
| 34  | CF    | 134 | GLU  |
| 34  | CF    | 141 | ILE  |
| 34  | CF    | 149 | VAL  |
| 34  | CF    | 152 | LEU  |
| 34  | CF    | 174 | ASP  |
| 35  | CG    | 11  | VAL  |
| 35  | CG    | 18  | LYS  |
| 35  | CG    | 155 | GLU  |
| 36  | CH    | 7   | ASP  |
| 36  | CH    | 15  | LEU  |
| 36  | CH    | 17  | ASP  |
| 36  | CH    | 21  | VAL  |
| 36  | CH    | 48  | GLU  |
| 36  | CH    | 51  | ARG  |
| 36  | CH    | 53  | GLU  |
| 36  | CH    | 55  | GLU  |
| 36  | CH    | 62  | LEU  |
| 36  | CH    | 75  | LEU  |
| 36  | CH    | 121 | VAL  |
| 36  | CH    | 127 | GLU  |
| 36  | CH    | 145 | ASN  |
| 37  | CJ    | 11  | LEU  |
| 37  | CJ    | 13  | VAL  |
| 37  | CJ    | 28  | LEU  |
| 37  | CJ    | 113 | LYS  |
| 38  | CK    | 5   | THR  |
| 38  | CK    | 9   | GLU  |
| 38  | CK    | 30  | THR  |
| 38  | CK    | 39  | LYS  |
| 38  | CK    | 124 | VAL  |
| 38  | CK    | 142 | ILE  |
| 39  | CL    | 35  | VAL  |
| 39  | CL    | 58  | LEU  |
| 39  | CL    | 98  | ARG  |
| 39  | CL    | 113 | MET  |
| 40  | CM    | 2   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | CM    | 21  | ARG  |
| 40  | CM    | 93  | ASN  |
| 40  | CM    | 94  | THR  |
| 40  | CM    | 100 | ILE  |
| 40  | CM    | 115 | GLU  |
| 41  | CN    | 6   | ARG  |
| 41  | CN    | 20  | LEU  |
| 41  | CN    | 59  | ARG  |
| 41  | CN    | 78  | LEU  |
| 42  | CO    | 2   | ARG  |
| 42  | CO    | 14  | SER  |
| 42  | CO    | 71  | ARG  |
| 42  | CO    | 76  | VAL  |
| 42  | CO    | 95  | THR  |
| 43  | CP    | 18  | LEU  |
| 43  | CP    | 31  | THR  |
| 43  | CP    | 38  | GLN  |
| 43  | CP    | 49  | VAL  |
| 43  | CP    | 56  | LYS  |
| 43  | CP    | 78  | VAL  |
| 44  | CQ    | 2   | SER  |
| 44  | CQ    | 26  | VAL  |
| 44  | CQ    | 39  | ARG  |
| 44  | CQ    | 40  | LEU  |
| 44  | CQ    | 102 | GLU  |
| 44  | CQ    | 114 | LEU  |
| 45  | CR    | 16  | LYS  |
| 45  | CR    | 51  | ARG  |
| 45  | CR    | 52  | GLN  |
| 46  | CS    | 12  | HIS  |
| 46  | CS    | 45  | GLU  |
| 46  | CS    | 48  | LYS  |
| 46  | CS    | 51  | VAL  |
| 46  | CS    | 102 | SER  |
| 47  | CT    | 7   | HIS  |
| 47  | CT    | 19  | LEU  |
| 47  | CT    | 29  | VAL  |
| 47  | CT    | 86  | MET  |
| 47  | CT    | 97  | LEU  |
| 48  | CU    | 1   | MET  |
| 48  | CU    | 2   | ILE  |
| 48  | CU    | 3   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | CU    | 10  | VAL  |
| 48  | CU    | 24  | MET  |
| 48  | CU    | 30  | ILE  |
| 48  | CU    | 49  | LYS  |
| 48  | CU    | 69  | ARG  |
| 49  | CV    | 61  | LYS  |
| 49  | CV    | 72  | ILE  |
| 49  | CV    | 81  | ASP  |
| 49  | CV    | 98  | SER  |
| 50  | CW    | 1   | MET  |
| 50  | CW    | 7   | GLU  |
| 50  | CW    | 10  | LYS  |
| 51  | CX    | 82  | ILE  |
| 52  | CY    | 25  | THR  |
| 52  | CY    | 35  | SER  |
| 52  | CY    | 48  | THR  |
| 52  | CY    | 71  | LEU  |
| 53  | CZ    | 18  | LEU  |
| 53  | CZ    | 19  | LEU  |
| 53  | CZ    | 38  | GLN  |
| 53  | CZ    | 58  | ASN  |
| 33  | DE    | 12  | LEU  |
| 33  | DE    | 107 | SER  |
| 33  | DE    | 127 | GLU  |
| 33  | DE    | 189 | THR  |
| 34  | DF    | 10  | ASP  |
| 34  | DF    | 57  | LEU  |
| 34  | DF    | 72  | LYS  |
| 34  | DF    | 94  | GLU  |
| 34  | DF    | 106 | ILE  |
| 34  | DF    | 117 | LEU  |
| 34  | DF    | 134 | GLU  |
| 34  | DF    | 141 | ILE  |
| 34  | DF    | 149 | VAL  |
| 34  | DF    | 152 | LEU  |
| 34  | DF    | 174 | ASP  |
| 35  | DG    | 3   | ARG  |
| 35  | DG    | 11  | VAL  |
| 35  | DG    | 18  | LYS  |
| 35  | DG    | 56  | ASP  |
| 35  | DG    | 155 | GLU  |
| 36  | DH    | 7   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | DH    | 15  | LEU  |
| 36  | DH    | 17  | ASP  |
| 36  | DH    | 21  | VAL  |
| 36  | DH    | 48  | GLU  |
| 36  | DH    | 53  | GLU  |
| 36  | DH    | 57  | LYS  |
| 36  | DH    | 58  | LEU  |
| 36  | DH    | 60  | GLU  |
| 36  | DH    | 75  | LEU  |
| 36  | DH    | 121 | VAL  |
| 36  | DH    | 127 | GLU  |
| 36  | DH    | 145 | ASN  |
| 37  | DJ    | 11  | LEU  |
| 37  | DJ    | 13  | VAL  |
| 37  | DJ    | 28  | LEU  |
| 37  | DJ    | 113 | LYS  |
| 38  | DK    | 124 | VAL  |
| 38  | DK    | 142 | ILE  |
| 39  | DL    | 58  | LEU  |
| 39  | DL    | 76  | VAL  |
| 39  | DL    | 110 | GLU  |
| 39  | DL    | 113 | MET  |
| 39  | DL    | 123 | LEU  |
| 40  | DM    | 2   | ARG  |
| 40  | DM    | 91  | ASP  |
| 40  | DM    | 94  | THR  |
| 40  | DM    | 115 | GLU  |
| 41  | DN    | 58  | LYS  |
| 41  | DN    | 59  | ARG  |
| 41  | DN    | 100 | LYS  |
| 42  | DO    | 2   | ARG  |
| 42  | DO    | 14  | SER  |
| 42  | DO    | 76  | VAL  |
| 43  | DP    | 31  | THR  |
| 43  | DP    | 49  | VAL  |
| 43  | DP    | 78  | VAL  |
| 44  | DQ    | 26  | VAL  |
| 44  | DQ    | 102 | GLU  |
| 45  | DR    | 41  | LYS  |
| 45  | DR    | 51  | ARG  |
| 46  | DS    | 102 | SER  |
| 47  | DT    | 86  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | DU    | 1   | MET  |
| 48  | DU    | 3   | ARG  |
| 48  | DU    | 10  | VAL  |
| 49  | DV    | 52  | LEU  |
| 49  | DV    | 61  | LYS  |
| 50  | DW    | 7   | GLU  |
| 50  | DW    | 53  | LYS  |
| 51  | DX    | 82  | ILE  |
| 52  | DY    | 25  | THR  |
| 52  | DY    | 35  | SER  |
| 53  | DZ    | 19  | LEU  |
| 53  | DZ    | 38  | GLN  |
| 54  | DI    | 7   | ASP  |
| 54  | DI    | 16  | SER  |
| 54  | DI    | 53  | ARG  |
| 54  | DI    | 64  | VAL  |
| 54  | DI    | 117 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 18  | HIS  |
| 2   | AB    | 93  | ASN  |
| 2   | AB    | 94  | HIS  |
| 2   | AB    | 120 | GLN  |
| 4   | AD    | 136 | GLN  |
| 5   | AE    | 89  | HIS  |
| 6   | AF    | 63  | ASN  |
| 7   | AG    | 97  | ASN  |
| 7   | AG    | 142 | HIS  |
| 8   | AH    | 4   | GLN  |
| 10  | AJ    | 58  | ASN  |
| 20  | AT    | 48  | GLN  |
| 20  | AT    | 78  | ASN  |
| 22  | C1    | 6   | ASN  |
| 22  | C1    | 38  | HIS  |
| 2   | BB    | 39  | HIS  |
| 2   | BB    | 93  | ASN  |
| 2   | BB    | 94  | HIS  |
| 2   | BB    | 120 | GLN  |
| 2   | BB    | 168 | HIS  |
| 4   | BD    | 131 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | BE    | 70  | ASN  |
| 5   | BE    | 89  | HIS  |
| 5   | BE    | 122 | ASN  |
| 7   | BG    | 97  | ASN  |
| 8   | BH    | 4   | GLN  |
| 8   | BH    | 38  | ASN  |
| 17  | BQ    | 51  | ASN  |
| 20  | BT    | 3   | ASN  |
| 24  | D3    | 26  | ASN  |
| 25  | D4    | 43  | HIS  |
| 29  | CC    | 142 | HIS  |
| 29  | DC    | 142 | HIS  |
| 33  | CE    | 115 | GLN  |
| 35  | CG    | 38  | ASN  |
| 38  | CK    | 138 | GLN  |
| 43  | CP    | 100 | HIS  |
| 48  | CU    | 28  | ASN  |
| 49  | CV    | 74  | ASN  |
| 51  | CX    | 57  | HIS  |
| 53  | CZ    | 45  | GLN  |
| 49  | DV    | 54  | GLN  |
| 54  | DI    | 122 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1530/1534 (99%) | 239 (15%)         | 0               |
| 1   | BA    | 1529/1534 (99%) | 246 (16%)         | 0               |
| 28  | CB    | 117/120 (97%)   | 11 (9%)           | 0               |
| 28  | DB    | 119/120 (99%)   | 9 (7%)            | 0               |
| 31  | CA    | 2892/2904 (99%) | 426 (14%)         | 0               |
| 55  | DA    | 2880/2904 (99%) | 367 (12%)         | 0               |
| All | All   | 9067/9116 (99%) | 1298 (14%)        | 0               |

All (1298) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 4   | U    |
| 1   | AA    | 5   | U    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 22  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 32  | A    |
| 1   | AA    | 39  | G    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 50  | A    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 52  | C    |
| 1   | AA    | 69  | G    |
| 1   | AA    | 71  | A    |
| 1   | AA    | 72  | A    |
| 1   | AA    | 74  | A    |
| 1   | AA    | 80  | A    |
| 1   | AA    | 81  | A    |
| 1   | AA    | 82  | G    |
| 1   | AA    | 83  | C    |
| 1   | AA    | 85  | U    |
| 1   | AA    | 86  | G    |
| 1   | AA    | 88  | U    |
| 1   | AA    | 89  | U    |
| 1   | AA    | 90  | C    |
| 1   | AA    | 92  | U    |
| 1   | AA    | 94  | G    |
| 1   | AA    | 95  | C    |
| 1   | AA    | 108 | G    |
| 1   | AA    | 120 | A    |
| 1   | AA    | 130 | A    |
| 1   | AA    | 131 | A    |
| 1   | AA    | 137 | U    |
| 1   | AA    | 141 | G    |
| 1   | AA    | 142 | G    |
| 1   | AA    | 143 | A    |
| 1   | AA    | 144 | G    |
| 1   | AA    | 149 | A    |
| 1   | AA    | 159 | G    |
| 1   | AA    | 163 | C    |
| 1   | AA    | 168 | G    |
| 1   | AA    | 177 | G    |
| 1   | AA    | 183 | C    |
| 1   | AA    | 197 | A    |
| 1   | AA    | 205 | A    |
| 1   | AA    | 210 | C    |
| 1   | AA    | 211 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 212 | G    |
| 1   | AA    | 226 | G    |
| 1   | AA    | 240 | G    |
| 1   | AA    | 245 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 250 | A    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 321 | A    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 329 | A    |
| 1   | AA    | 330 | C    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 346 | G    |
| 1   | AA    | 348 | G    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 373 | A    |
| 1   | AA    | 384 | G    |
| 1   | AA    | 398 | U    |
| 1   | AA    | 406 | G    |
| 1   | AA    | 411 | A    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 424 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 436 | C    |
| 1   | AA    | 457 | G    |
| 1   | AA    | 458 | U    |
| 1   | AA    | 463 | U    |
| 1   | AA    | 466 | A    |
| 1   | AA    | 467 | U    |
| 1   | AA    | 468 | A    |
| 1   | AA    | 474 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 481 | G    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 486 | U    |
| 1   | AA    | 495 | A    |
| 1   | AA    | 509 | A    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 527 | G7M  |
| 1   | AA    | 531 | U    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 564 | C    |
| 1   | AA    | 568 | G    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 576 | C    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 615 | G    |
| 1   | AA    | 633 | G    |
| 1   | AA    | 650 | G    |
| 1   | AA    | 653 | U    |
| 1   | AA    | 661 | G    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 695 | A    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |
| 1   | AA    | 723 | U    |
| 1   | AA    | 734 | G    |
| 1   | AA    | 748 | G    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 814 | A    |
| 1   | AA    | 815 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 821 | G    |
| 1   | AA    | 828 | U    |
| 1   | AA    | 836 | G    |
| 1   | AA    | 841 | C    |
| 1   | AA    | 842 | U    |
| 1   | AA    | 843 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 844  | G    |
| 1   | AA    | 845  | A    |
| 1   | AA    | 914  | A    |
| 1   | AA    | 926  | G    |
| 1   | AA    | 927  | G    |
| 1   | AA    | 934  | C    |
| 1   | AA    | 935  | A    |
| 1   | AA    | 960  | U    |
| 1   | AA    | 966  | 2MG  |
| 1   | AA    | 969  | A    |
| 1   | AA    | 971  | G    |
| 1   | AA    | 975  | A    |
| 1   | AA    | 976  | G    |
| 1   | AA    | 977  | A    |
| 1   | AA    | 987  | G    |
| 1   | AA    | 993  | G    |
| 1   | AA    | 1004 | A    |
| 1   | AA    | 1009 | U    |
| 1   | AA    | 1015 | G    |
| 1   | AA    | 1019 | A    |
| 1   | AA    | 1024 | G    |
| 1   | AA    | 1026 | G    |
| 1   | AA    | 1027 | C    |
| 1   | AA    | 1028 | C    |
| 1   | AA    | 1029 | U    |
| 1   | AA    | 1030 | U    |
| 1   | AA    | 1031 | C    |
| 1   | AA    | 1032 | G    |
| 1   | AA    | 1033 | G    |
| 1   | AA    | 1036 | A    |
| 1   | AA    | 1037 | C    |
| 1   | AA    | 1043 | G    |
| 1   | AA    | 1053 | G    |
| 1   | AA    | 1054 | C    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1086 | U    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1098 | C    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1124 | G    |
| 1   | AA    | 1125 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1132 | C    |
| 1   | AA    | 1133 | G    |
| 1   | AA    | 1136 | C    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1141 | C    |
| 1   | AA    | 1142 | G    |
| 1   | AA    | 1143 | G    |
| 1   | AA    | 1145 | A    |
| 1   | AA    | 1152 | A    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1160 | G    |
| 1   | AA    | 1168 | U    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1196 | A    |
| 1   | AA    | 1197 | A    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1214 | C    |
| 1   | AA    | 1215 | G    |
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1236 | A    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1239 | A    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1257 | A    |
| 1   | AA    | 1260 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1281 | C    |
| 1   | AA    | 1286 | U    |
| 1   | AA    | 1287 | A    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1302 | C    |
| 1   | AA    | 1305 | G    |
| 1   | AA    | 1312 | G    |
| 1   | AA    | 1317 | C    |
| 1   | AA    | 1320 | C    |
| 1   | AA    | 1346 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1353 | G    |
| 1   | AA    | 1363 | A    |
| 1   | AA    | 1370 | G    |
| 1   | AA    | 1379 | G    |
| 1   | AA    | 1381 | U    |
| 1   | AA    | 1398 | A    |
| 1   | AA    | 1419 | G    |
| 1   | AA    | 1429 | A    |
| 1   | AA    | 1441 | A    |
| 1   | AA    | 1446 | A    |
| 1   | AA    | 1447 | A    |
| 1   | AA    | 1448 | C    |
| 1   | AA    | 1451 | U    |
| 1   | AA    | 1452 | C    |
| 1   | AA    | 1453 | G    |
| 1   | AA    | 1492 | A    |
| 1   | AA    | 1497 | G    |
| 1   | AA    | 1499 | A    |
| 1   | AA    | 1503 | A    |
| 1   | AA    | 1506 | U    |
| 1   | AA    | 1507 | A    |
| 1   | AA    | 1517 | G    |
| 1   | AA    | 1529 | G    |
| 1   | AA    | 1530 | G    |
| 1   | AA    | 1534 | A    |
| 1   | BA    | 4    | U    |
| 1   | BA    | 5    | U    |
| 1   | BA    | 9    | G    |
| 1   | BA    | 22   | G    |
| 1   | BA    | 32   | A    |
| 1   | BA    | 39   | G    |
| 1   | BA    | 47   | C    |
| 1   | BA    | 48   | C    |
| 1   | BA    | 50   | A    |
| 1   | BA    | 51   | A    |
| 1   | BA    | 52   | C    |
| 1   | BA    | 69   | G    |
| 1   | BA    | 71   | A    |
| 1   | BA    | 72   | A    |
| 1   | BA    | 74   | A    |
| 1   | BA    | 80   | A    |
| 1   | BA    | 82   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BA    | 83  | C    |
| 1   | BA    | 84  | U    |
| 1   | BA    | 85  | U    |
| 1   | BA    | 86  | G    |
| 1   | BA    | 87  | C    |
| 1   | BA    | 88  | U    |
| 1   | BA    | 89  | U    |
| 1   | BA    | 90  | C    |
| 1   | BA    | 92  | U    |
| 1   | BA    | 94  | G    |
| 1   | BA    | 95  | C    |
| 1   | BA    | 108 | G    |
| 1   | BA    | 120 | A    |
| 1   | BA    | 130 | A    |
| 1   | BA    | 131 | A    |
| 1   | BA    | 137 | U    |
| 1   | BA    | 141 | G    |
| 1   | BA    | 142 | G    |
| 1   | BA    | 143 | A    |
| 1   | BA    | 144 | G    |
| 1   | BA    | 149 | A    |
| 1   | BA    | 159 | G    |
| 1   | BA    | 163 | C    |
| 1   | BA    | 168 | G    |
| 1   | BA    | 177 | G    |
| 1   | BA    | 183 | C    |
| 1   | BA    | 197 | A    |
| 1   | BA    | 200 | G    |
| 1   | BA    | 205 | A    |
| 1   | BA    | 210 | C    |
| 1   | BA    | 211 | G    |
| 1   | BA    | 212 | G    |
| 1   | BA    | 226 | G    |
| 1   | BA    | 245 | U    |
| 1   | BA    | 247 | G    |
| 1   | BA    | 250 | A    |
| 1   | BA    | 251 | G    |
| 1   | BA    | 266 | G    |
| 1   | BA    | 267 | C    |
| 1   | BA    | 289 | G    |
| 1   | BA    | 321 | A    |
| 1   | BA    | 328 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BA    | 329 | A    |
| 1   | BA    | 330 | C    |
| 1   | BA    | 332 | G    |
| 1   | BA    | 346 | G    |
| 1   | BA    | 348 | G    |
| 1   | BA    | 352 | C    |
| 1   | BA    | 354 | G    |
| 1   | BA    | 367 | U    |
| 1   | BA    | 372 | C    |
| 1   | BA    | 373 | A    |
| 1   | BA    | 384 | G    |
| 1   | BA    | 398 | U    |
| 1   | BA    | 406 | G    |
| 1   | BA    | 412 | A    |
| 1   | BA    | 413 | G    |
| 1   | BA    | 414 | A    |
| 1   | BA    | 421 | U    |
| 1   | BA    | 422 | C    |
| 1   | BA    | 424 | G    |
| 1   | BA    | 429 | U    |
| 1   | BA    | 430 | A    |
| 1   | BA    | 436 | C    |
| 1   | BA    | 457 | G    |
| 1   | BA    | 458 | U    |
| 1   | BA    | 463 | U    |
| 1   | BA    | 467 | U    |
| 1   | BA    | 468 | A    |
| 1   | BA    | 474 | G    |
| 1   | BA    | 481 | G    |
| 1   | BA    | 484 | G    |
| 1   | BA    | 486 | U    |
| 1   | BA    | 495 | A    |
| 1   | BA    | 509 | A    |
| 1   | BA    | 511 | C    |
| 1   | BA    | 527 | G7M  |
| 1   | BA    | 531 | U    |
| 1   | BA    | 532 | A    |
| 1   | BA    | 533 | A    |
| 1   | BA    | 547 | A    |
| 1   | BA    | 559 | A    |
| 1   | BA    | 564 | C    |
| 1   | BA    | 568 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BA    | 572 | A    |
| 1   | BA    | 573 | A    |
| 1   | BA    | 576 | C    |
| 1   | BA    | 577 | G    |
| 1   | BA    | 615 | G    |
| 1   | BA    | 633 | G    |
| 1   | BA    | 650 | G    |
| 1   | BA    | 653 | U    |
| 1   | BA    | 661 | G    |
| 1   | BA    | 665 | A    |
| 1   | BA    | 695 | A    |
| 1   | BA    | 702 | A    |
| 1   | BA    | 703 | G    |
| 1   | BA    | 723 | U    |
| 1   | BA    | 734 | G    |
| 1   | BA    | 748 | G    |
| 1   | BA    | 755 | G    |
| 1   | BA    | 777 | A    |
| 1   | BA    | 793 | U    |
| 1   | BA    | 794 | A    |
| 1   | BA    | 814 | A    |
| 1   | BA    | 815 | A    |
| 1   | BA    | 817 | C    |
| 1   | BA    | 821 | G    |
| 1   | BA    | 828 | U    |
| 1   | BA    | 836 | G    |
| 1   | BA    | 839 | C    |
| 1   | BA    | 840 | C    |
| 1   | BA    | 841 | C    |
| 1   | BA    | 842 | U    |
| 1   | BA    | 843 | U    |
| 1   | BA    | 844 | G    |
| 1   | BA    | 845 | A    |
| 1   | BA    | 846 | G    |
| 1   | BA    | 914 | A    |
| 1   | BA    | 926 | G    |
| 1   | BA    | 927 | G    |
| 1   | BA    | 934 | C    |
| 1   | BA    | 935 | A    |
| 1   | BA    | 960 | U    |
| 1   | BA    | 966 | 2MG  |
| 1   | BA    | 969 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | BA    | 971  | G    |
| 1   | BA    | 975  | A    |
| 1   | BA    | 976  | G    |
| 1   | BA    | 977  | A    |
| 1   | BA    | 987  | G    |
| 1   | BA    | 993  | G    |
| 1   | BA    | 1004 | A    |
| 1   | BA    | 1008 | U    |
| 1   | BA    | 1009 | U    |
| 1   | BA    | 1015 | G    |
| 1   | BA    | 1019 | A    |
| 1   | BA    | 1024 | G    |
| 1   | BA    | 1026 | G    |
| 1   | BA    | 1027 | C    |
| 1   | BA    | 1028 | C    |
| 1   | BA    | 1029 | U    |
| 1   | BA    | 1030 | U    |
| 1   | BA    | 1031 | C    |
| 1   | BA    | 1032 | G    |
| 1   | BA    | 1033 | G    |
| 1   | BA    | 1036 | A    |
| 1   | BA    | 1037 | C    |
| 1   | BA    | 1043 | G    |
| 1   | BA    | 1046 | A    |
| 1   | BA    | 1053 | G    |
| 1   | BA    | 1054 | C    |
| 1   | BA    | 1065 | U    |
| 1   | BA    | 1070 | U    |
| 1   | BA    | 1086 | U    |
| 1   | BA    | 1094 | G    |
| 1   | BA    | 1095 | U    |
| 1   | BA    | 1098 | C    |
| 1   | BA    | 1101 | A    |
| 1   | BA    | 1124 | G    |
| 1   | BA    | 1125 | U    |
| 1   | BA    | 1132 | C    |
| 1   | BA    | 1133 | G    |
| 1   | BA    | 1136 | C    |
| 1   | BA    | 1137 | C    |
| 1   | BA    | 1138 | G    |
| 1   | BA    | 1139 | G    |
| 1   | BA    | 1140 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | BA    | 1141 | C    |
| 1   | BA    | 1142 | G    |
| 1   | BA    | 1143 | G    |
| 1   | BA    | 1145 | A    |
| 1   | BA    | 1152 | A    |
| 1   | BA    | 1159 | U    |
| 1   | BA    | 1160 | G    |
| 1   | BA    | 1168 | U    |
| 1   | BA    | 1196 | A    |
| 1   | BA    | 1197 | A    |
| 1   | BA    | 1212 | U    |
| 1   | BA    | 1213 | A    |
| 1   | BA    | 1214 | C    |
| 1   | BA    | 1215 | G    |
| 1   | BA    | 1225 | A    |
| 1   | BA    | 1226 | C    |
| 1   | BA    | 1227 | A    |
| 1   | BA    | 1236 | A    |
| 1   | BA    | 1238 | A    |
| 1   | BA    | 1239 | A    |
| 1   | BA    | 1256 | A    |
| 1   | BA    | 1257 | A    |
| 1   | BA    | 1260 | G    |
| 1   | BA    | 1280 | A    |
| 1   | BA    | 1281 | C    |
| 1   | BA    | 1286 | U    |
| 1   | BA    | 1287 | A    |
| 1   | BA    | 1300 | G    |
| 1   | BA    | 1302 | C    |
| 1   | BA    | 1305 | G    |
| 1   | BA    | 1312 | G    |
| 1   | BA    | 1317 | C    |
| 1   | BA    | 1320 | C    |
| 1   | BA    | 1346 | A    |
| 1   | BA    | 1353 | G    |
| 1   | BA    | 1362 | A    |
| 1   | BA    | 1363 | A    |
| 1   | BA    | 1370 | G    |
| 1   | BA    | 1379 | G    |
| 1   | BA    | 1381 | U    |
| 1   | BA    | 1398 | A    |
| 1   | BA    | 1419 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | BA    | 1429 | A    |
| 1   | BA    | 1441 | A    |
| 1   | BA    | 1446 | A    |
| 1   | BA    | 1447 | A    |
| 1   | BA    | 1448 | C    |
| 1   | BA    | 1451 | U    |
| 1   | BA    | 1452 | C    |
| 1   | BA    | 1453 | G    |
| 1   | BA    | 1492 | A    |
| 1   | BA    | 1493 | A    |
| 1   | BA    | 1497 | G    |
| 1   | BA    | 1499 | A    |
| 1   | BA    | 1503 | A    |
| 1   | BA    | 1506 | U    |
| 1   | BA    | 1507 | A    |
| 1   | BA    | 1517 | G    |
| 1   | BA    | 1529 | G    |
| 1   | BA    | 1530 | G    |
| 1   | BA    | 1534 | A    |
| 28  | CB    | 9    | G    |
| 28  | CB    | 25   | U    |
| 28  | CB    | 35   | C    |
| 28  | CB    | 45   | A    |
| 28  | CB    | 56   | G    |
| 28  | CB    | 57   | A    |
| 28  | CB    | 88   | C    |
| 28  | CB    | 89   | U    |
| 28  | CB    | 90   | C    |
| 28  | CB    | 99   | A    |
| 28  | CB    | 109  | A    |
| 31  | CA    | 10   | A    |
| 31  | CA    | 14   | A    |
| 31  | CA    | 34   | U    |
| 31  | CA    | 36   | G    |
| 31  | CA    | 42   | A    |
| 31  | CA    | 46   | G    |
| 31  | CA    | 49   | A    |
| 31  | CA    | 58   | G    |
| 31  | CA    | 63   | A    |
| 31  | CA    | 71   | A    |
| 31  | CA    | 74   | A    |
| 31  | CA    | 75   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | CA    | 80  | G    |
| 31  | CA    | 83  | A    |
| 31  | CA    | 84  | A    |
| 31  | CA    | 101 | A    |
| 31  | CA    | 102 | U    |
| 31  | CA    | 118 | A    |
| 31  | CA    | 119 | A    |
| 31  | CA    | 120 | U    |
| 31  | CA    | 138 | U    |
| 31  | CA    | 139 | U    |
| 31  | CA    | 140 | C    |
| 31  | CA    | 141 | G    |
| 31  | CA    | 142 | A    |
| 31  | CA    | 143 | C    |
| 31  | CA    | 196 | A    |
| 31  | CA    | 199 | A    |
| 31  | CA    | 200 | U    |
| 31  | CA    | 215 | G    |
| 31  | CA    | 216 | A    |
| 31  | CA    | 221 | A    |
| 31  | CA    | 222 | A    |
| 31  | CA    | 248 | G    |
| 31  | CA    | 265 | A    |
| 31  | CA    | 266 | G    |
| 31  | CA    | 272 | A    |
| 31  | CA    | 276 | U    |
| 31  | CA    | 277 | G    |
| 31  | CA    | 278 | A    |
| 31  | CA    | 279 | A    |
| 31  | CA    | 285 | G    |
| 31  | CA    | 311 | A    |
| 31  | CA    | 329 | G    |
| 31  | CA    | 330 | A    |
| 31  | CA    | 343 | C    |
| 31  | CA    | 346 | A    |
| 31  | CA    | 352 | A    |
| 31  | CA    | 353 | C    |
| 31  | CA    | 362 | A    |
| 31  | CA    | 371 | A    |
| 31  | CA    | 372 | G    |
| 31  | CA    | 385 | C    |
| 31  | CA    | 386 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | CA    | 399 | U    |
| 31  | CA    | 404 | A    |
| 31  | CA    | 405 | U    |
| 31  | CA    | 411 | G    |
| 31  | CA    | 420 | C    |
| 31  | CA    | 424 | G    |
| 31  | CA    | 425 | G    |
| 31  | CA    | 451 | U    |
| 31  | CA    | 480 | A    |
| 31  | CA    | 481 | G    |
| 31  | CA    | 491 | G    |
| 31  | CA    | 503 | A    |
| 31  | CA    | 504 | A    |
| 31  | CA    | 505 | A    |
| 31  | CA    | 508 | A    |
| 31  | CA    | 517 | C    |
| 31  | CA    | 531 | C    |
| 31  | CA    | 532 | A    |
| 31  | CA    | 543 | G    |
| 31  | CA    | 544 | C    |
| 31  | CA    | 546 | U    |
| 31  | CA    | 547 | A    |
| 31  | CA    | 549 | G    |
| 31  | CA    | 550 | C    |
| 31  | CA    | 551 | G    |
| 31  | CA    | 555 | G    |
| 31  | CA    | 556 | A    |
| 31  | CA    | 563 | A    |
| 31  | CA    | 571 | U    |
| 31  | CA    | 573 | U    |
| 31  | CA    | 575 | A    |
| 31  | CA    | 586 | A    |
| 31  | CA    | 603 | A    |
| 31  | CA    | 613 | A    |
| 31  | CA    | 614 | A    |
| 31  | CA    | 615 | U    |
| 31  | CA    | 627 | A    |
| 31  | CA    | 637 | A    |
| 31  | CA    | 645 | C    |
| 31  | CA    | 647 | G    |
| 31  | CA    | 654 | A    |
| 31  | CA    | 655 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | CA    | 670 | A    |
| 31  | CA    | 684 | G    |
| 31  | CA    | 685 | A    |
| 31  | CA    | 686 | U    |
| 31  | CA    | 695 | G    |
| 31  | CA    | 717 | C    |
| 31  | CA    | 730 | A    |
| 31  | CA    | 740 | C    |
| 31  | CA    | 746 | PSU  |
| 31  | CA    | 747 | 5MU  |
| 31  | CA    | 775 | G    |
| 31  | CA    | 776 | G    |
| 31  | CA    | 782 | A    |
| 31  | CA    | 784 | G    |
| 31  | CA    | 785 | G    |
| 31  | CA    | 792 | A    |
| 31  | CA    | 802 | A    |
| 31  | CA    | 805 | G    |
| 31  | CA    | 812 | C    |
| 31  | CA    | 819 | A    |
| 31  | CA    | 827 | U    |
| 31  | CA    | 828 | U    |
| 31  | CA    | 845 | A    |
| 31  | CA    | 846 | U    |
| 31  | CA    | 847 | U    |
| 31  | CA    | 858 | G    |
| 31  | CA    | 859 | G    |
| 31  | CA    | 878 | A    |
| 31  | CA    | 883 | G    |
| 31  | CA    | 896 | A    |
| 31  | CA    | 897 | C    |
| 31  | CA    | 910 | A    |
| 31  | CA    | 914 | G    |
| 31  | CA    | 915 | C    |
| 31  | CA    | 931 | U    |
| 31  | CA    | 932 | U    |
| 31  | CA    | 941 | A    |
| 31  | CA    | 946 | C    |
| 31  | CA    | 953 | G    |
| 31  | CA    | 961 | C    |
| 31  | CA    | 974 | G    |
| 31  | CA    | 983 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 984  | A    |
| 31  | CA    | 985  | C    |
| 31  | CA    | 995  | C    |
| 31  | CA    | 996  | A    |
| 31  | CA    | 1012 | U    |
| 31  | CA    | 1013 | C    |
| 31  | CA    | 1022 | G    |
| 31  | CA    | 1026 | G    |
| 31  | CA    | 1033 | U    |
| 31  | CA    | 1040 | A    |
| 31  | CA    | 1045 | C    |
| 31  | CA    | 1046 | A    |
| 31  | CA    | 1047 | G    |
| 31  | CA    | 1057 | A    |
| 31  | CA    | 1061 | U    |
| 31  | CA    | 1070 | A    |
| 31  | CA    | 1083 | U    |
| 31  | CA    | 1088 | A    |
| 31  | CA    | 1089 | A    |
| 31  | CA    | 1090 | A    |
| 31  | CA    | 1091 | G    |
| 31  | CA    | 1096 | A    |
| 31  | CA    | 1097 | U    |
| 31  | CA    | 1111 | A    |
| 31  | CA    | 1112 | G    |
| 31  | CA    | 1122 | G    |
| 31  | CA    | 1128 | G    |
| 31  | CA    | 1129 | A    |
| 31  | CA    | 1132 | U    |
| 31  | CA    | 1133 | A    |
| 31  | CA    | 1135 | C    |
| 31  | CA    | 1136 | G    |
| 31  | CA    | 1142 | A    |
| 31  | CA    | 1168 | G    |
| 31  | CA    | 1169 | A    |
| 31  | CA    | 1170 | C    |
| 31  | CA    | 1171 | G    |
| 31  | CA    | 1172 | C    |
| 31  | CA    | 1175 | A    |
| 31  | CA    | 1176 | U    |
| 31  | CA    | 1177 | G    |
| 31  | CA    | 1179 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 1180 | U    |
| 31  | CA    | 1186 | G    |
| 31  | CA    | 1210 | G    |
| 31  | CA    | 1212 | G    |
| 31  | CA    | 1236 | G    |
| 31  | CA    | 1238 | G    |
| 31  | CA    | 1253 | A    |
| 31  | CA    | 1256 | G    |
| 31  | CA    | 1266 | G    |
| 31  | CA    | 1271 | G    |
| 31  | CA    | 1272 | A    |
| 31  | CA    | 1273 | U    |
| 31  | CA    | 1300 | G    |
| 31  | CA    | 1301 | A    |
| 31  | CA    | 1313 | U    |
| 31  | CA    | 1320 | C    |
| 31  | CA    | 1321 | A    |
| 31  | CA    | 1328 | A    |
| 31  | CA    | 1352 | U    |
| 31  | CA    | 1365 | A    |
| 31  | CA    | 1376 | C    |
| 31  | CA    | 1379 | U    |
| 31  | CA    | 1380 | G    |
| 31  | CA    | 1383 | A    |
| 31  | CA    | 1391 | U    |
| 31  | CA    | 1395 | A    |
| 31  | CA    | 1416 | G    |
| 31  | CA    | 1417 | C    |
| 31  | CA    | 1419 | A    |
| 31  | CA    | 1420 | A    |
| 31  | CA    | 1428 | C    |
| 31  | CA    | 1437 | C    |
| 31  | CA    | 1452 | G    |
| 31  | CA    | 1453 | A    |
| 31  | CA    | 1460 | U    |
| 31  | CA    | 1482 | G    |
| 31  | CA    | 1490 | A    |
| 31  | CA    | 1491 | G    |
| 31  | CA    | 1493 | C    |
| 31  | CA    | 1494 | A    |
| 31  | CA    | 1497 | U    |
| 31  | CA    | 1509 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 1510 | G    |
| 31  | CA    | 1515 | A    |
| 31  | CA    | 1523 | U    |
| 31  | CA    | 1532 | A    |
| 31  | CA    | 1534 | U    |
| 31  | CA    | 1535 | A    |
| 31  | CA    | 1536 | C    |
| 31  | CA    | 1537 | G    |
| 31  | CA    | 1565 | C    |
| 31  | CA    | 1566 | A    |
| 31  | CA    | 1569 | A    |
| 31  | CA    | 1578 | U    |
| 31  | CA    | 1583 | A    |
| 31  | CA    | 1585 | C    |
| 31  | CA    | 1607 | C    |
| 31  | CA    | 1608 | A    |
| 31  | CA    | 1647 | U    |
| 31  | CA    | 1648 | U    |
| 31  | CA    | 1649 | G    |
| 31  | CA    | 1674 | G    |
| 31  | CA    | 1695 | G    |
| 31  | CA    | 1715 | G    |
| 31  | CA    | 1729 | U    |
| 31  | CA    | 1730 | C    |
| 31  | CA    | 1731 | G    |
| 31  | CA    | 1732 | C    |
| 31  | CA    | 1738 | G    |
| 31  | CA    | 1744 | A    |
| 31  | CA    | 1750 | G    |
| 31  | CA    | 1764 | C    |
| 31  | CA    | 1773 | A    |
| 31  | CA    | 1782 | U    |
| 31  | CA    | 1800 | C    |
| 31  | CA    | 1801 | A    |
| 31  | CA    | 1808 | A    |
| 31  | CA    | 1816 | C    |
| 31  | CA    | 1822 | C    |
| 31  | CA    | 1829 | A    |
| 31  | CA    | 1869 | G    |
| 31  | CA    | 1870 | C    |
| 31  | CA    | 1871 | A    |
| 31  | CA    | 1872 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 1873 | G    |
| 31  | CA    | 1900 | A    |
| 31  | CA    | 1906 | G    |
| 31  | CA    | 1907 | G    |
| 31  | CA    | 1914 | C    |
| 31  | CA    | 1929 | G    |
| 31  | CA    | 1930 | G    |
| 31  | CA    | 1931 | U    |
| 31  | CA    | 1937 | A    |
| 31  | CA    | 1938 | A    |
| 31  | CA    | 1955 | U    |
| 31  | CA    | 1967 | C    |
| 31  | CA    | 1970 | A    |
| 31  | CA    | 1972 | G    |
| 31  | CA    | 1991 | U    |
| 31  | CA    | 1993 | U    |
| 31  | CA    | 1997 | C    |
| 31  | CA    | 2022 | U    |
| 31  | CA    | 2023 | C    |
| 31  | CA    | 2031 | A    |
| 31  | CA    | 2033 | A    |
| 31  | CA    | 2036 | C    |
| 31  | CA    | 2043 | C    |
| 31  | CA    | 2055 | C    |
| 31  | CA    | 2056 | G    |
| 31  | CA    | 2060 | A    |
| 31  | CA    | 2061 | G    |
| 31  | CA    | 2062 | A    |
| 31  | CA    | 2069 | G7M  |
| 31  | CA    | 2072 | C    |
| 31  | CA    | 2080 | A    |
| 31  | CA    | 2093 | G    |
| 31  | CA    | 2095 | A    |
| 31  | CA    | 2100 | G    |
| 31  | CA    | 2102 | G    |
| 31  | CA    | 2108 | A    |
| 31  | CA    | 2110 | G    |
| 31  | CA    | 2111 | U    |
| 31  | CA    | 2112 | G    |
| 31  | CA    | 2113 | U    |
| 31  | CA    | 2115 | G    |
| 31  | CA    | 2117 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 2118 | U    |
| 31  | CA    | 2119 | A    |
| 31  | CA    | 2123 | G    |
| 31  | CA    | 2124 | G    |
| 31  | CA    | 2125 | G    |
| 31  | CA    | 2126 | A    |
| 31  | CA    | 2127 | G    |
| 31  | CA    | 2128 | G    |
| 31  | CA    | 2131 | U    |
| 31  | CA    | 2132 | U    |
| 31  | CA    | 2133 | G    |
| 31  | CA    | 2146 | C    |
| 31  | CA    | 2147 | A    |
| 31  | CA    | 2157 | G    |
| 31  | CA    | 2158 | A    |
| 31  | CA    | 2159 | G    |
| 31  | CA    | 2160 | C    |
| 31  | CA    | 2162 | G    |
| 31  | CA    | 2164 | C    |
| 31  | CA    | 2165 | C    |
| 31  | CA    | 2171 | A    |
| 31  | CA    | 2172 | U    |
| 31  | CA    | 2173 | A    |
| 31  | CA    | 2174 | C    |
| 31  | CA    | 2178 | C    |
| 31  | CA    | 2183 | A    |
| 31  | CA    | 2190 | G    |
| 31  | CA    | 2198 | A    |
| 31  | CA    | 2203 | U    |
| 31  | CA    | 2204 | G    |
| 31  | CA    | 2211 | A    |
| 31  | CA    | 2225 | A    |
| 31  | CA    | 2226 | C    |
| 31  | CA    | 2238 | G    |
| 31  | CA    | 2239 | G    |
| 31  | CA    | 2259 | U    |
| 31  | CA    | 2268 | A    |
| 31  | CA    | 2280 | G    |
| 31  | CA    | 2283 | C    |
| 31  | CA    | 2287 | A    |
| 31  | CA    | 2305 | U    |
| 31  | CA    | 2311 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 2322 | A    |
| 31  | CA    | 2326 | C    |
| 31  | CA    | 2327 | A    |
| 31  | CA    | 2333 | A    |
| 31  | CA    | 2335 | A    |
| 31  | CA    | 2345 | G    |
| 31  | CA    | 2347 | C    |
| 31  | CA    | 2350 | C    |
| 31  | CA    | 2354 | C    |
| 31  | CA    | 2361 | G    |
| 31  | CA    | 2383 | G    |
| 31  | CA    | 2385 | C    |
| 31  | CA    | 2388 | A    |
| 31  | CA    | 2402 | U    |
| 31  | CA    | 2403 | C    |
| 31  | CA    | 2406 | A    |
| 31  | CA    | 2423 | U    |
| 31  | CA    | 2424 | C    |
| 31  | CA    | 2425 | A    |
| 31  | CA    | 2426 | A    |
| 31  | CA    | 2429 | G    |
| 31  | CA    | 2430 | A    |
| 31  | CA    | 2435 | A    |
| 31  | CA    | 2441 | U    |
| 31  | CA    | 2448 | A    |
| 31  | CA    | 2465 | C    |
| 31  | CA    | 2476 | A    |
| 31  | CA    | 2491 | U    |
| 31  | CA    | 2502 | G    |
| 31  | CA    | 2505 | G    |
| 31  | CA    | 2518 | A    |
| 31  | CA    | 2529 | G    |
| 31  | CA    | 2535 | G    |
| 31  | CA    | 2547 | A    |
| 31  | CA    | 2554 | U    |
| 31  | CA    | 2556 | C    |
| 31  | CA    | 2566 | A    |
| 31  | CA    | 2567 | G    |
| 31  | CA    | 2573 | C    |
| 31  | CA    | 2578 | G    |
| 31  | CA    | 2582 | G    |
| 31  | CA    | 2585 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | CA    | 2603 | G    |
| 31  | CA    | 2609 | U    |
| 31  | CA    | 2613 | U    |
| 31  | CA    | 2629 | U    |
| 31  | CA    | 2630 | G    |
| 31  | CA    | 2646 | C    |
| 31  | CA    | 2661 | G    |
| 31  | CA    | 2663 | G    |
| 31  | CA    | 2681 | C    |
| 31  | CA    | 2682 | A    |
| 31  | CA    | 2689 | U    |
| 31  | CA    | 2690 | U    |
| 31  | CA    | 2714 | G    |
| 31  | CA    | 2718 | G    |
| 31  | CA    | 2726 | A    |
| 31  | CA    | 2744 | G    |
| 31  | CA    | 2748 | A    |
| 31  | CA    | 2769 | U    |
| 31  | CA    | 2778 | A    |
| 31  | CA    | 2791 | G    |
| 31  | CA    | 2794 | C    |
| 31  | CA    | 2799 | A    |
| 31  | CA    | 2820 | A    |
| 31  | CA    | 2835 | A    |
| 31  | CA    | 2836 | U    |
| 31  | CA    | 2850 | A    |
| 31  | CA    | 2861 | U    |
| 31  | CA    | 2865 | U    |
| 31  | CA    | 2867 | G    |
| 31  | CA    | 2883 | A    |
| 31  | CA    | 2884 | U    |
| 31  | CA    | 2886 | A    |
| 31  | CA    | 2887 | A    |
| 31  | CA    | 2891 | U    |
| 31  | CA    | 2903 | U    |
| 31  | CA    | 2904 | U    |
| 28  | DB    | 25   | U    |
| 28  | DB    | 35   | C    |
| 28  | DB    | 45   | A    |
| 28  | DB    | 56   | G    |
| 28  | DB    | 57   | A    |
| 28  | DB    | 88   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DB    | 89  | U    |
| 28  | DB    | 90  | C    |
| 28  | DB    | 109 | A    |
| 55  | DA    | 10  | A    |
| 55  | DA    | 12  | U    |
| 55  | DA    | 34  | U    |
| 55  | DA    | 46  | G    |
| 55  | DA    | 63  | A    |
| 55  | DA    | 71  | A    |
| 55  | DA    | 74  | A    |
| 55  | DA    | 75  | G    |
| 55  | DA    | 80  | G    |
| 55  | DA    | 84  | A    |
| 55  | DA    | 101 | A    |
| 55  | DA    | 102 | U    |
| 55  | DA    | 118 | A    |
| 55  | DA    | 119 | A    |
| 55  | DA    | 120 | U    |
| 55  | DA    | 138 | U    |
| 55  | DA    | 139 | U    |
| 55  | DA    | 140 | C    |
| 55  | DA    | 141 | G    |
| 55  | DA    | 142 | A    |
| 55  | DA    | 143 | C    |
| 55  | DA    | 196 | A    |
| 55  | DA    | 199 | A    |
| 55  | DA    | 200 | U    |
| 55  | DA    | 215 | G    |
| 55  | DA    | 216 | A    |
| 55  | DA    | 221 | A    |
| 55  | DA    | 222 | A    |
| 55  | DA    | 248 | G    |
| 55  | DA    | 265 | A    |
| 55  | DA    | 266 | G    |
| 55  | DA    | 272 | A    |
| 55  | DA    | 276 | U    |
| 55  | DA    | 277 | G    |
| 55  | DA    | 278 | A    |
| 55  | DA    | 279 | A    |
| 55  | DA    | 285 | G    |
| 55  | DA    | 302 | C    |
| 55  | DA    | 311 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | DA    | 329 | G    |
| 55  | DA    | 330 | A    |
| 55  | DA    | 343 | C    |
| 55  | DA    | 346 | A    |
| 55  | DA    | 352 | A    |
| 55  | DA    | 353 | C    |
| 55  | DA    | 362 | A    |
| 55  | DA    | 370 | G    |
| 55  | DA    | 372 | G    |
| 55  | DA    | 386 | G    |
| 55  | DA    | 399 | U    |
| 55  | DA    | 411 | G    |
| 55  | DA    | 412 | A    |
| 55  | DA    | 420 | C    |
| 55  | DA    | 424 | G    |
| 55  | DA    | 425 | G    |
| 55  | DA    | 451 | U    |
| 55  | DA    | 480 | A    |
| 55  | DA    | 481 | G    |
| 55  | DA    | 491 | G    |
| 55  | DA    | 504 | A    |
| 55  | DA    | 505 | A    |
| 55  | DA    | 508 | A    |
| 55  | DA    | 531 | C    |
| 55  | DA    | 532 | A    |
| 55  | DA    | 543 | G    |
| 55  | DA    | 544 | C    |
| 55  | DA    | 546 | U    |
| 55  | DA    | 547 | A    |
| 55  | DA    | 548 | G    |
| 55  | DA    | 549 | G    |
| 55  | DA    | 550 | C    |
| 55  | DA    | 551 | G    |
| 55  | DA    | 563 | A    |
| 55  | DA    | 573 | U    |
| 55  | DA    | 575 | A    |
| 55  | DA    | 586 | A    |
| 55  | DA    | 603 | A    |
| 55  | DA    | 613 | A    |
| 55  | DA    | 614 | A    |
| 55  | DA    | 615 | U    |
| 55  | DA    | 627 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 637  | A    |
| 55  | DA    | 645  | C    |
| 55  | DA    | 647  | G    |
| 55  | DA    | 654  | A    |
| 55  | DA    | 655  | A    |
| 55  | DA    | 686  | U    |
| 55  | DA    | 717  | C    |
| 55  | DA    | 730  | A    |
| 55  | DA    | 747  | 5MU  |
| 55  | DA    | 764  | A    |
| 55  | DA    | 765  | C    |
| 55  | DA    | 775  | G    |
| 55  | DA    | 776  | G    |
| 55  | DA    | 782  | A    |
| 55  | DA    | 784  | G    |
| 55  | DA    | 785  | G    |
| 55  | DA    | 790  | U    |
| 55  | DA    | 792  | A    |
| 55  | DA    | 805  | G    |
| 55  | DA    | 812  | C    |
| 55  | DA    | 827  | U    |
| 55  | DA    | 828  | U    |
| 55  | DA    | 858  | G    |
| 55  | DA    | 859  | G    |
| 55  | DA    | 860  | U    |
| 55  | DA    | 878  | A    |
| 55  | DA    | 883  | G    |
| 55  | DA    | 885  | C    |
| 55  | DA    | 896  | A    |
| 55  | DA    | 897  | C    |
| 55  | DA    | 910  | A    |
| 55  | DA    | 914  | G    |
| 55  | DA    | 915  | C    |
| 55  | DA    | 927  | A    |
| 55  | DA    | 931  | U    |
| 55  | DA    | 932  | U    |
| 55  | DA    | 946  | C    |
| 55  | DA    | 961  | C    |
| 55  | DA    | 974  | G    |
| 55  | DA    | 983  | A    |
| 55  | DA    | 996  | A    |
| 55  | DA    | 1012 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 1013 | C    |
| 55  | DA    | 1022 | G    |
| 55  | DA    | 1026 | G    |
| 55  | DA    | 1033 | U    |
| 55  | DA    | 1040 | A    |
| 55  | DA    | 1047 | G    |
| 55  | DA    | 1057 | A    |
| 55  | DA    | 1061 | U    |
| 55  | DA    | 1070 | A    |
| 55  | DA    | 1083 | U    |
| 55  | DA    | 1088 | A    |
| 55  | DA    | 1089 | A    |
| 55  | DA    | 1090 | A    |
| 55  | DA    | 1091 | G    |
| 55  | DA    | 1096 | A    |
| 55  | DA    | 1097 | U    |
| 55  | DA    | 1112 | G    |
| 55  | DA    | 1132 | U    |
| 55  | DA    | 1133 | A    |
| 55  | DA    | 1135 | C    |
| 55  | DA    | 1136 | G    |
| 55  | DA    | 1142 | A    |
| 55  | DA    | 1168 | G    |
| 55  | DA    | 1172 | C    |
| 55  | DA    | 1174 | U    |
| 55  | DA    | 1175 | A    |
| 55  | DA    | 1176 | U    |
| 55  | DA    | 1177 | G    |
| 55  | DA    | 1180 | U    |
| 55  | DA    | 1187 | G    |
| 55  | DA    | 1237 | A    |
| 55  | DA    | 1238 | G    |
| 55  | DA    | 1253 | A    |
| 55  | DA    | 1256 | G    |
| 55  | DA    | 1271 | G    |
| 55  | DA    | 1272 | A    |
| 55  | DA    | 1273 | U    |
| 55  | DA    | 1300 | G    |
| 55  | DA    | 1301 | A    |
| 55  | DA    | 1329 | U    |
| 55  | DA    | 1352 | U    |
| 55  | DA    | 1365 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 1379 | U    |
| 55  | DA    | 1383 | A    |
| 55  | DA    | 1391 | U    |
| 55  | DA    | 1416 | G    |
| 55  | DA    | 1417 | C    |
| 55  | DA    | 1427 | A    |
| 55  | DA    | 1428 | C    |
| 55  | DA    | 1434 | A    |
| 55  | DA    | 1435 | G    |
| 55  | DA    | 1452 | G    |
| 55  | DA    | 1453 | A    |
| 55  | DA    | 1460 | U    |
| 55  | DA    | 1482 | G    |
| 55  | DA    | 1490 | A    |
| 55  | DA    | 1491 | G    |
| 55  | DA    | 1493 | C    |
| 55  | DA    | 1494 | A    |
| 55  | DA    | 1497 | U    |
| 55  | DA    | 1508 | A    |
| 55  | DA    | 1509 | A    |
| 55  | DA    | 1510 | G    |
| 55  | DA    | 1515 | A    |
| 55  | DA    | 1523 | U    |
| 55  | DA    | 1532 | A    |
| 55  | DA    | 1534 | U    |
| 55  | DA    | 1535 | A    |
| 55  | DA    | 1536 | C    |
| 55  | DA    | 1537 | G    |
| 55  | DA    | 1566 | A    |
| 55  | DA    | 1569 | A    |
| 55  | DA    | 1578 | U    |
| 55  | DA    | 1583 | A    |
| 55  | DA    | 1585 | C    |
| 55  | DA    | 1607 | C    |
| 55  | DA    | 1608 | A    |
| 55  | DA    | 1616 | A    |
| 55  | DA    | 1647 | U    |
| 55  | DA    | 1648 | U    |
| 55  | DA    | 1649 | G    |
| 55  | DA    | 1674 | G    |
| 55  | DA    | 1715 | G    |
| 55  | DA    | 1729 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 1730 | C    |
| 55  | DA    | 1731 | G    |
| 55  | DA    | 1732 | C    |
| 55  | DA    | 1738 | G    |
| 55  | DA    | 1744 | A    |
| 55  | DA    | 1764 | C    |
| 55  | DA    | 1773 | A    |
| 55  | DA    | 1782 | U    |
| 55  | DA    | 1800 | C    |
| 55  | DA    | 1801 | A    |
| 55  | DA    | 1808 | A    |
| 55  | DA    | 1816 | C    |
| 55  | DA    | 1829 | A    |
| 55  | DA    | 1869 | G    |
| 55  | DA    | 1870 | C    |
| 55  | DA    | 1871 | A    |
| 55  | DA    | 1872 | A    |
| 55  | DA    | 1873 | G    |
| 55  | DA    | 1906 | G    |
| 55  | DA    | 1907 | G    |
| 55  | DA    | 1913 | A    |
| 55  | DA    | 1914 | C    |
| 55  | DA    | 1929 | G    |
| 55  | DA    | 1930 | G    |
| 55  | DA    | 1931 | U    |
| 55  | DA    | 1937 | A    |
| 55  | DA    | 1938 | A    |
| 55  | DA    | 1955 | U    |
| 55  | DA    | 1965 | C    |
| 55  | DA    | 1967 | C    |
| 55  | DA    | 1970 | A    |
| 55  | DA    | 1972 | G    |
| 55  | DA    | 1991 | U    |
| 55  | DA    | 1993 | U    |
| 55  | DA    | 1997 | C    |
| 55  | DA    | 2023 | C    |
| 55  | DA    | 2031 | A    |
| 55  | DA    | 2033 | A    |
| 55  | DA    | 2043 | C    |
| 55  | DA    | 2055 | C    |
| 55  | DA    | 2056 | G    |
| 55  | DA    | 2060 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 2061 | G    |
| 55  | DA    | 2062 | A    |
| 55  | DA    | 2069 | G7M  |
| 55  | DA    | 2097 | A    |
| 55  | DA    | 2100 | G    |
| 55  | DA    | 2102 | G    |
| 55  | DA    | 2105 | U    |
| 55  | DA    | 2111 | U    |
| 55  | DA    | 2112 | G    |
| 55  | DA    | 2113 | U    |
| 55  | DA    | 2116 | G    |
| 55  | DA    | 2117 | A    |
| 55  | DA    | 2118 | U    |
| 55  | DA    | 2119 | A    |
| 55  | DA    | 2120 | G    |
| 55  | DA    | 2123 | G    |
| 55  | DA    | 2125 | G    |
| 55  | DA    | 2126 | A    |
| 55  | DA    | 2128 | G    |
| 55  | DA    | 2131 | U    |
| 55  | DA    | 2132 | U    |
| 55  | DA    | 2133 | G    |
| 55  | DA    | 2134 | A    |
| 55  | DA    | 2135 | A    |
| 55  | DA    | 2145 | C    |
| 55  | DA    | 2146 | C    |
| 55  | DA    | 2148 | G    |
| 55  | DA    | 2158 | A    |
| 55  | DA    | 2159 | G    |
| 55  | DA    | 2160 | C    |
| 55  | DA    | 2161 | C    |
| 55  | DA    | 2162 | G    |
| 55  | DA    | 2163 | A    |
| 55  | DA    | 2164 | C    |
| 55  | DA    | 2165 | C    |
| 55  | DA    | 2167 | U    |
| 55  | DA    | 2168 | G    |
| 55  | DA    | 2169 | A    |
| 55  | DA    | 2170 | A    |
| 55  | DA    | 2171 | A    |
| 55  | DA    | 2172 | U    |
| 55  | DA    | 2173 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 2177 | C    |
| 55  | DA    | 2178 | C    |
| 55  | DA    | 2179 | C    |
| 55  | DA    | 2181 | U    |
| 55  | DA    | 2183 | A    |
| 55  | DA    | 2185 | U    |
| 55  | DA    | 2190 | G    |
| 55  | DA    | 2198 | A    |
| 55  | DA    | 2204 | G    |
| 55  | DA    | 2211 | A    |
| 55  | DA    | 2225 | A    |
| 55  | DA    | 2238 | G    |
| 55  | DA    | 2239 | G    |
| 55  | DA    | 2268 | A    |
| 55  | DA    | 2283 | C    |
| 55  | DA    | 2286 | G    |
| 55  | DA    | 2287 | A    |
| 55  | DA    | 2305 | U    |
| 55  | DA    | 2308 | G    |
| 55  | DA    | 2312 | U    |
| 55  | DA    | 2324 | U    |
| 55  | DA    | 2325 | G    |
| 55  | DA    | 2333 | A    |
| 55  | DA    | 2335 | A    |
| 55  | DA    | 2347 | C    |
| 55  | DA    | 2383 | G    |
| 55  | DA    | 2385 | C    |
| 55  | DA    | 2402 | U    |
| 55  | DA    | 2403 | C    |
| 55  | DA    | 2406 | A    |
| 55  | DA    | 2407 | A    |
| 55  | DA    | 2423 | U    |
| 55  | DA    | 2424 | C    |
| 55  | DA    | 2425 | A    |
| 55  | DA    | 2431 | U    |
| 55  | DA    | 2435 | A    |
| 55  | DA    | 2441 | U    |
| 55  | DA    | 2448 | A    |
| 55  | DA    | 2476 | A    |
| 55  | DA    | 2491 | U    |
| 55  | DA    | 2502 | G    |
| 55  | DA    | 2505 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | DA    | 2518 | A    |
| 55  | DA    | 2529 | G    |
| 55  | DA    | 2535 | G    |
| 55  | DA    | 2547 | A    |
| 55  | DA    | 2556 | C    |
| 55  | DA    | 2566 | A    |
| 55  | DA    | 2567 | G    |
| 55  | DA    | 2573 | C    |
| 55  | DA    | 2574 | G    |
| 55  | DA    | 2585 | U    |
| 55  | DA    | 2603 | G    |
| 55  | DA    | 2609 | U    |
| 55  | DA    | 2613 | U    |
| 55  | DA    | 2629 | U    |
| 55  | DA    | 2630 | G    |
| 55  | DA    | 2661 | G    |
| 55  | DA    | 2663 | G    |
| 55  | DA    | 2689 | U    |
| 55  | DA    | 2690 | U    |
| 55  | DA    | 2714 | G    |
| 55  | DA    | 2726 | A    |
| 55  | DA    | 2744 | G    |
| 55  | DA    | 2748 | A    |
| 55  | DA    | 2765 | A    |
| 55  | DA    | 2778 | A    |
| 55  | DA    | 2791 | G    |
| 55  | DA    | 2798 | U    |
| 55  | DA    | 2799 | A    |
| 55  | DA    | 2811 | G    |
| 55  | DA    | 2820 | A    |
| 55  | DA    | 2821 | A    |
| 55  | DA    | 2836 | U    |
| 55  | DA    | 2867 | G    |
| 55  | DA    | 2891 | U    |

There are no RNA pucker outliers to report.

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

75 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 |
| 1   | 2MG  | AA    | 1207 | 1    | 19,26,27     | 1.11 | 2 (10%)  | 20,38,41    | 2.41 | 4 (20%)  |
| 1   | 4OC  | AA    | 1402 | 1    | 16,23,24     | 0.83 | 0        | 19,32,35    | 0.92 | 1 (5%)   |
| 1   | 5MC  | AA    | 1407 | 1    | 15,22,23     | 0.91 | 1 (6%)   | 17,32,35    | 0.76 | 1 (5%)   |
| 1   | UR3  | AA    | 1498 | 1    | 14,22,23     | 0.86 | 0        | 16,32,35    | 0.51 | 0        |
| 1   | 2MG  | AA    | 1516 | 1    | 19,26,27     | 1.32 | 2 (10%)  | 20,38,41    | 2.36 | 4 (20%)  |
| 1   | MA6  | AA    | 1518 | 1    | 16,26,27     | 0.72 | 0        | 18,38,41    | 0.92 | 1 (5%)   |
| 1   | MA6  | AA    | 1519 | 1    | 16,26,27     | 0.68 | 0        | 18,38,41    | 1.26 | 1 (5%)   |
| 1   | PSU  | AA    | 516  | 1,56 | 16,21,22     | 1.13 | 2 (12%)  | 20,30,33    | 5.94 | 4 (20%)  |
| 1   | G7M  | AA    | 527  | 1    | 19,26,27     | 1.25 | 2 (10%)  | 19,39,42    | 3.06 | 4 (21%)  |
| 1   | 2MG  | AA    | 966  | 1    | 19,26,27     | 1.20 | 2 (10%)  | 20,38,41    | 2.33 | 3 (15%)  |
| 1   | 5MC  | AA    | 967  | 1    | 15,22,23     | 0.86 | 1 (6%)   | 17,32,35    | 0.70 | 1 (5%)   |
| 12  | D2T  | AL    | 89   | 12   | 5,9,10       | 1.06 | 1 (20%)  | 3,11,13     | 1.76 | 1 (33%)  |
| 1   | 2MG  | BA    | 1207 | 1    | 19,26,27     | 1.18 | 2 (10%)  | 20,38,41    | 2.40 | 4 (20%)  |
| 1   | 4OC  | BA    | 1402 | 1    | 16,23,24     | 0.88 | 0        | 19,32,35    | 0.89 | 1 (5%)   |
| 1   | 5MC  | BA    | 1407 | 1    | 15,22,23     | 0.92 | 1 (6%)   | 17,32,35    | 0.75 | 1 (5%)   |
| 1   | UR3  | BA    | 1498 | 1    | 14,22,23     | 1.13 | 2 (14%)  | 16,32,35    | 0.42 | 0        |
| 1   | 2MG  | BA    | 1516 | 1    | 19,26,27     | 1.21 | 2 (10%)  | 20,38,41    | 2.38 | 4 (20%)  |
| 1   | MA6  | BA    | 1518 | 1    | 16,26,27     | 0.71 | 0        | 18,38,41    | 0.94 | 1 (5%)   |
| 1   | MA6  | BA    | 1519 | 1    | 16,26,27     | 0.62 | 0        | 18,38,41    | 1.25 | 1 (5%)   |
| 1   | PSU  | BA    | 516  | 1    | 16,21,22     | 1.20 | 2 (12%)  | 20,30,33    | 5.97 | 4 (20%)  |
| 1   | G7M  | BA    | 527  | 1    | 19,26,27     | 1.29 | 3 (15%)  | 19,39,42    | 3.17 | 4 (21%)  |
| 1   | 2MG  | BA    | 966  | 1    | 19,26,27     | 1.09 | 2 (10%)  | 20,38,41    | 2.37 | 4 (20%)  |
| 1   | 5MC  | BA    | 967  | 1    | 15,22,23     | 0.87 | 1 (6%)   | 17,32,35    | 0.68 | 1 (5%)   |
| 12  | D2T  | BL    | 89   | 12   | 5,9,10       | 1.42 | 1 (20%)  | 3,11,13     | 1.92 | 1 (33%)  |
| 31  | 6MZ  | CA    | 1618 | 31   | 18,25,26     | 0.92 | 1 (5%)   | 16,36,39    | 1.28 | 2 (12%)  |
| 31  | 2MG  | CA    | 1835 | 31   | 19,26,27     | 1.13 | 1 (5%)   | 20,38,41    | 2.32 | 4 (20%)  |
| 31  | PSU  | CA    | 1911 | 31   | 16,21,22     | 1.15 | 2 (12%)  | 20,30,33    | 5.93 | 4 (20%)  |
| 31  | 3TD  | CA    | 1915 | 31   | 16,22,23     | 0.99 | 2 (12%)  | 19,32,35    | 1.51 | 2 (10%)  |
| 31  | PSU  | CA    | 1917 | 31   | 16,21,22     | 1.14 | 2 (12%)  | 20,30,33    | 5.99 | 4 (20%)  |
| 31  | 5MU  | CA    | 1939 | 31   | 14,22,23     | 1.26 | 2 (14%)  | 16,32,35    | 4.22 | 3 (18%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | 5MC  | CA    | 1962 | 31    | 15,22,23     | 0.89 | 2 (13%)  | 17,32,35    | 0.63 | 1 (5%)   |
| 31  | 6MZ  | CA    | 2030 | 31    | 18,25,26     | 0.82 | 0        | 16,36,39    | 1.23 | 2 (12%)  |
| 31  | G7M  | CA    | 2069 | 31    | 19,26,27     | 1.01 | 2 (10%)  | 19,39,42    | 2.91 | 4 (21%)  |
| 31  | OMG  | CA    | 2251 | 31    | 18,26,27     | 1.18 | 2 (11%)  | 22,38,41    | 2.41 | 4 (18%)  |
| 31  | 2MG  | CA    | 2445 | 31    | 19,26,27     | 1.48 | 3 (15%)  | 20,38,41    | 2.39 | 4 (20%)  |
| 31  | PSU  | CA    | 2457 | 31    | 16,21,22     | 1.30 | 3 (18%)  | 20,30,33    | 5.94 | 4 (20%)  |
| 31  | OMC  | CA    | 2498 | 31,56 | 15,22,23     | 1.08 | 2 (13%)  | 19,31,34    | 0.56 | 0        |
| 31  | 2MA  | CA    | 2503 | 31    | 18,25,26     | 0.93 | 0        | 17,37,40    | 0.87 | 0        |
| 31  | PSU  | CA    | 2504 | 31    | 16,21,22     | 1.25 | 3 (18%)  | 20,30,33    | 5.93 | 4 (20%)  |
| 31  | OMU  | CA    | 2552 | 31    | 14,22,23     | 1.17 | 2 (14%)  | 18,31,34    | 3.64 | 2 (11%)  |
| 31  | PSU  | CA    | 2580 | 31    | 16,21,22     | 1.31 | 3 (18%)  | 20,30,33    | 5.97 | 5 (25%)  |
| 31  | PSU  | CA    | 2605 | 31    | 16,21,22     | 1.11 | 2 (12%)  | 20,30,33    | 5.96 | 5 (25%)  |
| 31  | 1MG  | CA    | 745  | 31    | 18,26,27     | 1.23 | 1 (5%)   | 18,39,42    | 1.17 | 2 (11%)  |
| 31  | PSU  | CA    | 746  | 31,56 | 16,21,22     | 1.32 | 3 (18%)  | 20,30,33    | 5.97 | 4 (20%)  |
| 31  | 5MU  | CA    | 747  | 31    | 14,22,23     | 1.17 | 1 (7%)   | 16,32,35    | 4.23 | 3 (18%)  |
| 31  | PSU  | CA    | 955  | 31    | 16,21,22     | 1.13 | 2 (12%)  | 20,30,33    | 5.95 | 4 (20%)  |
| 41  | 4D4  | CN    | 81   | 41    | 10,11,12     | 2.06 | 3 (30%)  | 7,13,15     | 2.56 | 2 (28%)  |
| 55  | 6MZ  | DA    | 1618 | 55    | 18,25,26     | 1.11 | 1 (5%)   | 16,36,39    | 1.92 | 2 (12%)  |
| 55  | 2MG  | DA    | 1835 | 55    | 19,26,27     | 1.06 | 1 (5%)   | 20,38,41    | 2.37 | 4 (20%)  |
| 55  | PSU  | DA    | 1911 | 55    | 16,21,22     | 1.11 | 2 (12%)  | 20,30,33    | 5.91 | 4 (20%)  |
| 55  | 3TD  | DA    | 1915 | 55    | 16,22,23     | 0.95 | 2 (12%)  | 19,32,35    | 1.55 | 2 (10%)  |
| 55  | PSU  | DA    | 1917 | 55    | 16,21,22     | 1.25 | 2 (12%)  | 20,30,33    | 5.97 | 4 (20%)  |
| 55  | 5MU  | DA    | 1939 | 55    | 14,22,23     | 1.17 | 1 (7%)   | 16,32,35    | 4.24 | 3 (18%)  |
| 55  | 5MC  | DA    | 1962 | 55    | 15,22,23     | 1.04 | 3 (20%)  | 17,32,35    | 0.69 | 0        |
| 55  | 6MZ  | DA    | 2030 | 55    | 18,25,26     | 1.13 | 1 (5%)   | 16,36,39    | 1.10 | 1 (6%)   |
| 55  | G7M  | DA    | 2069 | 55    | 19,26,27     | 1.14 | 2 (10%)  | 19,39,42    | 2.87 | 4 (21%)  |
| 55  | OMG  | DA    | 2251 | 55    | 18,26,27     | 1.05 | 1 (5%)   | 22,38,41    | 2.36 | 4 (18%)  |
| 55  | 2MG  | DA    | 2445 | 55    | 19,26,27     | 1.24 | 3 (15%)  | 20,38,41    | 2.55 | 4 (20%)  |
| 55  | H2U  | DA    | 2449 | 55    | 17,21,22     | 0.51 | 0        | 21,30,33    | 0.62 | 0        |
| 55  | PSU  | DA    | 2457 | 55    | 16,21,22     | 1.08 | 2 (12%)  | 20,30,33    | 5.93 | 4 (20%)  |
| 55  | OMC  | DA    | 2498 | 55,56 | 15,22,23     | 0.85 | 1 (6%)   | 19,31,34    | 0.73 | 0        |
| 55  | 2MA  | DA    | 2503 | 55,56 | 18,25,26     | 0.87 | 0        | 17,37,40    | 0.96 | 1 (5%)   |
| 55  | PSU  | DA    | 2504 | 55    | 16,21,22     | 1.45 | 3 (18%)  | 20,30,33    | 5.99 | 4 (20%)  |
| 55  | OMU  | DA    | 2552 | 55    | 14,22,23     | 1.21 | 2 (14%)  | 18,31,34    | 3.64 | 2 (11%)  |
| 55  | PSU  | DA    | 2580 | 55    | 16,21,22     | 1.49 | 4 (25%)  | 20,30,33    | 5.97 | 5 (25%)  |

| Mol | Type | Chain | Res    | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | PSU  | DA    | 2604   | 55    | 16,21,22     | 1.35 | 3 (18%)  | 20,30,33    | 5.93 | 4 (20%)  |
| 55  | PSU  | DA    | 2605   | 55    | 16,21,22     | 1.16 | 2 (12%)  | 20,30,33    | 5.94 | 4 (20%)  |
| 55  | 1MG  | DA    | 745    | 55    | 18,26,27     | 1.38 | 3 (16%)  | 18,39,42    | 1.27 | 3 (16%)  |
| 55  | PSU  | DA    | 746    | 55,56 | 16,21,22     | 1.62 | 4 (25%)  | 20,30,33    | 5.94 | 4 (20%)  |
| 55  | 5MU  | DA    | 747    | 55    | 14,22,23     | 1.30 | 2 (14%)  | 16,32,35    | 4.17 | 3 (18%)  |
| 55  | PSU  | DA    | 955    | 55    | 16,21,22     | 1.43 | 3 (18%)  | 20,30,33    | 5.96 | 5 (25%)  |
| 32  | MEQ  | DD    | 150[A] | 32    | 9,9,10       | 0.89 | 1 (11%)  | 7,10,12     | 0.96 | 1 (14%)  |
| 32  | MEQ  | DD    | 150[B] | 32    | 9,9,10       | 2.40 | 2 (22%)  | 7,10,12     | 1.55 | 1 (14%)  |
| 41  | 4D4  | DN    | 81[A]  | -     | 10,11,12     | 2.20 | 3 (30%)  | 7,13,15     | 2.33 | 2 (28%)  |
| 41  | 4D4  | DN    | 81[B]  | -     | 10,11,12     | 1.54 | 2 (20%)  | 7,13,15     | 2.61 | 2 (28%)  |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 2MG  | AA    | 1207 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 4OC  | AA    | 1402 | 1    | -       | 0/7/29/30 | 0/2/2/2 |
| 1   | 5MC  | AA    | 1407 | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | UR3  | AA    | 1498 | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 2MG  | AA    | 1516 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | MA6  | AA    | 1518 | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | MA6  | AA    | 1519 | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | PSU  | AA    | 516  | 1,56 | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | G7M  | AA    | 527  | 1    | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | 2MG  | AA    | 966  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 5MC  | AA    | 967  | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 12  | D2T  | AL    | 89   | 12   | -       | 0/2/12/14 | 0/0/0/0 |
| 1   | 2MG  | BA    | 1207 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 4OC  | BA    | 1402 | 1    | -       | 0/7/29/30 | 0/2/2/2 |
| 1   | 5MC  | BA    | 1407 | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | UR3  | BA    | 1498 | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 2MG  | BA    | 1516 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | MA6  | BA    | 1518 | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | MA6  | BA    | 1519 | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | PSU  | BA    | 516  | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | G7M  | BA    | 527  | 1    | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | 2MG  | BA    | 966  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 5MC  | BA    | 967  | 1    | -       | 0/3/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 12  | D2T  | BL    | 89   | 12    | -       | 0/2/12/14  | 0/0/0/0 |
| 31  | 6MZ  | CA    | 1618 | 31    | -       | 0/5/27/28  | 0/3/3/3 |
| 31  | 2MG  | CA    | 1835 | 31    | -       | 0/5/27/28  | 0/3/3/3 |
| 31  | PSU  | CA    | 1911 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | 3TD  | CA    | 1915 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | PSU  | CA    | 1917 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | 5MU  | CA    | 1939 | 31    | -       | 0/3/25/26  | 0/2/2/2 |
| 31  | 5MC  | CA    | 1962 | 31    | -       | 0/3/25/26  | 0/2/2/2 |
| 31  | 6MZ  | CA    | 2030 | 31    | -       | 0/5/27/28  | 0/3/3/3 |
| 31  | G7M  | CA    | 2069 | 31    | -       | 0/3/25/26  | 0/3/3/3 |
| 31  | OMG  | CA    | 2251 | 31    | -       | 0/5/27/28  | 0/3/3/3 |
| 31  | 2MG  | CA    | 2445 | 31    | -       | 0/5/27/28  | 0/3/3/3 |
| 31  | PSU  | CA    | 2457 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | OMC  | CA    | 2498 | 31,56 | -       | 0/5/27/28  | 0/2/2/2 |
| 31  | 2MA  | CA    | 2503 | 31    | -       | 0/3/25/26  | 0/3/3/3 |
| 31  | PSU  | CA    | 2504 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | OMU  | CA    | 2552 | 31    | -       | 0/5/27/28  | 0/2/2/2 |
| 31  | PSU  | CA    | 2580 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | PSU  | CA    | 2605 | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | 1MG  | CA    | 745  | 31    | -       | 0/3/25/26  | 0/3/3/3 |
| 31  | PSU  | CA    | 746  | 31,56 | -       | 0/7/25/26  | 0/2/2/2 |
| 31  | 5MU  | CA    | 747  | 31    | -       | 0/3/25/26  | 0/2/2/2 |
| 31  | PSU  | CA    | 955  | 31    | -       | 0/7/25/26  | 0/2/2/2 |
| 41  | 4D4  | CN    | 81   | 41    | -       | 0/10/12/14 | 0/0/0/0 |
| 55  | 6MZ  | DA    | 1618 | 55    | -       | 0/5/27/28  | 0/3/3/3 |
| 55  | 2MG  | DA    | 1835 | 55    | -       | 0/5/27/28  | 0/3/3/3 |
| 55  | PSU  | DA    | 1911 | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 3TD  | DA    | 1915 | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | DA    | 1917 | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU  | DA    | 1939 | 55    | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | 5MC  | DA    | 1962 | 55    | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | 6MZ  | DA    | 2030 | 55    | -       | 0/5/27/28  | 0/3/3/3 |
| 55  | G7M  | DA    | 2069 | 55    | -       | 0/3/25/26  | 0/3/3/3 |
| 55  | OMG  | DA    | 2251 | 55    | -       | 0/5/27/28  | 0/3/3/3 |
| 55  | 2MG  | DA    | 2445 | 55    | -       | 0/5/27/28  | 0/3/3/3 |
| 55  | H2U  | DA    | 2449 | 55    | -       | 0/7/38/39  | 0/2/2/2 |
| 55  | PSU  | DA    | 2457 | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | OMC  | DA    | 2498 | 55,56 | -       | 0/5/27/28  | 0/2/2/2 |
| 55  | 2MA  | DA    | 2503 | 55,56 | -       | 0/3/25/26  | 0/3/3/3 |
| 55  | PSU  | DA    | 2504 | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | OMU  | DA    | 2552 | 55    | -       | 0/5/27/28  | 0/2/2/2 |
| 55  | PSU  | DA    | 2580 | 55    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res    | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|--------|-------|---------|------------|---------|
| 55  | PSU  | DA    | 2604   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | DA    | 2605   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 1MG  | DA    | 745    | 55    | -       | 0/3/25/26  | 0/3/3/3 |
| 55  | PSU  | DA    | 746    | 55,56 | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU  | DA    | 747    | 55    | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | PSU  | DA    | 955    | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MEQ  | DD    | 150[A] | 32    | -       | 0/7/9/11   | 0/0/0/0 |
| 32  | MEQ  | DD    | 150[B] | 32    | -       | 0/7/9/11   | 0/0/0/0 |
| 41  | 4D4  | DN    | 81[A]  | -     | -       | 0/10/12/14 | 0/0/0/0 |
| 41  | 4D4  | DN    | 81[B]  | -     | -       | 0/10/12/14 | 0/0/0/0 |

All (129) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | DA    | 2030 | 6MZ  | O5'-C5' | -3.71 | 1.39        | 1.44     |
| 31  | CA    | 2445 | 2MG  | O5'-C5' | -3.38 | 1.40        | 1.44     |
| 55  | DA    | 1618 | 6MZ  | O5'-C5' | -3.37 | 1.40        | 1.44     |
| 55  | DA    | 2504 | PSU  | O5'-C5' | -3.30 | 1.40        | 1.44     |
| 55  | DA    | 746  | PSU  | C2'-C1' | -3.17 | 1.50        | 1.53     |
| 1   | BA    | 527  | G7M  | O5'-C5' | -2.98 | 1.40        | 1.44     |
| 55  | DA    | 746  | PSU  | O4'-C1' | -2.91 | 1.40        | 1.44     |
| 31  | CA    | 2457 | PSU  | O5'-C5' | -2.82 | 1.40        | 1.44     |
| 55  | DA    | 2580 | PSU  | O4'-C1' | -2.72 | 1.40        | 1.44     |
| 1   | AA    | 527  | G7M  | O5'-C5' | -2.66 | 1.41        | 1.44     |
| 55  | DA    | 955  | PSU  | C2'-C1' | -2.59 | 1.51        | 1.53     |
| 55  | DA    | 747  | 5MU  | O5'-C5' | -2.56 | 1.41        | 1.44     |
| 31  | CA    | 2504 | PSU  | O5'-C5' | -2.56 | 1.41        | 1.44     |
| 55  | DA    | 2069 | G7M  | O5'-C5' | -2.54 | 1.41        | 1.44     |
| 31  | CA    | 746  | PSU  | O4'-C1' | -2.53 | 1.40        | 1.44     |
| 31  | CA    | 2498 | OMC  | O5'-C5' | -2.46 | 1.41        | 1.44     |
| 55  | DA    | 2580 | PSU  | C6-C5   | -2.41 | 1.35        | 1.38     |
| 55  | DA    | 2604 | PSU  | O5'-C5' | -2.34 | 1.41        | 1.44     |
| 55  | DA    | 745  | 1MG  | C8-N7   | -2.34 | 1.30        | 1.34     |
| 55  | DA    | 2580 | PSU  | C5-C1'  | -2.30 | 1.50        | 1.52     |
| 55  | DA    | 2457 | PSU  | C6-C5   | -2.30 | 1.35        | 1.38     |
| 31  | CA    | 1915 | 3TD  | C6-C5   | -2.29 | 1.35        | 1.38     |
| 31  | CA    | 1618 | 6MZ  | O5'-C5' | -2.27 | 1.41        | 1.44     |
| 31  | CA    | 2580 | PSU  | O5'-C5' | -2.24 | 1.41        | 1.44     |
| 55  | DA    | 2604 | PSU  | C6-C5   | -2.21 | 1.35        | 1.38     |
| 55  | DA    | 1911 | PSU  | C6-C5   | -2.20 | 1.35        | 1.38     |
| 55  | DA    | 746  | PSU  | C6-C5   | -2.20 | 1.35        | 1.38     |
| 55  | DA    | 2504 | PSU  | C6-C5   | -2.20 | 1.35        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 31  | CA    | 2504   | PSU  | C6-C5   | -2.20 | 1.35        | 1.38     |
| 1   | BA    | 516    | PSU  | C6-C5   | -2.19 | 1.35        | 1.38     |
| 31  | CA    | 2580   | PSU  | C6-C5   | -2.17 | 1.35        | 1.38     |
| 55  | DA    | 1915   | 3TD  | C6-C5   | -2.16 | 1.35        | 1.38     |
| 55  | DA    | 2445   | 2MG  | O3'-C3' | -2.15 | 1.38        | 1.43     |
| 55  | DA    | 1917   | PSU  | C6-C5   | -2.13 | 1.35        | 1.38     |
| 31  | CA    | 746    | PSU  | C6-C5   | -2.13 | 1.35        | 1.38     |
| 31  | CA    | 2605   | PSU  | C6-C5   | -2.13 | 1.35        | 1.38     |
| 31  | CA    | 955    | PSU  | C6-C5   | -2.12 | 1.35        | 1.38     |
| 55  | DA    | 955    | PSU  | C6-C5   | -2.12 | 1.35        | 1.38     |
| 31  | CA    | 2457   | PSU  | C6-C5   | -2.12 | 1.35        | 1.38     |
| 31  | CA    | 1917   | PSU  | C6-C5   | -2.11 | 1.35        | 1.38     |
| 55  | DA    | 2605   | PSU  | C6-C5   | -2.10 | 1.35        | 1.38     |
| 31  | CA    | 1962   | 5MC  | C6-C5   | -2.10 | 1.34        | 1.40     |
| 1   | AA    | 1407   | 5MC  | C6-C5   | -2.09 | 1.34        | 1.40     |
| 1   | BA    | 967    | 5MC  | C6-C5   | -2.08 | 1.34        | 1.40     |
| 1   | AA    | 516    | PSU  | C6-C5   | -2.07 | 1.35        | 1.38     |
| 1   | AA    | 967    | 5MC  | C6-C5   | -2.07 | 1.34        | 1.40     |
| 1   | BA    | 1407   | 5MC  | C6-C5   | -2.06 | 1.34        | 1.40     |
| 55  | DA    | 1962   | 5MC  | C6-C5   | -2.06 | 1.34        | 1.40     |
| 31  | CA    | 1911   | PSU  | C6-C5   | -2.06 | 1.35        | 1.38     |
| 55  | DA    | 1962   | 5MC  | O5'-C5' | -2.03 | 1.41        | 1.44     |
| 31  | CA    | 2069   | G7M  | O5'-C5' | -2.02 | 1.41        | 1.44     |
| 31  | CA    | 1939   | 5MU  | O5'-C5' | -2.02 | 1.41        | 1.44     |
| 55  | DA    | 1962   | 5MC  | C5-C4   | 2.01  | 1.44        | 1.41     |
| 31  | CA    | 1962   | 5MC  | C5-C4   | 2.03  | 1.44        | 1.41     |
| 55  | DA    | 2552   | OMU  | C6-N1   | 2.04  | 1.38        | 1.35     |
| 1   | BA    | 527    | G7M  | C6-C5   | 2.04  | 1.45        | 1.41     |
| 55  | DA    | 2498   | OMC  | O4'-C1' | 2.07  | 1.44        | 1.41     |
| 1   | BA    | 1498   | UR3  | C6-N1   | 2.08  | 1.38        | 1.35     |
| 41  | CN    | 81     | 4D4  | CZ-NH1  | 2.11  | 1.43        | 1.34     |
| 31  | CA    | 2498   | OMC  | C6-N1   | 2.11  | 1.38        | 1.35     |
| 41  | DN    | 81[A]  | 4D4  | CZ-NH1  | 2.15  | 1.43        | 1.34     |
| 32  | DD    | 150[A] | MEQ  | CA-C    | 2.17  | 1.53        | 1.50     |
| 12  | AL    | 89     | D2T  | CA-C    | 2.17  | 1.53        | 1.50     |
| 55  | DA    | 1915   | 3TD  | C4-N3   | 2.18  | 1.41        | 1.38     |
| 1   | BA    | 966    | 2MG  | C6-C5   | 2.27  | 1.45        | 1.41     |
| 31  | CA    | 2552   | OMU  | C6-N1   | 2.30  | 1.38        | 1.35     |
| 31  | CA    | 1915   | 3TD  | C4-N3   | 2.31  | 1.41        | 1.38     |
| 31  | CA    | 2251   | OMG  | C6-C5   | 2.31  | 1.45        | 1.41     |
| 1   | AA    | 1207   | 2MG  | C6-C5   | 2.35  | 1.45        | 1.41     |
| 55  | DA    | 745    | 1MG  | C6-N1   | 2.38  | 1.41        | 1.38     |

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| Mol | Chain | Res   | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|-------|------|-------------|----------|
| 41  | DN    | 81[B] | 4D4  | CA-C  | 2.46 | 1.53        | 1.50     |
| 55  | DA    | 2445  | 2MG  | C6-C5 | 2.60 | 1.46        | 1.41     |
| 41  | CN    | 81    | 4D4  | CA-C  | 2.60 | 1.53        | 1.50     |
| 55  | DA    | 2580  | PSU  | C4-N3 | 2.64 | 1.37        | 1.33     |
| 1   | BA    | 1498  | UR3  | C4-N3 | 2.65 | 1.42        | 1.38     |
| 41  | DN    | 81[A] | 4D4  | CA-C  | 2.69 | 1.53        | 1.50     |
| 55  | DA    | 2457  | PSU  | C4-N3 | 2.75 | 1.38        | 1.33     |
| 1   | BA    | 1207  | 2MG  | C6-C5 | 2.76 | 1.46        | 1.41     |
| 1   | BA    | 1516  | 2MG  | C6-C5 | 2.83 | 1.46        | 1.41     |
| 55  | DA    | 2604  | PSU  | C4-N3 | 2.85 | 1.38        | 1.33     |
| 1   | AA    | 966   | 2MG  | C6-C5 | 2.85 | 1.46        | 1.41     |
| 55  | DA    | 2445  | 2MG  | C6-N1 | 2.97 | 1.38        | 1.33     |
| 12  | BL    | 89    | D2T  | CA-C  | 2.98 | 1.54        | 1.50     |
| 55  | DA    | 746   | PSU  | C4-N3 | 3.02 | 1.38        | 1.33     |
| 1   | BA    | 527   | G7M  | C6-N1 | 3.02 | 1.38        | 1.33     |
| 55  | DA    | 1835  | 2MG  | C6-N1 | 3.06 | 1.38        | 1.33     |
| 55  | DA    | 747   | 5MU  | C4-N3 | 3.07 | 1.38        | 1.33     |
| 55  | DA    | 1939  | 5MU  | C4-N3 | 3.08 | 1.38        | 1.33     |
| 31  | CA    | 2552  | OMU  | C4-N3 | 3.08 | 1.38        | 1.33     |
| 1   | AA    | 527   | G7M  | C6-N1 | 3.11 | 1.38        | 1.33     |
| 31  | CA    | 2504  | PSU  | C4-N3 | 3.12 | 1.38        | 1.33     |
| 55  | DA    | 2552  | OMU  | C4-N3 | 3.13 | 1.38        | 1.33     |
| 55  | DA    | 2605  | PSU  | C4-N3 | 3.13 | 1.38        | 1.33     |
| 31  | CA    | 2069  | G7M  | C6-N1 | 3.13 | 1.38        | 1.33     |
| 55  | DA    | 1917  | PSU  | C4-N3 | 3.21 | 1.38        | 1.33     |
| 55  | DA    | 1911  | PSU  | C4-N3 | 3.21 | 1.38        | 1.33     |
| 31  | CA    | 2605  | PSU  | C4-N3 | 3.21 | 1.38        | 1.33     |
| 31  | CA    | 2445  | 2MG  | C6-C5 | 3.21 | 1.47        | 1.41     |
| 31  | CA    | 2457  | PSU  | C4-N3 | 3.22 | 1.38        | 1.33     |
| 55  | DA    | 2504  | PSU  | C4-N3 | 3.22 | 1.38        | 1.33     |
| 31  | CA    | 1917  | PSU  | C4-N3 | 3.23 | 1.38        | 1.33     |
| 31  | CA    | 2580  | PSU  | C4-N3 | 3.24 | 1.38        | 1.33     |
| 1   | BA    | 516   | PSU  | C4-N3 | 3.25 | 1.38        | 1.33     |
| 55  | DA    | 2069  | G7M  | C6-N1 | 3.25 | 1.38        | 1.33     |
| 1   | BA    | 966   | 2MG  | C6-N1 | 3.26 | 1.39        | 1.33     |
| 1   | AA    | 1207  | 2MG  | C6-N1 | 3.28 | 1.39        | 1.33     |
| 31  | CA    | 747   | 5MU  | C4-N3 | 3.29 | 1.39        | 1.33     |
| 31  | CA    | 955   | PSU  | C4-N3 | 3.29 | 1.39        | 1.33     |
| 1   | AA    | 516   | PSU  | C4-N3 | 3.30 | 1.39        | 1.33     |
| 31  | CA    | 746   | PSU  | C4-N3 | 3.30 | 1.39        | 1.33     |
| 31  | CA    | 1835  | 2MG  | C6-N1 | 3.32 | 1.39        | 1.33     |
| 55  | DA    | 2251  | OMG  | C6-N1 | 3.33 | 1.39        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|------|-------------|----------|
| 55  | DA    | 955    | PSU  | C4-N3 | 3.35 | 1.39        | 1.33     |
| 31  | CA    | 1911   | PSU  | C4-N3 | 3.35 | 1.39        | 1.33     |
| 31  | CA    | 2251   | OMG  | C6-N1 | 3.36 | 1.39        | 1.33     |
| 1   | BA    | 1516   | 2MG  | C6-N1 | 3.38 | 1.39        | 1.33     |
| 1   | AA    | 1516   | 2MG  | C6-C5 | 3.39 | 1.47        | 1.41     |
| 31  | CA    | 1939   | 5MU  | C4-N3 | 3.40 | 1.39        | 1.33     |
| 1   | AA    | 1516   | 2MG  | C6-N1 | 3.40 | 1.39        | 1.33     |
| 1   | BA    | 1207   | 2MG  | C6-N1 | 3.41 | 1.39        | 1.33     |
| 31  | CA    | 2445   | 2MG  | C6-N1 | 3.42 | 1.39        | 1.33     |
| 1   | AA    | 966    | 2MG  | C6-N1 | 3.42 | 1.39        | 1.33     |
| 55  | DA    | 745    | 1MG  | C6-C5 | 3.50 | 1.47        | 1.41     |
| 32  | DD    | 150[B] | MEQ  | CA-C  | 3.62 | 1.55        | 1.50     |
| 41  | DN    | 81[B]  | 4D4  | CZ-NE | 3.76 | 1.40        | 1.33     |
| 31  | CA    | 745    | 1MG  | C6-C5 | 4.00 | 1.48        | 1.41     |
| 41  | CN    | 81     | 4D4  | CZ-NE | 5.46 | 1.44        | 1.33     |
| 41  | DN    | 81[A]  | 4D4  | CZ-NE | 5.93 | 1.45        | 1.33     |
| 32  | DD    | 150[B] | MEQ  | CB-CA | 6.05 | 1.61        | 1.53     |

All (197) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1   | BA    | 516  | PSU  | N1-C2-N3 | -19.01 | 114.73      | 128.40   |
| 55  | DA    | 2504 | PSU  | N1-C2-N3 | -19.00 | 114.74      | 128.40   |
| 31  | CA    | 1917 | PSU  | N1-C2-N3 | -18.94 | 114.78      | 128.40   |
| 31  | CA    | 2605 | PSU  | N1-C2-N3 | -18.93 | 114.78      | 128.40   |
| 31  | CA    | 746  | PSU  | N1-C2-N3 | -18.93 | 114.78      | 128.40   |
| 31  | CA    | 2580 | PSU  | N1-C2-N3 | -18.90 | 114.81      | 128.40   |
| 55  | DA    | 1917 | PSU  | N1-C2-N3 | -18.85 | 114.84      | 128.40   |
| 31  | CA    | 1911 | PSU  | N1-C2-N3 | -18.84 | 114.85      | 128.40   |
| 31  | CA    | 955  | PSU  | N1-C2-N3 | -18.84 | 114.85      | 128.40   |
| 55  | DA    | 1911 | PSU  | N1-C2-N3 | -18.83 | 114.86      | 128.40   |
| 31  | CA    | 2504 | PSU  | N1-C2-N3 | -18.81 | 114.87      | 128.40   |
| 1   | AA    | 516  | PSU  | N1-C2-N3 | -18.81 | 114.87      | 128.40   |
| 31  | CA    | 2457 | PSU  | N1-C2-N3 | -18.80 | 114.88      | 128.40   |
| 55  | DA    | 2457 | PSU  | N1-C2-N3 | -18.78 | 114.89      | 128.40   |
| 55  | DA    | 2580 | PSU  | N1-C2-N3 | -18.76 | 114.91      | 128.40   |
| 55  | DA    | 2605 | PSU  | N1-C2-N3 | -18.75 | 114.92      | 128.40   |
| 55  | DA    | 955  | PSU  | N1-C2-N3 | -18.75 | 114.92      | 128.40   |
| 55  | DA    | 746  | PSU  | N1-C2-N3 | -18.74 | 114.92      | 128.40   |
| 55  | DA    | 2604 | PSU  | N1-C2-N3 | -18.70 | 114.95      | 128.40   |
| 55  | DA    | 746  | PSU  | C5-C4-N3 | -12.55 | 115.14      | 125.43   |
| 1   | AA    | 516  | PSU  | C5-C4-N3 | -12.51 | 115.17      | 125.43   |

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| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 55  | DA    | 2580 | PSU  | C5-C4-N3 | -12.50 | 115.17      | 125.43   |
| 55  | DA    | 955  | PSU  | C5-C4-N3 | -12.50 | 115.18      | 125.43   |
| 31  | CA    | 1917 | PSU  | C5-C4-N3 | -12.49 | 115.18      | 125.43   |
| 31  | CA    | 2457 | PSU  | C5-C4-N3 | -12.48 | 115.19      | 125.43   |
| 31  | CA    | 746  | PSU  | C5-C4-N3 | -12.48 | 115.20      | 125.43   |
| 55  | DA    | 1917 | PSU  | C5-C4-N3 | -12.47 | 115.20      | 125.43   |
| 55  | DA    | 2504 | PSU  | C5-C4-N3 | -12.45 | 115.22      | 125.43   |
| 1   | BA    | 516  | PSU  | C5-C4-N3 | -12.44 | 115.22      | 125.43   |
| 31  | CA    | 2580 | PSU  | C5-C4-N3 | -12.41 | 115.25      | 125.43   |
| 31  | CA    | 1911 | PSU  | C5-C4-N3 | -12.40 | 115.26      | 125.43   |
| 31  | CA    | 955  | PSU  | C5-C4-N3 | -12.37 | 115.28      | 125.43   |
| 31  | CA    | 2504 | PSU  | C5-C4-N3 | -12.34 | 115.31      | 125.43   |
| 55  | DA    | 2457 | PSU  | C5-C4-N3 | -12.31 | 115.33      | 125.43   |
| 31  | CA    | 2605 | PSU  | C5-C4-N3 | -12.25 | 115.38      | 125.43   |
| 55  | DA    | 2605 | PSU  | C5-C4-N3 | -12.25 | 115.38      | 125.43   |
| 55  | DA    | 1911 | PSU  | C5-C4-N3 | -12.24 | 115.39      | 125.43   |
| 55  | DA    | 2604 | PSU  | C5-C4-N3 | -12.23 | 115.39      | 125.43   |
| 31  | CA    | 2069 | G7M  | C5-C6-N1 | -9.17  | 110.43      | 123.48   |
| 55  | DA    | 1939 | 5MU  | C5-C4-N3 | -9.11  | 115.19      | 125.24   |
| 31  | CA    | 747  | 5MU  | C5-C4-N3 | -9.11  | 115.20      | 125.24   |
| 31  | CA    | 1939 | 5MU  | C5-C4-N3 | -9.09  | 115.22      | 125.24   |
| 1   | AA    | 527  | G7M  | C5-C6-N1 | -9.06  | 110.58      | 123.48   |
| 55  | DA    | 2069 | G7M  | C5-C6-N1 | -9.00  | 110.67      | 123.48   |
| 1   | BA    | 527  | G7M  | C5-C6-N1 | -9.00  | 110.67      | 123.48   |
| 55  | DA    | 747  | 5MU  | C5-C4-N3 | -8.99  | 115.33      | 125.24   |
| 55  | DA    | 2445 | 2MG  | C5-C6-N1 | -8.31  | 111.65      | 123.48   |
| 31  | CA    | 2445 | 2MG  | C5-C6-N1 | -7.99  | 112.11      | 123.48   |
| 1   | AA    | 1207 | 2MG  | C5-C6-N1 | -7.96  | 112.16      | 123.48   |
| 1   | AA    | 966  | 2MG  | C5-C6-N1 | -7.86  | 112.30      | 123.48   |
| 31  | CA    | 2251 | OMG  | C5-C6-N1 | -7.76  | 112.44      | 123.48   |
| 1   | BA    | 966  | 2MG  | C5-C6-N1 | -7.75  | 112.45      | 123.48   |
| 1   | BA    | 1207 | 2MG  | C5-C6-N1 | -7.69  | 112.54      | 123.48   |
| 31  | CA    | 1835 | 2MG  | C5-C6-N1 | -7.60  | 112.67      | 123.48   |
| 55  | DA    | 1835 | 2MG  | C5-C6-N1 | -7.56  | 112.72      | 123.48   |
| 1   | BA    | 1516 | 2MG  | C5-C6-N1 | -7.55  | 112.73      | 123.48   |
| 1   | AA    | 1516 | 2MG  | C5-C6-N1 | -7.41  | 112.93      | 123.48   |
| 55  | DA    | 2251 | OMG  | C5-C6-N1 | -7.40  | 112.94      | 123.48   |
| 1   | BA    | 527  | G7M  | C6-C5-C4 | -7.21  | 113.67      | 120.84   |
| 1   | AA    | 527  | G7M  | C6-C5-C4 | -6.53  | 114.35      | 120.84   |
| 31  | CA    | 2069 | G7M  | C6-C5-C4 | -5.01  | 115.86      | 120.84   |
| 55  | DA    | 2069 | G7M  | C6-C5-C4 | -4.86  | 116.01      | 120.84   |
| 1   | AA    | 1519 | MA6  | N1-C6-N6 | -4.64  | 112.08      | 117.00   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | BA    | 1519   | MA6  | N1-C6-N6    | -4.53 | 112.19      | 117.00   |
| 1   | AA    | 1516   | 2MG  | C6-C5-C4    | -3.76 | 117.11      | 120.84   |
| 41  | DN    | 81[B]  | 4D4  | NH1-CZ-NE   | -3.66 | 110.65      | 119.30   |
| 1   | BA    | 1516   | 2MG  | C6-C5-C4    | -3.57 | 117.30      | 120.84   |
| 55  | DA    | 2069   | G7M  | N3-C2-N1    | -3.55 | 122.27      | 127.46   |
| 31  | CA    | 2552   | OMU  | C5-C4-N3    | -3.46 | 114.85      | 123.12   |
| 55  | DA    | 2552   | OMU  | C5-C4-N3    | -3.45 | 114.89      | 123.12   |
| 31  | CA    | 745    | 1MG  | C6-C5-C4    | -3.43 | 117.56      | 119.92   |
| 1   | BA    | 1207   | 2MG  | C6-C5-C4    | -3.41 | 117.46      | 120.84   |
| 1   | AA    | 527    | G7M  | N3-C2-N1    | -3.40 | 122.49      | 127.46   |
| 55  | DA    | 2445   | 2MG  | C6-C5-C4    | -3.34 | 117.52      | 120.84   |
| 31  | CA    | 2069   | G7M  | N3-C2-N1    | -3.30 | 122.64      | 127.46   |
| 1   | BA    | 527    | G7M  | N3-C2-N1    | -3.27 | 122.68      | 127.46   |
| 55  | DA    | 1835   | 2MG  | C6-C5-C4    | -3.26 | 117.61      | 120.84   |
| 41  | CN    | 81     | 4D4  | NH1-CZ-NE   | -3.25 | 111.64      | 119.30   |
| 31  | CA    | 2445   | 2MG  | C6-C5-C4    | -3.23 | 117.63      | 120.84   |
| 1   | AA    | 966    | 2MG  | C6-C5-C4    | -3.20 | 117.66      | 120.84   |
| 55  | DA    | 745    | 1MG  | C6-C5-C4    | -3.08 | 117.80      | 119.92   |
| 31  | CA    | 2251   | OMG  | C6-C5-C4    | -3.08 | 117.78      | 120.84   |
| 1   | AA    | 1207   | 2MG  | C6-C5-C4    | -3.07 | 117.79      | 120.84   |
| 1   | BA    | 966    | 2MG  | C6-C5-C4    | -3.01 | 117.85      | 120.84   |
| 55  | DA    | 745    | 1MG  | C5-C6-N1    | -3.00 | 114.85      | 118.28   |
| 55  | DA    | 1915   | 3TD  | C5-C4-N3    | -2.99 | 116.14      | 118.69   |
| 55  | DA    | 2251   | OMG  | N3-C2-N1    | -2.95 | 123.15      | 127.46   |
| 31  | CA    | 1915   | 3TD  | C5-C4-N3    | -2.95 | 116.18      | 118.69   |
| 31  | CA    | 1835   | 2MG  | C6-C5-C4    | -2.88 | 117.98      | 120.84   |
| 31  | CA    | 745    | 1MG  | C5-C6-N1    | -2.86 | 115.00      | 118.28   |
| 41  | DN    | 81[A]  | 4D4  | NH1-CZ-NE   | -2.74 | 112.83      | 119.30   |
| 55  | DA    | 2251   | OMG  | C6-C5-C4    | -2.72 | 118.14      | 120.84   |
| 31  | CA    | 2251   | OMG  | N3-C2-N1    | -2.72 | 123.48      | 127.46   |
| 1   | BA    | 1518   | MA6  | N1-C6-N6    | -2.50 | 114.34      | 117.00   |
| 32  | DD    | 150[A] | MEQ  | O-C-CA      | -2.29 | 118.70      | 125.02   |
| 1   | AA    | 1518   | MA6  | N1-C6-N6    | -2.13 | 114.74      | 117.00   |
| 31  | CA    | 2605   | PSU  | C4-C5-C1'   | -2.12 | 117.05      | 121.15   |
| 55  | DA    | 745    | 1MG  | O4'-C4'-C3' | -2.11 | 100.97      | 105.17   |
| 55  | DA    | 955    | PSU  | C3'-C2'-C1' | -2.03 | 99.60       | 101.93   |
| 55  | DA    | 2580   | PSU  | O4'-C1'-C2' | 2.10  | 107.82      | 104.45   |
| 31  | CA    | 1962   | 5MC  | CM5-C5-C6   | 2.10  | 122.87      | 118.67   |
| 55  | DA    | 2503   | 2MA  | CM2-C2-N3   | 2.12  | 120.67      | 117.22   |
| 55  | DA    | 1939   | 5MU  | C5M-C5-C6   | 2.12  | 122.91      | 118.67   |
| 55  | DA    | 747    | 5MU  | C5M-C5-C6   | 2.16  | 122.98      | 118.67   |
| 1   | BA    | 1407   | 5MC  | CM5-C5-C6   | 2.18  | 123.01      | 118.67   |

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| Mol | Chain | Res    | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|------|-------------|----------|
| 1   | AA    | 1407   | 5MC  | CM5-C5-C6   | 2.18 | 123.02      | 118.67   |
| 1   | BA    | 967    | 5MC  | CM5-C5-C6   | 2.20 | 123.06      | 118.67   |
| 31  | CA    | 1939   | 5MU  | C5M-C5-C6   | 2.20 | 123.07      | 118.67   |
| 31  | CA    | 747    | 5MU  | C5M-C5-C6   | 2.21 | 123.09      | 118.67   |
| 1   | AA    | 967    | 5MC  | CM5-C5-C6   | 2.24 | 123.13      | 118.67   |
| 31  | CA    | 2580   | PSU  | O4'-C1'-C2' | 2.24 | 108.06      | 104.45   |
| 31  | CA    | 2030   | 6MZ  | C9-N6-C6    | 2.40 | 124.91      | 122.85   |
| 55  | DA    | 2445   | 2MG  | N2-C2-N3    | 2.43 | 119.31      | 116.95   |
| 31  | CA    | 2445   | 2MG  | N2-C2-N3    | 2.43 | 119.31      | 116.95   |
| 12  | AL    | 89     | D2T  | C-CA-N      | 2.43 | 114.77      | 109.86   |
| 1   | BA    | 1516   | 2MG  | N2-C2-N3    | 2.62 | 119.50      | 116.95   |
| 1   | AA    | 1516   | 2MG  | N2-C2-N3    | 2.62 | 119.50      | 116.95   |
| 1   | AA    | 1207   | 2MG  | N2-C2-N3    | 2.78 | 119.65      | 116.95   |
| 12  | BL    | 89     | D2T  | C-CA-N      | 2.81 | 115.54      | 109.86   |
| 1   | BA    | 1207   | 2MG  | N2-C2-N3    | 2.89 | 119.76      | 116.95   |
| 31  | CA    | 1835   | 2MG  | N2-C2-N3    | 2.89 | 119.76      | 116.95   |
| 1   | BA    | 966    | 2MG  | N2-C2-N3    | 2.89 | 119.76      | 116.95   |
| 55  | DA    | 1618   | 6MZ  | C2-N1-C6    | 2.92 | 118.43      | 116.53   |
| 55  | DA    | 1835   | 2MG  | N2-C2-N3    | 2.93 | 119.80      | 116.95   |
| 1   | BA    | 1402   | 4OC  | CM4-N4-C4   | 3.02 | 125.55      | 122.94   |
| 55  | DA    | 2030   | 6MZ  | C2-N1-C6    | 3.22 | 118.63      | 116.53   |
| 31  | CA    | 2030   | 6MZ  | C2-N1-C6    | 3.23 | 118.63      | 116.53   |
| 31  | CA    | 1618   | 6MZ  | C2-N1-C6    | 3.23 | 118.63      | 116.53   |
| 1   | AA    | 1402   | 4OC  | CM4-N4-C4   | 3.27 | 125.77      | 122.94   |
| 31  | CA    | 1618   | 6MZ  | C9-N6-C6    | 3.31 | 125.69      | 122.85   |
| 32  | DD    | 150[B] | MEQ  | CB-CG-CD    | 3.70 | 121.54      | 113.18   |
| 55  | DA    | 2605   | PSU  | C6-N1-C2    | 4.53 | 122.61      | 115.36   |
| 55  | DA    | 955    | PSU  | C6-N1-C2    | 4.56 | 122.65      | 115.36   |
| 31  | CA    | 2504   | PSU  | C6-N1-C2    | 4.57 | 122.67      | 115.36   |
| 55  | DA    | 746    | PSU  | C6-N1-C2    | 4.57 | 122.68      | 115.36   |
| 55  | DA    | 2604   | PSU  | C6-N1-C2    | 4.58 | 122.69      | 115.36   |
| 1   | BA    | 516    | PSU  | C6-N1-C2    | 4.58 | 122.69      | 115.36   |
| 31  | CA    | 1917   | PSU  | C6-N1-C2    | 4.58 | 122.70      | 115.36   |
| 31  | CA    | 746    | PSU  | C6-N1-C2    | 4.59 | 122.70      | 115.36   |
| 55  | DA    | 1911   | PSU  | C6-N1-C2    | 4.59 | 122.71      | 115.36   |
| 31  | CA    | 955    | PSU  | C6-N1-C2    | 4.60 | 122.72      | 115.36   |
| 31  | CA    | 2457   | PSU  | C6-N1-C2    | 4.60 | 122.73      | 115.36   |
| 55  | DA    | 2457   | PSU  | C6-N1-C2    | 4.61 | 122.73      | 115.36   |
| 1   | AA    | 516    | PSU  | C6-N1-C2    | 4.61 | 122.73      | 115.36   |
| 55  | DA    | 1917   | PSU  | C6-N1-C2    | 4.61 | 122.74      | 115.36   |
| 31  | CA    | 1911   | PSU  | C6-N1-C2    | 4.62 | 122.75      | 115.36   |
| 55  | DA    | 2580   | PSU  | C6-N1-C2    | 4.62 | 122.76      | 115.36   |

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| Mol | Chain | Res   | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 31  | CA    | 2580  | PSU  | C6-N1-C2  | 4.62  | 122.76      | 115.36   |
| 31  | CA    | 2605  | PSU  | C6-N1-C2  | 4.64  | 122.78      | 115.36   |
| 55  | DA    | 2504  | PSU  | C6-N1-C2  | 4.70  | 122.88      | 115.36   |
| 1   | AA    | 1516  | 2MG  | C6-N1-C2  | 5.07  | 124.27      | 115.18   |
| 41  | DN    | 81[A] | 4D4  | NE-CZ-NH2 | 5.09  | 129.72      | 120.58   |
| 31  | CA    | 1835  | 2MG  | C6-N1-C2  | 5.11  | 124.33      | 115.18   |
| 1   | AA    | 966   | 2MG  | C6-N1-C2  | 5.17  | 124.43      | 115.18   |
| 1   | BA    | 1516  | 2MG  | C6-N1-C2  | 5.19  | 124.47      | 115.18   |
| 31  | CA    | 2445  | 2MG  | C6-N1-C2  | 5.24  | 124.57      | 115.18   |
| 1   | BA    | 966   | 2MG  | C6-N1-C2  | 5.25  | 124.58      | 115.18   |
| 55  | DA    | 1835  | 2MG  | C6-N1-C2  | 5.26  | 124.60      | 115.18   |
| 1   | BA    | 1207  | 2MG  | C6-N1-C2  | 5.30  | 124.67      | 115.18   |
| 31  | CA    | 1915  | 3TD  | C6-N1-C2  | 5.32  | 123.87      | 115.36   |
| 1   | AA    | 1207  | 2MG  | C6-N1-C2  | 5.36  | 124.78      | 115.18   |
| 55  | DA    | 1915  | 3TD  | C6-N1-C2  | 5.40  | 124.00      | 115.36   |
| 41  | DN    | 81[B] | 4D4  | NE-CZ-NH2 | 5.45  | 130.36      | 120.58   |
| 41  | CN    | 81    | 4D4  | NE-CZ-NH2 | 5.58  | 130.60      | 120.58   |
| 1   | AA    | 527   | G7M  | C6-N1-C2  | 5.62  | 124.14      | 116.06   |
| 55  | DA    | 2069  | G7M  | C6-N1-C2  | 5.74  | 124.31      | 116.06   |
| 1   | BA    | 527   | G7M  | C6-N1-C2  | 5.92  | 124.57      | 116.06   |
| 31  | CA    | 2069  | G7M  | C6-N1-C2  | 5.96  | 124.64      | 116.06   |
| 55  | DA    | 2445  | 2MG  | C6-N1-C2  | 6.00  | 125.92      | 115.18   |
| 55  | DA    | 2251  | OMG  | C6-N1-C2  | 6.15  | 124.91      | 116.06   |
| 31  | CA    | 2251  | OMG  | C6-N1-C2  | 6.41  | 125.28      | 116.06   |
| 55  | DA    | 1618  | 6MZ  | C9-N6-C6  | 6.61  | 128.52      | 122.85   |
| 55  | DA    | 2604  | PSU  | C4-N3-C2  | 12.83 | 126.38      | 115.16   |
| 55  | DA    | 955   | PSU  | C4-N3-C2  | 12.89 | 126.43      | 115.16   |
| 55  | DA    | 1911  | PSU  | C4-N3-C2  | 12.89 | 126.43      | 115.16   |
| 31  | CA    | 2605  | PSU  | C4-N3-C2  | 12.89 | 126.44      | 115.16   |
| 31  | CA    | 955   | PSU  | C4-N3-C2  | 12.89 | 126.44      | 115.16   |
| 31  | CA    | 1911  | PSU  | C4-N3-C2  | 12.91 | 126.45      | 115.16   |
| 31  | CA    | 746   | PSU  | C4-N3-C2  | 12.94 | 126.47      | 115.16   |
| 31  | CA    | 2580  | PSU  | C4-N3-C2  | 12.95 | 126.48      | 115.16   |
| 1   | AA    | 516   | PSU  | C4-N3-C2  | 12.96 | 126.49      | 115.16   |
| 31  | CA    | 2504  | PSU  | C4-N3-C2  | 12.97 | 126.50      | 115.16   |
| 55  | DA    | 746   | PSU  | C4-N3-C2  | 12.98 | 126.51      | 115.16   |
| 31  | CA    | 2457  | PSU  | C4-N3-C2  | 12.98 | 126.51      | 115.16   |
| 55  | DA    | 2580  | PSU  | C4-N3-C2  | 12.98 | 126.51      | 115.16   |
| 55  | DA    | 1917  | PSU  | C4-N3-C2  | 12.99 | 126.52      | 115.16   |
| 55  | DA    | 2605  | PSU  | C4-N3-C2  | 13.00 | 126.53      | 115.16   |
| 1   | BA    | 516   | PSU  | C4-N3-C2  | 13.05 | 126.57      | 115.16   |
| 55  | DA    | 2504  | PSU  | C4-N3-C2  | 13.06 | 126.58      | 115.16   |

*Continued on next page...*



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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 55  | DA    | 2457 | PSU  | C4-N3-C2 | 13.07 | 126.59      | 115.16   |
| 31  | CA    | 1917 | PSU  | C4-N3-C2 | 13.12 | 126.63      | 115.16   |
| 55  | DA    | 747  | 5MU  | C4-N3-C2 | 13.65 | 127.10      | 115.16   |
| 31  | CA    | 1939 | 5MU  | C4-N3-C2 | 13.87 | 127.29      | 115.16   |
| 31  | CA    | 747  | 5MU  | C4-N3-C2 | 13.87 | 127.29      | 115.16   |
| 55  | DA    | 1939 | 5MU  | C4-N3-C2 | 13.87 | 127.29      | 115.16   |
| 31  | CA    | 2552 | OMU  | C4-N3-C2 | 14.94 | 126.96      | 114.13   |
| 55  | DA    | 2552 | OMU  | C4-N3-C2 | 14.94 | 126.97      | 114.13   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 13 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 1   | AA    | 1518   | MA6  | 1       | 0            |
| 1   | AA    | 1519   | MA6  | 1       | 0            |
| 1   | BA    | 1518   | MA6  | 1       | 0            |
| 1   | BA    | 1519   | MA6  | 1       | 0            |
| 31  | CA    | 2030   | 6MZ  | 2       | 0            |
| 31  | CA    | 2445   | 2MG  | 1       | 0            |
| 31  | CA    | 2503   | 2MA  | 1       | 0            |
| 31  | CA    | 747    | 5MU  | 1       | 0            |
| 55  | DA    | 2030   | 6MZ  | 1       | 0            |
| 55  | DA    | 2445   | 2MG  | 1       | 0            |
| 55  | DA    | 2449   | H2U  | 1       | 0            |
| 55  | DA    | 2498   | OMC  | 1       | 0            |
| 55  | DA    | 747    | 5MU  | 1       | 0            |
| 32  | DD    | 150[B] | MEQ  | 1       | 0            |
| 41  | DN    | 81[B]  | 4D4  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 554 ligands modelled in this entry, 472 are monoatomic - leaving 82 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$ |
| 57  | PG4  | AA    | 1670 | -    | 12,12,12     | 0.27 | 0           | 11,11,11    | 0.40 | 0           |
| 58  | MPD  | AA    | 1671 | -    | 7,7,7        | 0.69 | 0           | 9,10,10     | 0.42 | 0           |
| 59  | PUT  | AA    | 1672 | -    | 5,5,5        | 0.23 | 0           | 4,4,4       | 0.22 | 0           |
| 59  | PUT  | AA    | 1673 | -    | 5,5,5        | 0.17 | 0           | 4,4,4       | 0.18 | 0           |
| 59  | PUT  | AA    | 1674 | -    | 5,5,5        | 0.17 | 0           | 4,4,4       | 0.17 | 0           |
| 59  | PUT  | AA    | 1675 | -    | 5,5,5        | 0.22 | 0           | 4,4,4       | 0.26 | 0           |
| 58  | MPD  | AA    | 1676 | -    | 7,7,7        | 0.59 | 0           | 9,10,10     | 0.38 | 0           |
| 60  | T1C  | AA    | 1677 | 56   | 44,45,45     | 0.99 | 3 (6%)      | 53,72,72    | 1.44 | 4 (7%)      |
| 62  | PEG  | AL    | 201  | -    | 6,6,6        | 0.25 | 0           | 5,5,5       | 0.12 | 0           |
| 57  | PG4  | BA    | 1642 | -    | 12,12,12     | 0.21 | 0           | 11,11,11    | 0.21 | 0           |
| 60  | T1C  | BA    | 1643 | 56   | 44,45,45     | 0.97 | 3 (6%)      | 53,72,72    | 1.42 | 3 (5%)      |
| 63  | EDO  | D1    | 101  | -    | 3,3,3        | 0.66 | 0           | 2,2,2       | 0.16 | 0           |
| 64  | PGE  | D1    | 102  | -    | 9,9,9        | 0.30 | 0           | 8,8,8       | 0.29 | 0           |
| 62  | PEG  | D1    | 103  | -    | 6,6,6        | 0.44 | 0           | 5,5,5       | 0.14 | 0           |
| 64  | PGE  | D3    | 101  | -    | 9,9,9        | 0.30 | 0           | 8,8,8       | 0.22 | 0           |
| 62  | PEG  | D3    | 102  | -    | 6,6,6        | 0.33 | 0           | 5,5,5       | 0.23 | 0           |
| 63  | EDO  | DA    | 3001 | -    | 3,3,3        | 0.84 | 0           | 2,2,2       | 0.12 | 0           |
| 59  | PUT  | DA    | 3002 | -    | 5,5,5        | 0.19 | 0           | 4,4,4       | 0.10 | 0           |
| 63  | EDO  | DA    | 3003 | -    | 3,3,3        | 0.76 | 0           | 2,2,2       | 0.14 | 0           |
| 63  | EDO  | DA    | 3004 | -    | 3,3,3        | 0.73 | 0           | 2,2,2       | 0.14 | 0           |
| 65  | SPD  | DA    | 3183 | -    | 9,9,9        | 0.13 | 0           | 8,8,8       | 0.18 | 0           |
| 59  | PUT  | DA    | 3184 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.19 | 0           |
| 66  | 1PE  | DA    | 3185 | -    | 15,15,15     | 0.16 | 0           | 14,14,14    | 0.15 | 0           |
| 64  | PGE  | DA    | 3186 | -    | 9,9,9        | 0.36 | 0           | 8,8,8       | 0.54 | 0           |
| 65  | SPD  | DA    | 3187 | -    | 9,9,9        | 0.17 | 0           | 8,8,8       | 0.42 | 0           |
| 59  | PUT  | DA    | 3188 | -    | 5,5,5        | 0.43 | 0           | 4,4,4       | 0.28 | 0           |
| 59  | PUT  | DA    | 3189 | -    | 5,5,5        | 0.47 | 0           | 4,4,4       | 0.47 | 0           |
| 58  | MPD  | DA    | 3190 | -    | 7,7,7        | 0.47 | 0           | 9,10,10     | 0.43 | 0           |
| 67  | ACY  | DA    | 3191 | -    | 1,3,3        | 2.13 | 1 (100%)    | 0,3,3       | 0.00 | -           |
| 58  | MPD  | DA    | 3192 | -    | 7,7,7        | 0.68 | 0           | 9,10,10     | 0.74 | 0           |
| 57  | PG4  | DA    | 3193 | -    | 12,12,12     | 0.30 | 0           | 11,11,11    | 0.42 | 0           |
| 63  | EDO  | DA    | 3194 | -    | 3,3,3        | 0.65 | 0           | 2,2,2       | 0.09 | 0           |
| 59  | PUT  | DA    | 3195 | -    | 5,5,5        | 0.32 | 0           | 4,4,4       | 0.56 | 0           |
| 67  | ACY  | DA    | 3196 | -    | 1,3,3        | 3.00 | 1 (100%)    | 0,3,3       | 0.00 | -           |
| 63  | EDO  | DA    | 3197 | -    | 3,3,3        | 0.64 | 0           | 2,2,2       | 0.25 | 0           |
| 63  | EDO  | DA    | 3198 | -    | 3,3,3        | 0.67 | 0           | 2,2,2       | 0.39 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 62  | PEG  | DA    | 3199 | -    | 6,6,6        | 0.30 | 0        | 5,5,5       | 0.20 | 0        |
| 62  | PEG  | DA    | 3200 | -    | 6,6,6        | 0.52 | 0        | 5,5,5       | 0.26 | 0        |
| 67  | ACY  | DA    | 3201 | -    | 1,3,3        | 1.98 | 0        | 0,3,3       | 0.00 | -        |
| 66  | 1PE  | DA    | 3202 | -    | 15,15,15     | 0.36 | 0        | 14,14,14    | 0.39 | 0        |
| 58  | MPD  | DA    | 3203 | -    | 7,7,7        | 0.88 | 0        | 9,10,10     | 0.58 | 0        |
| 59  | PUT  | DA    | 3204 | -    | 5,5,5        | 0.36 | 0        | 4,4,4       | 0.32 | 0        |
| 65  | SPD  | DA    | 3205 | -    | 9,9,9        | 0.24 | 0        | 8,8,8       | 0.20 | 0        |
| 58  | MPD  | DA    | 3206 | -    | 7,7,7        | 1.01 | 1 (14%)  | 9,10,10     | 0.48 | 0        |
| 63  | EDO  | DA    | 3207 | -    | 3,3,3        | 0.70 | 0        | 2,2,2       | 0.18 | 0        |
| 63  | EDO  | DA    | 3208 | -    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.32 | 0        |
| 58  | MPD  | DA    | 3209 | -    | 7,7,7        | 0.70 | 0        | 9,10,10     | 0.37 | 0        |
| 68  | GUN  | DA    | 3210 | -    | 9,12,12      | 2.11 | 2 (22%)  | 8,17,17     | 3.97 | 4 (50%)  |
| 59  | PUT  | DA    | 3211 | -    | 5,5,5        | 0.32 | 0        | 4,4,4       | 0.19 | 0        |
| 59  | PUT  | DA    | 3212 | -    | 5,5,5        | 0.38 | 0        | 4,4,4       | 0.34 | 0        |
| 64  | PGE  | DA    | 3213 | -    | 9,9,9        | 0.16 | 0        | 8,8,8       | 0.17 | 0        |
| 63  | EDO  | DA    | 3214 | -    | 3,3,3        | 0.66 | 0        | 2,2,2       | 0.26 | 0        |
| 57  | PG4  | DA    | 3215 | -    | 12,12,12     | 0.17 | 0        | 11,11,11    | 0.13 | 0        |
| 64  | PGE  | DA    | 3216 | -    | 9,9,9        | 0.14 | 0        | 8,8,8       | 0.25 | 0        |
| 62  | PEG  | DA    | 3217 | -    | 6,6,6        | 0.30 | 0        | 5,5,5       | 0.07 | 0        |
| 59  | PUT  | DA    | 3218 | -    | 5,5,5        | 0.14 | 0        | 4,4,4       | 0.14 | 0        |
| 69  | TRS  | DA    | 3219 | -    | 7,7,7        | 0.46 | 0        | 9,9,9       | 0.43 | 0        |
| 59  | PUT  | DA    | 3220 | -    | 5,5,5        | 0.20 | 0        | 4,4,4       | 0.16 | 0        |
| 59  | PUT  | DA    | 3221 | -    | 5,5,5        | 0.46 | 0        | 4,4,4       | 0.68 | 0        |
| 59  | PUT  | DA    | 3222 | -    | 5,5,5        | 0.28 | 0        | 4,4,4       | 0.32 | 0        |
| 65  | SPD  | DA    | 3223 | -    | 9,9,9        | 0.19 | 0        | 8,8,8       | 0.68 | 0        |
| 64  | PGE  | DA    | 3224 | -    | 9,9,9        | 0.25 | 0        | 8,8,8       | 0.17 | 0        |
| 62  | PEG  | DA    | 3225 | -    | 6,6,6        | 0.50 | 0        | 5,5,5       | 0.25 | 0        |
| 62  | PEG  | DA    | 3226 | -    | 6,6,6        | 0.43 | 0        | 5,5,5       | 0.26 | 0        |
| 63  | EDO  | DB    | 210  | -    | 3,3,3        | 0.60 | 0        | 2,2,2       | 0.25 | 0        |
| 63  | EDO  | DB    | 211  | -    | 3,3,3        | 0.60 | 0        | 2,2,2       | 0.20 | 0        |
| 64  | PGE  | DD    | 301  | -    | 9,9,9        | 0.29 | 0        | 8,8,8       | 0.32 | 0        |
| 58  | MPD  | DE    | 301  | -    | 7,7,7        | 0.84 | 0        | 9,10,10     | 0.71 | 0        |
| 58  | MPD  | DE    | 302  | -    | 7,7,7        | 0.89 | 1 (14%)  | 9,10,10     | 0.43 | 0        |
| 58  | MPD  | DK    | 201  | -    | 7,7,7        | 0.73 | 0        | 9,10,10     | 0.25 | 0        |
| 62  | PEG  | DL    | 201  | -    | 6,6,6        | 0.14 | 0        | 5,5,5       | 0.12 | 0        |
| 58  | MPD  | DN    | 201  | -    | 7,7,7        | 1.07 | 1 (14%)  | 9,10,10     | 0.54 | 0        |
| 62  | PEG  | DP    | 201  | -    | 6,6,6        | 0.30 | 0        | 5,5,5       | 0.15 | 0        |
| 62  | PEG  | DQ    | 201  | -    | 6,6,6        | 0.21 | 0        | 5,5,5       | 0.14 | 0        |
| 57  | PG4  | DQ    | 202  | -    | 12,12,12     | 0.16 | 0        | 11,11,11    | 0.15 | 0        |
| 57  | PG4  | DR    | 202  | -    | 12,12,12     | 0.43 | 0        | 11,11,11    | 0.53 | 0        |
| 64  | PGE  | DS    | 201  | -    | 9,9,9        | 0.48 | 0        | 8,8,8       | 0.47 | 0        |
| 57  | PG4  | DS    | 202  | -    | 12,12,12     | 0.47 | 0        | 11,11,11    | 0.42 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | MPD  | DS    | 203 | -    | 7,7,7        | 0.39 | 0        | 9,10,10     | 0.65 | 0        |
| 58  | MPD  | DT    | 201 | -    | 7,7,7        | 0.60 | 0        | 9,10,10     | 0.17 | 0        |
| 58  | MPD  | DT    | 202 | -    | 7,7,7        | 0.81 | 0        | 9,10,10     | 0.39 | 0        |
| 64  | PGE  | DU    | 101 | -    | 9,9,9        | 0.26 | 0        | 8,8,8       | 0.36 | 0        |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 57  | PG4  | AA    | 1670 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 58  | MPD  | AA    | 1671 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 59  | PUT  | AA    | 1672 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | AA    | 1673 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | AA    | 1674 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | AA    | 1675 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 58  | MPD  | AA    | 1676 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 60  | T1C  | AA    | 1677 | 56   | -       | 0/22/80/80 | 0/4/4/4 |
| 62  | PEG  | AL    | 201  | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 57  | PG4  | BA    | 1642 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 60  | T1C  | BA    | 1643 | 56   | -       | 0/22/80/80 | 0/4/4/4 |
| 63  | EDO  | D1    | 101  | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 64  | PGE  | D1    | 102  | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 62  | PEG  | D1    | 103  | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 64  | PGE  | D3    | 101  | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 62  | PEG  | D3    | 102  | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 63  | EDO  | DA    | 3001 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 59  | PUT  | DA    | 3002 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 63  | EDO  | DA    | 3003 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 63  | EDO  | DA    | 3004 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 65  | SPD  | DA    | 3183 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 59  | PUT  | DA    | 3184 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 66  | 1PE  | DA    | 3185 | -    | -       | 0/13/13/13 | 0/0/0/0 |
| 64  | PGE  | DA    | 3186 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 65  | SPD  | DA    | 3187 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 59  | PUT  | DA    | 3188 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | DA    | 3189 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 58  | MPD  | DA    | 3190 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 67  | ACY  | DA    | 3191 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 58  | MPD  | DA    | 3192 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 57  | PG4  | DA    | 3193 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 63  | EDO  | DA    | 3194 | -    | -       | 0/1/1/1    | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 59  | PUT  | DA    | 3195 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 67  | ACY  | DA    | 3196 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 63  | EDO  | DA    | 3197 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 63  | EDO  | DA    | 3198 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 62  | PEG  | DA    | 3199 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 62  | PEG  | DA    | 3200 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 67  | ACY  | DA    | 3201 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 66  | 1PE  | DA    | 3202 | -    | -       | 0/13/13/13 | 0/0/0/0 |
| 58  | MPD  | DA    | 3203 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 59  | PUT  | DA    | 3204 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 65  | SPD  | DA    | 3205 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 58  | MPD  | DA    | 3206 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 63  | EDO  | DA    | 3207 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 63  | EDO  | DA    | 3208 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 58  | MPD  | DA    | 3209 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 68  | GUN  | DA    | 3210 | -    | -       | 0/0/0/0    | 0/2/2/2 |
| 59  | PUT  | DA    | 3211 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | DA    | 3212 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 64  | PGE  | DA    | 3213 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 63  | EDO  | DA    | 3214 | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 57  | PG4  | DA    | 3215 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 64  | PGE  | DA    | 3216 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 62  | PEG  | DA    | 3217 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 59  | PUT  | DA    | 3218 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 69  | TRS  | DA    | 3219 | -    | -       | 0/9/9/9    | 0/0/0/0 |
| 59  | PUT  | DA    | 3220 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | DA    | 3221 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 59  | PUT  | DA    | 3222 | -    | -       | 0/3/3/3    | 0/0/0/0 |
| 65  | SPD  | DA    | 3223 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 64  | PGE  | DA    | 3224 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 62  | PEG  | DA    | 3225 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 62  | PEG  | DA    | 3226 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 63  | EDO  | DB    | 210  | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 63  | EDO  | DB    | 211  | -    | -       | 0/1/1/1    | 0/0/0/0 |
| 64  | PGE  | DD    | 301  | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 58  | MPD  | DE    | 301  | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 58  | MPD  | DE    | 302  | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 58  | MPD  | DK    | 201  | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 62  | PEG  | DL    | 201  | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 58  | MPD  | DN    | 201  | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 62  | PEG  | DP    | 201  | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 62  | PEG  | DQ    | 201  | -    | -       | 0/4/4/4    | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 57  | PG4  | DQ    | 202 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 57  | PG4  | DR    | 202 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 64  | PGE  | DS    | 201 | -    | -       | 0/7/7/7    | 0/0/0/0 |
| 57  | PG4  | DS    | 202 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 58  | MPD  | DS    | 203 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 58  | MPD  | DT    | 201 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 58  | MPD  | DT    | 202 | -    | -       | 0/5/5/5    | 0/0/0/0 |
| 64  | PGE  | DU    | 101 | -    | -       | 0/7/7/7    | 0/0/0/0 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 67  | DA    | 3191 | ACY  | CH3-C  | 2.13 | 1.51        | 1.48     |
| 58  | DE    | 302  | MPD  | C3-C2  | 2.15 | 1.59        | 1.53     |
| 60  | BA    | 1643 | T1C  | C7-C61 | 2.26 | 1.43        | 1.40     |
| 60  | AA    | 1677 | T1C  | C7-C61 | 2.36 | 1.43        | 1.40     |
| 58  | DA    | 3206 | MPD  | C3-C2  | 2.36 | 1.60        | 1.53     |
| 58  | DN    | 201  | MPD  | C3-C2  | 2.52 | 1.60        | 1.53     |
| 60  | AA    | 1677 | T1C  | C7-N7  | 2.53 | 1.49        | 1.42     |
| 60  | BA    | 1643 | T1C  | C7-N7  | 2.60 | 1.49        | 1.42     |
| 60  | AA    | 1677 | T1C  | C4-C3  | 2.85 | 1.57        | 1.52     |
| 67  | DA    | 3196 | ACY  | CH3-C  | 3.00 | 1.52        | 1.48     |
| 60  | BA    | 1643 | T1C  | C4-C3  | 3.25 | 1.58        | 1.52     |
| 68  | DA    | 3210 | GUN  | C6-N1  | 3.29 | 1.39        | 1.33     |
| 68  | DA    | 3210 | GUN  | C6-C5  | 4.79 | 1.50        | 1.41     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 68  | DA    | 3210 | GUN  | C5-C6-N1    | -8.05 | 112.02      | 123.48   |
| 60  | BA    | 1643 | T1C  | C8-C9-C10   | -4.41 | 115.88      | 120.58   |
| 60  | AA    | 1677 | T1C  | C8-C9-C10   | -3.98 | 116.33      | 120.58   |
| 68  | DA    | 3210 | GUN  | C6-C5-C4    | -3.42 | 117.44      | 120.84   |
| 68  | DA    | 3210 | GUN  | N3-C2-N1    | -2.39 | 123.97      | 127.46   |
| 60  | AA    | 1677 | T1C  | C5-C51-C1B  | 2.11  | 113.26      | 109.47   |
| 60  | AA    | 1677 | T1C  | C6-C61-C1A  | 2.31  | 122.38      | 118.10   |
| 60  | BA    | 1643 | T1C  | C61-C7-N7   | 2.33  | 121.01      | 118.93   |
| 68  | DA    | 3210 | GUN  | C6-N1-C2    | 6.30  | 125.12      | 116.06   |
| 60  | AA    | 1677 | T1C  | C92-N92-C93 | 6.95  | 124.40      | 115.76   |
| 60  | BA    | 1643 | T1C  | C92-N92-C93 | 7.08  | 124.57      | 115.76   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 48 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57  | AA    | 1670 | PG4  | 1       | 0            |
| 64  | D1    | 102  | PGE  | 2       | 0            |
| 62  | D1    | 103  | PEG  | 1       | 0            |
| 62  | D3    | 102  | PEG  | 2       | 0            |
| 59  | DA    | 3189 | PUT  | 1       | 0            |
| 58  | DA    | 3190 | MPD  | 1       | 0            |
| 58  | DA    | 3192 | MPD  | 2       | 0            |
| 57  | DA    | 3193 | PG4  | 1       | 0            |
| 63  | DA    | 3194 | EDO  | 1       | 0            |
| 59  | DA    | 3195 | PUT  | 3       | 0            |
| 63  | DA    | 3197 | EDO  | 1       | 0            |
| 62  | DA    | 3200 | PEG  | 1       | 0            |
| 58  | DA    | 3203 | MPD  | 2       | 0            |
| 59  | DA    | 3212 | PUT  | 1       | 0            |
| 64  | DA    | 3213 | PGE  | 1       | 0            |
| 57  | DA    | 3215 | PG4  | 1       | 0            |
| 64  | DA    | 3216 | PGE  | 1       | 0            |
| 59  | DA    | 3218 | PUT  | 1       | 0            |
| 69  | DA    | 3219 | TRS  | 1       | 0            |
| 59  | DA    | 3221 | PUT  | 3       | 0            |
| 59  | DA    | 3222 | PUT  | 1       | 0            |
| 65  | DA    | 3223 | SPD  | 4       | 0            |
| 64  | DA    | 3224 | PGE  | 3       | 0            |
| 63  | DB    | 211  | EDO  | 1       | 0            |
| 64  | DD    | 301  | PGE  | 2       | 0            |
| 58  | DN    | 201  | MPD  | 1       | 0            |
| 62  | DP    | 201  | PEG  | 1       | 0            |
| 57  | DR    | 202  | PG4  | 5       | 0            |
| 57  | DS    | 202  | PG4  | 1       | 0            |
| 64  | DU    | 101  | PGE  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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   | AA    | 1523/1534 (99%) | 0.70   | 103 (6%) 18 10 | 46, 105, 241, 293     | 0     |
| 1   | BA    | 1522/1534 (99%) | 1.53   | 399 (26%) 1 0  | 61, 140, 279, 284     | 0     |
| 2   | AB    | 224/224 (100%)  | 1.63   | 72 (32%) 0 0   | 83, 127, 202, 270     | 0     |
| 2   | BB    | 224/224 (100%)  | 1.76   | 78 (34%) 0 0   | 99, 144, 211, 261     | 0     |
| 3   | AC    | 206/206 (100%)  | 0.83   | 30 (14%) 3 1   | 80, 108, 141, 163     | 0     |
| 3   | BC    | 206/206 (100%)  | 2.64   | 116 (56%) 0 0  | 115, 151, 190, 231    | 0     |
| 4   | AD    | 205/205 (100%)  | 0.62   | 18 (8%) 11 6   | 64, 103, 131, 154     | 0     |
| 4   | BD    | 205/205 (100%)  | 0.20   | 1 (0%) 90 79   | 61, 81, 107, 131      | 0     |
| 5   | AE    | 155/155 (100%)  | 0.77   | 13 (8%) 12 6   | 67, 91, 133, 169      | 0     |
| 5   | BE    | 150/155 (96%)   | 1.17   | 33 (22%) 1 1   | 77, 97, 144, 227      | 0     |
| 6   | AF    | 106/106 (100%)  | 0.83   | 19 (17%) 2 1   | 82, 105, 128, 142     | 0     |
| 6   | BF    | 100/106 (94%)   | 0.98   | 14 (14%) 3 1   | 86, 121, 146, 154     | 0     |
| 7   | AG    | 151/151 (100%)  | 2.15   | 66 (43%) 0 0   | 107, 137, 166, 179    | 0     |
| 7   | BG    | 151/151 (100%)  | 5.30   | 125 (82%) 0 0  | 147, 203, 218, 228    | 0     |
| 8   | AH    | 129/129 (100%)  | 0.64   | 9 (6%) 17 10   | 71, 91, 118, 136      | 0     |
| 8   | BH    | 129/129 (100%)  | 1.02   | 24 (18%) 1 1   | 91, 116, 150, 168     | 0     |
| 9   | AI    | 127/127 (100%)  | 2.31   | 59 (46%) 0 0   | 96, 132, 169, 200     | 0     |
| 9   | BI    | 127/127 (100%)  | 3.78   | 77 (60%) 0 0   | 138, 176, 209, 229    | 0     |
| 10  | AJ    | 99/99 (100%)    | 2.03   | 41 (41%) 0 0   | 94, 121, 153, 168     | 0     |
| 10  | BJ    | 98/99 (98%)     | 4.86   | 78 (79%) 0 0   | 141, 171, 197, 207    | 0     |
| 11  | AK    | 117/117 (100%)  | 1.61   | 35 (29%) 1 0   | 68, 112, 147, 163     | 0     |
| 11  | BK    | 117/117 (100%)  | 1.47   | 32 (27%) 1 0   | 83, 116, 148, 168     | 0     |
| 12  | AL    | 122/123 (99%)   | 0.60   | 4 (3%) 47 30   | 55, 72, 104, 132      | 0     |
| 12  | BL    | 122/123 (99%)   | 1.39   | 29 (23%) 1 1   | 79, 97, 118, 142      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2   | OWAB(Å²) |     | Q<0.9              |   |
|-----|-------|----------------|--------|-----------|----------|-----|--------------------|---|
| 13  | AM    | 114/114 (100%) | 2.48   | 57 (50%)  | 0        | 0   | 106, 131, 182, 202 | 0 |
| 13  | BM    | 114/114 (100%) | 5.55   | 105 (92%) | 0        | 0   | 203, 237, 245, 249 | 0 |
| 14  | AN    | 100/100 (100%) | 1.82   | 37 (37%)  | 0        | 0   | 90, 117, 206, 215  | 0 |
| 14  | BN    | 100/100 (100%) | 3.85   | 75 (75%)  | 0        | 0   | 132, 181, 239, 250 | 0 |
| 15  | AO    | 88/88 (100%)   | 0.69   | 10 (11%)  | 6        | 3   | 72, 94, 112, 132   | 0 |
| 15  | BO    | 88/88 (100%)   | 1.26   | 20 (22%)  | 1        | 1   | 79, 112, 132, 150  | 0 |
| 16  | AP    | 82/82 (100%)   | 1.27   | 19 (23%)  | 1        | 1   | 67, 86, 121, 139   | 0 |
| 16  | BP    | 82/82 (100%)   | 2.78   | 47 (57%)  | 0        | 0   | 94, 111, 157, 166  | 0 |
| 17  | AQ    | 80/80 (100%)   | 0.65   | 5 (6%)    | 21       | 12  | 70, 86, 119, 143   | 0 |
| 17  | BQ    | 80/80 (100%)   | 2.17   | 34 (42%)  | 0        | 0   | 100, 128, 151, 156 | 0 |
| 18  | AR    | 55/55 (100%)   | 1.21   | 12 (21%)  | 1        | 1   | 79, 99, 135, 164   | 0 |
| 18  | BR    | 55/55 (100%)   | 1.07   | 6 (10%)   | 6        | 4   | 80, 96, 129, 157   | 0 |
| 19  | AS    | 79/79 (100%)   | 1.56   | 24 (30%)  | 0        | 0   | 103, 119, 156, 164 | 0 |
| 19  | BS    | 79/79 (100%)   | 5.06   | 66 (83%)  | 0        | 0   | 215, 232, 243, 251 | 0 |
| 20  | AT    | 86/86 (100%)   | 1.04   | 9 (10%)   | 7        | 4   | 70, 85, 120, 133   | 0 |
| 20  | BT    | 85/86 (98%)    | 3.27   | 53 (62%)  | 0        | 0   | 108, 128, 165, 179 | 0 |
| 21  | AU    | 56/56 (100%)   | 1.59   | 17 (30%)  | 0        | 0   | 83, 123, 159, 172  | 0 |
| 21  | BU    | 56/56 (100%)   | 1.01   | 8 (14%)   | 3        | 1   | 80, 106, 149, 160  | 0 |
| 22  | C1    | 56/56 (100%)   | 3.35   | 39 (69%)  | 0        | 0   | 110, 150, 178, 195 | 0 |
| 22  | D1    | 56/56 (100%)   | 0.59   | 0         | 100      | 100 | 26, 46, 71, 102    | 0 |
| 23  | C2    | 50/51 (98%)    | 3.69   | 34 (68%)  | 0        | 0   | 133, 148, 161, 183 | 0 |
| 23  | D2    | 51/51 (100%)   | 0.72   | 5 (9%)    | 8        | 5   | 55, 69, 95, 110    | 0 |
| 24  | C3    | 46/46 (100%)   | 4.61   | 39 (84%)  | 0        | 0   | 108, 117, 127, 138 | 0 |
| 24  | D3    | 46/46 (100%)   | 0.61   | 2 (4%)    | 36       | 22  | 38, 46, 61, 104    | 0 |
| 25  | C4    | 64/64 (100%)   | 3.12   | 44 (68%)  | 0        | 0   | 112, 130, 142, 148 | 0 |
| 25  | D4    | 64/64 (100%)   | 0.58   | 0         | 100      | 100 | 36, 44, 53, 68     | 0 |
| 26  | C5    | 38/38 (100%)   | 2.72   | 23 (60%)  | 0        | 0   | 108, 122, 133, 143 | 0 |
| 26  | D5    | 38/38 (100%)   | 0.64   | 1 (2%)    | 56       | 37  | 43, 54, 68, 91     | 0 |
| 27  | C0    | 58/58 (100%)   | 3.37   | 40 (68%)  | 0        | 0   | 104, 121, 140, 143 | 0 |
| 27  | D0    | 58/58 (100%)   | 0.52   | 0         | 100      | 100 | 33, 40, 60, 72     | 0 |
| 28  | CB    | 118/120 (98%)  | 1.72   | 46 (38%)  | 0        | 0   | 140, 195, 250, 254 | 0 |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | DB    | 120/120 (100%)  | 0.31   | 0 100 100      | 33, 60, 99, 143       | 0     |
| 29  | CC    | 271/272 (99%)   | 1.49   | 87 (32%) 0 0   | 88, 119, 152, 165     | 0     |
| 29  | DC    | 271/272 (99%)   | 0.30   | 6 (2%) 62 43   | 31, 57, 83, 96        | 0     |
| 30  | CD    | 209/209 (100%)  | 2.99   | 130 (62%) 0 0  | 103, 134, 170, 190    | 0     |
| 31  | CA    | 2876/2904 (99%) | 1.90   | 1026 (35%) 0 0 | 73, 178, 274, 295     | 0     |
| 32  | DD    | 208/209 (99%)   | 0.16   | 0 100 100      | 22, 41, 69, 91        | 0     |
| 33  | CE    | 201/201 (100%)  | 3.31   | 141 (70%) 0 0  | 119, 167, 201, 218    | 0     |
| 33  | DE    | 201/201 (100%)  | 0.38   | 3 (1%) 74 55   | 31, 59, 101, 141      | 0     |
| 34  | CF    | 177/178 (99%)   | 4.97   | 153 (86%) 0 0  | 204, 217, 226, 233    | 0     |
| 34  | DF    | 177/178 (99%)   | 0.68   | 16 (9%) 10 6   | 58, 84, 125, 138      | 0     |
| 35  | CG    | 176/176 (100%)  | 4.32   | 144 (81%) 0 0  | 140, 181, 219, 228    | 0     |
| 35  | DG    | 176/176 (100%)  | 0.34   | 8 (4%) 34 21   | 49, 73, 99, 128       | 0     |
| 36  | CH    | 149/149 (100%)  | 2.35   | 80 (53%) 0 0   | 86, 156, 175, 183     | 0     |
| 36  | DH    | 149/149 (100%)  | 2.11   | 63 (42%) 0 0   | 79, 157, 193, 208     | 0     |
| 37  | CJ    | 134/134 (100%)  | 7.53   | 127 (94%) 0 0  | 236, 253, 264, 272    | 0     |
| 37  | DJ    | 134/134 (100%)  | 5.80   | 110 (82%) 0 0  | 204, 229, 238, 246    | 0     |
| 38  | CK    | 142/142 (100%)  | 2.30   | 71 (50%) 0 0   | 105, 129, 168, 221    | 0     |
| 38  | DK    | 142/142 (100%)  | 0.12   | 0 100 100      | 25, 37, 61, 75        | 0     |
| 39  | CL    | 122/123 (99%)   | 1.69   | 41 (33%) 0 0   | 95, 116, 149, 167     | 0     |
| 39  | DL    | 123/123 (100%)  | 0.09   | 0 100 100      | 30, 46, 71, 109       | 0     |
| 40  | CM    | 144/144 (100%)  | 4.10   | 116 (80%) 0 0  | 113, 163, 214, 236    | 0     |
| 40  | DM    | 144/144 (100%)  | 0.32   | 3 (2%) 64 45   | 21, 58, 88, 117       | 0     |
| 41  | CN    | 135/136 (99%)   | 1.38   | 35 (25%) 1 0   | 98, 119, 150, 189     | 0     |
| 41  | DN    | 135/136 (99%)   | -0.02  | 0 100 100      | 29, 43, 69, 88        | 0     |
| 42  | CO    | 120/125 (96%)   | 2.71   | 71 (59%) 0 0   | 110, 132, 155, 186    | 0     |
| 42  | DO    | 125/125 (100%)  | 0.22   | 1 (0%) 86 71   | 29, 39, 68, 111       | 0     |
| 43  | CP    | 116/117 (99%)   | 3.84   | 87 (75%) 0 0   | 147, 171, 185, 189    | 0     |
| 43  | DP    | 117/117 (100%)  | 0.28   | 0 100 100      | 47, 60, 87, 97        | 0     |
| 44  | CQ    | 114/114 (100%)  | 2.53   | 65 (57%) 0 0   | 108, 126, 156, 172    | 0     |
| 44  | DQ    | 114/114 (100%)  | 0.14   | 3 (2%) 56 37   | 34, 52, 82, 114       | 0     |
| 45  | CR    | 117/117 (100%)  | 2.82   | 72 (61%) 0 0   | 98, 138, 174, 199     | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-------------------|--------|----------------|-----------------------|--------|
| 45  | DR    | 117/117 (100%)    | 0.29   | 1 (0%) 84 69   | 23, 33, 48, 70        | 0      |
| 46  | CS    | 103/103 (100%)    | 4.12   | 85 (82%) 0 0   | 114, 143, 185, 201    | 0      |
| 46  | DS    | 103/103 (100%)    | 0.13   | 1 (0%) 82 66   | 26, 45, 71, 93        | 0      |
| 47  | CT    | 110/110 (100%)    | 2.50   | 62 (56%) 0 0   | 109, 137, 180, 193    | 0      |
| 47  | DT    | 110/110 (100%)    | 0.10   | 1 (0%) 84 69   | 21, 36, 60, 118       | 0      |
| 48  | CU    | 93/93 (100%)      | 3.96   | 73 (78%) 0 0   | 131, 156, 184, 194    | 0      |
| 48  | DU    | 93/93 (100%)      | 0.63   | 5 (5%) 26 16   | 37, 60, 114, 130      | 0      |
| 49  | CV    | 102/103 (99%)     | 5.49   | 88 (86%) 0 0   | 119, 167, 203, 213    | 0      |
| 49  | DV    | 102/103 (99%)     | 0.55   | 11 (10%) 6 4   | 47, 64, 112, 144      | 0      |
| 50  | CW    | 94/94 (100%)      | 2.60   | 53 (56%) 0 0   | 125, 145, 165, 170    | 0      |
| 50  | DW    | 94/94 (100%)      | 0.06   | 0 100 100      | 38, 56, 80, 92        | 0      |
| 51  | CX    | 75/76 (98%)       | 2.93   | 39 (52%) 0 0   | 111, 134, 148, 178    | 0      |
| 51  | DX    | 76/76 (100%)      | 0.09   | 1 (1%) 77 59   | 31, 45, 69, 107       | 0      |
| 52  | CY    | 77/77 (100%)      | 1.92   | 32 (41%) 0 0   | 103, 122, 147, 168    | 0      |
| 52  | DY    | 77/77 (100%)      | 0.30   | 1 (1%) 77 59   | 37, 59, 92, 108       | 0      |
| 53  | CZ    | 62/62 (100%)      | 4.44   | 50 (80%) 0 0   | 134, 171, 184, 195    | 0      |
| 53  | DZ    | 62/62 (100%)      | 0.77   | 6 (9%) 8 5     | 52, 75, 111, 132      | 0      |
| 54  | DI    | 135/135 (100%)    | 2.40   | 71 (52%) 0 0   | 82, 158, 202, 211     | 1 (0%) |
| 55  | DA    | 2873/2904 (98%)   | 0.64   | 135 (4%) 32 20 | 22, 48, 215, 300      | 0      |
| All | All   | 20634/20751 (99%) | 1.61   | 5726 (27%) 1 0 | 21, 116, 247, 300     | 1 (0%) |

All (5726) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 37  | DJ    | 54  | PRO  | 42.5 |
| 37  | DJ    | 76  | ALA  | 23.0 |
| 9   | BI    | 128 | SER  | 22.9 |
| 37  | CJ    | 13  | VAL  | 22.8 |
| 37  | DJ    | 55  | ILE  | 21.9 |
| 37  | CJ    | 69  | PHE  | 21.4 |
| 37  | DJ    | 53  | LEU  | 21.2 |
| 37  | CJ    | 76  | ALA  | 20.8 |
| 37  | CJ    | 14  | ALA  | 18.3 |
| 34  | CF    | 128 | TYR  | 18.3 |
| 37  | CJ    | 11  | LEU  | 18.0 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | CJ    | 12   | GLN  | 18.0 |
| 37  | DJ    | 114  | ALA  | 17.9 |
| 9   | BI    | 16   | ALA  | 17.1 |
| 51  | CX    | 54   | GLY  | 16.3 |
| 37  | DJ    | 79   | LEU  | 16.2 |
| 49  | CV    | 80   | ALA  | 16.1 |
| 9   | BI    | 31   | ASN  | 16.1 |
| 10  | BJ    | 41   | PRO  | 16.0 |
| 49  | CV    | 31   | SER  | 15.7 |
| 31  | CA    | 2172 | U    | 15.3 |
| 9   | AI    | 130  | ARG  | 15.2 |
| 10  | BJ    | 74   | VAL  | 15.1 |
| 10  | BJ    | 8    | ILE  | 15.1 |
| 7   | BG    | 62   | PHE  | 14.9 |
| 37  | CJ    | 54   | PRO  | 14.9 |
| 55  | DA    | 2120 | G    | 14.7 |
| 7   | BG    | 65   | ALA  | 14.7 |
| 20  | BT    | 4    | ILE  | 14.6 |
| 37  | CJ    | 138  | LEU  | 14.6 |
| 37  | DJ    | 80   | LEU  | 14.5 |
| 49  | CV    | 20   | GLY  | 14.5 |
| 40  | CM    | 114  | GLY  | 14.5 |
| 34  | CF    | 85   | ILE  | 14.5 |
| 13  | BM    | 45   | ILE  | 14.3 |
| 1   | BA    | 211  | G    | 14.1 |
| 46  | CS    | 96   | VAL  | 14.0 |
| 31  | CA    | 1067 | A    | 14.0 |
| 49  | CV    | 13   | VAL  | 14.0 |
| 37  | CJ    | 57   | VAL  | 13.9 |
| 9   | BI    | 130  | ARG  | 13.9 |
| 37  | DJ    | 96   | ASP  | 13.7 |
| 7   | BG    | 52   | GLN  | 13.7 |
| 37  | CJ    | 55   | ILE  | 13.7 |
| 37  | DJ    | 135  | SER  | 13.7 |
| 37  | DJ    | 78   | VAL  | 13.6 |
| 10  | BJ    | 42   | LEU  | 13.5 |
| 33  | CE    | 55   | SER  | 13.5 |
| 10  | BJ    | 73   | LEU  | 13.4 |
| 37  | CJ    | 80   | LEU  | 13.3 |
| 19  | BS    | 48   | THR  | 13.2 |
| 40  | CM    | 80   | SER  | 13.2 |
| 31  | CA    | 1068 | G    | 13.2 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | CJ    | 82   | LYS  | 13.2 |
| 19  | BS    | 66   | MET  | 13.1 |
| 49  | CV    | 36   | VAL  | 13.1 |
| 34  | CF    | 156  | ILE  | 13.1 |
| 37  | DJ    | 13   | VAL  | 13.0 |
| 53  | CZ    | 45   | GLN  | 13.0 |
| 14  | BN    | 60   | GLN  | 13.0 |
| 9   | BI    | 17   | ALA  | 12.9 |
| 7   | BG    | 49   | THR  | 12.9 |
| 54  | DI    | 131  | THR  | 12.8 |
| 37  | CJ    | 129  | ILE  | 12.8 |
| 37  | CJ    | 17   | MET  | 12.8 |
| 7   | BG    | 111  | ARG  | 12.8 |
| 24  | C3    | 1    | MET  | 12.7 |
| 37  | CJ    | 99   | GLY  | 12.7 |
| 1   | BA    | 1307 | U    | 12.6 |
| 37  | DJ    | 88   | SER  | 12.6 |
| 37  | CJ    | 20   | PRO  | 12.6 |
| 37  | CJ    | 56   | PRO  | 12.6 |
| 37  | DJ    | 67   | PHE  | 12.5 |
| 34  | CF    | 76   | GLY  | 12.5 |
| 37  | CJ    | 21   | SER  | 12.5 |
| 30  | CD    | 4    | LEU  | 12.5 |
| 19  | BS    | 29   | LYS  | 12.4 |
| 48  | CU    | 83   | ALA  | 12.3 |
| 30  | CD    | 6    | GLY  | 12.3 |
| 34  | CF    | 157  | THR  | 12.3 |
| 33  | CE    | 172  | ALA  | 12.3 |
| 7   | BG    | 42   | ILE  | 12.3 |
| 1   | BA    | 1302 | C    | 12.3 |
| 48  | CU    | 43   | ILE  | 12.3 |
| 1   | AA    | 86   | G    | 12.3 |
| 13  | BM    | 46   | SER  | 12.2 |
| 13  | BM    | 105  | ASN  | 12.2 |
| 1   | BA    | 983  | A    | 12.2 |
| 1   | BA    | 1242 | G    | 12.2 |
| 53  | CZ    | 32   | ALA  | 12.2 |
| 7   | BG    | 133  | THR  | 12.1 |
| 40  | CM    | 101  | ILE  | 12.1 |
| 7   | BG    | 75   | VAL  | 12.1 |
| 34  | CF    | 40   | VAL  | 12.1 |
| 46  | CS    | 50   | GLY  | 12.1 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | CV    | 33   | LYS  | 12.1 |
| 13  | BM    | 10   | PRO  | 12.1 |
| 22  | C1    | 5    | GLN  | 12.0 |
| 48  | CU    | 60   | THR  | 12.0 |
| 35  | CG    | 32   | GLU  | 11.9 |
| 37  | CJ    | 23   | PRO  | 11.9 |
| 48  | CU    | 59   | ASN  | 11.9 |
| 1   | BA    | 1030 | U    | 11.8 |
| 1   | BA    | 1024 | G    | 11.8 |
| 31  | CA    | 2174 | C    | 11.8 |
| 9   | BI    | 67   | VAL  | 11.8 |
| 46  | CS    | 27   | ILE  | 11.7 |
| 35  | CG    | 40   | ALA  | 11.7 |
| 55  | DA    | 2163 | A    | 11.7 |
| 35  | CG    | 108  | GLY  | 11.6 |
| 1   | BA    | 1020 | G    | 11.6 |
| 37  | CJ    | 42   | PHE  | 11.6 |
| 23  | C2    | 24   | THR  | 11.5 |
| 7   | BG    | 116  | MET  | 11.5 |
| 49  | CV    | 39   | ILE  | 11.5 |
| 37  | CJ    | 139  | VAL  | 11.4 |
| 9   | BI    | 126  | GLN  | 11.4 |
| 13  | BM    | 95   | LEU  | 11.4 |
| 37  | CJ    | 51   | LYS  | 11.4 |
| 34  | CF    | 154  | ILE  | 11.4 |
| 37  | CJ    | 126  | THR  | 11.3 |
| 37  | CJ    | 59   | ILE  | 11.2 |
| 46  | CS    | 32   | THR  | 11.2 |
| 31  | CA    | 2110 | G    | 11.2 |
| 13  | BM    | 84   | GLY  | 11.2 |
| 34  | CF    | 97   | TRP  | 11.2 |
| 40  | CM    | 100  | ILE  | 11.2 |
| 49  | CV    | 78   | GLY  | 11.1 |
| 40  | CM    | 81   | ASP  | 11.1 |
| 1   | AA    | 1030 | U    | 11.1 |
| 31  | CA    | 931  | U    | 11.1 |
| 31  | CA    | 2126 | A    | 11.0 |
| 7   | BG    | 134  | ALA  | 11.0 |
| 37  | CJ    | 38   | PHE  | 11.0 |
| 13  | BM    | 32   | ALA  | 11.0 |
| 31  | CA    | 331  | C    | 10.9 |
| 1   | BA    | 209  | U    | 10.9 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | CW    | 57   | TYR  | 10.9 |
| 13  | BM    | 22   | ILE  | 10.9 |
| 34  | CF    | 65   | PRO  | 10.8 |
| 14  | BN    | 4    | GLN  | 10.8 |
| 1   | BA    | 1022 | A    | 10.8 |
| 35  | CG    | 33   | LEU  | 10.8 |
| 40  | CM    | 79   | LEU  | 10.8 |
| 31  | CA    | 1537 | G    | 10.7 |
| 37  | CJ    | 121  | ASP  | 10.7 |
| 13  | BM    | 23   | TYR  | 10.7 |
| 37  | CJ    | 120  | ALA  | 10.6 |
| 40  | CM    | 92   | LEU  | 10.6 |
| 20  | BT    | 3    | ASN  | 10.6 |
| 23  | C2    | 47   | VAL  | 10.6 |
| 53  | CZ    | 15   | ASN  | 10.6 |
| 14  | BN    | 36   | ALA  | 10.6 |
| 37  | CJ    | 97   | LYS  | 10.6 |
| 37  | DJ    | 12   | GLN  | 10.6 |
| 30  | CD    | 26   | VAL  | 10.5 |
| 1   | BA    | 1021 | A    | 10.5 |
| 49  | CV    | 35   | ILE  | 10.5 |
| 37  | CJ    | 132  | THR  | 10.4 |
| 22  | C1    | 3    | VAL  | 10.4 |
| 49  | CV    | 50   | PRO  | 10.4 |
| 37  | CJ    | 78   | VAL  | 10.4 |
| 7   | BG    | 43   | VAL  | 10.4 |
| 35  | CG    | 103  | ILE  | 10.4 |
| 37  | CJ    | 22   | PRO  | 10.3 |
| 37  | DJ    | 23   | PRO  | 10.3 |
| 34  | CF    | 106  | ILE  | 10.3 |
| 43  | CP    | 117  | PHE  | 10.3 |
| 35  | CG    | 148  | LEU  | 10.3 |
| 37  | DJ    | 138  | LEU  | 10.2 |
| 35  | CG    | 157  | TYR  | 10.2 |
| 37  | DJ    | 24   | VAL  | 10.2 |
| 31  | CA    | 1103 | A    | 10.2 |
| 9   | BI    | 11   | ARG  | 10.2 |
| 37  | CJ    | 130  | GLU  | 10.1 |
| 35  | CG    | 62   | TRP  | 10.1 |
| 1   | BA    | 1025 | U    | 10.1 |
| 7   | BG    | 73   | VAL  | 10.1 |
| 3   | BC    | 196  | ILE  | 10.1 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | CG    | 105  | LEU  | 10.0 |
| 37  | CJ    | 68   | THR  | 10.0 |
| 34  | CF    | 155  | THR  | 10.0 |
| 37  | CJ    | 87   | LYS  | 10.0 |
| 37  | CJ    | 43   | ASN  | 10.0 |
| 37  | CJ    | 94   | ASN  | 10.0 |
| 19  | BS    | 14   | HIS  | 10.0 |
| 7   | BG    | 103  | TRP  | 9.9  |
| 23  | C2    | 21   | TYR  | 9.9  |
| 54  | DI    | 128  | THR  | 9.9  |
| 7   | BG    | 91   | VAL  | 9.9  |
| 31  | CA    | 1087 | G    | 9.9  |
| 34  | CF    | 35   | THR  | 9.9  |
| 10  | BJ    | 26   | VAL  | 9.9  |
| 31  | CA    | 2125 | G    | 9.9  |
| 55  | DA    | 2121 | G    | 9.9  |
| 7   | BG    | 77   | SER  | 9.8  |
| 1   | BA    | 1305 | G    | 9.8  |
| 7   | BG    | 66   | LEU  | 9.8  |
| 22  | C1    | 2    | ALA  | 9.8  |
| 24  | C3    | 42   | LEU  | 9.8  |
| 37  | CJ    | 96   | ASP  | 9.7  |
| 13  | BM    | 5    | ALA  | 9.7  |
| 34  | CF    | 86   | GLY  | 9.7  |
| 30  | CD    | 10   | GLY  | 9.7  |
| 34  | CF    | 129  | SER  | 9.7  |
| 13  | BM    | 83   | LEU  | 9.7  |
| 31  | CA    | 1084 | A    | 9.7  |
| 7   | BG    | 69   | VAL  | 9.7  |
| 7   | BG    | 151  | PHE  | 9.7  |
| 19  | BS    | 38   | SER  | 9.7  |
| 1   | BA    | 1016 | A    | 9.6  |
| 22  | C1    | 6    | ASN  | 9.6  |
| 9   | AI    | 20   | PHE  | 9.6  |
| 13  | BM    | 33   | ILE  | 9.6  |
| 37  | CJ    | 98   | VAL  | 9.6  |
| 37  | CJ    | 89   | GLY  | 9.6  |
| 13  | BM    | 96   | PRO  | 9.6  |
| 13  | BM    | 39   | ILE  | 9.6  |
| 44  | CQ    | 85   | SER  | 9.6  |
| 31  | CA    | 1086 | A    | 9.5  |
| 1   | BA    | 204  | G    | 9.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | CM    | 82   | LEU  | 9.5  |
| 10  | BJ    | 40   | ILE  | 9.5  |
| 24  | C3    | 35   | ARG  | 9.4  |
| 37  | DJ    | 94   | ASN  | 9.4  |
| 19  | BS    | 49   | ILE  | 9.4  |
| 1   | AA    | 87   | C    | 9.4  |
| 49  | CV    | 87   | PHE  | 9.4  |
| 37  | CJ    | 61   | VAL  | 9.4  |
| 34  | CF    | 105  | THR  | 9.4  |
| 3   | BC    | 155  | GLY  | 9.4  |
| 9   | BI    | 32   | GLN  | 9.3  |
| 51  | CX    | 53   | CYS  | 9.3  |
| 13  | BM    | 19   | LEU  | 9.3  |
| 37  | CJ    | 28   | LEU  | 9.3  |
| 53  | CZ    | 29   | ARG  | 9.3  |
| 1   | BA    | 1274 | A    | 9.3  |
| 16  | BP    | 57   | ILE  | 9.3  |
| 43  | CP    | 40   | ILE  | 9.3  |
| 1   | BA    | 1222 | G    | 9.3  |
| 43  | CP    | 64   | TYR  | 9.2  |
| 10  | BJ    | 90   | LEU  | 9.2  |
| 1   | BA    | 985  | C    | 9.2  |
| 43  | CP    | 63   | LYS  | 9.2  |
| 46  | CS    | 88   | GLY  | 9.2  |
| 37  | DJ    | 36   | MET  | 9.2  |
| 10  | BJ    | 87   | LEU  | 9.1  |
| 34  | CF    | 117  | LEU  | 9.1  |
| 37  | DJ    | 133  | ALA  | 9.1  |
| 55  | DA    | 2124 | G    | 9.1  |
| 10  | BJ    | 76   | ILE  | 9.1  |
| 49  | CV    | 19   | LYS  | 9.1  |
| 3   | BC    | 193  | TYR  | 9.1  |
| 46  | CS    | 63   | VAL  | 9.1  |
| 7   | BG    | 71   | PRO  | 9.1  |
| 31  | CA    | 329  | G    | 9.1  |
| 18  | BR    | 20   | GLU  | 9.1  |
| 7   | BG    | 112  | GLY  | 9.1  |
| 31  | CA    | 2666 | C    | 9.1  |
| 3   | BC    | 197  | GLY  | 9.1  |
| 31  | CA    | 613  | A    | 9.1  |
| 19  | BS    | 28   | LYS  | 9.1  |
| 7   | BG    | 46   | ALA  | 9.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | BG    | 137  | LYS  | 9.1  |
| 20  | BT    | 60   | ARG  | 9.0  |
| 37  | CJ    | 71   | THR  | 9.0  |
| 14  | BN    | 72   | GLY  | 9.0  |
| 48  | CU    | 47   | VAL  | 9.0  |
| 24  | C3    | 17   | GLY  | 9.0  |
| 31  | CA    | 1066 | U    | 9.0  |
| 49  | CV    | 75   | ALA  | 9.0  |
| 55  | DA    | 2110 | G    | 8.9  |
| 13  | BM    | 48   | LEU  | 8.9  |
| 7   | BG    | 53   | ARG  | 8.9  |
| 1   | BA    | 1032 | G    | 8.9  |
| 53  | CZ    | 17   | GLU  | 8.9  |
| 49  | CV    | 14   | LEU  | 8.9  |
| 34  | CF    | 131  | GLY  | 8.9  |
| 49  | CV    | 79   | LYS  | 8.8  |
| 37  | CJ    | 90   | SER  | 8.8  |
| 9   | BI    | 66   | THR  | 8.8  |
| 49  | CV    | 29   | LEU  | 8.8  |
| 1   | BA    | 958  | A    | 8.8  |
| 34  | CF    | 153  | ASP  | 8.8  |
| 49  | CV    | 89   | ASP  | 8.8  |
| 49  | CV    | 3    | ALA  | 8.8  |
| 19  | BS    | 63   | THR  | 8.8  |
| 48  | CU    | 72   | GLN  | 8.8  |
| 46  | CS    | 20   | VAL  | 8.8  |
| 29  | CC    | 241  | GLY  | 8.8  |
| 19  | BS    | 31   | LEU  | 8.8  |
| 40  | CM    | 89   | VAL  | 8.8  |
| 29  | CC    | 239  | ASN  | 8.8  |
| 48  | CU    | 55   | VAL  | 8.7  |
| 27  | C0    | 56   | LYS  | 8.7  |
| 16  | BP    | 17   | TYR  | 8.7  |
| 13  | BM    | 64   | VAL  | 8.7  |
| 1   | BA    | 1271 | A    | 8.7  |
| 34  | CF    | 126  | GLY  | 8.7  |
| 1   | BA    | 1243 | C    | 8.7  |
| 24  | C3    | 18   | PHE  | 8.7  |
| 31  | CA    | 2665 | A    | 8.7  |
| 37  | CJ    | 75   | PRO  | 8.7  |
| 9   | BI    | 18   | ARG  | 8.7  |
| 10  | BJ    | 72   | ARG  | 8.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 40         | CM           | 78         | ARG         | 8.7         |
| 34         | CF           | 176        | PRO         | 8.7         |
| 37         | DJ           | 69         | PHE         | 8.6         |
| 10         | BJ           | 77         | VAL         | 8.6         |
| 54         | DI           | 130        | PRO         | 8.6         |
| 37         | CJ           | 60         | THR         | 8.6         |
| 31         | CA           | 1175       | A           | 8.6         |
| 34         | CF           | 132        | VAL         | 8.6         |
| 34         | CF           | 95         | ARG         | 8.6         |
| 10         | BJ           | 12         | ALA         | 8.6         |
| 24         | C3           | 7          | PRO         | 8.6         |
| 33         | CE           | 33         | VAL         | 8.6         |
| 37         | CJ           | 47         | ASP         | 8.6         |
| 37         | DJ           | 116        | ASP         | 8.6         |
| 19         | BS           | 37         | ARG         | 8.6         |
| 34         | CF           | 23         | ASN         | 8.6         |
| 1          | BA           | 1026       | G           | 8.6         |
| 13         | AM           | 30         | SER         | 8.6         |
| 37         | DJ           | 89         | GLY         | 8.6         |
| 34         | CF           | 130        | MET         | 8.6         |
| 37         | DJ           | 115        | ALA         | 8.6         |
| 7          | BG           | 45         | SER         | 8.6         |
| 49         | CV           | 98         | SER         | 8.6         |
| 48         | CU           | 10         | VAL         | 8.5         |
| 14         | BN           | 20         | TYR         | 8.5         |
| 33         | CE           | 143        | LEU         | 8.5         |
| 31         | CA           | 1211       | C           | 8.5         |
| 34         | CF           | 147        | ASP         | 8.5         |
| 14         | AN           | 21         | PHE         | 8.5         |
| 31         | CA           | 2123       | G           | 8.5         |
| 3          | BC           | 195        | VAL         | 8.5         |
| 49         | CV           | 32         | GLY         | 8.5         |
| 3          | BC           | 71         | ALA         | 8.5         |
| 35         | CG           | 52         | PHE         | 8.5         |
| 37         | DJ           | 59         | ILE         | 8.5         |
| 7          | BG           | 17         | LYS         | 8.5         |
| 1          | BA           | 1296       | C           | 8.5         |
| 31         | CA           | 1083       | U           | 8.5         |
| 35         | CG           | 43         | VAL         | 8.5         |
| 7          | BG           | 106        | GLU         | 8.5         |
| 9          | AI           | 21         | ILE         | 8.5         |
| 37         | DJ           | 20         | PRO         | 8.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 7          | BG           | 79         | ARG         | 8.4         |
| 37         | CJ           | 9          | VAL         | 8.4         |
| 37         | DJ           | 68         | THR         | 8.4         |
| 7          | BG           | 148        | ASN         | 8.4         |
| 9          | BI           | 68         | LYS         | 8.4         |
| 7          | BG           | 132        | GLY         | 8.4         |
| 34         | CF           | 144        | ASP         | 8.4         |
| 48         | CU           | 42         | GLU         | 8.4         |
| 13         | BM           | 40         | ALA         | 8.4         |
| 19         | BS           | 60         | VAL         | 8.3         |
| 23         | C2           | 36         | LEU         | 8.3         |
| 45         | CR           | 106        | PHE         | 8.3         |
| 49         | CV           | 81         | ASP         | 8.3         |
| 7          | BG           | 39         | ALA         | 8.3         |
| 50         | CW           | 94         | ALA         | 8.3         |
| 53         | CZ           | 33         | ALA         | 8.3         |
| 1          | BA           | 984        | C           | 8.3         |
| 19         | BS           | 5          | LEU         | 8.3         |
| 17         | BQ           | 70         | THR         | 8.3         |
| 51         | CX           | 33         | ALA         | 8.3         |
| 9          | BI           | 40         | GLY         | 8.3         |
| 10         | BJ           | 7          | ARG         | 8.3         |
| 34         | CF           | 80         | ARG         | 8.3         |
| 43         | CP           | 99         | TYR         | 8.3         |
| 1          | BA           | 942        | G           | 8.3         |
| 48         | CU           | 15         | HIS         | 8.3         |
| 49         | CV           | 48         | PRO         | 8.2         |
| 35         | CG           | 172        | LYS         | 8.2         |
| 10         | BJ           | 86         | ALA         | 8.2         |
| 19         | BS           | 24         | GLU         | 8.2         |
| 40         | CM           | 20         | GLY         | 8.2         |
| 13         | BM           | 2          | ALA         | 8.2         |
| 1          | BA           | 948        | C           | 8.2         |
| 24         | C3           | 30         | VAL         | 8.2         |
| 40         | CM           | 71         | ALA         | 8.2         |
| 7          | BG           | 4          | ARG         | 8.2         |
| 33         | CE           | 104        | ALA         | 8.2         |
| 31         | CA           | 75         | G           | 8.2         |
| 7          | BG           | 141        | VAL         | 8.2         |
| 43         | CP           | 51         | ALA         | 8.2         |
| 7          | BG           | 109        | ARG         | 8.2         |
| 14         | BN           | 35         | ASN         | 8.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | DJ    | 137  | GLY  | 8.2  |
| 43  | CP    | 24   | THR  | 8.2  |
| 9   | BI    | 127  | PHE  | 8.1  |
| 19  | BS    | 74   | PHE  | 8.1  |
| 31  | CA    | 1085 | A    | 8.1  |
| 42  | CO    | 111  | ALA  | 8.1  |
| 2   | BB    | 34   | ALA  | 8.1  |
| 37  | CJ    | 83   | ALA  | 8.1  |
| 44  | CQ    | 84   | ILE  | 8.1  |
| 3   | BC    | 119  | SER  | 8.1  |
| 55  | DA    | 2125 | G    | 8.1  |
| 23  | C2    | 52   | ALA  | 8.1  |
| 1   | BA    | 1241 | G    | 8.1  |
| 11  | BK    | 47   | ALA  | 8.0  |
| 13  | BM    | 55   | THR  | 8.0  |
| 33  | CE    | 173  | THR  | 8.0  |
| 19  | BS    | 32   | ARG  | 8.0  |
| 37  | CJ    | 33   | VAL  | 8.0  |
| 55  | DA    | 2174 | C    | 8.0  |
| 10  | BJ    | 94   | ALA  | 8.0  |
| 35  | CG    | 151  | TYR  | 8.0  |
| 10  | BJ    | 71   | LEU  | 8.0  |
| 48  | CU    | 46   | ALA  | 8.0  |
| 55  | DA    | 896  | A    | 8.0  |
| 19  | BS    | 39   | THR  | 8.0  |
| 48  | CU    | 61   | LEU  | 8.0  |
| 35  | CG    | 171  | THR  | 8.0  |
| 19  | BS    | 76   | PRO  | 8.0  |
| 55  | DA    | 1067 | A    | 8.0  |
| 49  | CV    | 88   | GLU  | 8.0  |
| 24  | C3    | 36   | ALA  | 7.9  |
| 1   | BA    | 82   | G    | 7.9  |
| 2   | AB    | 6    | MET  | 7.9  |
| 2   | AB    | 136  | MET  | 7.9  |
| 2   | AB    | 14   | VAL  | 7.9  |
| 1   | BA    | 1017 | U    | 7.9  |
| 16  | BP    | 80   | LYS  | 7.9  |
| 31  | CA    | 2124 | G    | 7.9  |
| 37  | CJ    | 133  | ALA  | 7.9  |
| 42  | CO    | 28   | LEU  | 7.9  |
| 55  | DA    | 2116 | G    | 7.9  |
| 40  | CM    | 8    | PRO  | 7.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | BG    | 144  | MET  | 7.9  |
| 14  | AN    | 23   | LYS  | 7.9  |
| 20  | BT    | 72   | ALA  | 7.9  |
| 33  | CE    | 150  | THR  | 7.9  |
| 1   | AA    | 1031 | C    | 7.9  |
| 35  | CG    | 111  | HIS  | 7.9  |
| 33  | CE    | 23   | PHE  | 7.9  |
| 1   | BA    | 80   | A    | 7.9  |
| 14  | AN    | 31   | ILE  | 7.9  |
| 24  | C3    | 33   | ARG  | 7.9  |
| 31  | CA    | 330  | A    | 7.9  |
| 13  | BM    | 47   | GLU  | 7.8  |
| 31  | CA    | 1078 | U    | 7.8  |
| 40  | CM    | 130  | GLY  | 7.8  |
| 1   | AA    | 1032 | G    | 7.8  |
| 7   | BG    | 54   | SER  | 7.8  |
| 36  | DH    | 137  | GLU  | 7.8  |
| 55  | DA    | 138  | U    | 7.8  |
| 9   | BI    | 14   | SER  | 7.8  |
| 43  | CP    | 54   | VAL  | 7.8  |
| 13  | AM    | 33   | ILE  | 7.8  |
| 3   | BC    | 198  | VAL  | 7.8  |
| 45  | CR    | 74   | ILE  | 7.8  |
| 13  | BM    | 85   | CYS  | 7.8  |
| 22  | C1    | 4    | GLN  | 7.7  |
| 7   | BG    | 41   | SER  | 7.7  |
| 13  | BM    | 25   | VAL  | 7.7  |
| 34  | CF    | 31   | VAL  | 7.7  |
| 35  | CG    | 169  | VAL  | 7.7  |
| 35  | CG    | 26   | ILE  | 7.7  |
| 16  | BP    | 52   | LEU  | 7.7  |
| 34  | CF    | 93   | GLY  | 7.7  |
| 40  | CM    | 10   | GLU  | 7.7  |
| 31  | CA    | 1167 | C    | 7.7  |
| 36  | CH    | 140  | ALA  | 7.7  |
| 33  | CE    | 47   | LYS  | 7.7  |
| 13  | AM    | 43   | VAL  | 7.7  |
| 37  | CJ    | 31   | GLN  | 7.7  |
| 40  | CM    | 120  | VAL  | 7.7  |
| 30  | CD    | 186  | LEU  | 7.7  |
| 43  | CP    | 65   | THR  | 7.7  |
| 55  | DA    | 2175 | C    | 7.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | C3    | 27   | GLY  | 7.7  |
| 37  | CJ    | 119  | GLY  | 7.7  |
| 10  | BJ    | 75   | ASP  | 7.6  |
| 13  | BM    | 29   | ARG  | 7.6  |
| 1   | BA    | 1031 | C    | 7.6  |
| 51  | CX    | 63   | ALA  | 7.6  |
| 7   | BG    | 87   | VAL  | 7.6  |
| 33  | CE    | 201  | ALA  | 7.6  |
| 3   | BC    | 192  | THR  | 7.6  |
| 37  | CJ    | 29   | GLY  | 7.6  |
| 50  | CW    | 6    | ALA  | 7.6  |
| 37  | DJ    | 66   | SER  | 7.6  |
| 29  | CC    | 27   | GLY  | 7.6  |
| 10  | BJ    | 22   | THR  | 7.6  |
| 14  | BN    | 2    | ALA  | 7.6  |
| 7   | BG    | 15   | ASP  | 7.6  |
| 2   | AB    | 135  | LEU  | 7.6  |
| 10  | BJ    | 95   | GLY  | 7.5  |
| 1   | BA    | 1028 | C    | 7.5  |
| 34  | CF    | 113  | ASP  | 7.5  |
| 34  | CF    | 34   | ILE  | 7.5  |
| 35  | CG    | 83   | PHE  | 7.5  |
| 53  | CZ    | 14   | LEU  | 7.5  |
| 31  | CA    | 2171 | A    | 7.5  |
| 46  | CS    | 59   | ILE  | 7.5  |
| 53  | CZ    | 49   | ASP  | 7.5  |
| 16  | BP    | 41   | PRO  | 7.5  |
| 14  | BN    | 54   | ASP  | 7.5  |
| 33  | CE    | 119  | ILE  | 7.5  |
| 34  | CF    | 152  | LEU  | 7.5  |
| 7   | AG    | 62   | PHE  | 7.5  |
| 31  | CA    | 1077 | A    | 7.5  |
| 1   | BA    | 953  | G    | 7.5  |
| 43  | CP    | 38   | GLN  | 7.5  |
| 55  | DA    | 2172 | U    | 7.5  |
| 35  | CG    | 106  | SER  | 7.5  |
| 7   | BG    | 105  | VAL  | 7.5  |
| 40  | CM    | 77   | ILE  | 7.5  |
| 1   | BA    | 949  | A    | 7.5  |
| 31  | CA    | 1069 | A    | 7.5  |
| 43  | CP    | 29   | HIS  | 7.5  |
| 2   | BB    | 135  | LEU  | 7.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2802 | G    | 7.5  |
| 9   | BI    | 64   | TYR  | 7.4  |
| 35  | CG    | 2    | SER  | 7.4  |
| 37  | CJ    | 24   | VAL  | 7.4  |
| 55  | DA    | 1065 | U    | 7.4  |
| 25  | C4    | 37   | ALA  | 7.4  |
| 1   | BA    | 1275 | A    | 7.4  |
| 36  | CH    | 11   | ASN  | 7.4  |
| 42  | CO    | 116  | VAL  | 7.4  |
| 37  | DJ    | 134  | ARG  | 7.4  |
| 40  | CM    | 102  | GLY  | 7.4  |
| 25  | C4    | 43   | HIS  | 7.4  |
| 13  | BM    | 24   | GLY  | 7.4  |
| 55  | DA    | 1172 | C    | 7.4  |
| 9   | BI    | 44   | ALA  | 7.4  |
| 37  | CJ    | 74   | PRO  | 7.4  |
| 34  | CF    | 28   | VAL  | 7.4  |
| 49  | CV    | 83   | VAL  | 7.4  |
| 53  | CZ    | 37   | LEU  | 7.4  |
| 31  | CA    | 2402 | U    | 7.4  |
| 34  | CF    | 83   | TYR  | 7.4  |
| 26  | C5    | 10   | LEU  | 7.4  |
| 1   | BA    | 959  | A    | 7.4  |
| 1   | BA    | 1314 | C    | 7.4  |
| 37  | CJ    | 73   | THR  | 7.4  |
| 29  | CC    | 233  | GLY  | 7.4  |
| 47  | CT    | 5    | ALA  | 7.4  |
| 31  | CA    | 1075 | C    | 7.4  |
| 47  | CT    | 84   | ARG  | 7.3  |
| 31  | CA    | 1065 | U    | 7.3  |
| 31  | CA    | 312  | G    | 7.3  |
| 20  | BT    | 79   | LEU  | 7.3  |
| 37  | DJ    | 77   | ALA  | 7.3  |
| 46  | CS    | 103  | ALA  | 7.3  |
| 34  | CF    | 151  | GLY  | 7.3  |
| 31  | CA    | 2163 | A    | 7.3  |
| 31  | CA    | 2173 | A    | 7.3  |
| 41  | CN    | 136  | MET  | 7.3  |
| 1   | AA    | 88   | U    | 7.3  |
| 31  | CA    | 2300 | C    | 7.3  |
| 53  | CZ    | 59   | GLU  | 7.3  |
| 37  | CJ    | 86   | ILE  | 7.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | BS    | 30   | PRO  | 7.3  |
| 1   | BA    | 1050 | G    | 7.3  |
| 9   | BI    | 5    | GLN  | 7.3  |
| 33  | CE    | 164  | LEU  | 7.3  |
| 33  | CE    | 144  | GLU  | 7.3  |
| 53  | CZ    | 31   | GLN  | 7.3  |
| 10  | BJ    | 101  | SER  | 7.3  |
| 34  | CF    | 39   | GLY  | 7.3  |
| 38  | CK    | 22   | GLY  | 7.3  |
| 2   | BB    | 14   | VAL  | 7.3  |
| 49  | CV    | 30   | SER  | 7.3  |
| 31  | CA    | 289  | G    | 7.3  |
| 34  | CF    | 173  | PHE  | 7.2  |
| 31  | CA    | 2891 | U    | 7.2  |
| 27  | C0    | 29   | LEU  | 7.2  |
| 3   | BC    | 156  | ARG  | 7.2  |
| 1   | BA    | 94   | G    | 7.2  |
| 33  | CE    | 200  | LEU  | 7.2  |
| 48  | CU    | 8    | LEU  | 7.2  |
| 49  | CV    | 52   | LEU  | 7.2  |
| 9   | BI    | 4    | ASN  | 7.2  |
| 7   | BG    | 16   | PRO  | 7.2  |
| 50  | CW    | 27   | PRO  | 7.2  |
| 31  | CA    | 2169 | A    | 7.2  |
| 13  | BM    | 101  | ARG  | 7.2  |
| 35  | CG    | 10   | VAL  | 7.2  |
| 31  | CA    | 878  | A    | 7.2  |
| 7   | BG    | 108  | ALA  | 7.2  |
| 10  | BJ    | 10   | LEU  | 7.2  |
| 43  | CP    | 115  | LEU  | 7.2  |
| 49  | CV    | 12   | ILE  | 7.2  |
| 1   | BA    | 954  | G    | 7.2  |
| 46  | CS    | 35   | PHE  | 7.2  |
| 14  | BN    | 68   | GLY  | 7.2  |
| 40  | CM    | 142  | ILE  | 7.2  |
| 37  | CJ    | 85   | GLY  | 7.2  |
| 35  | CG    | 86   | LYS  | 7.2  |
| 7   | BG    | 150  | ALA  | 7.2  |
| 24  | C3    | 32   | ALA  | 7.2  |
| 46  | CS    | 14   | VAL  | 7.2  |
| 53  | CZ    | 42   | LEU  | 7.2  |
| 26  | C5    | 32   | LYS  | 7.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | CU    | 87   | LEU  | 7.1  |
| 37  | DJ    | 84   | ALA  | 7.1  |
| 34  | CF    | 102  | ARG  | 7.1  |
| 37  | DJ    | 28   | LEU  | 7.1  |
| 23  | C2    | 37   | LYS  | 7.1  |
| 31  | CA    | 2797 | U    | 7.1  |
| 37  | CJ    | 95   | LYS  | 7.1  |
| 49  | CV    | 5    | ILE  | 7.1  |
| 1   | BA    | 1218 | C    | 7.1  |
| 31  | CA    | 1057 | A    | 7.1  |
| 37  | CJ    | 18   | ALA  | 7.1  |
| 1   | BA    | 1303 | C    | 7.1  |
| 55  | DA    | 2118 | U    | 7.1  |
| 19  | BS    | 61   | PHE  | 7.1  |
| 10  | BJ    | 91   | ASP  | 7.1  |
| 31  | CA    | 2121 | G    | 7.1  |
| 49  | CV    | 26   | LYS  | 7.1  |
| 34  | CF    | 174  | ASP  | 7.1  |
| 43  | CP    | 108  | ASP  | 7.1  |
| 55  | DA    | 2178 | C    | 7.1  |
| 39  | CL    | 110  | GLU  | 7.1  |
| 10  | AJ    | 6    | ILE  | 7.1  |
| 23  | C2    | 23   | THR  | 7.1  |
| 37  | DJ    | 52   | GLY  | 7.1  |
| 31  | CA    | 2175 | C    | 7.1  |
| 44  | CQ    | 97   | LEU  | 7.1  |
| 55  | DA    | 2111 | U    | 7.1  |
| 31  | CA    | 2127 | G    | 7.1  |
| 49  | CV    | 77   | THR  | 7.1  |
| 44  | CQ    | 95   | ALA  | 7.1  |
| 7   | BG    | 18   | PHE  | 7.1  |
| 1   | AA    | 81   | A    | 7.0  |
| 25  | C4    | 28   | ASN  | 7.0  |
| 37  | CJ    | 8    | TYR  | 7.0  |
| 53  | CZ    | 41   | HIS  | 7.0  |
| 37  | DJ    | 87   | LYS  | 7.0  |
| 49  | CV    | 38   | GLY  | 7.0  |
| 55  | DA    | 2167 | U    | 7.0  |
| 33  | CE    | 118  | LEU  | 7.0  |
| 35  | CG    | 9    | VAL  | 7.0  |
| 14  | BN    | 61   | ARG  | 7.0  |
| 40  | CM    | 28   | GLY  | 7.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2667 | C    | 7.0  |
| 3   | BC    | 79   | LYS  | 7.0  |
| 10  | BJ    | 11   | LYS  | 7.0  |
| 13  | BM    | 109  | ARG  | 7.0  |
| 43  | CP    | 39   | VAL  | 7.0  |
| 51  | CX    | 52   | GLY  | 7.0  |
| 33  | CE    | 183  | PHE  | 7.0  |
| 55  | DA    | 2166 | U    | 7.0  |
| 7   | BG    | 47   | LEU  | 7.0  |
| 7   | BG    | 129  | GLU  | 7.0  |
| 40  | CM    | 90   | VAL  | 7.0  |
| 20  | BT    | 75   | HIS  | 7.0  |
| 10  | AJ    | 42   | LEU  | 7.0  |
| 3   | BC    | 159  | GLY  | 7.0  |
| 10  | BJ    | 98   | VAL  | 7.0  |
| 1   | BA    | 203  | G    | 7.0  |
| 1   | BA    | 1304 | G    | 7.0  |
| 13  | BM    | 94   | GLY  | 7.0  |
| 27  | C0    | 24   | LEU  | 6.9  |
| 19  | BS    | 41   | PHE  | 6.9  |
| 34  | CF    | 158  | THR  | 6.9  |
| 30  | CD    | 44   | GLY  | 6.9  |
| 46  | CS    | 98   | ILE  | 6.9  |
| 1   | BA    | 79   | G    | 6.9  |
| 31  | CA    | 549  | G    | 6.9  |
| 34  | CF    | 175  | PHE  | 6.9  |
| 7   | BG    | 48   | GLU  | 6.9  |
| 37  | CJ    | 50   | GLU  | 6.9  |
| 54  | DI    | 134  | GLU  | 6.9  |
| 48  | CU    | 57   | VAL  | 6.9  |
| 31  | CA    | 1168 | G    | 6.9  |
| 31  | CA    | 1536 | C    | 6.9  |
| 34  | CF    | 121  | SER  | 6.9  |
| 14  | BN    | 53   | ARG  | 6.9  |
| 31  | CA    | 316  | C    | 6.9  |
| 31  | CA    | 1185 | G    | 6.9  |
| 31  | CA    | 2120 | G    | 6.9  |
| 35  | CG    | 45   | HIS  | 6.9  |
| 30  | CD    | 8    | LYS  | 6.9  |
| 26  | C5    | 38   | GLY  | 6.9  |
| 37  | CJ    | 93   | PRO  | 6.9  |
| 13  | BM    | 28   | THR  | 6.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | CJ    | 113  | LYS  | 6.9  |
| 19  | BS    | 80   | TYR  | 6.9  |
| 31  | CA    | 2168 | G    | 6.9  |
| 40  | CM    | 75   | ALA  | 6.8  |
| 9   | AI    | 90   | TYR  | 6.8  |
| 31  | CA    | 2119 | A    | 6.8  |
| 33  | CE    | 75   | SER  | 6.8  |
| 37  | CJ    | 123  | GLU  | 6.8  |
| 54  | DI    | 2    | ALA  | 6.8  |
| 7   | BG    | 30   | LEU  | 6.8  |
| 55  | DA    | 2176 | A    | 6.8  |
| 25  | C4    | 4    | ILE  | 6.8  |
| 27  | C0    | 43   | ALA  | 6.8  |
| 1   | BA    | 1023 | U    | 6.8  |
| 2   | AB    | 123  | ASP  | 6.8  |
| 2   | BB    | 186  | ILE  | 6.8  |
| 31  | CA    | 2170 | A    | 6.8  |
| 35  | CG    | 41   | VAL  | 6.8  |
| 46  | CS    | 101  | ILE  | 6.8  |
| 49  | CV    | 28   | VAL  | 6.8  |
| 16  | BP    | 60   | TRP  | 6.8  |
| 19  | BS    | 72   | GLY  | 6.8  |
| 35  | CG    | 30   | ASN  | 6.8  |
| 30  | CD    | 38   | LYS  | 6.8  |
| 37  | CJ    | 44   | ALA  | 6.8  |
| 43  | CP    | 107  | ALA  | 6.8  |
| 36  | DH    | 66   | ASN  | 6.8  |
| 13  | BM    | 63   | PHE  | 6.8  |
| 31  | CA    | 1210 | G    | 6.8  |
| 31  | CA    | 1076 | C    | 6.8  |
| 13  | BM    | 51   | GLY  | 6.8  |
| 34  | CF    | 75   | ALA  | 6.8  |
| 46  | CS    | 28   | ALA  | 6.8  |
| 55  | DA    | 2123 | G    | 6.8  |
| 31  | CA    | 1095 | A    | 6.8  |
| 20  | BT    | 56   | PRO  | 6.8  |
| 35  | CG    | 92   | VAL  | 6.8  |
| 37  | CJ    | 62   | TYR  | 6.8  |
| 33  | CE    | 24   | ASN  | 6.8  |
| 31  | CA    | 311  | A    | 6.8  |
| 2   | BB    | 201  | PRO  | 6.8  |
| 34  | CF    | 107  | ALA  | 6.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AM    | 19   | LEU  | 6.7  |
| 13  | BM    | 56   | LEU  | 6.7  |
| 25  | C4    | 40   | ARG  | 6.7  |
| 30  | CD    | 166  | GLY  | 6.7  |
| 31  | CA    | 877  | A    | 6.7  |
| 10  | BJ    | 102  | LEU  | 6.7  |
| 14  | BN    | 16   | LEU  | 6.7  |
| 31  | CA    | 1104 | C    | 6.7  |
| 7   | BG    | 107  | ALA  | 6.7  |
| 9   | BI    | 7    | TYR  | 6.7  |
| 31  | CA    | 356  | G    | 6.7  |
| 47  | CT    | 97   | LEU  | 6.7  |
| 31  | CA    | 12   | U    | 6.7  |
| 10  | BJ    | 6    | ILE  | 6.7  |
| 11  | AK    | 82   | LEU  | 6.7  |
| 47  | CT    | 86   | MET  | 6.7  |
| 10  | BJ    | 9    | ARG  | 6.7  |
| 20  | BT    | 76   | LYS  | 6.7  |
| 46  | CS    | 87   | GLN  | 6.7  |
| 3   | BC    | 53   | SER  | 6.7  |
| 13  | BM    | 31   | LYS  | 6.7  |
| 55  | DA    | 2127 | G    | 6.7  |
| 14  | BN    | 31   | ILE  | 6.7  |
| 46  | CS    | 78   | ARG  | 6.7  |
| 49  | CV    | 69   | ASN  | 6.7  |
| 35  | CG    | 51   | THR  | 6.7  |
| 35  | CG    | 84   | THR  | 6.7  |
| 42  | CO    | 120  | GLU  | 6.7  |
| 49  | DV    | 56   | GLY  | 6.7  |
| 31  | CA    | 2108 | A    | 6.7  |
| 53  | CZ    | 22   | LEU  | 6.7  |
| 30  | CD    | 96   | ILE  | 6.7  |
| 23  | C2    | 49   | TYR  | 6.6  |
| 1   | BA    | 1049 | U    | 6.6  |
| 31  | CA    | 1105 | U    | 6.6  |
| 53  | CZ    | 40   | SER  | 6.6  |
| 35  | CG    | 69   | ARG  | 6.6  |
| 31  | CA    | 267  | C    | 6.6  |
| 19  | BS    | 40   | ILE  | 6.6  |
| 10  | AJ    | 74   | VAL  | 6.6  |
| 7   | BG    | 101  | MET  | 6.6  |
| 13  | BM    | 6    | GLY  | 6.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | BA           | 1217       | C           | 6.6         |
| 2          | BB           | 35         | ARG         | 6.6         |
| 7          | BG           | 123        | GLU         | 6.6         |
| 34         | CF           | 55         | ALA         | 6.6         |
| 9          | BI           | 38         | TYR         | 6.6         |
| 35         | CG           | 58         | TYR         | 6.6         |
| 31         | CA           | 2128       | G           | 6.6         |
| 44         | CQ           | 110        | ILE         | 6.6         |
| 37         | DJ           | 73         | THR         | 6.6         |
| 10         | BJ           | 82         | LYS         | 6.6         |
| 20         | BT           | 24         | ARG         | 6.6         |
| 31         | CA           | 1535       | A           | 6.6         |
| 3          | BC           | 154        | SER         | 6.6         |
| 13         | BM           | 35         | ALA         | 6.6         |
| 53         | CZ           | 24         | GLU         | 6.6         |
| 1          | BA           | 1004       | A           | 6.6         |
| 13         | BM           | 12         | HIS         | 6.6         |
| 14         | BN           | 52         | PRO         | 6.6         |
| 40         | CM           | 85         | VAL         | 6.6         |
| 14         | BN           | 27         | LEU         | 6.6         |
| 37         | DJ           | 99         | GLY         | 6.6         |
| 42         | CO           | 24         | MET         | 6.6         |
| 1          | BA           | 1331       | G           | 6.6         |
| 7          | AG           | 4          | ARG         | 6.6         |
| 1          | BA           | 1236       | A           | 6.6         |
| 9          | AI           | 129        | LYS         | 6.6         |
| 21         | AU           | 2          | PRO         | 6.5         |
| 54         | DI           | 121        | SER         | 6.5         |
| 1          | AA           | 1026       | G           | 6.5         |
| 43         | CP           | 103        | VAL         | 6.5         |
| 33         | CE           | 54         | GLY         | 6.5         |
| 49         | CV           | 95         | PHE         | 6.5         |
| 30         | CD           | 154        | LYS         | 6.5         |
| 27         | C0           | 23         | THR         | 6.5         |
| 35         | CG           | 102        | VAL         | 6.5         |
| 9          | AI           | 17         | ALA         | 6.5         |
| 31         | CA           | 846        | U           | 6.5         |
| 36         | CH           | 132        | PHE         | 6.5         |
| 30         | CD           | 201        | LEU         | 6.5         |
| 54         | DI           | 132        | TYR         | 6.5         |
| 17         | BQ           | 45         | HIS         | 6.5         |
| 1          | BA           | 1018       | G           | 6.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 38         | CK           | 35         | ARG         | 6.5         |
| 10         | BJ           | 100        | ILE         | 6.5         |
| 36         | CH           | 136        | SER         | 6.5         |
| 37         | CJ           | 122        | ILE         | 6.5         |
| 37         | CJ           | 131        | GLY         | 6.5         |
| 42         | CO           | 29         | VAL         | 6.5         |
| 51         | CX           | 26         | PHE         | 6.5         |
| 35         | CG           | 27         | LYS         | 6.5         |
| 37         | DJ           | 22         | PRO         | 6.5         |
| 8          | BH           | 55         | THR         | 6.5         |
| 31         | CA           | 1082       | U           | 6.5         |
| 1          | BA           | 78         | A           | 6.5         |
| 31         | CA           | 1169       | A           | 6.5         |
| 31         | CA           | 1213       | A           | 6.5         |
| 37         | DJ           | 14         | ALA         | 6.5         |
| 17         | BQ           | 73         | TRP         | 6.5         |
| 19         | BS           | 12         | ASP         | 6.5         |
| 45         | CR           | 90         | ILE         | 6.5         |
| 3          | BC           | 43         | LEU         | 6.5         |
| 43         | CP           | 25         | ARG         | 6.5         |
| 16         | BP           | 81         | ALA         | 6.5         |
| 31         | CA           | 2161       | C           | 6.5         |
| 1          | BA           | 85         | U           | 6.5         |
| 55         | DA           | 1062       | G           | 6.5         |
| 25         | C4           | 41         | LYS         | 6.5         |
| 13         | BM           | 108        | THR         | 6.5         |
| 31         | CA           | 409        | G           | 6.5         |
| 35         | CG           | 7          | ALA         | 6.5         |
| 13         | BM           | 79         | ARG         | 6.4         |
| 33         | CE           | 193        | VAL         | 6.4         |
| 35         | CG           | 112        | PRO         | 6.4         |
| 7          | BG           | 38         | THR         | 6.4         |
| 9          | BI           | 9          | THR         | 6.4         |
| 1          | BA           | 1276       | G           | 6.4         |
| 10         | BJ           | 38         | GLY         | 6.4         |
| 31         | CA           | 1870       | C           | 6.4         |
| 13         | BM           | 21         | SER         | 6.4         |
| 34         | CF           | 136        | ILE         | 6.4         |
| 37         | CJ           | 84         | ALA         | 6.4         |
| 7          | BG           | 8          | GLY         | 6.4         |
| 10         | BJ           | 25         | ILE         | 6.4         |
| 31         | CA           | 2803       | G           | 6.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | CV    | 40   | ASN  | 6.4  |
| 47  | CT    | 105  | VAL  | 6.4  |
| 51  | CX    | 59   | LEU  | 6.4  |
| 14  | BN    | 22   | ALA  | 6.4  |
| 31  | CA    | 885  | C    | 6.4  |
| 34  | CF    | 122  | PHE  | 6.4  |
| 27  | C0    | 8    | THR  | 6.4  |
| 37  | CJ    | 79   | LEU  | 6.4  |
| 1   | BA    | 989  | U    | 6.4  |
| 34  | CF    | 84   | PRO  | 6.4  |
| 12  | AL    | 124  | ALA  | 6.4  |
| 43  | CP    | 46   | GLU  | 6.4  |
| 14  | AN    | 47   | LYS  | 6.3  |
| 37  | DJ    | 11   | LEU  | 6.3  |
| 55  | DA    | 1064 | C    | 6.3  |
| 7   | BG    | 115  | SER  | 6.3  |
| 22  | C1    | 46   | ASP  | 6.3  |
| 24  | C3    | 31   | LEU  | 6.3  |
| 35  | CG    | 17   | VAL  | 6.3  |
| 13  | BM    | 98   | ARG  | 6.3  |
| 54  | DI    | 96   | PHE  | 6.3  |
| 9   | AI    | 128  | SER  | 6.3  |
| 47  | CT    | 47   | VAL  | 6.3  |
| 25  | C4    | 36   | LYS  | 6.3  |
| 27  | C0    | 34   | HIS  | 6.3  |
| 34  | CF    | 41   | GLY  | 6.3  |
| 37  | CJ    | 32   | GLY  | 6.3  |
| 33  | CE    | 128  | ALA  | 6.3  |
| 37  | CJ    | 77   | ALA  | 6.3  |
| 31  | CA    | 81   | G    | 6.3  |
| 31  | CA    | 1238 | G    | 6.3  |
| 34  | CF    | 92   | ARG  | 6.3  |
| 37  | CJ    | 58   | VAL  | 6.3  |
| 37  | CJ    | 81   | LYS  | 6.3  |
| 42  | CO    | 118  | ARG  | 6.3  |
| 2   | BB    | 12   | ALA  | 6.3  |
| 7   | BG    | 145  | ALA  | 6.3  |
| 35  | CG    | 80   | THR  | 6.3  |
| 43  | CP    | 92   | PHE  | 6.3  |
| 15  | BO    | 17   | ARG  | 6.3  |
| 34  | CF    | 94   | GLU  | 6.3  |
| 43  | CP    | 66   | GLY  | 6.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | BA    | 1321 | U    | 6.3  |
| 31  | CA    | 1094 | U    | 6.3  |
| 34  | CF    | 69   | LYS  | 6.3  |
| 7   | AG    | 42   | ILE  | 6.3  |
| 7   | AG    | 66   | LEU  | 6.3  |
| 37  | DJ    | 19   | ASN  | 6.3  |
| 2   | AB    | 74   | ARG  | 6.3  |
| 37  | CJ    | 46   | THR  | 6.3  |
| 45  | CR    | 98   | ILE  | 6.3  |
| 31  | CA    | 1107 | G    | 6.3  |
| 43  | CP    | 52   | SER  | 6.3  |
| 44  | CQ    | 22   | PRO  | 6.3  |
| 35  | CG    | 107  | LEU  | 6.3  |
| 13  | BM    | 65   | VAL  | 6.3  |
| 1   | AA    | 85   | U    | 6.3  |
| 1   | AA    | 844  | G    | 6.3  |
| 30  | CD    | 77   | ARG  | 6.2  |
| 37  | CJ    | 67   | PHE  | 6.2  |
| 13  | BM    | 103  | LYS  | 6.2  |
| 49  | CV    | 4    | LYS  | 6.2  |
| 13  | BM    | 93   | ARG  | 6.2  |
| 9   | AI    | 6    | TYR  | 6.2  |
| 31  | CA    | 2860 | A    | 6.2  |
| 40  | CM    | 113  | ALA  | 6.2  |
| 30  | CD    | 97   | SER  | 6.2  |
| 37  | DJ    | 74   | PRO  | 6.2  |
| 36  | CH    | 72   | ILE  | 6.2  |
| 40  | CM    | 88   | GLY  | 6.2  |
| 35  | CG    | 174  | ALA  | 6.2  |
| 37  | CJ    | 70   | VAL  | 6.2  |
| 31  | CA    | 930  | G    | 6.2  |
| 34  | CF    | 143  | TYR  | 6.2  |
| 53  | CZ    | 56   | LEU  | 6.2  |
| 7   | BG    | 35   | LYS  | 6.2  |
| 43  | CP    | 27   | VAL  | 6.2  |
| 10  | BJ    | 80   | THR  | 6.2  |
| 51  | CX    | 62   | LYS  | 6.2  |
| 2   | BB    | 20   | THR  | 6.2  |
| 13  | BM    | 36   | ALA  | 6.2  |
| 40  | CM    | 117  | THR  | 6.2  |
| 37  | CJ    | 19   | ASN  | 6.2  |
| 51  | CX    | 32   | LEU  | 6.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | CZ    | 18   | LEU  | 6.2  |
| 30  | CD    | 74   | GLU  | 6.2  |
| 55  | DA    | 884  | U    | 6.2  |
| 2   | BB    | 67   | ILE  | 6.2  |
| 34  | CF    | 60   | ILE  | 6.2  |
| 40  | CM    | 126  | ARG  | 6.1  |
| 13  | AM    | 99   | GLY  | 6.1  |
| 55  | DA    | 883  | G    | 6.1  |
| 13  | BM    | 99   | GLY  | 6.1  |
| 14  | BN    | 8    | ALA  | 6.1  |
| 7   | BG    | 72   | THR  | 6.1  |
| 40  | CM    | 19   | LEU  | 6.1  |
| 50  | CW    | 89   | ILE  | 6.1  |
| 33  | CE    | 154  | ASP  | 6.1  |
| 14  | BN    | 18   | ASP  | 6.1  |
| 19  | BS    | 21   | LYS  | 6.1  |
| 20  | BT    | 34   | LYS  | 6.1  |
| 7   | BG    | 50   | LEU  | 6.1  |
| 38  | CK    | 93   | ILE  | 6.1  |
| 10  | AJ    | 35   | GLN  | 6.1  |
| 13  | BM    | 43   | VAL  | 6.1  |
| 49  | CV    | 25   | VAL  | 6.1  |
| 33  | CE    | 89   | PRO  | 6.1  |
| 1   | BA    | 1270 | G    | 6.1  |
| 24  | C3    | 28   | ARG  | 6.1  |
| 45  | CR    | 73   | GLY  | 6.1  |
| 13  | BM    | 30   | SER  | 6.1  |
| 24  | C3    | 26   | ASN  | 6.1  |
| 33  | CE    | 131  | THR  | 6.1  |
| 40  | CM    | 107  | PHE  | 6.1  |
| 44  | CQ    | 27   | GLU  | 6.1  |
| 2   | BB    | 21   | ARG  | 6.1  |
| 23  | C2    | 43   | VAL  | 6.1  |
| 18  | BR    | 51   | TYR  | 6.1  |
| 1   | BA    | 1005 | A    | 6.1  |
| 31  | CA    | 1106 | G    | 6.1  |
| 34  | CF    | 164  | GLU  | 6.1  |
| 37  | CJ    | 30   | GLN  | 6.1  |
| 30  | CD    | 9    | VAL  | 6.1  |
| 37  | DJ    | 98   | VAL  | 6.1  |
| 43  | CP    | 78   | VAL  | 6.1  |
| 35  | CG    | 82   | GLY  | 6.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 13         | BM           | 54         | ASP         | 6.1         |
| 43         | CP           | 105        | ALA         | 6.1         |
| 49         | CV           | 51         | ALA         | 6.1         |
| 1          | BA           | 1019       | A           | 6.1         |
| 7          | AG           | 79         | ARG         | 6.1         |
| 31         | CA           | 344        | A           | 6.1         |
| 43         | CP           | 106        | LEU         | 6.1         |
| 37         | DJ           | 117        | MET         | 6.1         |
| 40         | CM           | 135        | ILE         | 6.1         |
| 29         | CC           | 234        | GLY         | 6.0         |
| 20         | BT           | 63         | ALA         | 6.0         |
| 1          | BA           | 1306       | A           | 6.0         |
| 23         | C2           | 45         | GLN         | 6.0         |
| 55         | DA           | 2122       | U           | 6.0         |
| 54         | DI           | 38         | MET         | 6.0         |
| 27         | C0           | 55         | VAL         | 6.0         |
| 36         | CH           | 130        | VAL         | 6.0         |
| 43         | CP           | 41         | ALA         | 6.0         |
| 31         | CA           | 1217       | U           | 6.0         |
| 43         | CP           | 87         | ILE         | 6.0         |
| 16         | BP           | 54         | LEU         | 6.0         |
| 19         | BS           | 52         | HIS         | 6.0         |
| 40         | CM           | 133        | ALA         | 6.0         |
| 31         | CA           | 476        | G           | 6.0         |
| 13         | BM           | 41         | GLU         | 6.0         |
| 16         | BP           | 20         | VAL         | 6.0         |
| 29         | CC           | 242        | LYS         | 6.0         |
| 9          | BI           | 90         | TYR         | 6.0         |
| 10         | AJ           | 73         | LEU         | 6.0         |
| 10         | BJ           | 21         | ALA         | 6.0         |
| 1          | BA           | 208        | U           | 6.0         |
| 2          | BB           | 40         | ILE         | 6.0         |
| 7          | BG           | 58         | GLU         | 6.0         |
| 31         | CA           | 2892       | G           | 6.0         |
| 46         | CS           | 55         | ASP         | 6.0         |
| 1          | BA           | 1201       | A           | 6.0         |
| 1          | BA           | 1280       | A           | 6.0         |
| 31         | CA           | 1088       | A           | 6.0         |
| 49         | CV           | 6          | ARG         | 6.0         |
| 37         | CJ           | 118        | THR         | 6.0         |
| 31         | CA           | 2107       | G           | 6.0         |
| 45         | CR           | 29         | SER         | 6.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | C4    | 61   | CYS  | 6.0  |
| 38  | CK    | 119  | PHE  | 6.0  |
| 14  | BN    | 55   | SER  | 6.0  |
| 7   | BG    | 99   | LEU  | 6.0  |
| 46  | CS    | 18   | GLN  | 6.0  |
| 22  | C1    | 35   | GLY  | 6.0  |
| 19  | BS    | 77   | THR  | 5.9  |
| 7   | AG    | 109  | ARG  | 5.9  |
| 17  | BQ    | 63   | GLU  | 5.9  |
| 22  | C1    | 34   | SER  | 5.9  |
| 29  | CC    | 245  | VAL  | 5.9  |
| 35  | CG    | 152  | ARG  | 5.9  |
| 46  | CS    | 61   | ALA  | 5.9  |
| 15  | BO    | 89   | ARG  | 5.9  |
| 10  | AJ    | 75   | ASP  | 5.9  |
| 23  | C2    | 18   | GLY  | 5.9  |
| 46  | CS    | 22   | LEU  | 5.9  |
| 29  | CC    | 244  | PRO  | 5.9  |
| 35  | CG    | 8    | PRO  | 5.9  |
| 37  | CJ    | 27   | ALA  | 5.9  |
| 45  | CR    | 71   | GLN  | 5.9  |
| 37  | CJ    | 53   | LEU  | 5.9  |
| 43  | CP    | 62   | LEU  | 5.9  |
| 55  | DA    | 2115 | G    | 5.9  |
| 3   | BC    | 126  | ARG  | 5.9  |
| 1   | BA    | 950  | U    | 5.9  |
| 48  | CU    | 85   | VAL  | 5.9  |
| 23  | C2    | 53   | LYS  | 5.9  |
| 51  | CX    | 55   | ARG  | 5.9  |
| 23  | C2    | 15   | ALA  | 5.9  |
| 37  | CJ    | 41   | ALA  | 5.9  |
| 31  | CA    | 2118 | U    | 5.9  |
| 34  | CF    | 165  | GLU  | 5.9  |
| 31  | CA    | 345  | A    | 5.9  |
| 45  | CR    | 33   | ARG  | 5.9  |
| 37  | DJ    | 38   | PHE  | 5.9  |
| 19  | BS    | 6    | LYS  | 5.9  |
| 13  | BM    | 86   | TYR  | 5.9  |
| 52  | CY    | 78   | TYR  | 5.9  |
| 16  | BP    | 16   | PHE  | 5.9  |
| 30  | CD    | 82   | PHE  | 5.9  |
| 20  | BT    | 73   | ALA  | 5.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | CS    | 31   | GLU  | 5.9  |
| 31  | CA    | 896  | A    | 5.8  |
| 31  | CA    | 2150 | C    | 5.8  |
| 35  | CG    | 31   | GLY  | 5.9  |
| 44  | CQ    | 9    | GLU  | 5.8  |
| 54  | DI    | 129  | LEU  | 5.8  |
| 1   | BA    | 1235 | U    | 5.8  |
| 10  | BJ    | 89   | ARG  | 5.8  |
| 30  | CD    | 185  | ASN  | 5.8  |
| 31  | CA    | 1064 | C    | 5.8  |
| 49  | CV    | 73   | PHE  | 5.8  |
| 11  | BK    | 55   | SER  | 5.8  |
| 19  | BS    | 27   | ASP  | 5.8  |
| 52  | CY    | 49   | LEU  | 5.8  |
| 37  | CJ    | 91   | GLY  | 5.8  |
| 14  | BN    | 37   | SER  | 5.8  |
| 47  | CT    | 101  | SER  | 5.8  |
| 41  | CN    | 16   | ARG  | 5.8  |
| 7   | BG    | 152  | ALA  | 5.8  |
| 2   | BB    | 187  | VAL  | 5.8  |
| 9   | AI    | 19   | VAL  | 5.8  |
| 25  | C4    | 2    | PRO  | 5.8  |
| 31  | CA    | 1215 | G    | 5.8  |
| 35  | CG    | 121  | ILE  | 5.8  |
| 36  | DH    | 74   | ALA  | 5.8  |
| 36  | DH    | 70   | GLU  | 5.8  |
| 46  | CS    | 62   | GLU  | 5.8  |
| 55  | DA    | 1068 | G    | 5.8  |
| 2   | AB    | 131  | LYS  | 5.8  |
| 17  | BQ    | 17   | MET  | 5.8  |
| 33  | CE    | 138  | LEU  | 5.8  |
| 34  | CF    | 170  | LEU  | 5.8  |
| 36  | CH    | 15   | LEU  | 5.8  |
| 10  | BJ    | 19   | ASP  | 5.8  |
| 25  | C4    | 27   | ALA  | 5.8  |
| 9   | AI    | 104  | VAL  | 5.8  |
| 48  | CU    | 34   | VAL  | 5.8  |
| 42  | CO    | 119  | SER  | 5.8  |
| 55  | DA    | 879  | G    | 5.8  |
| 7   | BG    | 60   | GLU  | 5.8  |
| 30  | CD    | 30   | GLU  | 5.8  |
| 35  | CG    | 56   | ASP  | 5.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | CR    | 91   | ASP  | 5.8  |
| 37  | CJ    | 135  | SER  | 5.8  |
| 43  | CP    | 67   | ASN  | 5.8  |
| 37  | DJ    | 100  | LYS  | 5.8  |
| 7   | BG    | 88   | PRO  | 5.8  |
| 55  | DA    | 2165 | C    | 5.8  |
| 20  | BT    | 49   | LYS  | 5.7  |
| 2   | AB    | 46   | THR  | 5.7  |
| 9   | BI    | 81   | HIS  | 5.7  |
| 2   | AB    | 4    | VAL  | 5.7  |
| 34  | CF    | 135  | GLN  | 5.7  |
| 35  | CG    | 4    | VAL  | 5.7  |
| 35  | CG    | 162  | VAL  | 5.7  |
| 49  | CV    | 70   | VAL  | 5.7  |
| 53  | CZ    | 11   | VAL  | 5.7  |
| 30  | CD    | 76   | GLY  | 5.7  |
| 37  | DJ    | 85   | GLY  | 5.7  |
| 47  | CT    | 43   | ALA  | 5.7  |
| 49  | CV    | 64   | ALA  | 5.7  |
| 13  | AM    | 16   | VAL  | 5.7  |
| 1   | BA    | 213  | G    | 5.7  |
| 51  | CX    | 60   | PHE  | 5.7  |
| 46  | CS    | 49   | ILE  | 5.7  |
| 49  | CV    | 71   | ALA  | 5.7  |
| 43  | CP    | 26   | LEU  | 5.7  |
| 34  | CF    | 79   | ILE  | 5.7  |
| 47  | CT    | 82   | MET  | 5.7  |
| 50  | CW    | 1    | MET  | 5.7  |
| 39  | CL    | 68   | GLY  | 5.7  |
| 31  | CA    | 1214 | A    | 5.7  |
| 37  | DJ    | 103  | ARG  | 5.7  |
| 37  | CJ    | 125  | MET  | 5.7  |
| 1   | BA    | 987  | G    | 5.7  |
| 31  | CA    | 317  | G    | 5.7  |
| 37  | DJ    | 110  | ALA  | 5.7  |
| 44  | CQ    | 115  | ASN  | 5.7  |
| 44  | CQ    | 8    | LEU  | 5.7  |
| 1   | BA    | 196  | A    | 5.7  |
| 9   | BI    | 125  | PRO  | 5.7  |
| 35  | CG    | 54   | PRO  | 5.7  |
| 7   | BG    | 140  | ASP  | 5.7  |
| 30  | CD    | 43   | ASP  | 5.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | CE    | 98   | LYS  | 5.7  |
| 48  | CU    | 1    | MET  | 5.7  |
| 31  | CA    | 1049 | C    | 5.7  |
| 37  | CJ    | 124  | ALA  | 5.7  |
| 51  | CX    | 61   | ALA  | 5.7  |
| 3   | BC    | 106  | VAL  | 5.7  |
| 31  | CA    | 2162 | G    | 5.7  |
| 35  | CG    | 110  | SER  | 5.7  |
| 35  | CG    | 67   | THR  | 5.7  |
| 37  | CJ    | 45   | LYS  | 5.7  |
| 29  | CC    | 249  | GLY  | 5.7  |
| 35  | CG    | 78   | GLY  | 5.7  |
| 37  | DJ    | 50   | GLU  | 5.7  |
| 1   | BA    | 1029 | U    | 5.7  |
| 1   | BA    | 1126 | U    | 5.7  |
| 1   | BA    | 1240 | U    | 5.7  |
| 35  | CG    | 35   | ARG  | 5.7  |
| 27  | C0    | 9    | GLN  | 5.7  |
| 31  | CA    | 1606 | C    | 5.7  |
| 33  | CE    | 178  | VAL  | 5.7  |
| 25  | C4    | 64   | TYR  | 5.7  |
| 31  | CA    | 646  | U    | 5.7  |
| 30  | CD    | 3    | GLY  | 5.7  |
| 31  | CA    | 514  | A    | 5.6  |
| 34  | CF    | 110  | ARG  | 5.6  |
| 24  | C3    | 37   | LYS  | 5.6  |
| 31  | CA    | 1174 | U    | 5.6  |
| 55  | DA    | 2109 | U    | 5.6  |
| 7   | BG    | 83   | SER  | 5.6  |
| 35  | CG    | 104  | ASN  | 5.6  |
| 19  | BS    | 59   | PRO  | 5.6  |
| 36  | DH    | 94   | ILE  | 5.6  |
| 33  | CE    | 17   | THR  | 5.6  |
| 27  | C0    | 27   | LEU  | 5.6  |
| 50  | CW    | 42   | LEU  | 5.6  |
| 1   | BA    | 90   | C    | 5.6  |
| 10  | BJ    | 39   | PRO  | 5.6  |
| 30  | CD    | 200  | ASP  | 5.6  |
| 13  | AM    | 64   | VAL  | 5.6  |
| 30  | CD    | 203  | VAL  | 5.6  |
| 37  | DJ    | 71   | THR  | 5.6  |
| 33  | CE    | 101  | TYR  | 5.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | BG    | 76   | LYS  | 5.6  |
| 31  | CA    | 1046 | A    | 5.6  |
| 36  | DH    | 63   | ALA  | 5.6  |
| 25  | C4    | 22   | PHE  | 5.6  |
| 1   | AA    | 82   | G    | 5.6  |
| 34  | CF    | 43   | ALA  | 5.6  |
| 1   | BA    | 81   | A    | 5.6  |
| 29  | CC    | 240  | PHE  | 5.6  |
| 30  | CD    | 5    | VAL  | 5.6  |
| 19  | BS    | 71   | LEU  | 5.6  |
| 31  | CA    | 328  | U    | 5.6  |
| 42  | CO    | 56   | LYS  | 5.6  |
| 45  | CR    | 6    | ARG  | 5.6  |
| 47  | CT    | 103  | ILE  | 5.6  |
| 31  | CA    | 2628 | C    | 5.6  |
| 37  | DJ    | 27   | ALA  | 5.6  |
| 1   | BA    | 102  | G    | 5.6  |
| 1   | BA    | 202  | G    | 5.6  |
| 1   | BA    | 1221 | G    | 5.6  |
| 13  | BM    | 76   | SER  | 5.6  |
| 31  | CA    | 546  | U    | 5.6  |
| 34  | CF    | 32   | GLU  | 5.6  |
| 13  | BM    | 14   | HIS  | 5.5  |
| 41  | CN    | 17   | ASN  | 5.5  |
| 49  | DV    | 53   | ASN  | 5.5  |
| 7   | AG    | 82   | GLY  | 5.5  |
| 9   | BI    | 15   | SER  | 5.5  |
| 31  | CA    | 45   | G    | 5.5  |
| 30  | CD    | 151  | THR  | 5.5  |
| 34  | CF    | 99   | PHE  | 5.5  |
| 37  | DJ    | 8    | TYR  | 5.5  |
| 1   | AA    | 1027 | C    | 5.5  |
| 10  | BJ    | 27   | GLU  | 5.5  |
| 31  | CA    | 355  | U    | 5.5  |
| 46  | CS    | 94   | THR  | 5.5  |
| 29  | CC    | 48   | ARG  | 5.5  |
| 11  | AK    | 19   | GLY  | 5.5  |
| 35  | CG    | 57   | GLY  | 5.5  |
| 35  | CG    | 117  | LEU  | 5.5  |
| 1   | BA    | 1333 | A    | 5.5  |
| 55  | DA    | 1077 | A    | 5.5  |
| 45  | CR    | 118  | ALA  | 5.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 48         | CU           | 35         | ALA         | 5.5         |
| 24         | C3           | 16         | HIS         | 5.5         |
| 36         | CH           | 142        | VAL         | 5.5         |
| 38         | CK           | 139        | VAL         | 5.5         |
| 3          | BC           | 206        | GLU         | 5.5         |
| 1          | BA           | 1237       | C           | 5.5         |
| 7          | BG           | 5          | ARG         | 5.5         |
| 31         | CA           | 1872       | A           | 5.5         |
| 37         | CJ           | 15         | ALA         | 5.5         |
| 55         | DA           | 1098       | A           | 5.5         |
| 3          | BC           | 39         | VAL         | 5.5         |
| 34         | CF           | 37         | ASN         | 5.5         |
| 44         | CQ           | 12         | GLN         | 5.5         |
| 49         | CV           | 66         | GLN         | 5.5         |
| 1          | BA           | 4          | U           | 5.5         |
| 9          | BI           | 30         | ILE         | 5.5         |
| 49         | CV           | 18         | ASP         | 5.5         |
| 33         | CE           | 142        | ALA         | 5.5         |
| 9          | BI           | 58         | VAL         | 5.5         |
| 10         | AJ           | 76         | ILE         | 5.5         |
| 2          | BB           | 37         | LYS         | 5.5         |
| 3          | BC           | 76         | VAL         | 5.5         |
| 7          | BG           | 89         | VAL         | 5.5         |
| 27         | C0           | 48         | ILE         | 5.5         |
| 31         | CA           | 291        | G           | 5.5         |
| 35         | CG           | 160        | LYS         | 5.5         |
| 51         | CX           | 56         | ASP         | 5.5         |
| 3          | BC           | 111        | LEU         | 5.5         |
| 53         | CZ           | 47         | ARG         | 5.5         |
| 10         | BJ           | 99         | GLN         | 5.5         |
| 42         | CO           | 62         | ASN         | 5.5         |
| 37         | CJ           | 128        | SER         | 5.5         |
| 1          | BA           | 1245       | C           | 5.5         |
| 31         | CA           | 327        | G           | 5.5         |
| 31         | CA           | 879        | G           | 5.5         |
| 23         | C2           | 44         | ARG         | 5.4         |
| 31         | CA           | 1518       | C           | 5.5         |
| 14         | BN           | 11         | VAL         | 5.4         |
| 1          | BA           | 955        | U           | 5.4         |
| 3          | BC           | 120        | ILE         | 5.4         |
| 31         | CA           | 74         | A           | 5.4         |
| 30         | CD           | 180        | VAL         | 5.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 548  | G    | 5.4  |
| 23  | C2    | 46   | HIS  | 5.4  |
| 7   | BG    | 119  | ARG  | 5.4  |
| 7   | BG    | 118  | LEU  | 5.4  |
| 10  | BJ    | 93   | ALA  | 5.4  |
| 31  | CA    | 1089 | A    | 5.4  |
| 31  | CA    | 335  | C    | 5.4  |
| 34  | CF    | 74   | VAL  | 5.4  |
| 1   | BA    | 844  | G    | 5.4  |
| 10  | BJ    | 81   | GLU  | 5.4  |
| 31  | CA    | 1212 | G    | 5.4  |
| 31  | CA    | 2801 | G    | 5.4  |
| 34  | CF    | 18   | THR  | 5.4  |
| 19  | AS    | 55   | ARG  | 5.4  |
| 30  | CD    | 46   | ARG  | 5.4  |
| 7   | BG    | 130  | ASN  | 5.4  |
| 37  | CJ    | 52   | GLY  | 5.4  |
| 13  | AM    | 44   | LYS  | 5.4  |
| 22  | C1    | 27   | SER  | 5.4  |
| 31  | CA    | 892  | A    | 5.4  |
| 31  | CA    | 1048 | A    | 5.4  |
| 46  | CS    | 25   | LEU  | 5.4  |
| 40  | CM    | 45   | GLY  | 5.4  |
| 34  | CF    | 77   | PHE  | 5.4  |
| 2   | BB    | 82   | ASP  | 5.4  |
| 13  | BM    | 74   | SER  | 5.4  |
| 30  | CD    | 41   | ALA  | 5.4  |
| 40  | CM    | 131  | ALA  | 5.4  |
| 45  | CR    | 99   | ALA  | 5.4  |
| 14  | BN    | 45   | VAL  | 5.4  |
| 42  | CO    | 63   | ARG  | 5.4  |
| 1   | BA    | 1273 | C    | 5.4  |
| 31  | CA    | 183  | C    | 5.4  |
| 38  | CK    | 97   | PRO  | 5.4  |
| 50  | CW    | 29   | ILE  | 5.4  |
| 54  | DI    | 84   | TYR  | 5.4  |
| 43  | CP    | 69   | ASP  | 5.4  |
| 43  | CP    | 110  | ALA  | 5.4  |
| 36  | DH    | 138  | VAL  | 5.4  |
| 1   | BA    | 974  | A    | 5.4  |
| 35  | CG    | 109  | PHE  | 5.4  |
| 13  | AM    | 5    | ALA  | 5.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 13         | AM           | 32         | ALA         | 5.4         |
| 31         | CA           | 626        | A           | 5.4         |
| 12         | BL           | 124        | ALA         | 5.4         |
| 1          | AA           | 1020       | G           | 5.4         |
| 9          | BI           | 10         | GLY         | 5.4         |
| 51         | CX           | 57         | HIS         | 5.4         |
| 55         | DA           | 1061       | U           | 5.4         |
| 14         | BN           | 5          | SER         | 5.3         |
| 19         | BS           | 68         | GLY         | 5.3         |
| 1          | BA           | 1244       | G           | 5.3         |
| 34         | CF           | 177        | PHE         | 5.3         |
| 36         | DH           | 139        | PHE         | 5.3         |
| 39         | CL           | 37         | ASP         | 5.3         |
| 7          | AG           | 69         | VAL         | 5.3         |
| 35         | CG           | 132        | VAL         | 5.3         |
| 37         | DJ           | 104        | ALA         | 5.3         |
| 48         | CU           | 58         | VAL         | 5.3         |
| 37         | DJ           | 48         | SER         | 5.3         |
| 27         | C0           | 7          | ILE         | 5.3         |
| 1          | BA           | 1297       | G           | 5.3         |
| 14         | BN           | 49         | GLN         | 5.3         |
| 45         | CR           | 81         | ASN         | 5.3         |
| 9          | AI           | 127        | PHE         | 5.3         |
| 9          | BI           | 20         | PHE         | 5.3         |
| 31         | CA           | 1873       | G           | 5.3         |
| 34         | CF           | 25         | VAL         | 5.3         |
| 49         | CV           | 49         | VAL         | 5.3         |
| 55         | DA           | 882        | G           | 5.3         |
| 27         | C0           | 10         | THR         | 5.3         |
| 37         | DJ           | 132        | THR         | 5.3         |
| 37         | CJ           | 136        | MET         | 5.3         |
| 49         | CV           | 43         | LYS         | 5.3         |
| 34         | CF           | 119        | ALA         | 5.3         |
| 31         | CA           | 420        | C           | 5.3         |
| 33         | CE           | 197        | GLU         | 5.3         |
| 35         | CG           | 161        | GLY         | 5.3         |
| 37         | DJ           | 43         | ASN         | 5.3         |
| 1          | BA           | 1015       | G           | 5.3         |
| 33         | CE           | 72         | SER         | 5.3         |
| 10         | BJ           | 37         | ARG         | 5.3         |
| 19         | BS           | 58         | VAL         | 5.3         |
| 1          | BA           | 988        | G           | 5.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 1216 | G    | 5.3  |
| 36  | CH    | 133  | GLN  | 5.3  |
| 30  | CD    | 31   | ALA  | 5.3  |
| 34  | CF    | 26   | MET  | 5.3  |
| 9   | AI    | 5    | GLN  | 5.3  |
| 49  | CV    | 15   | THR  | 5.3  |
| 1   | BA    | 1148 | U    | 5.3  |
| 42  | CO    | 83   | LEU  | 5.3  |
| 46  | CS    | 54   | VAL  | 5.3  |
| 27  | C0    | 44   | ILE  | 5.2  |
| 35  | CG    | 81   | GLU  | 5.2  |
| 35  | CG    | 131  | ILE  | 5.2  |
| 14  | BN    | 6    | MET  | 5.2  |
| 37  | DJ    | 131  | GLY  | 5.2  |
| 10  | BJ    | 85   | ASP  | 5.2  |
| 13  | BM    | 58   | ASP  | 5.2  |
| 36  | CH    | 74   | ALA  | 5.2  |
| 46  | CS    | 33   | VAL  | 5.2  |
| 48  | CU    | 36   | LYS  | 5.2  |
| 13  | BM    | 77   | ILE  | 5.2  |
| 40  | CM    | 115  | GLU  | 5.2  |
| 13  | BM    | 34   | LEU  | 5.2  |
| 31  | CA    | 268  | C    | 5.2  |
| 35  | CG    | 59   | ALA  | 5.2  |
| 50  | CW    | 69   | GLU  | 5.2  |
| 47  | CT    | 85   | ILE  | 5.2  |
| 34  | CF    | 81   | GLN  | 5.2  |
| 55  | DA    | 2168 | G    | 5.2  |
| 31  | CA    | 2651 | C    | 5.2  |
| 7   | BG    | 110  | LYS  | 5.2  |
| 20  | BT    | 38   | ALA  | 5.2  |
| 48  | CU    | 37   | ASP  | 5.2  |
| 23  | C2    | 39   | PHE  | 5.2  |
| 16  | BP    | 42   | ILE  | 5.2  |
| 14  | BN    | 43   | ASN  | 5.2  |
| 15  | AO    | 17   | ARG  | 5.2  |
| 31  | CA    | 138  | U    | 5.2  |
| 7   | BG    | 80   | VAL  | 5.2  |
| 37  | DJ    | 10   | LYS  | 5.2  |
| 1   | BA    | 101  | A    | 5.2  |
| 7   | BG    | 113  | ASP  | 5.2  |
| 13  | AM    | 11   | ASP  | 5.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | BT    | 53   | GLU  | 5.2  |
| 31  | CA    | 1171 | G    | 5.2  |
| 52  | CY    | 35   | SER  | 5.2  |
| 13  | AM    | 7    | ILE  | 5.2  |
| 38  | CK    | 142  | ILE  | 5.2  |
| 44  | CQ    | 4    | ILE  | 5.2  |
| 9   | BI    | 8    | GLY  | 5.2  |
| 6   | AF    | 61   | LEU  | 5.2  |
| 17  | BQ    | 50   | ASN  | 5.2  |
| 21  | AU    | 11   | PRO  | 5.2  |
| 27  | C0    | 53   | PHE  | 5.2  |
| 31  | CA    | 893  | C    | 5.2  |
| 31  | CA    | 1166 | G    | 5.2  |
| 33  | CE    | 88   | ARG  | 5.2  |
| 3   | BC    | 77   | ILE  | 5.2  |
| 9   | BI    | 37   | GLN  | 5.2  |
| 40  | CM    | 35   | HIS  | 5.2  |
| 12  | BL    | 70   | GLU  | 5.2  |
| 34  | CF    | 56   | ASP  | 5.2  |
| 55  | DA    | 2106 | U    | 5.2  |
| 31  | CA    | 1047 | G    | 5.2  |
| 31  | CA    | 1271 | G    | 5.2  |
| 43  | CP    | 30   | ARG  | 5.2  |
| 1   | BA    | 207  | C    | 5.1  |
| 1   | BA    | 1336 | C    | 5.1  |
| 13  | AM    | 4    | ILE  | 5.1  |
| 53  | CZ    | 21   | LEU  | 5.1  |
| 9   | BI    | 41   | ARG  | 5.1  |
| 31  | CA    | 408  | G    | 5.1  |
| 48  | CU    | 16   | VAL  | 5.1  |
| 30  | CD    | 153  | GLY  | 5.1  |
| 46  | CS    | 100  | GLY  | 5.1  |
| 3   | BC    | 124  | LEU  | 5.1  |
| 24  | C3    | 34   | ARG  | 5.1  |
| 40  | CM    | 74   | THR  | 5.1  |
| 53  | CZ    | 28   | LEU  | 5.1  |
| 37  | DJ    | 51   | LYS  | 5.1  |
| 39  | CL    | 33   | ALA  | 5.1  |
| 54  | DI    | 124  | ASP  | 5.1  |
| 13  | BM    | 113  | ARG  | 5.1  |
| 14  | BN    | 13   | ARG  | 5.1  |
| 34  | CF    | 4    | LEU  | 5.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2177 | C    | 5.1  |
| 33  | CE    | 48   | THR  | 5.1  |
| 51  | CX    | 58   | THR  | 5.1  |
| 9   | BI    | 103  | PHE  | 5.1  |
| 48  | CU    | 84   | TYR  | 5.1  |
| 19  | BS    | 50   | ALA  | 5.1  |
| 49  | CV    | 84   | GLY  | 5.1  |
| 34  | CF    | 91   | LEU  | 5.1  |
| 7   | BG    | 131  | LYS  | 5.1  |
| 13  | BM    | 104  | THR  | 5.1  |
| 14  | BN    | 58   | SER  | 5.1  |
| 30  | CD    | 133  | THR  | 5.1  |
| 33  | CE    | 124  | PHE  | 5.1  |
| 46  | CS    | 83   | TYR  | 5.1  |
| 1   | BA    | 977  | A    | 5.1  |
| 7   | BG    | 102  | ARG  | 5.1  |
| 3   | BC    | 103  | ILE  | 5.1  |
| 7   | AG    | 151  | PHE  | 5.1  |
| 50  | CW    | 91   | PHE  | 5.1  |
| 26  | C5    | 20   | ASP  | 5.1  |
| 52  | CY    | 34   | HIS  | 5.1  |
| 48  | CU    | 75   | GLY  | 5.1  |
| 20  | BT    | 64   | LYS  | 5.1  |
| 33  | CE    | 73   | ILE  | 5.1  |
| 34  | CF    | 67   | ILE  | 5.1  |
| 35  | CG    | 141  | ILE  | 5.1  |
| 17  | BQ    | 44   | LEU  | 5.1  |
| 44  | CQ    | 74   | PHE  | 5.1  |
| 51  | CX    | 83   | GLU  | 5.1  |
| 52  | CY    | 45   | ARG  | 5.1  |
| 1   | BA    | 1312 | G    | 5.1  |
| 34  | CF    | 172  | ALA  | 5.1  |
| 49  | CV    | 76   | ALA  | 5.1  |
| 31  | CA    | 501  | A    | 5.1  |
| 31  | CA    | 513  | A    | 5.1  |
| 37  | DJ    | 106  | LEU  | 5.1  |
| 19  | BS    | 57   | HIS  | 5.1  |
| 48  | CU    | 24   | MET  | 5.1  |
| 38  | CK    | 128  | ASN  | 5.0  |
| 31  | CA    | 2904 | U    | 5.0  |
| 36  | DH    | 65   | ALA  | 5.0  |
| 34  | CF    | 68   | THR  | 5.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | BN    | 9    | ARG  | 5.0  |
| 22  | C1    | 36   | GLU  | 5.0  |
| 30  | CD    | 152  | PRO  | 5.0  |
| 37  | DJ    | 49   | ILE  | 5.0  |
| 13  | AM    | 25   | VAL  | 5.0  |
| 51  | CX    | 34   | GLY  | 5.0  |
| 34  | CF    | 38   | MET  | 5.0  |
| 36  | CH    | 67   | ALA  | 5.0  |
| 45  | CR    | 113  | ALA  | 5.0  |
| 14  | BN    | 30   | ILE  | 5.0  |
| 16  | BP    | 50   | THR  | 5.0  |
| 37  | DJ    | 60   | THR  | 5.0  |
| 1   | BA    | 222  | C    | 5.0  |
| 36  | DH    | 132  | PHE  | 5.0  |
| 7   | AG    | 53   | ARG  | 5.0  |
| 13  | BM    | 81   | MET  | 5.0  |
| 33  | CE    | 11   | ALA  | 5.0  |
| 24  | C3    | 12   | ARG  | 5.0  |
| 47  | CT    | 6    | LYS  | 5.0  |
| 51  | CX    | 25   | ARG  | 5.0  |
| 53  | CZ    | 54   | LYS  | 5.0  |
| 54  | DI    | 40   | GLU  | 5.0  |
| 19  | BS    | 25   | SER  | 5.0  |
| 19  | BS    | 42   | PRO  | 5.0  |
| 35  | CG    | 25   | THR  | 5.0  |
| 37  | DJ    | 42   | PHE  | 5.0  |
| 10  | BJ    | 34   | ALA  | 5.0  |
| 20  | BT    | 46   | ALA  | 5.0  |
| 20  | BT    | 50   | ALA  | 5.0  |
| 2   | BB    | 9    | MET  | 5.0  |
| 40  | CM    | 144  | GLU  | 5.0  |
| 31  | CA    | 103  | A    | 5.0  |
| 33  | CE    | 157  | LEU  | 5.0  |
| 1   | BA    | 83   | C    | 5.0  |
| 1   | BA    | 962  | C    | 5.0  |
| 7   | BG    | 82   | GLY  | 5.0  |
| 7   | AG    | 5    | ARG  | 5.0  |
| 1   | BA    | 1309 | G    | 5.0  |
| 31  | CA    | 332  | A    | 5.0  |
| 53  | CZ    | 6    | LEU  | 5.0  |
| 55  | DA    | 654  | A    | 5.0  |
| 3   | BC    | 73   | PRO  | 5.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | AH    | 2    | SER  | 5.0  |
| 14  | BN    | 24   | ARG  | 5.0  |
| 43  | CP    | 88   | LYS  | 5.0  |
| 53  | CZ    | 63   | ALA  | 5.0  |
| 13  | BM    | 4    | ILE  | 5.0  |
| 55  | DA    | 2141 | G    | 5.0  |
| 42  | CO    | 36   | THR  | 5.0  |
| 38  | CK    | 136  | GLN  | 5.0  |
| 7   | AG    | 134  | ALA  | 5.0  |
| 1   | AA    | 1025 | U    | 5.0  |
| 31  | CA    | 369  | U    | 5.0  |
| 44  | CQ    | 59   | PHE  | 5.0  |
| 7   | BG    | 68   | ASN  | 5.0  |
| 11  | AK    | 81   | ASN  | 5.0  |
| 30  | CD    | 25   | THR  | 5.0  |
| 27  | C0    | 2    | ALA  | 5.0  |
| 30  | CD    | 47   | ALA  | 5.0  |
| 44  | CQ    | 111  | LYS  | 5.0  |
| 50  | CW    | 58   | SER  | 4.9  |
| 13  | BM    | 11   | ASP  | 4.9  |
| 40  | CM    | 108  | ALA  | 4.9  |
| 43  | CP    | 93   | ASP  | 4.9  |
| 48  | CU    | 12   | ARG  | 4.9  |
| 16  | BP    | 39   | PHE  | 4.9  |
| 9   | AI    | 32   | GLN  | 4.9  |
| 30  | CD    | 199  | SER  | 4.9  |
| 33  | CE    | 32   | VAL  | 4.9  |
| 13  | AM    | 36   | ALA  | 4.9  |
| 14  | BN    | 33   | ASP  | 4.9  |
| 19  | AS    | 39   | THR  | 4.9  |
| 46  | CS    | 26   | ASP  | 4.9  |
| 1   | BA    | 1034 | G    | 4.9  |
| 22  | C1    | 55   | ILE  | 4.9  |
| 31  | CA    | 357  | C    | 4.9  |
| 2   | BB    | 39   | HIS  | 4.9  |
| 11  | BK    | 21   | ALA  | 4.9  |
| 3   | BC    | 144  | LEU  | 4.9  |
| 45  | CR    | 94   | ILE  | 4.9  |
| 2   | AB    | 139  | ARG  | 4.9  |
| 17  | BQ    | 46   | VAL  | 4.9  |
| 7   | AG    | 58   | GLU  | 4.9  |
| 9   | BI    | 92   | GLU  | 4.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 48   | ILE  | 4.9  |
| 48  | CU    | 2    | ILE  | 4.9  |
| 55  | DA    | 885  | C    | 4.9  |
| 3   | BC    | 107  | ARG  | 4.9  |
| 27  | C0    | 42   | PRO  | 4.9  |
| 37  | CJ    | 92   | LYS  | 4.9  |
| 31  | CA    | 431  | U    | 4.9  |
| 35  | CG    | 77   | ILE  | 4.9  |
| 36  | CH    | 58   | LEU  | 4.9  |
| 43  | CP    | 58   | ILE  | 4.9  |
| 49  | CV    | 82   | ARG  | 4.9  |
| 31  | CA    | 262  | A    | 4.9  |
| 10  | AJ    | 36   | VAL  | 4.9  |
| 17  | BQ    | 78   | VAL  | 4.9  |
| 31  | CA    | 882  | G    | 4.9  |
| 31  | CA    | 2808 | G    | 4.9  |
| 14  | BN    | 40   | ASP  | 4.9  |
| 41  | CN    | 79   | ALA  | 4.9  |
| 13  | AM    | 45   | ILE  | 4.9  |
| 13  | BM    | 80   | LEU  | 4.9  |
| 45  | CR    | 26   | GLY  | 4.9  |
| 31  | CA    | 2180 | U    | 4.9  |
| 55  | DA    | 1094 | U    | 4.9  |
| 53  | CZ    | 36   | GLN  | 4.9  |
| 31  | CA    | 2800 | A    | 4.9  |
| 55  | DA    | 892  | A    | 4.9  |
| 7   | AG    | 59   | LEU  | 4.9  |
| 31  | CA    | 1056 | G    | 4.9  |
| 31  | CA    | 1235 | G    | 4.9  |
| 49  | CV    | 47   | LYS  | 4.9  |
| 11  | BK    | 64   | GLN  | 4.9  |
| 9   | AI    | 55   | VAL  | 4.9  |
| 3   | BC    | 42   | TYR  | 4.9  |
| 17  | BQ    | 6    | ARG  | 4.9  |
| 31  | CA    | 505  | A    | 4.9  |
| 42  | CO    | 93   | GLY  | 4.9  |
| 37  | DJ    | 113  | LYS  | 4.9  |
| 31  | CA    | 1863 | G    | 4.9  |
| 37  | CJ    | 37   | GLU  | 4.8  |
| 35  | CG    | 127  | THR  | 4.8  |
| 48  | CU    | 31   | VAL  | 4.8  |
| 37  | DJ    | 75   | PRO  | 4.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | CK    | 47   | HIS  | 4.8  |
| 27  | C0    | 32   | ILE  | 4.8  |
| 52  | CY    | 46   | PHE  | 4.8  |
| 31  | CA    | 1234 | U    | 4.8  |
| 31  | CA    | 2106 | U    | 4.8  |
| 3   | BC    | 80   | LYS  | 4.8  |
| 34  | CF    | 47   | LYS  | 4.8  |
| 36  | DH    | 96   | THR  | 4.8  |
| 1   | BA    | 1209 | C    | 4.8  |
| 36  | DH    | 107  | GLY  | 4.8  |
| 20  | BT    | 67   | ILE  | 4.8  |
| 55  | DA    | 1066 | U    | 4.8  |
| 7   | BG    | 122  | ASN  | 4.8  |
| 13  | BM    | 61   | ALA  | 4.8  |
| 30  | CD    | 45   | TYR  | 4.8  |
| 55  | DA    | 2132 | U    | 4.8  |
| 9   | AI    | 22   | LYS  | 4.8  |
| 34  | CF    | 30   | ARG  | 4.8  |
| 37  | DJ    | 40   | LYS  | 4.8  |
| 14  | BN    | 32   | SER  | 4.8  |
| 37  | CJ    | 88   | SER  | 4.8  |
| 30  | CD    | 60   | VAL  | 4.8  |
| 7   | AG    | 106  | GLU  | 4.8  |
| 19  | BS    | 34   | TRP  | 4.8  |
| 6   | BF    | 39   | LEU  | 4.8  |
| 30  | CD    | 101  | PHE  | 4.8  |
| 30  | CD    | 132  | ALA  | 4.8  |
| 19  | BS    | 55   | ARG  | 4.8  |
| 31  | CA    | 343  | C    | 4.8  |
| 54  | DI    | 101  | LYS  | 4.8  |
| 1   | AA    | 1022 | A    | 4.8  |
| 33  | CE    | 186  | VAL  | 4.8  |
| 3   | BC    | 203  | PHE  | 4.8  |
| 30  | CD    | 35   | THR  | 4.8  |
| 40  | CM    | 70   | LYS  | 4.8  |
| 10  | AJ    | 7    | ARG  | 4.8  |
| 13  | BM    | 52   | GLN  | 4.8  |
| 18  | AR    | 51   | TYR  | 4.8  |
| 1   | BA    | 1340 | A    | 4.8  |
| 31  | CA    | 101  | A    | 4.8  |
| 40  | CM    | 132  | ARG  | 4.8  |
| 46  | CS    | 13   | ARG  | 4.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | CF    | 10   | ASP  | 4.8  |
| 41  | CN    | 72   | PRO  | 4.8  |
| 31  | CA    | 895  | U    | 4.8  |
| 31  | CA    | 336  | C    | 4.8  |
| 31  | CA    | 1547 | C    | 4.8  |
| 55  | DA    | 2177 | C    | 4.8  |
| 35  | CG    | 175  | LYS  | 4.8  |
| 40  | CM    | 21   | ARG  | 4.8  |
| 9   | BI    | 107  | ASP  | 4.8  |
| 35  | CG    | 94   | TYR  | 4.8  |
| 31  | CA    | 315  | G    | 4.8  |
| 13  | BM    | 69   | LEU  | 4.8  |
| 41  | CN    | 41   | LEU  | 4.8  |
| 43  | CP    | 59   | ALA  | 4.8  |
| 1   | BA    | 1219 | A    | 4.8  |
| 16  | BP    | 9    | HIS  | 4.8  |
| 38  | CK    | 21   | THR  | 4.8  |
| 14  | BN    | 34   | VAL  | 4.7  |
| 7   | AG    | 7    | ILE  | 4.7  |
| 10  | BJ    | 35   | GLN  | 4.7  |
| 16  | BP    | 53   | ASP  | 4.7  |
| 36  | DH    | 56   | ALA  | 4.7  |
| 1   | BA    | 1341 | U    | 4.7  |
| 54  | DI    | 114  | GLU  | 4.7  |
| 34  | CF    | 8    | TYR  | 4.7  |
| 2   | AB    | 210  | VAL  | 4.7  |
| 16  | BP    | 19   | VAL  | 4.7  |
| 47  | CT    | 83   | LYS  | 4.7  |
| 40  | CM    | 72   | ALA  | 4.7  |
| 30  | CD    | 83   | ARG  | 4.7  |
| 34  | CF    | 42   | GLU  | 4.7  |
| 31  | CA    | 214  | G    | 4.7  |
| 31  | CA    | 2877 | G    | 4.7  |
| 48  | CU    | 81   | LYS  | 4.7  |
| 55  | DA    | 2126 | A    | 4.7  |
| 45  | CR    | 38   | ALA  | 4.7  |
| 45  | CR    | 95   | LEU  | 4.7  |
| 2   | AB    | 44   | GLU  | 4.7  |
| 47  | CT    | 4    | ILE  | 4.7  |
| 11  | BK    | 30   | THR  | 4.7  |
| 26  | C5    | 1    | MET  | 4.7  |
| 7   | AG    | 65   | ALA  | 4.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | BG    | 78   | ARG  | 4.7  |
| 13  | AM    | 40   | ALA  | 4.7  |
| 19  | BS    | 3    | ARG  | 4.7  |
| 35  | CG    | 24   | ILE  | 4.7  |
| 20  | BT    | 8    | LYS  | 4.7  |
| 29  | CC    | 232  | HIS  | 4.7  |
| 9   | BI    | 43   | THR  | 4.7  |
| 1   | BA    | 1231 | G    | 4.7  |
| 25  | C4    | 14   | PHE  | 4.7  |
| 41  | CN    | 80   | VAL  | 4.7  |
| 7   | AG    | 68   | ASN  | 4.7  |
| 30  | CD    | 90   | PHE  | 4.7  |
| 43  | CP    | 53   | THR  | 4.7  |
| 2   | AB    | 117  | LEU  | 4.7  |
| 13  | BM    | 13   | LYS  | 4.7  |
| 30  | CD    | 187  | LEU  | 4.7  |
| 31  | CA    | 2627 | G    | 4.7  |
| 31  | CA    | 318  | C    | 4.7  |
| 55  | DA    | 1089 | A    | 4.7  |
| 36  | CH    | 137  | GLU  | 4.7  |
| 2   | BB    | 32   | PHE  | 4.7  |
| 14  | BN    | 21   | PHE  | 4.7  |
| 10  | BJ    | 92   | LEU  | 4.7  |
| 36  | DH    | 124  | THR  | 4.7  |
| 39  | CL    | 3    | GLN  | 4.7  |
| 55  | DA    | 1063 | G    | 4.7  |
| 49  | CV    | 55   | PRO  | 4.7  |
| 55  | DA    | 2164 | C    | 4.7  |
| 55  | DA    | 1060 | U    | 4.7  |
| 39  | CL    | 111  | LYS  | 4.7  |
| 2   | BB    | 10   | LEU  | 4.7  |
| 36  | DH    | 125  | THR  | 4.7  |
| 33  | CE    | 22   | ASP  | 4.7  |
| 53  | CZ    | 35   | GLY  | 4.7  |
| 1   | BA    | 1033 | G    | 4.7  |
| 1   | BA    | 1224 | U    | 4.7  |
| 31  | CA    | 1868 | C    | 4.7  |
| 31  | CA    | 2122 | U    | 4.7  |
| 35  | CG    | 126  | PRO  | 4.7  |
| 1   | BA    | 1534 | A    | 4.7  |
| 55  | DA    | 2117 | A    | 4.7  |
| 24  | C3    | 22   | MET  | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 29   | VAL  | 4.6  |
| 36  | CH    | 135  | HIS  | 4.6  |
| 40  | CM    | 127  | VAL  | 4.6  |
| 51  | CX    | 23   | VAL  | 4.6  |
| 13  | AM    | 26   | GLY  | 4.6  |
| 22  | C1    | 44   | THR  | 4.6  |
| 40  | CM    | 76   | GLU  | 4.6  |
| 14  | AN    | 100  | SER  | 4.6  |
| 43  | CP    | 49   | VAL  | 4.6  |
| 48  | CU    | 62   | VAL  | 4.6  |
| 49  | CV    | 11   | VAL  | 4.6  |
| 21  | AU    | 16   | LEU  | 4.6  |
| 2   | BB    | 33   | GLY  | 4.6  |
| 34  | CF    | 150  | ARG  | 4.6  |
| 54  | DI    | 94   | ARG  | 4.6  |
| 37  | DJ    | 37   | GLU  | 4.6  |
| 31  | CA    | 850  | U    | 4.6  |
| 30  | CD    | 1    | MET  | 4.6  |
| 31  | CA    | 313  | G    | 4.6  |
| 33  | CE    | 127  | GLU  | 4.6  |
| 13  | BM    | 70   | ARG  | 4.6  |
| 27  | C0    | 12   | SER  | 4.6  |
| 7   | BG    | 63   | GLU  | 4.6  |
| 11  | AK    | 43   | GLY  | 4.6  |
| 50  | CW    | 67   | GLY  | 4.6  |
| 43  | CP    | 36   | TYR  | 4.6  |
| 1   | BA    | 205  | A    | 4.6  |
| 47  | CT    | 94   | ASP  | 4.6  |
| 1   | BA    | 951  | G    | 4.6  |
| 31  | CA    | 1530 | G    | 4.6  |
| 33  | CE    | 43   | THR  | 4.6  |
| 31  | CA    | 1534 | U    | 4.6  |
| 22  | C1    | 15   | MET  | 4.6  |
| 33  | CE    | 134  | LEU  | 4.6  |
| 36  | DH    | 87   | GLU  | 4.6  |
| 36  | DH    | 136  | SER  | 4.6  |
| 7   | BG    | 98   | ALA  | 4.6  |
| 38  | CK    | 55   | ILE  | 4.6  |
| 40  | CM    | 137  | ALA  | 4.6  |
| 35  | CG    | 44   | LYS  | 4.6  |
| 43  | CP    | 33   | ARG  | 4.6  |
| 1   | BA    | 981  | U    | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 880  | G    | 4.6  |
| 31  | CA    | 1074 | G    | 4.6  |
| 33  | CE    | 177  | PRO  | 4.6  |
| 13  | BM    | 50   | GLU  | 4.6  |
| 29  | CC    | 47   | GLY  | 4.6  |
| 44  | CQ    | 13   | MET  | 4.6  |
| 35  | CG    | 6    | LYS  | 4.6  |
| 43  | CP    | 109  | ALA  | 4.6  |
| 47  | CT    | 92   | ARG  | 4.6  |
| 3   | BC    | 109  | PRO  | 4.6  |
| 25  | C4    | 46   | PRO  | 4.6  |
| 43  | CP    | 104  | GLN  | 4.6  |
| 51  | CX    | 42   | GLY  | 4.6  |
| 33  | CE    | 15   | SER  | 4.6  |
| 1   | BA    | 972  | C    | 4.6  |
| 42  | CO    | 114  | GLU  | 4.6  |
| 7   | AG    | 6    | VAL  | 4.6  |
| 17  | BQ    | 8    | LEU  | 4.6  |
| 25  | C4    | 38   | THR  | 4.6  |
| 31  | CA    | 44   | A    | 4.6  |
| 39  | CL    | 69   | VAL  | 4.6  |
| 45  | CR    | 7    | GLY  | 4.6  |
| 33  | CE    | 100  | MET  | 4.6  |
| 1   | BA    | 68   | G    | 4.6  |
| 31  | CA    | 88   | G    | 4.6  |
| 31  | CA    | 2630 | G    | 4.6  |
| 1   | BA    | 1027 | C    | 4.6  |
| 43  | CP    | 97   | PHE  | 4.6  |
| 1   | BA    | 89   | U    | 4.6  |
| 21  | AU    | 9    | ASN  | 4.5  |
| 1   | AA    | 78   | A    | 4.5  |
| 24  | C3    | 43   | THR  | 4.5  |
| 38  | CK    | 137  | PRO  | 4.5  |
| 35  | CG    | 75   | MET  | 4.5  |
| 20  | BT    | 31   | PHE  | 4.5  |
| 33  | CE    | 103  | GLY  | 4.5  |
| 36  | CH    | 61   | VAL  | 4.5  |
| 1   | BA    | 946  | A    | 4.5  |
| 38  | CK    | 42   | ALA  | 4.5  |
| 45  | CR    | 17   | ILE  | 4.5  |
| 7   | AG    | 54   | SER  | 4.5  |
| 11  | AK    | 18   | ASP  | 4.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 17  | BQ    | 72   | SER  | 4.5  |
| 7   | AG    | 26   | PHE  | 4.5  |
| 3   | BC    | 78   | GLY  | 4.5  |
| 31  | CA    | 314  | C    | 4.5  |
| 31  | CA    | 1059 | G    | 4.5  |
| 45  | CR    | 37   | GLN  | 4.5  |
| 55  | DA    | 881  | G    | 4.5  |
| 19  | BS    | 11   | ILE  | 4.5  |
| 39  | CL    | 38   | ILE  | 4.5  |
| 50  | CW    | 48   | MET  | 4.5  |
| 54  | DI    | 135  | ALA  | 4.5  |
| 13  | BM    | 42   | ASP  | 4.5  |
| 37  | CJ    | 64   | ASP  | 4.5  |
| 2   | BB    | 16   | PHE  | 4.5  |
| 26  | C5    | 33   | HIS  | 4.5  |
| 37  | DJ    | 107  | GLN  | 4.5  |
| 48  | CU    | 76   | ARG  | 4.5  |
| 31  | CA    | 281  | C    | 4.5  |
| 31  | CA    | 2116 | G    | 4.5  |
| 37  | DJ    | 33   | VAL  | 4.5  |
| 7   | AG    | 8    | GLY  | 4.5  |
| 33  | CE    | 42   | GLY  | 4.5  |
| 7   | AG    | 141  | VAL  | 4.5  |
| 30  | CD    | 73   | VAL  | 4.5  |
| 31  | CA    | 1061 | U    | 4.5  |
| 35  | CG    | 76   | VAL  | 4.5  |
| 54  | DI    | 133  | GLU  | 4.5  |
| 33  | CE    | 199  | MET  | 4.5  |
| 47  | CT    | 54   | ALA  | 4.5  |
| 48  | DU    | 1    | MET  | 4.5  |
| 34  | CF    | 100  | PHE  | 4.5  |
| 47  | CT    | 48   | LYS  | 4.5  |
| 9   | AI    | 63   | LEU  | 4.5  |
| 13  | AM    | 48   | LEU  | 4.5  |
| 50  | CW    | 64   | VAL  | 4.5  |
| 43  | CP    | 56   | LYS  | 4.5  |
| 5   | BE    | 140  | THR  | 4.5  |
| 40  | CM    | 121  | THR  | 4.5  |
| 9   | BI    | 98   | LEU  | 4.5  |
| 49  | CV    | 42   | VAL  | 4.5  |
| 13  | AM    | 39   | ILE  | 4.5  |
| 31  | CA    | 816  | C    | 4.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | BS    | 44   | MET  | 4.5  |
| 16  | AP    | 16   | PHE  | 4.5  |
| 31  | CA    | 1093 | G    | 4.5  |
| 31  | CA    | 1407 | G    | 4.5  |
| 16  | BP    | 56   | ARG  | 4.5  |
| 31  | CA    | 2181 | U    | 4.5  |
| 54  | DI    | 136  | ILE  | 4.5  |
| 2   | BB    | 206  | ALA  | 4.5  |
| 31  | CA    | 876  | C    | 4.5  |
| 31  | CA    | 2178 | C    | 4.5  |
| 34  | CF    | 14   | LYS  | 4.5  |
| 1   | BA    | 941  | G    | 4.5  |
| 38  | CK    | 40   | HIS  | 4.5  |
| 13  | AM    | 115  | PRO  | 4.4  |
| 15  | BO    | 19   | ALA  | 4.4  |
| 14  | BN    | 73   | PHE  | 4.4  |
| 31  | CA    | 1233 | C    | 4.4  |
| 35  | CG    | 38   | ASN  | 4.4  |
| 37  | CJ    | 25   | GLY  | 4.4  |
| 40  | CM    | 124  | GLY  | 4.4  |
| 55  | DA    | 2161 | C    | 4.4  |
| 37  | DJ    | 127  | ARG  | 4.4  |
| 35  | CG    | 129  | THR  | 4.4  |
| 36  | CH    | 110  | VAL  | 4.4  |
| 31  | CA    | 1984 | G    | 4.4  |
| 7   | BG    | 86   | GLN  | 4.4  |
| 2   | AB    | 7    | ARG  | 4.4  |
| 26  | C5    | 19   | ARG  | 4.4  |
| 33  | CE    | 49   | ARG  | 4.4  |
| 34  | CF    | 112  | ARG  | 4.4  |
| 49  | CV    | 21   | LYS  | 4.4  |
| 34  | CF    | 49   | LEU  | 4.4  |
| 42  | CO    | 76   | VAL  | 4.4  |
| 49  | CV    | 67   | VAL  | 4.4  |
| 42  | CO    | 113  | ILE  | 4.4  |
| 34  | CF    | 11   | GLU  | 4.4  |
| 26  | C5    | 12   | ARG  | 4.4  |
| 30  | CD    | 184  | ARG  | 4.4  |
| 35  | CG    | 156  | PRO  | 4.4  |
| 37  | DJ    | 92   | LYS  | 4.4  |
| 33  | CE    | 180  | LEU  | 4.4  |
| 10  | BJ    | 32   | THR  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | BG    | 90   | GLU  | 4.4  |
| 13  | BM    | 49   | SER  | 4.4  |
| 27  | C0    | 39   | GLU  | 4.4  |
| 37  | CJ    | 127  | ARG  | 4.4  |
| 38  | CK    | 98   | GLU  | 4.4  |
| 49  | CV    | 63   | ALA  | 4.4  |
| 2   | AB    | 9    | MET  | 4.4  |
| 40  | CM    | 91   | ASP  | 4.4  |
| 1   | BA    | 1003 | G    | 4.4  |
| 40  | CM    | 122  | VAL  | 4.4  |
| 1   | BA    | 1125 | U    | 4.4  |
| 9   | BI    | 79   | ILE  | 4.4  |
| 16  | BP    | 51   | ARG  | 4.4  |
| 41  | CN    | 73   | ILE  | 4.4  |
| 51  | CX    | 37   | ILE  | 4.4  |
| 7   | AG    | 52   | GLN  | 4.4  |
| 43  | CP    | 32   | PRO  | 4.4  |
| 51  | CX    | 64   | ASP  | 4.4  |
| 9   | BI    | 129  | LYS  | 4.4  |
| 31  | CA    | 413  | C    | 4.4  |
| 33  | CE    | 122  | GLU  | 4.4  |
| 55  | DA    | 897  | C    | 4.4  |
| 1   | BA    | 842  | U    | 4.4  |
| 11  | AK    | 97   | ILE  | 4.4  |
| 2   | BB    | 213  | TYR  | 4.4  |
| 34  | CF    | 27   | GLN  | 4.4  |
| 46  | CS    | 15   | SER  | 4.4  |
| 46  | CS    | 29   | THR  | 4.4  |
| 20  | BT    | 9    | LYS  | 4.4  |
| 3   | BC    | 102  | ASN  | 4.4  |
| 10  | BJ    | 96   | VAL  | 4.4  |
| 1   | AA    | 1001 | C    | 4.4  |
| 55  | DA    | 893  | C    | 4.4  |
| 49  | CV    | 72   | ILE  | 4.4  |
| 8   | BH    | 130  | ALA  | 4.4  |
| 19  | AS    | 56   | GLN  | 4.4  |
| 31  | CA    | 2799 | A    | 4.4  |
| 14  | BN    | 63   | ARG  | 4.4  |
| 54  | DI    | 72   | LEU  | 4.4  |
| 35  | CG    | 48   | ASN  | 4.4  |
| 15  | BO    | 15   | PHE  | 4.4  |
| 19  | BS    | 56   | GLN  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | BM    | 75   | MET  | 4.4  |
| 8   | AH    | 121  | LEU  | 4.4  |
| 12  | BL    | 81   | LEU  | 4.4  |
| 30  | CD    | 84   | LEU  | 4.3  |
| 40  | CM    | 30   | THR  | 4.3  |
| 13  | BM    | 62   | LYS  | 4.3  |
| 11  | BK    | 110  | ILE  | 4.3  |
| 17  | BQ    | 21   | ILE  | 4.3  |
| 36  | CH    | 94   | ILE  | 4.3  |
| 44  | CQ    | 50   | ILE  | 4.3  |
| 9   | AI    | 59   | GLU  | 4.3  |
| 14  | AN    | 25   | ALA  | 4.3  |
| 40  | CM    | 7    | SER  | 4.3  |
| 42  | CO    | 79   | LEU  | 4.3  |
| 1   | BA    | 1239 | A    | 4.3  |
| 1   | BA    | 1013 | G    | 4.3  |
| 31  | CA    | 2668 | G    | 4.3  |
| 40  | CM    | 139  | GLY  | 4.3  |
| 7   | BG    | 9    | GLN  | 4.3  |
| 34  | CF    | 101  | GLU  | 4.3  |
| 31  | CA    | 1079 | C    | 4.3  |
| 34  | CF    | 22   | TYR  | 4.3  |
| 31  | CA    | 1090 | A    | 4.3  |
| 31  | CA    | 1015 | U    | 4.3  |
| 33  | CE    | 175  | ILE  | 4.3  |
| 31  | CA    | 124  | G    | 4.3  |
| 30  | CD    | 55   | LYS  | 4.3  |
| 37  | DJ    | 97   | LYS  | 4.3  |
| 20  | BT    | 59   | ASP  | 4.3  |
| 20  | BT    | 68   | HIS  | 4.3  |
| 2   | AB    | 27   | MET  | 4.3  |
| 7   | BG    | 44   | TYR  | 4.3  |
| 35  | CG    | 166  | ASP  | 4.3  |
| 23  | C2    | 22   | THR  | 4.3  |
| 35  | CG    | 113  | VAL  | 4.3  |
| 51  | CX    | 41   | ARG  | 4.3  |
| 52  | CY    | 47   | VAL  | 4.3  |
| 2   | BB    | 164  | ILE  | 4.3  |
| 12  | BL    | 108  | LYS  | 4.3  |
| 31  | CA    | 1073 | A    | 4.3  |
| 31  | CA    | 2657 | A    | 4.3  |
| 7   | BG    | 120  | LEU  | 4.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | CO    | 94   | TYR  | 4.3  |
| 45  | CR    | 117  | LEU  | 4.3  |
| 13  | BM    | 90   | ARG  | 4.3  |
| 13  | BM    | 111  | GLY  | 4.3  |
| 31  | CA    | 475  | C    | 4.3  |
| 2   | AB    | 37   | LYS  | 4.3  |
| 9   | AI    | 89   | GLU  | 4.3  |
| 33  | CE    | 121  | VAL  | 4.3  |
| 19  | BS    | 43   | ASN  | 4.3  |
| 45  | CR    | 30   | ARG  | 4.3  |
| 49  | DV    | 52   | LEU  | 4.3  |
| 28  | CB    | 24   | G    | 4.3  |
| 31  | CA    | 1279 | G    | 4.3  |
| 31  | CA    | 2693 | G    | 4.3  |
| 14  | BN    | 10   | GLU  | 4.3  |
| 19  | BS    | 23   | VAL  | 4.3  |
| 30  | CD    | 50   | VAL  | 4.3  |
| 40  | CM    | 38   | GLN  | 4.3  |
| 45  | CR    | 101  | PHE  | 4.3  |
| 46  | CS    | 6    | GLN  | 4.3  |
| 17  | BQ    | 74   | THR  | 4.3  |
| 34  | CF    | 171  | ALA  | 4.3  |
| 1   | BA    | 1150 | A    | 4.3  |
| 3   | BC    | 112  | ASP  | 4.3  |
| 33  | CE    | 147  | LEU  | 4.3  |
| 1   | AA    | 1033 | G    | 4.3  |
| 1   | BA    | 1272 | G    | 4.3  |
| 1   | BA    | 1281 | C    | 4.3  |
| 31  | CA    | 2164 | C    | 4.3  |
| 55  | DA    | 2146 | C    | 4.3  |
| 2   | BB    | 131  | LYS  | 4.3  |
| 3   | BC    | 50   | ALA  | 4.3  |
| 36  | DH    | 89   | LYS  | 4.3  |
| 19  | BS    | 13   | LEU  | 4.3  |
| 49  | CV    | 56   | GLY  | 4.3  |
| 1   | BA    | 1035 | A    | 4.3  |
| 14  | BN    | 71   | HIS  | 4.3  |
| 31  | CA    | 1548 | A    | 4.3  |
| 22  | C1    | 8    | PRO  | 4.3  |
| 40  | CM    | 119  | PRO  | 4.3  |
| 41  | CN    | 12   | MET  | 4.3  |
| 50  | CW    | 2    | PHE  | 4.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | BI    | 21   | ILE  | 4.3  |
| 25  | C4    | 45   | ARG  | 4.3  |
| 31  | CA    | 280  | U    | 4.3  |
| 31  | CA    | 884  | U    | 4.3  |
| 55  | DA    | 2105 | U    | 4.3  |
| 27  | C0    | 25   | LEU  | 4.2  |
| 51  | CX    | 85   | GLU  | 4.2  |
| 33  | CE    | 126  | VAL  | 4.2  |
| 38  | CK    | 118  | MET  | 4.2  |
| 1   | BA    | 250  | A    | 4.2  |
| 25  | C4    | 25   | LYS  | 4.2  |
| 46  | CS    | 60   | LYS  | 4.2  |
| 1   | BA    | 952  | U    | 4.2  |
| 1   | BA    | 1007 | U    | 4.2  |
| 6   | BF    | 97   | THR  | 4.2  |
| 16  | AP    | 47   | GLU  | 4.2  |
| 31  | CA    | 1112 | G    | 4.2  |
| 15  | BO    | 75   | VAL  | 4.2  |
| 24  | C3    | 5    | PHE  | 4.2  |
| 25  | C4    | 35   | LYS  | 4.2  |
| 36  | CH    | 139  | PHE  | 4.2  |
| 37  | CJ    | 36   | MET  | 4.2  |
| 49  | CV    | 85   | PHE  | 4.2  |
| 49  | DV    | 49   | VAL  | 4.2  |
| 20  | BT    | 36   | TYR  | 4.2  |
| 49  | DV    | 51   | ALA  | 4.2  |
| 15  | BO    | 21   | ASP  | 4.2  |
| 1   | BA    | 1310 | G    | 4.2  |
| 24  | C3    | 13   | ASN  | 4.2  |
| 9   | BI    | 48   | VAL  | 4.2  |
| 16  | AP    | 39   | PHE  | 4.2  |
| 33  | CE    | 28   | VAL  | 4.2  |
| 34  | CF    | 114  | PHE  | 4.2  |
| 40  | CM    | 50   | PHE  | 4.2  |
| 11  | AK    | 110  | ILE  | 4.2  |
| 9   | BI    | 94   | LEU  | 4.2  |
| 28  | CB    | 63   | C    | 4.2  |
| 31  | CA    | 1874 | C    | 4.2  |
| 43  | CP    | 70   | ALA  | 4.2  |
| 48  | CU    | 33   | LYS  | 4.2  |
| 49  | CV    | 2    | ALA  | 4.2  |
| 54  | DI    | 3    | LEU  | 4.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | AT    | 80   | THR  | 4.2  |
| 31  | CA    | 180  | G    | 4.2  |
| 31  | CA    | 1444 | G    | 4.2  |
| 35  | CG    | 125  | CYS  | 4.2  |
| 19  | BS    | 65   | GLU  | 4.2  |
| 35  | CG    | 173  | GLU  | 4.2  |
| 3   | BC    | 108  | LYS  | 4.2  |
| 31  | CA    | 810  | U    | 4.2  |
| 48  | CU    | 44   | LYS  | 4.2  |
| 11  | BK    | 67   | ALA  | 4.2  |
| 35  | CG    | 21   | GLY  | 4.2  |
| 40  | CM    | 83   | ALA  | 4.2  |
| 1   | AA    | 1000 | A    | 4.2  |
| 10  | AJ    | 102  | LEU  | 4.2  |
| 9   | AI    | 88   | MET  | 4.2  |
| 37  | CJ    | 117  | MET  | 4.2  |
| 42  | CO    | 1    | MET  | 4.2  |
| 13  | BM    | 44   | LYS  | 4.2  |
| 44  | CQ    | 5    | ILE  | 4.2  |
| 49  | CV    | 65   | ILE  | 4.2  |
| 31  | CA    | 2032 | G    | 4.2  |
| 45  | CR    | 25   | TYR  | 4.2  |
| 47  | CT    | 95   | ARG  | 4.2  |
| 34  | CF    | 36   | LEU  | 4.2  |
| 1   | AA    | 1277 | C    | 4.2  |
| 1   | BA    | 1230 | C    | 4.2  |
| 13  | BM    | 102  | THR  | 4.2  |
| 49  | CV    | 62   | GLU  | 4.2  |
| 36  | DH    | 99   | ILE  | 4.2  |
| 6   | AF    | 37   | HIS  | 4.2  |
| 46  | CS    | 82   | HIS  | 4.2  |
| 46  | CS    | 30   | GLY  | 4.2  |
| 9   | AI    | 97   | GLU  | 4.2  |
| 34  | CF    | 64   | LYS  | 4.2  |
| 1   | AA    | 1036 | A    | 4.2  |
| 5   | BE    | 120  | VAL  | 4.2  |
| 5   | BE    | 80   | THR  | 4.2  |
| 37  | CJ    | 34   | ASN  | 4.2  |
| 30  | CD    | 59   | ARG  | 4.2  |
| 8   | BH    | 122  | GLY  | 4.2  |
| 46  | CS    | 92   | TRP  | 4.2  |
| 37  | DJ    | 81   | LYS  | 4.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 45         | CR           | 18         | LEU         | 4.2         |
| 33         | CE           | 140        | ASP         | 4.2         |
| 14         | AN           | 37         | SER         | 4.2         |
| 1          | BA           | 1001       | C           | 4.2         |
| 1          | BA           | 1210       | C           | 4.2         |
| 31         | CA           | 2165       | C           | 4.2         |
| 35         | CG           | 90         | VAL         | 4.2         |
| 53         | CZ           | 48         | ARG         | 4.2         |
| 19         | AS           | 49         | ILE         | 4.2         |
| 37         | CJ           | 35         | ILE         | 4.2         |
| 38         | CK           | 54         | ILE         | 4.2         |
| 37         | CJ           | 16         | GLY         | 4.2         |
| 36         | DH           | 67         | ALA         | 4.1         |
| 40         | CM           | 84         | LYS         | 4.2         |
| 7          | AG           | 23         | LEU         | 4.1         |
| 11         | BK           | 68         | GLU         | 4.1         |
| 30         | CD           | 39         | ASP         | 4.1         |
| 3          | BC           | 179        | ARG         | 4.1         |
| 10         | AJ           | 45         | ARG         | 4.1         |
| 33         | CE           | 10         | SER         | 4.1         |
| 31         | CA           | 638        | G           | 4.1         |
| 31         | CA           | 1041       | G           | 4.1         |
| 1          | AA           | 1037       | C           | 4.1         |
| 55         | DA           | 2171       | A           | 4.1         |
| 1          | AA           | 89         | U           | 4.1         |
| 14         | BN           | 39         | GLU         | 4.1         |
| 9          | AI           | 39         | PHE         | 4.1         |
| 9          | BI           | 33         | ARG         | 4.1         |
| 7          | AG           | 110        | LYS         | 4.1         |
| 13         | AM           | 13         | LYS         | 4.1         |
| 54         | DI           | 123        | ILE         | 4.1         |
| 30         | CD           | 121        | THR         | 4.1         |
| 34         | CF           | 139        | PRO         | 4.1         |
| 40         | CM           | 5          | THR         | 4.1         |
| 13         | AM           | 35         | ALA         | 4.1         |
| 33         | CE           | 35         | TYR         | 4.1         |
| 43         | CP           | 102        | ARG         | 4.1         |
| 46         | CS           | 24         | LYS         | 4.1         |
| 37         | DJ           | 57         | VAL         | 4.1         |
| 4          | AD           | 39         | GLY         | 4.1         |
| 31         | CA           | 1533       | C           | 4.1         |
| 34         | CF           | 29         | PRO         | 4.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AM    | 34   | LEU  | 4.1  |
| 28  | CB    | 22   | U    | 4.1  |
| 31  | CA    | 799  | G    | 4.1  |
| 40  | CM    | 138  | ALA  | 4.1  |
| 38  | CK    | 141  | ASP  | 4.1  |
| 13  | BM    | 38   | GLY  | 4.1  |
| 22  | C1    | 51   | GLY  | 4.1  |
| 37  | CJ    | 137  | GLY  | 4.1  |
| 46  | CS    | 46   | GLU  | 4.1  |
| 12  | BL    | 50   | ARG  | 4.1  |
| 45  | CR    | 92   | ARG  | 4.1  |
| 7   | AG    | 50   | LEU  | 4.1  |
| 9   | BI    | 121  | ALA  | 4.1  |
| 31  | CA    | 1531 | C    | 4.1  |
| 31  | CA    | 2111 | U    | 4.1  |
| 54  | DI    | 106  | PHE  | 4.1  |
| 1   | BA    | 1048 | G    | 4.1  |
| 33  | CE    | 176  | ASP  | 4.1  |
| 13  | BM    | 53   | ILE  | 4.1  |
| 46  | CS    | 37   | GLU  | 4.1  |
| 54  | DI    | 66   | GLY  | 4.1  |
| 44  | CQ    | 72   | ARG  | 4.1  |
| 48  | CU    | 80   | TRP  | 4.1  |
| 1   | BA    | 982  | U    | 4.1  |
| 2   | AB    | 214  | LEU  | 4.1  |
| 7   | BG    | 26   | PHE  | 4.1  |
| 31  | CA    | 1732 | C    | 4.1  |
| 8   | BH    | 90   | ASP  | 4.1  |
| 17  | BQ    | 23   | VAL  | 4.1  |
| 19  | BS    | 81   | ARG  | 4.1  |
| 2   | AB    | 132  | LYS  | 4.1  |
| 34  | CF    | 141  | ILE  | 4.1  |
| 35  | CG    | 158  | LYS  | 4.1  |
| 11  | AK    | 100  | LEU  | 4.1  |
| 37  | CJ    | 115  | ALA  | 4.1  |
| 41  | CN    | 78   | LEU  | 4.1  |
| 2   | AB    | 16   | PHE  | 4.1  |
| 3   | BC    | 118  | ASP  | 4.1  |
| 28  | CB    | 97   | C    | 4.1  |
| 31  | CA    | 1044 | C    | 4.1  |
| 3   | BC    | 204  | LYS  | 4.1  |
| 7   | AG    | 64   | VAL  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | BI    | 117  | GLY  | 4.1  |
| 31  | CA    | 85   | G    | 4.1  |
| 31  | CA    | 866  | A    | 4.1  |
| 31  | CA    | 2835 | A    | 4.1  |
| 31  | CA    | 2872 | A    | 4.1  |
| 55  | DA    | 277  | G    | 4.1  |
| 8   | BH    | 121  | LEU  | 4.1  |
| 30  | CD    | 95   | SER  | 4.1  |
| 31  | CA    | 545  | U    | 4.1  |
| 45  | CR    | 35   | ALA  | 4.1  |
| 9   | BI    | 124  | ARG  | 4.1  |
| 36  | DH    | 127  | GLU  | 4.1  |
| 7   | AG    | 49   | THR  | 4.1  |
| 28  | CB    | 37   | C    | 4.1  |
| 11  | AK    | 84   | VAL  | 4.1  |
| 33  | CE    | 196  | VAL  | 4.1  |
| 36  | CH    | 134  | VAL  | 4.1  |
| 17  | BQ    | 61   | ILE  | 4.1  |
| 1   | AA    | 412  | A    | 4.1  |
| 3   | BC    | 172  | ARG  | 4.0  |
| 30  | CD    | 80   | TRP  | 4.1  |
| 31  | CA    | 1142 | A    | 4.1  |
| 31  | CA    | 2167 | U    | 4.1  |
| 33  | CE    | 76   | PRO  | 4.0  |
| 37  | CJ    | 66   | SER  | 4.1  |
| 21  | AU    | 36   | GLU  | 4.0  |
| 47  | CT    | 99   | ARG  | 4.0  |
| 40  | CM    | 52   | GLY  | 4.0  |
| 46  | CS    | 51   | VAL  | 4.0  |
| 7   | AG    | 116  | MET  | 4.0  |
| 14  | BN    | 47   | LYS  | 4.0  |
| 41  | CN    | 116  | ALA  | 4.0  |
| 43  | CP    | 61   | GLN  | 4.0  |
| 31  | CA    | 1325 | U    | 4.0  |
| 31  | CA    | 477  | A    | 4.0  |
| 35  | CG    | 154  | PRO  | 4.0  |
| 39  | CL    | 89   | ASN  | 4.0  |
| 1   | AA    | 1276 | G    | 4.0  |
| 3   | BC    | 194  | GLY  | 4.0  |
| 19  | BS    | 26   | GLY  | 4.0  |
| 33  | CE    | 64   | GLY  | 4.0  |
| 10  | AJ    | 8    | ILE  | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | CR    | 65   | ILE  | 4.0  |
| 2   | AB    | 10   | LEU  | 4.0  |
| 49  | CV    | 22   | ARG  | 4.0  |
| 14  | BN    | 15   | ALA  | 4.0  |
| 49  | CV    | 27   | ASN  | 4.0  |
| 1   | BA    | 945  | G    | 4.0  |
| 31  | CA    | 2383 | G    | 4.0  |
| 29  | CC    | 101  | ARG  | 4.0  |
| 33  | CE    | 12   | LEU  | 4.0  |
| 34  | CF    | 98   | GLU  | 4.0  |
| 36  | CH    | 122  | LEU  | 4.0  |
| 53  | CZ    | 5    | GLU  | 4.0  |
| 7   | BG    | 51   | ALA  | 4.0  |
| 19  | BS    | 75   | ALA  | 4.0  |
| 33  | CE    | 50   | ALA  | 4.0  |
| 37  | CJ    | 104  | ALA  | 4.0  |
| 44  | CQ    | 91   | ALA  | 4.0  |
| 50  | CW    | 37   | PRO  | 4.0  |
| 35  | CG    | 73   | ASN  | 4.0  |
| 3   | BC    | 200  | VAL  | 4.0  |
| 44  | CQ    | 26   | VAL  | 4.0  |
| 33  | CE    | 67   | ARG  | 4.0  |
| 54  | DI    | 88   | HIS  | 4.0  |
| 31  | CA    | 801  | G    | 4.0  |
| 36  | CH    | 127  | GLU  | 4.0  |
| 43  | CP    | 60   | GLU  | 4.0  |
| 1   | BA    | 194  | C    | 4.0  |
| 1   | BA    | 1226 | C    | 4.0  |
| 42  | CO    | 20   | MET  | 4.0  |
| 23  | C2    | 31   | PRO  | 4.0  |
| 7   | AG    | 105  | VAL  | 4.0  |
| 6   | AF    | 36   | ILE  | 4.0  |
| 48  | CU    | 30   | ILE  | 4.0  |
| 1   | BA    | 174  | A    | 4.0  |
| 1   | BA    | 460  | A    | 4.0  |
| 31  | CA    | 1143 | A    | 4.0  |
| 45  | CR    | 45   | TYR  | 4.0  |
| 55  | DA    | 2114 | A    | 4.0  |
| 14  | BN    | 3    | LYS  | 4.0  |
| 23  | C2    | 29   | THR  | 4.0  |
| 11  | AK    | 21   | ALA  | 4.0  |
| 31  | CA    | 290  | U    | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 1018 | U    | 4.0  |
| 35  | CG    | 91   | GLY  | 4.0  |
| 40  | CM    | 34   | GLY  | 4.0  |
| 2   | AB    | 36   | ASN  | 4.0  |
| 33  | CE    | 171  | ASP  | 4.0  |
| 13  | BM    | 16   | VAL  | 4.0  |
| 37  | DJ    | 61   | VAL  | 4.0  |
| 45  | CR    | 39   | VAL  | 4.0  |
| 16  | AP    | 4    | ILE  | 4.0  |
| 44  | CQ    | 99   | TYR  | 4.0  |
| 1   | BA    | 1038 | C    | 4.0  |
| 22  | C1    | 33   | THR  | 4.0  |
| 29  | CC    | 225  | MET  | 4.0  |
| 31  | CA    | 603  | A    | 4.0  |
| 31  | CA    | 224  | U    | 4.0  |
| 31  | CA    | 1406 | U    | 4.0  |
| 1   | BA    | 944  | G    | 4.0  |
| 31  | CA    | 2367 | G    | 4.0  |
| 7   | AG    | 48   | GLU  | 4.0  |
| 14  | AN    | 27   | LEU  | 4.0  |
| 15  | AO    | 69   | TYR  | 4.0  |
| 35  | CG    | 50   | LEU  | 4.0  |
| 9   | AI    | 16   | ALA  | 4.0  |
| 36  | DH    | 123  | ARG  | 4.0  |
| 35  | CG    | 49   | THR  | 4.0  |
| 50  | CW    | 28   | ALA  | 4.0  |
| 55  | DA    | 1847 | A    | 4.0  |
| 31  | CA    | 259  | G    | 4.0  |
| 31  | CA    | 1731 | G    | 4.0  |
| 31  | CA    | 2819 | G    | 4.0  |
| 34  | CF    | 149  | VAL  | 4.0  |
| 44  | CQ    | 92   | VAL  | 4.0  |
| 13  | BM    | 100  | GLN  | 4.0  |
| 30  | CD    | 75   | ALA  | 4.0  |
| 33  | CE    | 135  | ALA  | 4.0  |
| 13  | AM    | 31   | LYS  | 3.9  |
| 31  | CA    | 222  | A    | 3.9  |
| 36  | DH    | 142  | VAL  | 3.9  |
| 1   | BA    | 976  | G    | 3.9  |
| 31  | CA    | 361  | G    | 3.9  |
| 31  | CA    | 2895 | G    | 3.9  |
| 42  | CO    | 101  | GLY  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | CP    | 22   | GLY  | 3.9  |
| 43  | CP    | 101  | GLY  | 3.9  |
| 2   | AB    | 49   | MET  | 3.9  |
| 2   | BB    | 134  | ALA  | 3.9  |
| 46  | CS    | 1    | MET  | 3.9  |
| 47  | CT    | 98   | LYS  | 3.9  |
| 48  | CU    | 82   | LYS  | 3.9  |
| 1   | AA    | 1004 | A    | 3.9  |
| 36  | CH    | 108  | VAL  | 3.9  |
| 49  | DV    | 55   | PRO  | 3.9  |
| 49  | CV    | 86   | ARG  | 3.9  |
| 2   | AB    | 85   | LEU  | 3.9  |
| 7   | BG    | 23   | LEU  | 3.9  |
| 34  | CF    | 127  | ASN  | 3.9  |
| 14  | BN    | 7    | LYS  | 3.9  |
| 22  | C1    | 37   | LYS  | 3.9  |
| 30  | CD    | 86   | GLU  | 3.9  |
| 36  | CH    | 70   | GLU  | 3.9  |
| 1   | BA    | 1041 | G    | 3.9  |
| 13  | BM    | 106  | ALA  | 3.9  |
| 31  | CA    | 989  | G    | 3.9  |
| 31  | CA    | 1202 | G    | 3.9  |
| 31  | CA    | 2833 | U    | 3.9  |
| 23  | C2    | 40   | ASP  | 3.9  |
| 46  | CS    | 99   | THR  | 3.9  |
| 49  | CV    | 94   | ARG  | 3.9  |
| 31  | CA    | 2176 | A    | 3.9  |
| 29  | CC    | 236  | GLU  | 3.9  |
| 37  | DJ    | 21   | SER  | 3.9  |
| 20  | BT    | 45   | ALA  | 3.9  |
| 33  | CE    | 26   | ALA  | 3.9  |
| 38  | CK    | 94   | ALA  | 3.9  |
| 1   | BA    | 1127 | G    | 3.9  |
| 36  | CH    | 68   | ARG  | 3.9  |
| 52  | CY    | 18   | ARG  | 3.9  |
| 20  | BT    | 35   | VAL  | 3.9  |
| 21  | AU    | 13   | ASP  | 3.9  |
| 34  | CF    | 12   | VAL  | 3.9  |
| 27  | C0    | 41   | THR  | 3.9  |
| 47  | CT    | 16   | LYS  | 3.9  |
| 16  | AP    | 45   | GLU  | 3.9  |
| 31  | CA    | 76   | C    | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | CM    | 3    | LEU  | 3.9  |
| 35  | CG    | 96   | ALA  | 3.9  |
| 26  | C5    | 25   | VAL  | 3.9  |
| 29  | CC    | 172  | VAL  | 3.9  |
| 34  | CF    | 142  | ASP  | 3.9  |
| 31  | CA    | 805  | G    | 3.9  |
| 1   | BA    | 1277 | C    | 3.9  |
| 31  | CA    | 1043 | C    | 3.9  |
| 2   | AB    | 42   | ASN  | 3.9  |
| 1   | BA    | 1254 | A    | 3.9  |
| 14  | BN    | 59   | ARG  | 3.9  |
| 53  | DZ    | 63   | ALA  | 3.9  |
| 55  | DA    | 2119 | A    | 3.9  |
| 3   | BC    | 56   | VAL  | 3.9  |
| 3   | BC    | 116  | VAL  | 3.9  |
| 8   | BH    | 110  | VAL  | 3.9  |
| 1   | BA    | 1253 | G    | 3.9  |
| 2   | BB    | 212  | LEU  | 3.9  |
| 3   | BC    | 171  | GLY  | 3.9  |
| 30  | CD    | 188  | LEU  | 3.9  |
| 55  | DA    | 2128 | G    | 3.9  |
| 1   | BA    | 175  | C    | 3.9  |
| 20  | BT    | 5    | LYS  | 3.9  |
| 35  | CG    | 20   | ASN  | 3.9  |
| 3   | BC    | 117  | ALA  | 3.9  |
| 7   | BG    | 121  | ALA  | 3.9  |
| 14  | AN    | 5    | SER  | 3.9  |
| 16  | BP    | 58   | ALA  | 3.9  |
| 35  | CG    | 68   | ALA  | 3.9  |
| 1   | BA    | 325  | A    | 3.9  |
| 31  | CA    | 213  | A    | 3.9  |
| 31  | CA    | 423  | A    | 3.9  |
| 31  | CA    | 1395 | A    | 3.9  |
| 48  | CU    | 56   | GLU  | 3.9  |
| 50  | CW    | 7    | GLU  | 3.9  |
| 13  | AM    | 24   | GLY  | 3.9  |
| 35  | CG    | 66   | GLY  | 3.9  |
| 38  | CK    | 23   | LYS  | 3.9  |
| 14  | BN    | 50   | THR  | 3.9  |
| 22  | C1    | 26   | THR  | 3.9  |
| 31  | CA    | 1017 | G    | 3.9  |
| 31  | CA    | 2876 | G    | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | AB    | 12   | ALA  | 3.9  |
| 20  | AT    | 87   | ALA  | 3.9  |
| 42  | CO    | 107  | ASN  | 3.9  |
| 17  | BQ    | 5    | ILE  | 3.9  |
| 27  | C0    | 57   | VAL  | 3.9  |
| 50  | CW    | 45   | ASP  | 3.9  |
| 3   | BC    | 54   | ARG  | 3.9  |
| 40  | CM    | 65   | GLY  | 3.9  |
| 9   | AI    | 51   | PRO  | 3.9  |
| 39  | CL    | 48   | PRO  | 3.9  |
| 7   | BG    | 84   | THR  | 3.9  |
| 1   | BA    | 1214 | C    | 3.9  |
| 30  | CD    | 42   | ASN  | 3.9  |
| 31  | CA    | 2129 | C    | 3.9  |
| 55  | DA    | 2162 | G    | 3.9  |
| 31  | CA    | 1599 | U    | 3.8  |
| 34  | CF    | 120  | LYS  | 3.8  |
| 1   | AA    | 80   | A    | 3.8  |
| 1   | AA    | 1019 | A    | 3.8  |
| 35  | CG    | 37   | LEU  | 3.8  |
| 36  | CH    | 77   | THR  | 3.8  |
| 40  | CM    | 118  | THR  | 3.8  |
| 47  | CT    | 40   | ASN  | 3.8  |
| 53  | CZ    | 44   | LYS  | 3.8  |
| 3   | BC    | 122  | SER  | 3.8  |
| 1   | AA    | 1002 | G    | 3.8  |
| 1   | AA    | 1024 | G    | 3.8  |
| 1   | BA    | 108  | G    | 3.8  |
| 2   | AB    | 41   | ILE  | 3.8  |
| 49  | DV    | 54   | GLN  | 3.8  |
| 51  | CX    | 51   | VAL  | 3.8  |
| 31  | CA    | 308  | G    | 3.8  |
| 7   | BG    | 59   | LEU  | 3.8  |
| 31  | CA    | 2309 | A    | 3.8  |
| 38  | CK    | 78   | THR  | 3.8  |
| 48  | CU    | 71   | GLY  | 3.8  |
| 30  | CD    | 68   | PHE  | 3.8  |
| 1   | BA    | 165  | G    | 3.8  |
| 7   | BG    | 149  | LYS  | 3.8  |
| 31  | CA    | 1341 | G    | 3.8  |
| 10  | BJ    | 23   | ALA  | 3.8  |
| 1   | BA    | 1267 | C    | 3.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | BA           | 1364       | U           | 3.8         |
| 6          | AF           | 62         | MET         | 3.8         |
| 38         | CK           | 1          | MET         | 3.8         |
| 31         | CA           | 2045       | C           | 3.8         |
| 38         | CK           | 60         | ASP         | 3.8         |
| 38         | CK           | 64         | VAL         | 3.8         |
| 7          | BG           | 57         | SER         | 3.8         |
| 53         | CZ           | 8          | GLU         | 3.8         |
| 24         | C3           | 14         | ARG         | 3.8         |
| 46         | CS           | 52         | PRO         | 3.8         |
| 28         | CB           | 23         | G           | 3.8         |
| 19         | BS           | 22         | ALA         | 3.8         |
| 31         | CA           | 270        | A           | 3.8         |
| 10         | BJ           | 33         | GLY         | 3.8         |
| 26         | C5           | 2          | LYS         | 3.8         |
| 30         | CD           | 2          | ILE         | 3.8         |
| 33         | CE           | 168        | ASP         | 3.8         |
| 37         | CJ           | 116        | ASP         | 3.8         |
| 38         | CK           | 17         | VAL         | 3.8         |
| 45         | CR           | 14         | HIS         | 3.8         |
| 3          | AC           | 168        | TYR         | 3.8         |
| 16         | BP           | 77         | GLU         | 3.8         |
| 3          | BC           | 127        | ARG         | 3.8         |
| 10         | AJ           | 39         | PRO         | 3.8         |
| 7          | AG           | 39         | ALA         | 3.8         |
| 45         | CR           | 42         | ALA         | 3.8         |
| 2          | BB           | 89         | GLN         | 3.8         |
| 31         | CA           | 1524       | G           | 3.8         |
| 38         | CK           | 66         | GLY         | 3.8         |
| 2          | AB           | 8          | ASP         | 3.8         |
| 2          | AB           | 30         | PHE         | 3.8         |
| 2          | BB           | 36         | ASN         | 3.8         |
| 11         | BK           | 65         | VAL         | 3.8         |
| 46         | CS           | 64         | VAL         | 3.8         |
| 22         | C1           | 18         | SER         | 3.8         |
| 37         | CJ           | 26         | PRO         | 3.8         |
| 7          | BG           | 127        | ALA         | 3.8         |
| 16         | AP           | 43         | ALA         | 3.8         |
| 37         | DJ           | 124        | ALA         | 3.8         |
| 1          | BA           | 1002       | G           | 3.8         |
| 3          | BC           | 181        | ASP         | 3.8         |
| 14         | BN           | 69         | ARG         | 3.8         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | CB    | 98   | G    | 3.8  |
| 31  | CA    | 295  | G    | 3.8  |
| 31  | CA    | 474  | G    | 3.8  |
| 31  | CA    | 2491 | U    | 3.8  |
| 31  | CA    | 2890 | G    | 3.8  |
| 36  | DH    | 11   | ASN  | 3.8  |
| 26  | C5    | 8    | LYS  | 3.8  |
| 31  | CA    | 228  | C    | 3.8  |
| 2   | BB    | 44   | GLU  | 3.8  |
| 35  | CG    | 167  | GLU  | 3.8  |
| 33  | CE    | 148  | ILE  | 3.8  |
| 36  | CH    | 143  | ILE  | 3.8  |
| 44  | CQ    | 86   | VAL  | 3.8  |
| 46  | CS    | 58   | VAL  | 3.8  |
| 10  | AJ    | 10   | LEU  | 3.8  |
| 20  | BT    | 70   | ASN  | 3.8  |
| 22  | C1    | 19   | HIS  | 3.8  |
| 25  | C4    | 26   | HIS  | 3.8  |
| 31  | CA    | 233  | A    | 3.8  |
| 31  | CA    | 377  | G    | 3.8  |
| 41  | CN    | 84   | LYS  | 3.8  |
| 55  | DA    | 2133 | G    | 3.8  |
| 1   | BA    | 1265 | C    | 3.8  |
| 42  | CO    | 6    | SER  | 3.8  |
| 10  | AJ    | 5    | ARG  | 3.8  |
| 30  | CD    | 49   | GLN  | 3.8  |
| 53  | CZ    | 25   | GLN  | 3.8  |
| 36  | CH    | 91   | PHE  | 3.8  |
| 38  | CK    | 89   | PHE  | 3.8  |
| 49  | CV    | 93   | VAL  | 3.8  |
| 54  | DI    | 55   | VAL  | 3.8  |
| 46  | CS    | 19   | THR  | 3.7  |
| 1   | BA    | 172  | A    | 3.7  |
| 31  | CA    | 412  | A    | 3.7  |
| 31  | CA    | 1328 | A    | 3.7  |
| 28  | CB    | 51   | G    | 3.7  |
| 31  | CA    | 611  | C    | 3.7  |
| 37  | CJ    | 134  | ARG  | 3.7  |
| 55  | DA    | 880  | G    | 3.7  |
| 33  | CE    | 37   | ALA  | 3.7  |
| 17  | BQ    | 29   | VAL  | 3.7  |
| 33  | CE    | 14   | VAL  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 149  | ASN  | 3.7  |
| 7   | BG    | 85   | TYR  | 3.7  |
| 38  | CK    | 53   | TYR  | 3.7  |
| 38  | CK    | 95   | ARG  | 3.7  |
| 37  | DJ    | 128  | SER  | 3.7  |
| 1   | BA    | 1320 | C    | 3.7  |
| 46  | CS    | 42   | ALA  | 3.7  |
| 7   | BG    | 104  | ILE  | 3.7  |
| 13  | BM    | 97   | VAL  | 3.7  |
| 33  | CE    | 188  | MET  | 3.7  |
| 15  | BO    | 26   | GLU  | 3.7  |
| 50  | CW    | 79   | ARG  | 3.7  |
| 25  | C4    | 15   | LYS  | 3.7  |
| 42  | CO    | 7    | GLY  | 3.7  |
| 30  | CD    | 206  | ALA  | 3.7  |
| 36  | CH    | 14   | SER  | 3.7  |
| 28  | CB    | 19   | C    | 3.7  |
| 10  | AJ    | 77   | VAL  | 3.7  |
| 45  | CR    | 8    | VAL  | 3.7  |
| 51  | CX    | 38   | VAL  | 3.7  |
| 1   | BA    | 100  | G    | 3.7  |
| 31  | CA    | 495  | G    | 3.7  |
| 31  | CA    | 1245 | G    | 3.7  |
| 31  | CA    | 1653 | G    | 3.7  |
| 47  | CT    | 11   | ARG  | 3.7  |
| 22  | C1    | 57   | LYS  | 3.7  |
| 29  | CC    | 5    | LYS  | 3.7  |
| 37  | CJ    | 100  | LYS  | 3.7  |
| 27  | C0    | 20   | HIS  | 3.7  |
| 53  | CZ    | 58   | ASN  | 3.7  |
| 13  | BM    | 37   | ALA  | 3.7  |
| 14  | BN    | 99   | ALA  | 3.7  |
| 30  | CD    | 102  | ALA  | 3.7  |
| 1   | BA    | 1037 | C    | 3.7  |
| 31  | CA    | 1289 | C    | 3.7  |
| 31  | CA    | 2614 | A    | 3.7  |
| 40  | CM    | 95   | LEU  | 3.7  |
| 42  | CO    | 52   | ILE  | 3.7  |
| 9   | BI    | 91   | ASP  | 3.7  |
| 44  | CQ    | 93   | ARG  | 3.7  |
| 45  | CR    | 64   | ARG  | 3.7  |
| 26  | C5    | 13   | ASN  | 3.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 12         | BL           | 117        | TYR         | 3.7         |
| 33         | CE           | 13         | THR         | 3.7         |
| 40         | CM           | 15         | ALA         | 3.7         |
| 8          | BH           | 2          | SER         | 3.7         |
| 2          | BB           | 31         | ILE         | 3.7         |
| 2          | BB           | 41         | ILE         | 3.7         |
| 13         | AM           | 56         | LEU         | 3.7         |
| 14         | BN           | 12         | LYS         | 3.7         |
| 1          | BA           | 121        | U           | 3.7         |
| 1          | BA           | 1132       | C           | 3.7         |
| 2          | BB           | 6          | MET         | 3.7         |
| 11         | BK           | 85         | MET         | 3.7         |
| 33         | CE           | 7          | ASP         | 3.7         |
| 43         | CP           | 89         | ASP         | 3.7         |
| 55         | DA           | 2147       | A           | 3.7         |
| 1          | BA           | 212        | G           | 3.7         |
| 10         | BJ           | 20         | GLN         | 3.7         |
| 15         | BO           | 20         | ASN         | 3.7         |
| 19         | BS           | 69         | HIS         | 3.7         |
| 31         | CA           | 30         | G           | 3.7         |
| 52         | CY           | 20         | HIS         | 3.7         |
| 9          | BI           | 39         | PHE         | 3.7         |
| 13         | AM           | 10         | PRO         | 3.7         |
| 33         | CE           | 129        | PRO         | 3.7         |
| 37         | CJ           | 112        | THR         | 3.7         |
| 2          | AB           | 186        | ILE         | 3.7         |
| 10         | BJ           | 24         | GLU         | 3.7         |
| 30         | CD           | 34         | VAL         | 3.7         |
| 31         | CA           | 1045       | C           | 3.7         |
| 31         | CA           | 2796       | U           | 3.7         |
| 5          | BE           | 91         | GLY         | 3.7         |
| 31         | CA           | 53         | A           | 3.7         |
| 31         | CA           | 666        | A           | 3.7         |
| 14         | BN           | 62         | ASN         | 3.7         |
| 40         | CM           | 141        | LYS         | 3.7         |
| 13         | AM           | 15         | ALA         | 3.7         |
| 31         | CA           | 117        | G           | 3.7         |
| 33         | CE           | 190        | ALA         | 3.7         |
| 46         | CS           | 36         | ALA         | 3.7         |
| 2          | AB           | 47         | VAL         | 3.7         |
| 33         | CE           | 179        | SER         | 3.7         |
| 38         | CK           | 140        | LEU         | 3.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | BA    | 1313 | U    | 3.7  |
| 31  | CA    | 1060 | U    | 3.7  |
| 33  | DE    | 7    | ASP  | 3.7  |
| 42  | CO    | 117  | ASP  | 3.7  |
| 31  | CA    | 680  | C    | 3.7  |
| 31  | CA    | 1278 | C    | 3.7  |
| 18  | BR    | 48   | ARG  | 3.7  |
| 1   | BA    | 1036 | A    | 3.7  |
| 31  | CA    | 1608 | A    | 3.7  |
| 2   | AB    | 134  | ALA  | 3.7  |
| 4   | AD    | 113  | GLU  | 3.7  |
| 7   | BG    | 61   | ALA  | 3.7  |
| 10  | AJ    | 34   | ALA  | 3.7  |
| 46  | CS    | 12   | HIS  | 3.7  |
| 46  | CS    | 45   | GLU  | 3.7  |
| 54  | DI    | 104  | ALA  | 3.7  |
| 39  | CL    | 21   | CYS  | 3.7  |
| 46  | CS    | 75   | VAL  | 3.7  |
| 1   | BA    | 1266 | G    | 3.7  |
| 54  | DI    | 126  | LEU  | 3.7  |
| 2   | BB    | 123  | ASP  | 3.6  |
| 35  | CG    | 74   | SER  | 3.7  |
| 31  | CA    | 2629 | U    | 3.6  |
| 46  | CS    | 95   | ASP  | 3.6  |
| 10  | BJ    | 88   | MET  | 3.6  |
| 1   | BA    | 63   | C    | 3.6  |
| 31  | CA    | 353  | C    | 3.6  |
| 33  | CE    | 30   | GLN  | 3.6  |
| 3   | BC    | 160  | ALA  | 3.6  |
| 11  | AK    | 66   | ALA  | 3.6  |
| 19  | AS    | 57   | HIS  | 3.6  |
| 9   | BI    | 19   | VAL  | 3.6  |
| 30  | CD    | 27   | ILE  | 3.6  |
| 30  | CD    | 100  | LEU  | 3.6  |
| 35  | CG    | 133  | LEU  | 3.6  |
| 31  | CA    | 1309 | G    | 3.6  |
| 29  | CC    | 251  | GLN  | 3.6  |
| 1   | BA    | 210  | C    | 3.6  |
| 31  | CA    | 1207 | C    | 3.6  |
| 37  | DJ    | 83   | ALA  | 3.6  |
| 47  | CT    | 7    | HIS  | 3.6  |
| 16  | BP    | 36   | VAL  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 849  | A    | 3.6  |
| 37  | DJ    | 58   | VAL  | 3.6  |
| 55  | DA    | 2108 | A    | 3.6  |
| 42  | CO    | 105  | GLY  | 3.6  |
| 2   | AB    | 5    | SER  | 3.6  |
| 6   | AF    | 97   | THR  | 3.6  |
| 20  | BT    | 80   | THR  | 3.6  |
| 37  | CJ    | 48   | SER  | 3.6  |
| 33  | CE    | 16   | GLU  | 3.6  |
| 35  | CG    | 22   | GLN  | 3.6  |
| 9   | AI    | 83   | ILE  | 3.6  |
| 18  | AR    | 23   | TYR  | 3.6  |
| 45  | CR    | 34   | VAL  | 3.6  |
| 54  | DI    | 59   | LEU  | 3.6  |
| 1   | BA    | 986  | U    | 3.6  |
| 7   | AG    | 74   | GLU  | 3.6  |
| 3   | BC    | 70   | THR  | 3.6  |
| 24  | C3    | 24   | THR  | 3.6  |
| 34  | CF    | 96   | MET  | 3.6  |
| 35  | CG    | 128  | GLN  | 3.6  |
| 1   | AA    | 1281 | C    | 3.6  |
| 13  | BM    | 57   | ARG  | 3.6  |
| 31  | CA    | 1236 | G    | 3.6  |
| 42  | CO    | 103  | ARG  | 3.6  |
| 14  | BN    | 51   | LEU  | 3.6  |
| 2   | BB    | 13   | GLY  | 3.6  |
| 21  | AU    | 3    | VAL  | 3.6  |
| 33  | CE    | 77   | ILE  | 3.6  |
| 40  | CM    | 27   | LEU  | 3.6  |
| 40  | CM    | 116  | VAL  | 3.6  |
| 1   | AA    | 121  | U    | 3.6  |
| 31  | CA    | 2305 | U    | 3.6  |
| 36  | CH    | 109  | GLU  | 3.6  |
| 1   | BA    | 195  | A    | 3.6  |
| 14  | AN    | 66   | GLN  | 3.6  |
| 36  | CH    | 89   | LYS  | 3.6  |
| 7   | AG    | 18   | PHE  | 3.6  |
| 16  | BP    | 38   | PHE  | 3.6  |
| 47  | CT    | 3    | THR  | 3.6  |
| 48  | CU    | 29   | THR  | 3.6  |
| 2   | BB    | 139  | ARG  | 3.6  |
| 40  | CM    | 18   | ARG  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | CT    | 44   | ALA  | 3.6  |
| 4   | AD    | 21   | LEU  | 3.6  |
| 9   | AI    | 94   | LEU  | 3.6  |
| 11  | BK    | 86   | VAL  | 3.6  |
| 39  | CL    | 99   | ILE  | 3.6  |
| 10  | BJ    | 97   | ASP  | 3.6  |
| 14  | AN    | 101  | TRP  | 3.6  |
| 14  | BN    | 23   | LYS  | 3.6  |
| 33  | CE    | 132  | LYS  | 3.6  |
| 34  | CF    | 7    | TYR  | 3.6  |
| 40  | CM    | 62   | PRO  | 3.6  |
| 31  | CA    | 1647 | U    | 3.6  |
| 13  | BM    | 3    | ARG  | 3.6  |
| 31  | CA    | 2117 | A    | 3.6  |
| 35  | CG    | 5    | ALA  | 3.6  |
| 13  | BM    | 66   | GLU  | 3.6  |
| 28  | CB    | 110  | C    | 3.6  |
| 31  | CA    | 2364 | C    | 3.6  |
| 43  | CP    | 20   | GLU  | 3.6  |
| 1   | BA    | 1347 | G    | 3.6  |
| 31  | CA    | 512  | G    | 3.6  |
| 31  | CA    | 2109 | U    | 3.6  |
| 55  | DA    | 1059 | G    | 3.6  |
| 11  | AK    | 56   | ARG  | 3.6  |
| 36  | CH    | 27   | ARG  | 3.6  |
| 31  | CA    | 2792 | A    | 3.6  |
| 33  | CE    | 36   | ALA  | 3.6  |
| 2   | AB    | 221  | VAL  | 3.6  |
| 4   | AD    | 117  | LEU  | 3.6  |
| 33  | CE    | 4    | VAL  | 3.6  |
| 37  | CJ    | 49   | ILE  | 3.6  |
| 37  | DJ    | 129  | ILE  | 3.6  |
| 38  | CK    | 56   | VAL  | 3.6  |
| 2   | AB    | 15   | HIS  | 3.6  |
| 31  | CA    | 565  | C    | 3.6  |
| 36  | CH    | 128  | HIS  | 3.6  |
| 37  | DJ    | 93   | PRO  | 3.6  |
| 44  | CQ    | 24   | ASP  | 3.6  |
| 1   | AA    | 1015 | G    | 3.6  |
| 17  | BQ    | 53   | CYS  | 3.6  |
| 29  | CC    | 30   | PHE  | 3.6  |
| 31  | CA    | 1475 | G    | 3.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 7          | BG           | 74         | GLU         | 3.6         |
| 13         | BM           | 67         | GLY         | 3.6         |
| 30         | CD           | 91         | THR         | 3.6         |
| 33         | CE           | 34         | ALA         | 3.6         |
| 36         | DH           | 126        | GLY         | 3.6         |
| 11         | AK           | 129        | VAL         | 3.6         |
| 39         | CL           | 2          | ILE         | 3.6         |
| 10         | AJ           | 55         | PRO         | 3.6         |
| 10         | BJ           | 15         | HIS         | 3.6         |
| 22         | C1           | 42         | HIS         | 3.6         |
| 1          | BA           | 980        | C           | 3.5         |
| 31         | CA           | 11         | C           | 3.5         |
| 31         | CA           | 767        | U           | 3.5         |
| 40         | CM           | 106        | GLU         | 3.5         |
| 1          | BA           | 1006       | G           | 3.5         |
| 9          | AI           | 87         | LEU         | 3.5         |
| 28         | CB           | 21         | G           | 3.5         |
| 10         | BJ           | 28         | THR         | 3.5         |
| 14         | AN           | 67         | THR         | 3.5         |
| 14         | BN           | 79         | LEU         | 3.5         |
| 34         | DF           | 176        | PRO         | 3.5         |
| 48         | CU           | 28         | ASN         | 3.5         |
| 1          | BA           | 1325       | C           | 3.5         |
| 31         | CA           | 1320       | C           | 3.5         |
| 45         | CR           | 57         | PHE         | 3.5         |
| 3          | BC           | 129        | MET         | 3.5         |
| 36         | CH           | 60         | GLU         | 3.5         |
| 12         | BL           | 69         | GLY         | 3.5         |
| 34         | CF           | 62         | GLY         | 3.5         |
| 2          | BB           | 7          | ARG         | 3.5         |
| 7          | BG           | 37         | SER         | 3.5         |
| 7          | BG           | 125        | SER         | 3.5         |
| 13         | BM           | 73         | ILE         | 3.5         |
| 18         | AR           | 48         | ARG         | 3.5         |
| 19         | BS           | 4          | SER         | 3.5         |
| 34         | DF           | 80         | ARG         | 3.5         |
| 41         | CN           | 126        | ILE         | 3.5         |
| 43         | CP           | 111        | ARG         | 3.5         |
| 1          | BA           | 1323       | G           | 3.5         |
| 31         | CA           | 619        | G           | 3.5         |
| 1          | BA           | 216        | U           | 3.5         |
| 2          | AB           | 32         | PHE         | 3.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 31         | CA           | 1201       | U           | 3.5         |
| 42         | CO           | 11         | ASN         | 3.5         |
| 16         | BP           | 45         | GLU         | 3.5         |
| 46         | CS           | 79         | ARG         | 3.5         |
| 6          | AF           | 39         | LEU         | 3.5         |
| 3          | AC           | 195        | VAL         | 3.5         |
| 16         | AP           | 71         | VAL         | 3.5         |
| 19         | BS           | 35         | SER         | 3.5         |
| 30         | CD           | 146        | ILE         | 3.5         |
| 37         | CJ           | 101        | ILE         | 3.5         |
| 11         | AK           | 111        | THR         | 3.5         |
| 31         | CA           | 7          | G           | 3.5         |
| 9          | AI           | 31         | ASN         | 3.5         |
| 31         | CA           | 2654       | A           | 3.5         |
| 1          | BA           | 1327       | C           | 3.5         |
| 31         | CA           | 2047       | C           | 3.5         |
| 46         | CS           | 81         | LYS         | 3.5         |
| 36         | DH           | 105        | ALA         | 3.5         |
| 43         | CP           | 82         | ALA         | 3.5         |
| 46         | CS           | 39         | LEU         | 3.5         |
| 35         | DG           | 17         | VAL         | 3.5         |
| 50         | CW           | 63         | ILE         | 3.5         |
| 1          | BA           | 1295       | U           | 3.5         |
| 4          | AD           | 31         | LYS         | 3.5         |
| 28         | CB           | 117        | G           | 3.5         |
| 31         | CA           | 1734       | G           | 3.5         |
| 31         | CA           | 2502       | G           | 3.5         |
| 1          | BA           | 223        | A           | 3.5         |
| 31         | CA           | 508        | A           | 3.5         |
| 1          | BA           | 1208       | C           | 3.5         |
| 13         | BM           | 15         | ALA         | 3.5         |
| 19         | BS           | 51         | VAL         | 3.5         |
| 43         | CP           | 28         | VAL         | 3.5         |
| 35         | CG           | 130        | GLU         | 3.5         |
| 48         | CU           | 6          | ARG         | 3.5         |
| 1          | BA           | 957        | U           | 3.5         |
| 31         | CA           | 1864       | U           | 3.5         |
| 31         | CA           | 2783       | U           | 3.5         |
| 48         | DU           | 92         | ASN         | 3.5         |
| 1          | BA           | 1252       | A           | 3.5         |
| 25         | C4           | 29         | LEU         | 3.5         |
| 31         | CA           | 881        | G           | 3.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 31         | CA           | 1026       | G           | 3.5         |
| 31         | CA           | 1322       | A           | 3.5         |
| 35         | CG           | 79         | VAL         | 3.5         |
| 36         | DH           | 108        | VAL         | 3.5         |
| 20         | BT           | 71         | LYS         | 3.5         |
| 33         | CE           | 21         | ARG         | 3.5         |
| 34         | CF           | 133        | ARG         | 3.5         |
| 13         | AM           | 42         | ASP         | 3.5         |
| 45         | CR           | 102        | ASP         | 3.5         |
| 14         | BN           | 70         | PRO         | 3.5         |
| 31         | CA           | 2861       | U           | 3.5         |
| 41         | CN           | 99         | GLY         | 3.5         |
| 47         | CT           | 9          | HIS         | 3.5         |
| 27         | C0           | 17         | LEU         | 3.5         |
| 34         | CF           | 137        | ILE         | 3.5         |
| 35         | CG           | 136        | ALA         | 3.5         |
| 54         | DI           | 120        | ALA         | 3.5         |
| 1          | BA           | 979        | C           | 3.5         |
| 2          | BB           | 11         | LYS         | 3.5         |
| 7          | AG           | 43         | VAL         | 3.5         |
| 49         | CV           | 92         | LYS         | 3.5         |
| 9          | AI           | 85         | ARG         | 3.5         |
| 45         | CR           | 11         | ARG         | 3.5         |
| 50         | CW           | 12         | GLN         | 3.5         |
| 53         | CZ           | 38         | GLN         | 3.5         |
| 31         | CA           | 1869       | G           | 3.5         |
| 7          | AG           | 57         | SER         | 3.5         |
| 30         | CD           | 156        | PHE         | 3.5         |
| 1          | BA           | 88         | U           | 3.5         |
| 55         | DA           | 546        | U           | 3.5         |
| 36         | DH           | 77         | THR         | 3.5         |
| 22         | C1           | 32         | LYS         | 3.5         |
| 39         | CL           | 103        | VAL         | 3.5         |
| 20         | BT           | 51         | PHE         | 3.5         |
| 31         | CA           | 406        | G           | 3.5         |
| 31         | CA           | 1551       | A           | 3.5         |
| 9          | AI           | 24         | GLY         | 3.4         |
| 10         | AJ           | 33         | GLY         | 3.4         |
| 34         | CF           | 24         | SER         | 3.4         |
| 37         | DJ           | 90         | SER         | 3.4         |
| 40         | CM           | 42         | SER         | 3.4         |
| 1          | AA           | 1029       | U           | 3.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | AJ    | 43   | PRO  | 3.4  |
| 37  | DJ    | 46   | THR  | 3.4  |
| 47  | CT    | 39   | THR  | 3.4  |
| 11  | AK    | 47   | ALA  | 3.4  |
| 44  | CQ    | 43   | PHE  | 3.4  |
| 1   | BA    | 975  | A    | 3.4  |
| 31  | CA    | 126  | A    | 3.4  |
| 31  | CA    | 422  | A    | 3.4  |
| 36  | DH    | 95   | GLY  | 3.4  |
| 1   | BA    | 956  | U    | 3.4  |
| 31  | CA    | 405  | U    | 3.4  |
| 12  | BL    | 114  | ARG  | 3.4  |
| 13  | AM    | 57   | ARG  | 3.4  |
| 31  | CA    | 808  | G    | 3.4  |
| 50  | CW    | 11   | GLU  | 3.4  |
| 2   | BB    | 166  | ALA  | 3.4  |
| 13  | BM    | 60   | VAL  | 3.4  |
| 27  | C0    | 14   | ILE  | 3.4  |
| 30  | CD    | 36   | GLN  | 3.4  |
| 35  | CG    | 65   | ALA  | 3.4  |
| 30  | CD    | 98   | VAL  | 3.4  |
| 34  | DF    | 74   | VAL  | 3.4  |
| 1   | BA    | 206  | C    | 3.4  |
| 31  | CA    | 817  | C    | 3.4  |
| 54  | DI    | 36   | ASP  | 3.4  |
| 1   | BA    | 1330 | U    | 3.4  |
| 13  | BM    | 71   | ARG  | 3.4  |
| 44  | CQ    | 11   | GLU  | 3.4  |
| 7   | BG    | 2    | PRO  | 3.4  |
| 36  | CH    | 75   | LEU  | 3.4  |
| 1   | BA    | 1356 | G    | 3.4  |
| 30  | CD    | 167  | ASN  | 3.4  |
| 31  | CA    | 407  | G    | 3.4  |
| 31  | CA    | 539  | G    | 3.4  |
| 31  | CA    | 1042 | G    | 3.4  |
| 31  | CA    | 1250 | G    | 3.4  |
| 31  | CA    | 1332 | G    | 3.4  |
| 38  | CK    | 65   | THR  | 3.4  |
| 45  | DR    | 118  | ALA  | 3.4  |
| 55  | DA    | 1093 | G    | 3.4  |
| 36  | CH    | 144  | VAL  | 3.4  |
| 2   | AB    | 225  | ARG  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 28   | GLU  | 3.4  |
| 42  | CO    | 2    | ARG  | 3.4  |
| 50  | CW    | 43   | ASP  | 3.4  |
| 28  | CB    | 118  | C    | 3.4  |
| 31  | CA    | 1052 | C    | 3.4  |
| 31  | CA    | 2650 | U    | 3.4  |
| 9   | AI    | 54   | LEU  | 3.4  |
| 12  | BL    | 24   | LEU  | 3.4  |
| 47  | CT    | 87   | PRO  | 3.4  |
| 36  | CH    | 141  | LYS  | 3.4  |
| 48  | CU    | 68   | LYS  | 3.4  |
| 2   | AB    | 213  | TYR  | 3.4  |
| 31  | CA    | 1622 | G    | 3.4  |
| 31  | CA    | 1875 | G    | 3.4  |
| 31  | CA    | 2238 | G    | 3.4  |
| 40  | CM    | 128  | THR  | 3.4  |
| 5   | BE    | 109  | GLY  | 3.4  |
| 26  | C5    | 36   | ARG  | 3.4  |
| 29  | CC    | 235  | GLY  | 3.4  |
| 40  | CM    | 26   | GLY  | 3.4  |
| 1   | AA    | 83   | C    | 3.4  |
| 1   | BA    | 473  | U    | 3.4  |
| 14  | BN    | 97   | LYS  | 3.4  |
| 5   | AE    | 111  | MET  | 3.4  |
| 34  | CF    | 59   | ALA  | 3.4  |
| 5   | BE    | 123  | VAL  | 3.4  |
| 7   | BG    | 70   | ARG  | 3.4  |
| 31  | CA    | 309  | A    | 3.4  |
| 13  | AM    | 23   | TYR  | 3.4  |
| 14  | BN    | 67   | THR  | 3.4  |
| 44  | CQ    | 35   | GLY  | 3.4  |
| 48  | CU    | 4    | GLU  | 3.4  |
| 31  | CA    | 2405 | G    | 3.4  |
| 5   | BE    | 23   | LYS  | 3.4  |
| 33  | CE    | 63   | LYS  | 3.4  |
| 13  | BM    | 112  | PRO  | 3.4  |
| 17  | BQ    | 64   | CYS  | 3.4  |
| 36  | CH    | 117  | LEU  | 3.4  |
| 37  | CJ    | 39   | CYS  | 3.4  |
| 2   | BB    | 208  | ARG  | 3.4  |
| 21  | AU    | 17   | ARG  | 3.4  |
| 40  | CM    | 1    | MET  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | AN    | 54   | ASP  | 3.4  |
| 1   | BA    | 218  | U    | 3.4  |
| 1   | BA    | 1039 | G    | 3.4  |
| 1   | BA    | 1308 | U    | 3.4  |
| 31  | CA    | 1539 | U    | 3.4  |
| 2   | AB    | 35   | ARG  | 3.4  |
| 7   | BG    | 143  | ARG  | 3.4  |
| 31  | CA    | 334  | C    | 3.4  |
| 31  | CA    | 510  | C    | 3.4  |
| 31  | CA    | 2310 | C    | 3.4  |
| 5   | BE    | 46   | VAL  | 3.4  |
| 37  | DJ    | 136  | MET  | 3.4  |
| 41  | CN    | 36   | VAL  | 3.4  |
| 12  | BL    | 71   | GLY  | 3.4  |
| 24  | C3    | 11   | LYS  | 3.4  |
| 29  | DC    | 240  | PHE  | 3.4  |
| 37  | CJ    | 72   | LYS  | 3.4  |
| 40  | CM    | 24   | GLY  | 3.4  |
| 47  | CT    | 49   | LYS  | 3.4  |
| 49  | CV    | 44   | LYS  | 3.4  |
| 1   | BA    | 532  | A    | 3.4  |
| 1   | BA    | 969  | A    | 3.4  |
| 31  | CA    | 279  | A    | 3.4  |
| 31  | CA    | 478  | A    | 3.4  |
| 31  | CA    | 1609 | A    | 3.4  |
| 55  | DA    | 1088 | A    | 3.4  |
| 7   | AG    | 123  | GLU  | 3.4  |
| 16  | BP    | 11   | ALA  | 3.4  |
| 7   | AG    | 41   | SER  | 3.4  |
| 40  | CM    | 140  | GLY  | 3.4  |
| 29  | CC    | 213  | TRP  | 3.4  |
| 31  | CA    | 241  | A    | 3.3  |
| 55  | DA    | 1070 | A    | 3.3  |
| 2   | BB    | 145  | GLU  | 3.3  |
| 5   | BE    | 36   | LEU  | 3.3  |
| 54  | DI    | 47   | GLU  | 3.3  |
| 34  | CF    | 138  | PHE  | 3.3  |
| 38  | CK    | 105  | VAL  | 3.3  |
| 43  | CP    | 44   | GLY  | 3.3  |
| 44  | CQ    | 30   | VAL  | 3.3  |
| 48  | CU    | 67   | VAL  | 3.3  |
| 1   | BA    | 1139 | G    | 3.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | BA           | 1334       | G           | 3.3         |
| 1          | BA           | 1454       | G           | 3.3         |
| 3          | BC           | 164        | ARG         | 3.3         |
| 6          | AF           | 63         | ASN         | 3.3         |
| 17         | BQ           | 69         | LYS         | 3.3         |
| 1          | BA           | 1211       | U           | 3.3         |
| 14         | AN           | 99         | ALA         | 3.3         |
| 37         | CJ           | 110        | ALA         | 3.3         |
| 37         | CJ           | 140        | VAL         | 3.3         |
| 45         | CR           | 27         | ALA         | 3.3         |
| 33         | CE           | 158        | PHE         | 3.3         |
| 39         | CL           | 112        | PHE         | 3.3         |
| 45         | CR           | 82         | GLY         | 3.3         |
| 29         | CC           | 230        | HIS         | 3.3         |
| 31         | CA           | 2691       | C           | 3.3         |
| 38         | CK           | 34         | ARG         | 3.3         |
| 1          | BA           | 1187       | G           | 3.3         |
| 31         | CA           | 266        | G           | 3.3         |
| 34         | CF           | 33         | LYS         | 3.3         |
| 20         | BT           | 13         | GLN         | 3.3         |
| 1          | BA           | 1014       | A           | 3.3         |
| 2          | AB           | 69         | PHE         | 3.3         |
| 11         | AK           | 102        | ALA         | 3.3         |
| 31         | CA           | 911        | A           | 3.3         |
| 42         | CO           | 84         | GLY         | 3.3         |
| 39         | CL           | 35         | VAL         | 3.3         |
| 39         | CL           | 83         | ALA         | 3.3         |
| 35         | CG           | 99         | LYS         | 3.3         |
| 40         | CM           | 13         | LYS         | 3.3         |
| 49         | CV           | 97         | LYS         | 3.3         |
| 51         | CX           | 68         | LYS         | 3.3         |
| 1          | AA           | 1028       | C           | 3.3         |
| 1          | BA           | 87         | C           | 3.3         |
| 31         | CA           | 57         | C           | 3.3         |
| 33         | CE           | 165        | HIS         | 3.3         |
| 34         | CF           | 134        | GLU         | 3.3         |
| 55         | DA           | 141        | G           | 3.3         |
| 1          | BA           | 1247       | U           | 3.3         |
| 31         | CA           | 139        | U           | 3.3         |
| 31         | CA           | 150        | U           | 3.3         |
| 10         | AJ           | 37         | ARG         | 3.3         |
| 11         | BK           | 45         | ALA         | 3.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | AO    | 89   | ARG  | 3.3  |
| 30  | CD    | 162  | ALA  | 3.3  |
| 33  | CE    | 151  | GLY  | 3.3  |
| 41  | CN    | 11   | LYS  | 3.3  |
| 44  | CQ    | 33   | VAL  | 3.3  |
| 47  | CT    | 8    | ARG  | 3.3  |
| 53  | CZ    | 2    | LYS  | 3.3  |
| 53  | CZ    | 13   | GLU  | 3.3  |
| 1   | BA    | 330  | C    | 3.3  |
| 7   | AG    | 140  | ASP  | 3.3  |
| 31  | CA    | 1607 | C    | 3.3  |
| 1   | BA    | 275  | G    | 3.3  |
| 1   | BA    | 847  | G    | 3.3  |
| 9   | BI    | 85   | ARG  | 3.3  |
| 31  | CA    | 914  | G    | 3.3  |
| 31  | CA    | 2159 | G    | 3.3  |
| 31  | CA    | 2455 | G    | 3.3  |
| 36  | CH    | 83   | LYS  | 3.3  |
| 33  | CE    | 182  | ALA  | 3.3  |
| 46  | CS    | 38   | VAL  | 3.3  |
| 3   | BC    | 167  | TRP  | 3.3  |
| 49  | CV    | 101  | GLU  | 3.3  |
| 15  | BO    | 18   | ASP  | 3.3  |
| 36  | DH    | 86   | ASP  | 3.3  |
| 9   | BI    | 95   | ARG  | 3.3  |
| 10  | BJ    | 45   | ARG  | 3.3  |
| 25  | C4    | 3    | LYS  | 3.3  |
| 31  | CA    | 31   | C    | 3.3  |
| 37  | DJ    | 34   | ASN  | 3.3  |
| 31  | CA    | 1880 | U    | 3.3  |
| 7   | BG    | 117  | ALA  | 3.3  |
| 36  | DH    | 147  | VAL  | 3.3  |
| 45  | CR    | 68   | ALA  | 3.3  |
| 1   | AA    | 1034 | G    | 3.3  |
| 1   | BA    | 933  | G    | 3.3  |
| 1   | BA    | 978  | A    | 3.3  |
| 2   | BB    | 15   | HIS  | 3.3  |
| 40  | CM    | 129  | LYS  | 3.3  |
| 43  | CP    | 34   | HIS  | 3.3  |
| 25  | C4    | 44   | LEU  | 3.3  |
| 44  | CQ    | 101  | ARG  | 3.3  |
| 46  | CS    | 7    | SER  | 3.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | AC           | 155        | GLY         | 3.3         |
| 3          | BC           | 145        | GLY         | 3.3         |
| 17         | AQ           | 53         | CYS         | 3.3         |
| 31         | CA           | 1600       | C           | 3.3         |
| 31         | CA           | 1986       | C           | 3.3         |
| 36         | DH           | 92         | GLY         | 3.3         |
| 10         | AJ           | 25         | ILE         | 3.3         |
| 36         | DH           | 143        | ILE         | 3.3         |
| 12         | BL           | 23         | ALA         | 3.3         |
| 15         | BO           | 12         | VAL         | 3.3         |
| 3          | BC           | 26         | THR         | 3.3         |
| 10         | BJ           | 43         | PRO         | 3.3         |
| 1          | BA           | 86         | G           | 3.3         |
| 30         | CD           | 204        | LYS         | 3.3         |
| 31         | CA           | 271        | G           | 3.3         |
| 31         | CA           | 1022       | G           | 3.3         |
| 31         | CA           | 1277       | G           | 3.3         |
| 31         | CA           | 2004       | G           | 3.3         |
| 31         | CA           | 2363       | G           | 3.3         |
| 35         | CG           | 116        | GLN         | 3.3         |
| 31         | CA           | 1373       | A           | 3.3         |
| 34         | DF           | 39         | GLY         | 3.3         |
| 1          | BA           | 153        | C           | 3.3         |
| 1          | BA           | 186        | C           | 3.3         |
| 3          | BC           | 37         | PHE         | 3.3         |
| 3          | BC           | 170        | GLU         | 3.3         |
| 30         | CD           | 202        | ILE         | 3.3         |
| 31         | CA           | 1730       | C           | 3.3         |
| 40         | CM           | 143        | GLU         | 3.3         |
| 50         | CW           | 56         | PHE         | 3.3         |
| 11         | AK           | 99         | ALA         | 3.3         |
| 30         | CD           | 197        | THR         | 3.3         |
| 38         | CK           | 92         | MET         | 3.3         |
| 10         | AJ           | 31         | ARG         | 3.3         |
| 3          | BC           | 190        | HIS         | 3.3         |
| 7          | BG           | 55         | GLY         | 3.3         |
| 11         | AK           | 42         | LEU         | 3.3         |
| 11         | BK           | 43         | GLY         | 3.3         |
| 25         | C4           | 9          | GLY         | 3.3         |
| 31         | CA           | 1239       | G           | 3.3         |
| 40         | CM           | 61         | LEU         | 3.3         |
| 44         | CQ           | 40         | LEU         | 3.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | CU    | 32   | LEU  | 3.3  |
| 31  | CA    | 1326 | U    | 3.2  |
| 37  | DJ    | 62   | TYR  | 3.2  |
| 54  | DI    | 98   | GLU  | 3.2  |
| 1   | BA    | 1269 | A    | 3.2  |
| 31  | CA    | 515  | A    | 3.2  |
| 31  | CA    | 1205 | A    | 3.2  |
| 48  | CU    | 74   | ILE  | 3.2  |
| 55  | DA    | 1057 | A    | 3.2  |
| 23  | C2    | 12   | VAL  | 3.2  |
| 13  | AM    | 101  | ARG  | 3.2  |
| 5   | BE    | 103  | THR  | 3.2  |
| 3   | AC    | 82   | GLU  | 3.2  |
| 8   | BH    | 89   | LYS  | 3.2  |
| 52  | CY    | 44   | LYS  | 3.2  |
| 11  | AK    | 32   | VAL  | 3.2  |
| 12  | BL    | 93   | VAL  | 3.2  |
| 31  | CA    | 421  | C    | 3.2  |
| 31  | CA    | 550  | C    | 3.2  |
| 31  | CA    | 1764 | C    | 3.2  |
| 31  | CA    | 2412 | A    | 3.2  |
| 33  | CE    | 102  | ARG  | 3.2  |
| 36  | CH    | 123  | ARG  | 3.2  |
| 41  | CN    | 40   | ARG  | 3.2  |
| 50  | CW    | 50   | MET  | 3.2  |
| 53  | DZ    | 39   | GLN  | 3.2  |
| 3   | BC    | 85   | GLU  | 3.2  |
| 19  | AS    | 27   | ASP  | 3.2  |
| 21  | BU    | 16   | LEU  | 3.2  |
| 35  | CG    | 138  | LYS  | 3.2  |
| 49  | CV    | 60   | GLU  | 3.2  |
| 53  | CZ    | 60   | LYS  | 3.2  |
| 2   | AB    | 60   | ILE  | 3.2  |
| 7   | BG    | 7    | ILE  | 3.2  |
| 16  | AP    | 17   | TYR  | 3.2  |
| 21  | AU    | 4    | ILE  | 3.2  |
| 24  | C3    | 41   | ARG  | 3.2  |
| 31  | CA    | 894  | U    | 3.2  |
| 31  | CA    | 1173 | U    | 3.2  |
| 39  | CL    | 24   | VAL  | 3.2  |
| 28  | CB    | 56   | G    | 3.2  |
| 31  | CA    | 375  | G    | 3.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 31         | CA           | 2525       | G           | 3.2         |
| 31         | CA           | 2862       | G           | 3.2         |
| 1          | AA           | 1332       | A           | 3.2         |
| 25         | C4           | 49         | MET         | 3.2         |
| 53         | CZ           | 30         | MET         | 3.2         |
| 55         | DA           | 613        | A           | 3.2         |
| 2          | AB           | 211        | THR         | 3.2         |
| 3          | BC           | 183        | ASP         | 3.2         |
| 33         | CE           | 56         | GLY         | 3.2         |
| 34         | CF           | 169        | LEU         | 3.2         |
| 43         | CP           | 75         | GLY         | 3.2         |
| 25         | C4           | 42         | ARG         | 3.2         |
| 36         | DH           | 135        | HIS         | 3.2         |
| 42         | CO           | 100        | CYS         | 3.2         |
| 38         | CK           | 15         | TRP         | 3.2         |
| 51         | CX           | 36         | ILE         | 3.2         |
| 2          | BB           | 210        | VAL         | 3.2         |
| 36         | CH           | 65         | ALA         | 3.2         |
| 47         | CT           | 56         | ALA         | 3.2         |
| 48         | CU           | 92         | ASN         | 3.2         |
| 1          | AA           | 984        | C           | 3.2         |
| 1          | BA           | 1355       | G           | 3.2         |
| 7          | BG           | 14         | PRO         | 3.2         |
| 31         | CA           | 2152       | G           | 3.2         |
| 31         | CA           | 2732       | G           | 3.2         |
| 47         | CT           | 2          | GLU         | 3.2         |
| 1          | AA           | 1170       | A           | 3.2         |
| 27         | C0           | 33         | GLY         | 3.2         |
| 31         | CA           | 182        | A           | 3.2         |
| 31         | CA           | 1253       | A           | 3.2         |
| 55         | DA           | 2170       | A           | 3.2         |
| 52         | CY           | 48         | THR         | 3.2         |
| 21         | AU           | 19         | PHE         | 3.2         |
| 31         | CA           | 2807       | U           | 3.2         |
| 9          | AI           | 64         | TYR         | 3.2         |
| 11         | BK           | 102        | ALA         | 3.2         |
| 43         | CP           | 50         | ALA         | 3.2         |
| 43         | CP           | 74         | VAL         | 3.2         |
| 44         | CQ           | 3          | ASN         | 3.2         |
| 45         | CR           | 10         | ALA         | 3.2         |
| 45         | CR           | 93         | LYS         | 3.2         |
| 25         | C4           | 57         | LEU         | 3.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | CB    | 49   | C    | 3.2  |
| 35  | CG    | 16   | ASP  | 3.2  |
| 47  | CT    | 110  | ARG  | 3.2  |
| 1   | AA    | 79   | G    | 3.2  |
| 1   | AA    | 1127 | G    | 3.2  |
| 1   | BA    | 1362 | A    | 3.2  |
| 31  | CA    | 1133 | A    | 3.2  |
| 31  | CA    | 1643 | G    | 3.2  |
| 23  | C2    | 20   | PHE  | 3.2  |
| 41  | CN    | 24   | THR  | 3.2  |
| 1   | BA    | 91   | U    | 3.2  |
| 10  | AJ    | 56   | HIS  | 3.2  |
| 43  | CP    | 90   | VAL  | 3.2  |
| 55  | DA    | 2131 | U    | 3.2  |
| 33  | CE    | 8    | ALA  | 3.2  |
| 1   | BA    | 1141 | C    | 3.2  |
| 5   | BE    | 144  | LEU  | 3.2  |
| 50  | CW    | 68   | LYS  | 3.2  |
| 50  | CW    | 71   | LYS  | 3.2  |
| 52  | CY    | 77   | LYS  | 3.2  |
| 1   | BA    | 1145 | A    | 3.2  |
| 17  | BQ    | 42   | THR  | 3.2  |
| 2   | BB    | 199  | VAL  | 3.2  |
| 3   | AC    | 105  | GLU  | 3.2  |
| 11  | AK    | 45   | ALA  | 3.2  |
| 25  | C4    | 24   | HIS  | 3.2  |
| 30  | CD    | 88   | GLU  | 3.2  |
| 31  | CA    | 29   | U    | 3.2  |
| 31  | CA    | 535  | G    | 3.2  |
| 31  | CA    | 1285 | A    | 3.2  |
| 31  | CA    | 929  | U    | 3.2  |
| 31  | CA    | 1538 | G    | 3.2  |
| 43  | CP    | 35   | ILE  | 3.2  |
| 35  | CG    | 63   | ALA  | 3.2  |
| 36  | CH    | 78   | VAL  | 3.2  |
| 46  | CS    | 34   | GLU  | 3.2  |
| 24  | C3    | 8    | SER  | 3.2  |
| 24  | C3    | 15   | SER  | 3.2  |
| 33  | CE    | 62   | GLN  | 3.2  |
| 37  | DJ    | 95   | LYS  | 3.2  |
| 46  | CS    | 76   | LYS  | 3.2  |
| 44  | CQ    | 16   | ASP  | 3.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 31         | CA           | 2815       | C           | 3.2         |
| 20         | BT           | 12         | ILE         | 3.2         |
| 30         | CD           | 14         | ILE         | 3.2         |
| 38         | CK           | 81         | ILE         | 3.2         |
| 54         | DI           | 11         | ILE         | 3.2         |
| 10         | BJ           | 36         | VAL         | 3.2         |
| 31         | CA           | 596        | U           | 3.2         |
| 13         | AM           | 29         | ARG         | 3.2         |
| 21         | AU           | 26         | ALA         | 3.2         |
| 31         | CA           | 1596       | A           | 3.2         |
| 35         | CG           | 145        | ALA         | 3.2         |
| 36         | CH           | 9          | VAL         | 3.2         |
| 31         | CA           | 2782       | G           | 3.2         |
| 36         | DH           | 128        | HIS         | 3.2         |
| 48         | CU           | 69         | ARG         | 3.2         |
| 55         | DA           | 2140       | G           | 3.2         |
| 30         | CD           | 148        | GLN         | 3.2         |
| 35         | CG           | 176        | LYS         | 3.2         |
| 49         | CV           | 53         | ASN         | 3.2         |
| 52         | CY           | 54         | LYS         | 3.2         |
| 16         | AP           | 74         | LEU         | 3.2         |
| 36         | DH           | 90         | LEU         | 3.2         |
| 39         | CL           | 56         | ASP         | 3.2         |
| 1          | AA           | 1282       | C           | 3.2         |
| 1          | BA           | 1262       | C           | 3.2         |
| 1          | BA           | 1383       | C           | 3.2         |
| 31         | CA           | 1172       | C           | 3.2         |
| 24         | C3           | 21         | ARG         | 3.1         |
| 41         | CN           | 74         | THR         | 3.1         |
| 31         | CA           | 2639       | A           | 3.1         |
| 1          | BA           | 177        | G           | 3.1         |
| 7          | AG           | 77         | SER         | 3.1         |
| 31         | CA           | 597        | G           | 3.1         |
| 31         | CA           | 1037       | G           | 3.1         |
| 31         | CA           | 2410       | G           | 3.1         |
| 36         | CH           | 6          | LEU         | 3.1         |
| 44         | CQ           | 31         | TRP         | 3.1         |
| 1          | BA           | 999        | C           | 3.1         |
| 13         | AM           | 17         | ILE         | 3.1         |
| 30         | CD           | 179        | ARG         | 3.1         |
| 28         | CB           | 4          | C           | 3.1         |
| 31         | CA           | 587        | C           | 3.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2260 | C    | 3.1  |
| 21  | AU    | 14   | VAL  | 3.1  |
| 38  | CK    | 124  | VAL  | 3.1  |
| 4   | AD    | 30   | THR  | 3.1  |
| 48  | CU    | 91   | GLN  | 3.1  |
| 1   | BA    | 1151 | A    | 3.1  |
| 20  | BT    | 21   | ASN  | 3.1  |
| 31  | CA    | 1525 | A    | 3.1  |
| 31  | CA    | 2346 | A    | 3.1  |
| 44  | DQ    | 2    | SER  | 3.1  |
| 53  | CZ    | 10   | SER  | 3.1  |
| 1   | BA    | 1144 | G    | 3.1  |
| 1   | BA    | 1215 | G    | 3.1  |
| 14  | AN    | 63   | ARG  | 3.1  |
| 34  | CF    | 163  | ASP  | 3.1  |
| 46  | CS    | 93   | PHE  | 3.1  |
| 1   | BA    | 1263 | C    | 3.1  |
| 2   | AB    | 53   | ALA  | 3.1  |
| 5   | AE    | 137  | VAL  | 3.1  |
| 12  | BL    | 119  | VAL  | 3.1  |
| 37  | DJ    | 70   | VAL  | 3.1  |
| 29  | CC    | 237  | GLY  | 3.1  |
| 40  | CM    | 134  | ALA  | 3.1  |
| 45  | CR    | 44   | GLN  | 3.1  |
| 34  | CF    | 5    | HIS  | 3.1  |
| 34  | DF    | 83   | TYR  | 3.1  |
| 36  | CH    | 90   | LEU  | 3.1  |
| 38  | CK    | 125  | TYR  | 3.1  |
| 39  | CL    | 109  | SER  | 3.1  |
| 41  | CN    | 88   | ASN  | 3.1  |
| 42  | CO    | 23   | ASN  | 3.1  |
| 54  | DI    | 5    | LEU  | 3.1  |
| 12  | AL    | 108  | LYS  | 3.1  |
| 42  | CO    | 39   | PRO  | 3.1  |
| 43  | CP    | 2    | ASP  | 3.1  |
| 31  | CA    | 1138 | G    | 3.1  |
| 12  | BL    | 113  | ALA  | 3.1  |
| 13  | AM    | 38   | GLY  | 3.1  |
| 22  | C1    | 54   | VAL  | 3.1  |
| 31  | CA    | 2786 | U    | 3.1  |
| 45  | CR    | 110  | VAL  | 3.1  |
| 1   | BA    | 1317 | C    | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 23  | C2    | 19   | HIS  | 3.1  |
| 43  | CP    | 100  | HIS  | 3.1  |
| 7   | BG    | 124  | LEU  | 3.1  |
| 18  | AR    | 55   | LEU  | 3.1  |
| 53  | CZ    | 4    | LYS  | 3.1  |
| 53  | CZ    | 7    | ARG  | 3.1  |
| 46  | CS    | 43   | ASN  | 3.1  |
| 21  | BU    | 2    | PRO  | 3.1  |
| 1   | BA    | 1000 | A    | 3.1  |
| 31  | CA    | 1321 | A    | 3.1  |
| 55  | DA    | 1175 | A    | 3.1  |
| 1   | BA    | 354  | G    | 3.1  |
| 3   | BC    | 180  | ALA  | 3.1  |
| 36  | CH    | 63   | ALA  | 3.1  |
| 44  | CQ    | 73   | VAL  | 3.1  |
| 4   | AD    | 154  | ARG  | 3.1  |
| 19  | BS    | 73   | GLU  | 3.1  |
| 25  | C4    | 39   | LYS  | 3.1  |
| 30  | CD    | 7    | LYS  | 3.1  |
| 45  | CR    | 89   | GLU  | 3.1  |
| 3   | AC    | 43   | LEU  | 3.1  |
| 34  | CF    | 51   | ASP  | 3.1  |
| 13  | BM    | 9    | ILE  | 3.1  |
| 26  | D5    | 38   | GLY  | 3.1  |
| 2   | AB    | 208  | ARG  | 3.1  |
| 7   | AG    | 61   | ALA  | 3.1  |
| 31  | CA    | 2814 | A    | 3.1  |
| 41  | CN    | 56   | ALA  | 3.1  |
| 42  | CO    | 91   | ALA  | 3.1  |
| 55  | DA    | 878  | A    | 3.1  |
| 31  | CA    | 288  | U    | 3.1  |
| 1   | BA    | 993  | G    | 3.1  |
| 1   | BA    | 1322 | C    | 3.1  |
| 3   | AC    | 190  | HIS  | 3.1  |
| 31  | CA    | 544  | C    | 3.1  |
| 31  | CA    | 1024 | G    | 3.1  |
| 9   | BI    | 6    | TYR  | 3.1  |
| 13  | BM    | 78   | LYS  | 3.1  |
| 34  | CF    | 9    | LYS  | 3.1  |
| 16  | BP    | 10   | GLY  | 3.1  |
| 7   | BG    | 64   | VAL  | 3.1  |
| 11  | AK    | 86   | VAL  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 84   | U    | 3.1  |
| 1   | BA    | 96   | U    | 3.1  |
| 14  | BN    | 17   | ALA  | 3.1  |
| 31  | CA    | 1108 | U    | 3.1  |
| 31  | CA    | 2245 | U    | 3.1  |
| 1   | AA    | 1492 | A    | 3.1  |
| 1   | BA    | 1368 | A    | 3.1  |
| 28  | CB    | 119  | A    | 3.1  |
| 31  | CA    | 1260 | A    | 3.1  |
| 36  | DH    | 15   | LEU  | 3.1  |
| 1   | BA    | 1342 | C    | 3.1  |
| 31  | CA    | 61   | C    | 3.1  |
| 31  | CA    | 1092 | C    | 3.1  |
| 29  | CC    | 26   | LYS  | 3.1  |
| 31  | CA    | 1225 | G    | 3.1  |
| 31  | CA    | 2325 | G    | 3.1  |
| 49  | CV    | 9    | ASP  | 3.1  |
| 55  | DA    | 2156 | G    | 3.1  |
| 13  | AM    | 21   | SER  | 3.1  |
| 23  | C2    | 6    | ARG  | 3.1  |
| 37  | DJ    | 86   | ILE  | 3.1  |
| 38  | CK    | 67   | ASN  | 3.1  |
| 6   | BF    | 10   | VAL  | 3.1  |
| 9   | BI    | 75   | GLN  | 3.1  |
| 30  | CD    | 94   | GLN  | 3.1  |
| 37  | CJ    | 108  | GLU  | 3.1  |
| 31  | CA    | 615  | U    | 3.1  |
| 44  | CQ    | 42   | ALA  | 3.1  |
| 55  | DA    | 2169 | A    | 3.1  |
| 1   | BA    | 1149 | C    | 3.1  |
| 3   | BC    | 36   | ASP  | 3.1  |
| 22  | C1    | 16   | ARG  | 3.1  |
| 1   | BA    | 963  | G    | 3.1  |
| 12  | BL    | 67   | ILE  | 3.1  |
| 20  | BT    | 48   | GLN  | 3.1  |
| 28  | CB    | 20   | G    | 3.1  |
| 31  | CA    | 748  | G    | 3.1  |
| 31  | CA    | 1016 | G    | 3.1  |
| 31  | CA    | 1517 | G    | 3.1  |
| 31  | CA    | 2115 | G    | 3.1  |
| 31  | CA    | 2526 | G    | 3.1  |
| 34  | CF    | 44   | ILE  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | DJ    | 118  | THR  | 3.1  |
| 9   | BI    | 86   | ALA  | 3.0  |
| 21  | BU    | 6    | VAL  | 3.0  |
| 31  | CA    | 1460 | U    | 3.0  |
| 36  | DH    | 100  | ALA  | 3.0  |
| 36  | CH    | 47   | PHE  | 3.0  |
| 40  | CM    | 64   | PHE  | 3.0  |
| 1   | BA    | 1204 | A    | 3.0  |
| 16  | BP    | 35   | ARG  | 3.0  |
| 30  | CD    | 134  | HIS  | 3.0  |
| 42  | CO    | 96   | ARG  | 3.0  |
| 45  | CR    | 53   | ARG  | 3.0  |
| 10  | AJ    | 100  | ILE  | 3.0  |
| 28  | CB    | 27   | C    | 3.0  |
| 31  | CA    | 151  | C    | 3.0  |
| 31  | CA    | 1319 | C    | 3.0  |
| 12  | BL    | 97   | THR  | 3.0  |
| 13  | AM    | 96   | PRO  | 3.0  |
| 43  | CP    | 47   | VAL  | 3.0  |
| 44  | CQ    | 17   | VAL  | 3.0  |
| 1   | BA    | 1370 | G    | 3.0  |
| 28  | CB    | 7    | G    | 3.0  |
| 31  | CA    | 1071 | G    | 3.0  |
| 31  | CA    | 2299 | U    | 3.0  |
| 3   | BC    | 72   | ARG  | 3.0  |
| 21  | AU    | 37   | PHE  | 3.0  |
| 46  | CS    | 5    | PHE  | 3.0  |
| 2   | AB    | 40   | ILE  | 3.0  |
| 31  | CA    | 443  | A    | 3.0  |
| 31  | CA    | 502  | A    | 3.0  |
| 31  | CA    | 2052 | A    | 3.0  |
| 31  | CA    | 2311 | A    | 3.0  |
| 31  | CA    | 2632 | A    | 3.0  |
| 36  | CH    | 13   | GLY  | 3.0  |
| 44  | CQ    | 23   | GLY  | 3.0  |
| 14  | BN    | 57   | PRO  | 3.0  |
| 31  | CA    | 1958 | C    | 3.0  |
| 31  | CA    | 2313 | C    | 3.0  |
| 41  | CN    | 77   | PRO  | 3.0  |
| 7   | AG    | 73   | VAL  | 3.0  |
| 54  | DI    | 80   | THR  | 3.0  |
| 31  | CA    | 1438 | U    | 3.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 9          | AI           | 95         | ARG         | 3.0         |
| 21         | BU           | 19         | PHE         | 3.0         |
| 25         | C4           | 8          | ARG         | 3.0         |
| 30         | CD           | 118        | PHE         | 3.0         |
| 31         | CA           | 376        | G           | 3.0         |
| 10         | BJ           | 56         | HIS         | 3.0         |
| 36         | DH           | 88         | GLY         | 3.0         |
| 38         | CK           | 138        | GLN         | 3.0         |
| 53         | DZ           | 38         | GLN         | 3.0         |
| 1          | BA           | 352        | C           | 3.0         |
| 11         | BK           | 84         | VAL         | 3.0         |
| 5          | BE           | 75         | ALA         | 3.0         |
| 12         | BL           | 48         | ALA         | 3.0         |
| 29         | CC           | 37         | ASN         | 3.0         |
| 31         | CA           | 257        | C           | 3.0         |
| 31         | CA           | 2248       | C           | 3.0         |
| 39         | CL           | 32         | TYR         | 3.0         |
| 36         | DH           | 64         | ALA         | 3.0         |
| 43         | CP           | 79         | ALA         | 3.0         |
| 36         | DH           | 12         | LEU         | 3.0         |
| 1          | AA           | 1187       | G           | 3.0         |
| 1          | BA           | 378        | G           | 3.0         |
| 31         | CA           | 1186       | G           | 3.0         |
| 31         | CA           | 2112       | G           | 3.0         |
| 36         | CH           | 16         | GLY         | 3.0         |
| 37         | DJ           | 47         | ASP         | 3.0         |
| 30         | CD           | 150        | GLN         | 3.0         |
| 37         | DJ           | 31         | GLN         | 3.0         |
| 2          | BB           | 217        | VAL         | 3.0         |
| 7          | AG           | 71         | PRO         | 3.0         |
| 9          | BI           | 123        | ARG         | 3.0         |
| 46         | CS           | 84         | ARG         | 3.0         |
| 5          | AE           | 19         | ASN         | 3.0         |
| 31         | CA           | 1532       | A           | 3.0         |
| 31         | CA           | 2453       | A           | 3.0         |
| 31         | CA           | 2660       | A           | 3.0         |
| 36         | CH           | 36         | ALA         | 3.0         |
| 1          | AA           | 1023       | U           | 3.0         |
| 10         | BJ           | 83         | THR         | 3.0         |
| 15         | BO           | 22         | THR         | 3.0         |
| 14         | BN           | 66         | GLN         | 3.0         |
| 1          | BA           | 104        | G           | 3.0         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 3          | BC           | 132        | ARG         | 3.0         |
| 31         | CA           | 494        | G           | 3.0         |
| 31         | CA           | 1983       | G           | 3.0         |
| 31         | CA           | 2633       | G           | 3.0         |
| 35         | CG           | 3          | ARG         | 3.0         |
| 42         | CO           | 33         | ILE         | 3.0         |
| 7          | BG           | 6          | VAL         | 3.0         |
| 36         | DH           | 25         | TYR         | 3.0         |
| 38         | CK           | 126        | ALA         | 3.0         |
| 42         | CO           | 25         | ALA         | 3.0         |
| 44         | CQ           | 34         | GLU         | 3.0         |
| 47         | CT           | 93         | ALA         | 3.0         |
| 1          | BA           | 1008       | U           | 3.0         |
| 1          | AA           | 77         | A           | 3.0         |
| 2          | AB           | 129        | LEU         | 3.0         |
| 29         | CC           | 223        | THR         | 3.0         |
| 31         | CA           | 310        | A           | 3.0         |
| 31         | CA           | 504        | A           | 3.0         |
| 53         | CZ           | 55         | THR         | 3.0         |
| 9          | AI           | 79         | ILE         | 3.0         |
| 40         | CM           | 41         | ARG         | 3.0         |
| 42         | CO           | 46         | ARG         | 3.0         |
| 3          | AC           | 66         | VAL         | 3.0         |
| 14         | BN           | 19         | LYS         | 3.0         |
| 43         | CP           | 68         | LYS         | 3.0         |
| 46         | CS           | 66         | HIS         | 3.0         |
| 49         | CV           | 17         | LYS         | 3.0         |
| 51         | CX           | 67         | VAL         | 3.0         |
| 1          | BA           | 1220       | G           | 3.0         |
| 31         | CA           | 245        | G           | 3.0         |
| 31         | CA           | 1252       | G           | 3.0         |
| 44         | CQ           | 108        | ALA         | 3.0         |
| 1          | BA           | 632        | U           | 3.0         |
| 1          | BA           | 1212       | U           | 3.0         |
| 31         | CA           | 665        | U           | 3.0         |
| 54         | DI           | 76         | PHE         | 3.0         |
| 1          | BA           | 176        | C           | 3.0         |
| 31         | CA           | 184        | C           | 3.0         |
| 31         | CA           | 902        | C           | 3.0         |
| 7          | AG           | 133        | THR         | 3.0         |
| 13         | AM           | 46         | SER         | 3.0         |
| 31         | CA           | 609        | A           | 3.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | CL    | 65   | THR  | 3.0  |
| 54  | DI    | 67   | THR  | 3.0  |
| 44  | CQ    | 109  | ARG  | 3.0  |
| 9   | AI    | 62   | ASP  | 3.0  |
| 25  | C4    | 47   | LYS  | 3.0  |
| 29  | CC    | 97   | LYS  | 3.0  |
| 40  | DM    | 104  | GLN  | 3.0  |
| 3   | AC    | 39   | VAL  | 3.0  |
| 49  | CV    | 34   | VAL  | 3.0  |
| 42  | CO    | 66   | ALA  | 3.0  |
| 31  | CA    | 1224 | U    | 3.0  |
| 50  | CW    | 26   | PHE  | 3.0  |
| 1   | BA    | 1337 | G    | 3.0  |
| 14  | BN    | 41   | ARG  | 3.0  |
| 31  | CA    | 1228 | G    | 3.0  |
| 31  | CA    | 2000 | C    | 3.0  |
| 31  | CA    | 2362 | C    | 3.0  |
| 31  | CA    | 2616 | C    | 3.0  |
| 19  | BS    | 18   | LYS  | 3.0  |
| 29  | CC    | 28   | LYS  | 3.0  |
| 1   | BA    | 1339 | A    | 3.0  |
| 31  | CA    | 272  | A    | 3.0  |
| 31  | CA    | 1652 | A    | 3.0  |
| 45  | CR    | 59   | GLN  | 3.0  |
| 30  | CD    | 155  | VAL  | 3.0  |
| 36  | DH    | 103  | VAL  | 3.0  |
| 40  | CM    | 110  | VAL  | 3.0  |
| 3   | BC    | 104  | ALA  | 2.9  |
| 24  | C3    | 23   | ALA  | 2.9  |
| 18  | AR    | 29   | LEU  | 2.9  |
| 42  | CO    | 112  | TYR  | 2.9  |
| 35  | CG    | 159  | GLY  | 2.9  |
| 42  | CO    | 26   | GLY  | 2.9  |
| 50  | CW    | 46   | LYS  | 2.9  |
| 52  | CY    | 55   | GLY  | 2.9  |
| 1   | BA    | 470  | C    | 2.9  |
| 1   | BA    | 1129 | C    | 2.9  |
| 31  | CA    | 236  | C    | 2.9  |
| 31  | CA    | 411  | G    | 2.9  |
| 31  | CA    | 540  | C    | 2.9  |
| 31  | CA    | 1295 | C    | 2.9  |
| 31  | CA    | 2078 | C    | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | AI    | 92   | GLU  | 2.9  |
| 35  | CG    | 64   | GLN  | 2.9  |
| 1   | AA    | 1021 | A    | 2.9  |
| 1   | BA    | 468  | A    | 2.9  |
| 9   | BI    | 122  | ARG  | 2.9  |
| 10  | BJ    | 70   | HIS  | 2.9  |
| 48  | CU    | 45   | ALA  | 2.9  |
| 51  | CX    | 84   | ALA  | 2.9  |
| 30  | CD    | 56   | LYS  | 2.9  |
| 31  | CA    | 1468 | U    | 2.9  |
| 44  | CQ    | 100  | LEU  | 2.9  |
| 3   | BC    | 158  | GLY  | 2.9  |
| 38  | CK    | 79   | GLY  | 2.9  |
| 55  | DA    | 2113 | U    | 2.9  |
| 12  | AL    | 70   | GLU  | 2.9  |
| 34  | CF    | 19   | GLU  | 2.9  |
| 3   | AC    | 68   | ILE  | 2.9  |
| 7   | BG    | 29   | ILE  | 2.9  |
| 31  | CA    | 1985 | C    | 2.9  |
| 36  | CH    | 125  | THR  | 2.9  |
| 28  | CB    | 96   | G    | 2.9  |
| 31  | CA    | 1529 | G    | 2.9  |
| 1   | BA    | 1248 | A    | 2.9  |
| 22  | C1    | 53   | LYS  | 2.9  |
| 37  | DJ    | 140  | VAL  | 2.9  |
| 45  | CR    | 70   | ARG  | 2.9  |
| 3   | BC    | 157  | LEU  | 2.9  |
| 22  | C1    | 45   | ALA  | 2.9  |
| 29  | CC    | 243  | HIS  | 2.9  |
| 34  | CF    | 20   | PHE  | 2.9  |
| 47  | CT    | 58   | ALA  | 2.9  |
| 54  | DI    | 127  | ALA  | 2.9  |
| 5   | BE    | 108  | GLY  | 2.9  |
| 7   | AG    | 132  | GLY  | 2.9  |
| 36  | CH    | 126  | GLY  | 2.9  |
| 54  | DI    | 119  | PRO  | 2.9  |
| 7   | BG    | 139  | GLU  | 2.9  |
| 30  | CD    | 183  | GLU  | 2.9  |
| 43  | CP    | 98   | GLN  | 2.9  |
| 1   | BA    | 54   | C    | 2.9  |
| 13  | AM    | 20   | THR  | 2.9  |
| 20  | BT    | 16   | LYS  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | C1    | 11   | SER  | 2.9  |
| 42  | CO    | 45   | ARG  | 2.9  |
| 6   | AF    | 96   | VAL  | 2.9  |
| 16  | AP    | 21   | VAL  | 2.9  |
| 36  | DH    | 110  | VAL  | 2.9  |
| 50  | CW    | 77   | VAL  | 2.9  |
| 1   | AA    | 963  | G    | 2.9  |
| 1   | BA    | 198  | G    | 2.9  |
| 3   | AC    | 189  | ALA  | 2.9  |
| 7   | AG    | 47   | LEU  | 2.9  |
| 19  | AS    | 47   | LEU  | 2.9  |
| 31  | CA    | 2365 | G    | 2.9  |
| 1   | BA    | 1205 | U    | 2.9  |
| 29  | CC    | 227  | PRO  | 2.9  |
| 31  | CA    | 941  | A    | 2.9  |
| 31  | CA    | 1583 | A    | 2.9  |
| 40  | CM    | 87   | GLY  | 2.9  |
| 16  | BP    | 40   | ASN  | 2.9  |
| 29  | CC    | 46   | ASN  | 2.9  |
| 11  | AK    | 80   | LYS  | 2.9  |
| 33  | CE    | 99   | LYS  | 2.9  |
| 52  | CY    | 61   | LYS  | 2.9  |
| 9   | AI    | 28   | ILE  | 2.9  |
| 10  | BJ    | 16   | ARG  | 2.9  |
| 13  | BM    | 17   | ILE  | 2.9  |
| 29  | CC    | 270  | ARG  | 2.9  |
| 37  | CJ    | 65   | ARG  | 2.9  |
| 39  | CL    | 49   | ARG  | 2.9  |
| 47  | CT    | 66   | ILE  | 2.9  |
| 2   | BB    | 80   | VAL  | 2.9  |
| 30  | CD    | 24   | VAL  | 2.9  |
| 31  | CA    | 32   | C    | 2.9  |
| 31  | CA    | 2896 | C    | 2.9  |
| 36  | CH    | 21   | VAL  | 2.9  |
| 50  | CW    | 3    | THR  | 2.9  |
| 9   | BI    | 63   | LEU  | 2.9  |
| 29  | CC    | 210  | ALA  | 2.9  |
| 34  | CF    | 45   | ALA  | 2.9  |
| 49  | CV    | 90   | GLY  | 2.9  |
| 50  | CW    | 74   | ALA  | 2.9  |
| 52  | CY    | 15   | GLY  | 2.9  |
| 18  | AR    | 20   | GLU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | BA    | 1375 | A    | 2.9  |
| 31  | CA    | 70   | G    | 2.9  |
| 7   | AG    | 137  | LYS  | 2.9  |
| 31  | CA    | 71   | A    | 2.9  |
| 31  | CA    | 612  | G    | 2.9  |
| 31  | CA    | 883  | G    | 2.9  |
| 31  | CA    | 1113 | U    | 2.9  |
| 31  | CA    | 1729 | U    | 2.9  |
| 31  | CA    | 1862 | G    | 2.9  |
| 49  | DV    | 48   | PRO  | 2.9  |
| 55  | DA    | 1058 | U    | 2.9  |
| 31  | CA    | 2158 | A    | 2.9  |
| 16  | BP    | 18   | GLN  | 2.9  |
| 13  | BM    | 82   | ASP  | 2.9  |
| 1   | AA    | 1320 | C    | 2.9  |
| 1   | BA    | 1369 | C    | 2.9  |
| 7   | BG    | 27   | VAL  | 2.9  |
| 6   | AF    | 42   | TRP  | 2.9  |
| 6   | BF    | 8    | PHE  | 2.9  |
| 10  | AJ    | 12   | ALA  | 2.9  |
| 13  | AM    | 37   | ALA  | 2.9  |
| 17  | BQ    | 67   | LEU  | 2.9  |
| 26  | C5    | 21   | GLY  | 2.9  |
| 34  | CF    | 168  | ALA  | 2.9  |
| 36  | CH    | 107  | GLY  | 2.9  |
| 42  | CO    | 70   | THR  | 2.9  |
| 31  | CA    | 598  | U    | 2.9  |
| 31  | CA    | 2878 | U    | 2.9  |
| 34  | CF    | 109  | PRO  | 2.9  |
| 40  | CM    | 29   | LYS  | 2.9  |
| 9   | AI    | 33   | ARG  | 2.9  |
| 24  | C3    | 39   | ARG  | 2.9  |
| 1   | BA    | 105  | G    | 2.9  |
| 1   | BA    | 134  | G    | 2.9  |
| 31  | CA    | 86   | G    | 2.9  |
| 31  | CA    | 127  | A    | 2.9  |
| 31  | CA    | 326  | G    | 2.9  |
| 31  | CA    | 1237 | A    | 2.9  |
| 31  | CA    | 1244 | A    | 2.9  |
| 31  | CA    | 1521 | G    | 2.9  |
| 31  | CA    | 1616 | A    | 2.9  |
| 31  | CA    | 2157 | G    | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2694 | G    | 2.9  |
| 5   | BE    | 78   | ASN  | 2.9  |
| 49  | CV    | 58   | ILE  | 2.9  |
| 26  | C5    | 3    | VAL  | 2.9  |
| 33  | CE    | 2    | GLU  | 2.9  |
| 41  | CN    | 101  | VAL  | 2.9  |
| 9   | AI    | 82   | GLY  | 2.9  |
| 14  | AN    | 32   | SER  | 2.9  |
| 19  | BS    | 47   | LEU  | 2.9  |
| 24  | D3    | 46   | LYS  | 2.9  |
| 38  | CK    | 20   | ALA  | 2.9  |
| 51  | CX    | 35   | SER  | 2.9  |
| 31  | CA    | 815  | C    | 2.9  |
| 31  | CA    | 1100 | C    | 2.9  |
| 31  | CA    | 2050 | C    | 2.9  |
| 49  | CV    | 46   | GLN  | 2.9  |
| 50  | CW    | 84   | PRO  | 2.9  |
| 55  | DA    | 2180 | U    | 2.9  |
| 1   | AA    | 959  | A    | 2.9  |
| 1   | BA    | 263  | A    | 2.9  |
| 1   | BA    | 1363 | A    | 2.9  |
| 31  | CA    | 2358 | A    | 2.9  |
| 31  | CA    | 2778 | A    | 2.9  |
| 36  | CH    | 4    | ILE  | 2.9  |
| 55  | DA    | 1090 | A    | 2.9  |
| 17  | AQ    | 4    | LYS  | 2.9  |
| 42  | CO    | 21   | PHE  | 2.9  |
| 6   | BF    | 38   | ARG  | 2.9  |
| 7   | BG    | 13   | LEU  | 2.9  |
| 36  | DH    | 82   | SER  | 2.9  |
| 38  | CK    | 108  | MET  | 2.9  |
| 9   | AI    | 18   | ARG  | 2.9  |
| 48  | CU    | 21   | SER  | 2.9  |
| 1   | BA    | 1140 | C    | 2.9  |
| 29  | DC    | 243  | HIS  | 2.9  |
| 31  | CA    | 653  | U    | 2.9  |
| 31  | CA    | 2903 | U    | 2.9  |
| 13  | AM    | 114  | LYS  | 2.9  |
| 14  | BN    | 76   | LYS  | 2.9  |
| 2   | BB    | 93   | ASN  | 2.9  |
| 5   | BE    | 148  | ASN  | 2.9  |
| 7   | BG    | 126  | ASP  | 2.9  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 40         | CM           | 111        | ILE         | 2.9         |
| 50         | CW           | 5          | ASN         | 2.9         |
| 1          | BA           | 1227       | A           | 2.9         |
| 31         | CA           | 196        | A           | 2.9         |
| 1          | BA           | 201        | G           | 2.9         |
| 1          | BA           | 1343       | G           | 2.9         |
| 1          | BA           | 1361       | G           | 2.9         |
| 6          | AF           | 66         | ALA         | 2.9         |
| 14         | AN           | 36         | ALA         | 2.9         |
| 30         | CD           | 138        | LEU         | 2.9         |
| 39         | CL           | 28         | SER         | 2.8         |
| 46         | CS           | 102        | SER         | 2.8         |
| 1          | AA           | 1148       | U           | 2.8         |
| 31         | CA           | 1542       | U           | 2.8         |
| 42         | CO           | 85         | PRO         | 2.8         |
| 53         | CZ           | 9          | LYS         | 2.8         |
| 21         | AU           | 39         | GLU         | 2.8         |
| 11         | AK           | 98         | ARG         | 2.8         |
| 24         | C3           | 9          | VAL         | 2.8         |
| 30         | CD           | 135        | GLY         | 2.8         |
| 34         | CF           | 13         | VAL         | 2.8         |
| 42         | CO           | 12         | ARG         | 2.8         |
| 40         | CM           | 112        | LEU         | 2.8         |
| 43         | CP           | 77         | ALA         | 2.8         |
| 3          | BC           | 51         | SER         | 2.8         |
| 10         | AJ           | 101        | SER         | 2.8         |
| 1          | AA           | 1125       | U           | 2.8         |
| 31         | CA           | 261        | G           | 2.8         |
| 31         | CA           | 273        | G           | 2.8         |
| 31         | CA           | 1523       | U           | 2.8         |
| 31         | CA           | 2302       | U           | 2.8         |
| 31         | CA           | 2847       | U           | 2.8         |
| 34         | CF           | 72         | LYS         | 2.8         |
| 46         | CS           | 11         | GLN         | 2.8         |
| 55         | DA           | 2107       | G           | 2.8         |
| 55         | DA           | 2159       | G           | 2.8         |
| 1          | AA           | 1302       | C           | 2.8         |
| 1          | BA           | 1228       | C           | 2.8         |
| 10         | BJ           | 50         | THR         | 2.8         |
| 19         | BS           | 33         | THR         | 2.8         |
| 31         | CA           | 623        | C           | 2.8         |
| 34         | CF           | 87         | CYS         | 2.8         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | DA    | 2153 | C    | 2.8  |
| 35  | CG    | 124  | GLU  | 2.8  |
| 3   | BC    | 65   | ARG  | 2.8  |
| 10  | BJ    | 31   | ARG  | 2.8  |
| 21  | BU    | 4    | ILE  | 2.8  |
| 15  | AO    | 21   | ASP  | 2.8  |
| 25  | C4    | 21   | GLY  | 2.8  |
| 17  | AQ    | 83   | VAL  | 2.8  |
| 21  | AU    | 12   | PHE  | 2.8  |
| 35  | CG    | 15   | VAL  | 2.8  |
| 44  | CQ    | 32   | VAL  | 2.8  |
| 54  | DI    | 35   | VAL  | 2.8  |
| 2   | AB    | 57   | LEU  | 2.8  |
| 36  | DH    | 6    | LEU  | 2.8  |
| 40  | CM    | 109  | LYS  | 2.8  |
| 20  | AT    | 55   | GLN  | 2.8  |
| 31  | CA    | 616  | A    | 2.8  |
| 31  | CA    | 1275 | A    | 2.8  |
| 1   | BA    | 961  | U    | 2.8  |
| 31  | CA    | 1176 | U    | 2.8  |
| 29  | CC    | 231  | PRO  | 2.8  |
| 31  | CA    | 215  | G    | 2.8  |
| 31  | CA    | 307  | G    | 2.8  |
| 31  | CA    | 2830 | C    | 2.8  |
| 41  | CN    | 23   | GLY  | 2.8  |
| 48  | CU    | 79   | ASP  | 2.8  |
| 33  | CE    | 96   | VAL  | 2.8  |
| 47  | CT    | 69   | LEU  | 2.8  |
| 33  | CE    | 39   | ALA  | 2.8  |
| 21  | AU    | 8    | GLU  | 2.8  |
| 11  | BK    | 98   | ARG  | 2.8  |
| 31  | CA    | 2147 | A    | 2.8  |
| 3   | BC    | 74   | GLY  | 2.8  |
| 18  | AR    | 59   | ILE  | 2.8  |
| 8   | AH    | 54   | ASP  | 2.8  |
| 31  | CA    | 561  | G    | 2.8  |
| 47  | CT    | 68   | ASP  | 2.8  |
| 33  | CE    | 60   | TRP  | 2.8  |
| 2   | BB    | 84   | ALA  | 2.8  |
| 20  | BT    | 11   | ALA  | 2.8  |
| 3   | BC    | 161  | GLU  | 2.8  |
| 23  | D2    | 45   | GLN  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | C4    | 60   | ALA  | 2.8  |
| 1   | BA    | 1264 | U    | 2.8  |
| 31  | CA    | 2149 | U    | 2.8  |
| 22  | C1    | 7    | LYS  | 2.8  |
| 36  | DH    | 141  | LYS  | 2.8  |
| 1   | AA    | 1441 | A    | 2.8  |
| 1   | BA    | 1238 | A    | 2.8  |
| 12  | BL    | 82   | ILE  | 2.8  |
| 13  | AM    | 104  | THR  | 2.8  |
| 35  | CG    | 19   | ILE  | 2.8  |
| 47  | CT    | 55   | ILE  | 2.8  |
| 50  | CW    | 40   | ILE  | 2.8  |
| 30  | CD    | 176  | ASP  | 2.8  |
| 31  | CA    | 128  | C    | 2.8  |
| 31  | CA    | 1909 | C    | 2.8  |
| 7   | AG    | 103  | TRP  | 2.8  |
| 10  | BJ    | 51   | VAL  | 2.8  |
| 38  | CK    | 74   | TYR  | 2.8  |
| 9   | BI    | 45   | ARG  | 2.8  |
| 12  | AL    | 73   | ASN  | 2.8  |
| 17  | BQ    | 60   | GLU  | 2.8  |
| 31  | CA    | 367  | G    | 2.8  |
| 31  | CA    | 2621 | G    | 2.8  |
| 20  | BT    | 61   | GLN  | 2.8  |
| 35  | CG    | 42   | GLU  | 2.8  |
| 43  | CP    | 37   | ALA  | 2.8  |
| 45  | CR    | 116  | ALA  | 2.8  |
| 27  | C0    | 54   | MET  | 2.8  |
| 52  | CY    | 56   | MET  | 2.8  |
| 1   | AA    | 1286 | U    | 2.8  |
| 16  | BP    | 12   | LYS  | 2.8  |
| 31  | CA    | 87   | U    | 2.8  |
| 46  | CS    | 48   | LYS  | 2.8  |
| 3   | BC    | 205  | GLY  | 2.8  |
| 9   | BI    | 69   | GLY  | 2.8  |
| 19  | AS    | 25   | SER  | 2.8  |
| 30  | CD    | 145  | SER  | 2.8  |
| 2   | AB    | 82   | ASP  | 2.8  |
| 31  | CA    | 2749 | A    | 2.8  |
| 34  | CF    | 6    | ASP  | 2.8  |
| 45  | CR    | 49   | ASP  | 2.8  |
| 5   | BE    | 124  | LEU  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | BR    | 40   | VAL  | 2.8  |
| 38  | CK    | 75   | TYR  | 2.8  |
| 41  | CN    | 26   | VAL  | 2.8  |
| 45  | CR    | 88   | VAL  | 2.8  |
| 51  | DX    | 10   | THR  | 2.8  |
| 21  | AU    | 38   | TYR  | 2.8  |
| 29  | CC    | 238  | ARG  | 2.8  |
| 31  | CA    | 264  | C    | 2.8  |
| 31  | CA    | 854  | C    | 2.8  |
| 31  | CA    | 1135 | C    | 2.8  |
| 44  | CQ    | 103  | ARG  | 2.8  |
| 3   | AC    | 104  | ALA  | 2.8  |
| 31  | CA    | 77   | G    | 2.8  |
| 31  | CA    | 178  | G    | 2.8  |
| 31  | CA    | 488  | G    | 2.8  |
| 31  | CA    | 1063 | G    | 2.8  |
| 31  | CA    | 1807 | G    | 2.8  |
| 31  | CA    | 2677 | G    | 2.8  |
| 31  | CA    | 2816 | G    | 2.8  |
| 31  | CA    | 235  | U    | 2.8  |
| 3   | AC    | 81   | GLY  | 2.8  |
| 2   | BB    | 91   | PHE  | 2.8  |
| 11  | AK    | 31   | ILE  | 2.8  |
| 34  | CF    | 82   | GLY  | 2.8  |
| 39  | CL    | 15   | GLY  | 2.8  |
| 5   | AE    | 10   | GLU  | 2.8  |
| 27  | C0    | 45   | ARG  | 2.8  |
| 54  | DI    | 7    | ASP  | 2.8  |
| 36  | CH    | 138  | VAL  | 2.8  |
| 1   | BA    | 1044 | A    | 2.8  |
| 29  | CC    | 18   | LYS  | 2.8  |
| 31  | CA    | 6    | A    | 2.8  |
| 31  | CA    | 368  | A    | 2.8  |
| 31  | CA    | 867  | C    | 2.8  |
| 31  | CA    | 1080 | A    | 2.8  |
| 31  | CA    | 1420 | A    | 2.8  |
| 50  | CW    | 10   | LYS  | 2.8  |
| 50  | CW    | 14   | LYS  | 2.8  |
| 25  | C4    | 65   | ALA  | 2.8  |
| 42  | CO    | 18   | GLN  | 2.8  |
| 34  | DF    | 38   | MET  | 2.8  |
| 1   | BA    | 1278 | G    | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 19   | GLY  | 2.8  |
| 31  | CA    | 168  | G    | 2.8  |
| 31  | CA    | 263  | G    | 2.8  |
| 31  | CA    | 390  | U    | 2.8  |
| 31  | CA    | 551  | G    | 2.8  |
| 31  | CA    | 1324 | G    | 2.8  |
| 11  | AK    | 34   | ILE  | 2.8  |
| 20  | BT    | 32   | ILE  | 2.8  |
| 34  | CF    | 71   | ARG  | 2.8  |
| 35  | CG    | 12   | PRO  | 2.8  |
| 47  | CT    | 96   | ILE  | 2.8  |
| 16  | BP    | 76   | LYS  | 2.8  |
| 46  | CS    | 23   | GLU  | 2.8  |
| 51  | CX    | 66   | LYS  | 2.8  |
| 3   | BC    | 87   | LEU  | 2.8  |
| 46  | CS    | 4    | VAL  | 2.8  |
| 11  | AK    | 33   | THR  | 2.8  |
| 1   | AA    | 962  | C    | 2.8  |
| 5   | BE    | 118  | ALA  | 2.8  |
| 31  | CA    | 240  | C    | 2.8  |
| 31  | CA    | 244  | A    | 2.7  |
| 31  | CA    | 440  | C    | 2.8  |
| 31  | CA    | 1330 | C    | 2.8  |
| 31  | CA    | 1871 | A    | 2.7  |
| 31  | CA    | 2179 | C    | 2.8  |
| 31  | CA    | 2376 | A    | 2.7  |
| 31  | CA    | 2716 | C    | 2.8  |
| 40  | CM    | 98   | ALA  | 2.8  |
| 50  | CW    | 54   | ALA  | 2.8  |
| 38  | CK    | 131  | ASN  | 2.7  |
| 40  | CM    | 4    | ASN  | 2.7  |
| 31  | CA    | 1004 | U    | 2.7  |
| 3   | AC    | 103  | ILE  | 2.7  |
| 4   | AD    | 160  | GLU  | 2.7  |
| 23  | C2    | 35   | GLU  | 2.7  |
| 1   | BA    | 1186 | G    | 2.7  |
| 38  | CK    | 71   | ASP  | 2.7  |
| 10  | AJ    | 98   | VAL  | 2.7  |
| 33  | CE    | 153  | LEU  | 2.7  |
| 3   | BC    | 123  | GLN  | 2.7  |
| 22  | C1    | 48   | TYR  | 2.7  |
| 25  | C4    | 6    | THR  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 71   | ALA  | 2.7  |
| 44  | CQ    | 25   | THR  | 2.7  |
| 7   | AG    | 144  | MET  | 2.7  |
| 1   | BA    | 109  | A    | 2.7  |
| 13  | AM    | 51   | GLY  | 2.7  |
| 20  | BT    | 52   | ASN  | 2.7  |
| 1   | BA    | 157  | U    | 2.7  |
| 31  | CA    | 1340 | U    | 2.7  |
| 31  | CA    | 2259 | U    | 2.7  |
| 33  | CE    | 114  | ARG  | 2.7  |
| 55  | DA    | 1078 | U    | 2.7  |
| 16  | BP    | 15   | PRO  | 2.7  |
| 5   | BE    | 149  | SER  | 2.7  |
| 6   | AF    | 89   | VAL  | 2.7  |
| 9   | AI    | 58   | VAL  | 2.7  |
| 9   | BI    | 34   | SER  | 2.7  |
| 14  | BN    | 14   | VAL  | 2.7  |
| 14  | BN    | 46   | LEU  | 2.7  |
| 29  | CC    | 202  | LEU  | 2.7  |
| 40  | CM    | 25   | SER  | 2.7  |
| 42  | CO    | 115  | LEU  | 2.7  |
| 54  | DI    | 33   | VAL  | 2.7  |
| 31  | CA    | 248  | G    | 2.7  |
| 31  | CA    | 1633 | G    | 2.7  |
| 31  | CA    | 2618 | G    | 2.7  |
| 55  | DA    | 1087 | G    | 2.7  |
| 42  | CO    | 77   | ALA  | 2.7  |
| 45  | CR    | 96   | ALA  | 2.7  |
| 16  | BP    | 5    | ARG  | 2.7  |
| 1   | BA    | 943  | U    | 2.7  |
| 20  | BT    | 78   | ASN  | 2.7  |
| 31  | CA    | 394  | C    | 2.7  |
| 31  | CA    | 584  | C    | 2.7  |
| 31  | CA    | 1658 | C    | 2.7  |
| 31  | CA    | 1708 | C    | 2.7  |
| 31  | CA    | 2793 | C    | 2.7  |
| 40  | CM    | 11   | GLY  | 2.7  |
| 46  | CS    | 56   | GLY  | 2.7  |
| 31  | CA    | 1467 | U    | 2.7  |
| 37  | DJ    | 108  | GLU  | 2.7  |
| 1   | BA    | 478  | A    | 2.7  |
| 13  | AM    | 63   | PHE  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 52   | A    | 2.7  |
| 31  | CA    | 227  | A    | 2.7  |
| 31  | CA    | 1111 | A    | 2.7  |
| 34  | DF    | 77   | PHE  | 2.7  |
| 15  | BO    | 29   | VAL  | 2.7  |
| 3   | BC    | 69   | HIS  | 2.7  |
| 25  | C4    | 23   | LYS  | 2.7  |
| 52  | CY    | 21   | ALA  | 2.7  |
| 1   | BA    | 377  | G    | 2.7  |
| 1   | BA    | 1057 | G    | 2.7  |
| 2   | BB    | 46   | THR  | 2.7  |
| 31  | CA    | 26   | G    | 2.7  |
| 31  | CA    | 43   | G    | 2.7  |
| 31  | CA    | 1311 | G    | 2.7  |
| 35  | CG    | 122  | THR  | 2.7  |
| 37  | DJ    | 25   | GLY  | 2.7  |
| 40  | CM    | 136  | GLU  | 2.7  |
| 55  | DA    | 2148 | G    | 2.7  |
| 1   | BA    | 1136 | C    | 2.7  |
| 30  | CD    | 126  | ASN  | 2.7  |
| 31  | CA    | 2334 | U    | 2.7  |
| 33  | CE    | 156  | ASN  | 2.7  |
| 5   | BE    | 150  | PRO  | 2.7  |
| 28  | CB    | 50   | A    | 2.7  |
| 31  | CA    | 256  | A    | 2.7  |
| 31  | CA    | 1496 | A    | 2.7  |
| 22  | C1    | 30   | VAL  | 2.7  |
| 37  | DJ    | 72   | LYS  | 2.7  |
| 54  | DI    | 29   | ASP  | 2.7  |
| 46  | CS    | 21   | ARG  | 2.7  |
| 38  | CK    | 134  | ALA  | 2.7  |
| 16  | BP    | 47   | GLU  | 2.7  |
| 16  | BP    | 62   | GLY  | 2.7  |
| 1   | BA    | 191  | G    | 2.7  |
| 2   | BB    | 42   | ASN  | 2.7  |
| 2   | BB    | 69   | PHE  | 2.7  |
| 35  | CG    | 36   | THR  | 2.7  |
| 3   | BC    | 202  | ILE  | 2.7  |
| 28  | CB    | 102  | G    | 2.7  |
| 31  | CA    | 93   | G    | 2.7  |
| 31  | CA    | 113  | U    | 2.7  |
| 31  | CA    | 333  | G    | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 536  | G    | 2.7  |
| 31  | CA    | 1963 | U    | 2.7  |
| 3   | AC    | 89   | LYS  | 2.7  |
| 26  | C5    | 15   | LYS  | 2.7  |
| 35  | CG    | 85   | LYS  | 2.7  |
| 1   | BA    | 71   | A    | 2.7  |
| 1   | BA    | 1188 | A    | 2.7  |
| 10  | AJ    | 62   | ARG  | 2.7  |
| 19  | AS    | 78   | ARG  | 2.7  |
| 25  | C4    | 30   | ARG  | 2.7  |
| 30  | CD    | 37   | VAL  | 2.7  |
| 33  | CE    | 195  | GLN  | 2.7  |
| 34  | DF    | 40   | VAL  | 2.7  |
| 36  | CH    | 12   | LEU  | 2.7  |
| 31  | CA    | 89   | A    | 2.7  |
| 40  | CM    | 123  | ARG  | 2.7  |
| 54  | DI    | 27   | VAL  | 2.7  |
| 55  | DA    | 1848 | A    | 2.7  |
| 26  | C5    | 6    | SER  | 2.7  |
| 35  | CG    | 28   | GLY  | 2.7  |
| 36  | DH    | 106  | ALA  | 2.7  |
| 37  | DJ    | 29   | GLY  | 2.7  |
| 40  | CM    | 40   | SER  | 2.7  |
| 42  | CO    | 59   | SER  | 2.7  |
| 44  | CQ    | 2    | SER  | 2.7  |
| 46  | CS    | 69   | GLY  | 2.7  |
| 3   | BC    | 147  | LYS  | 2.7  |
| 9   | AI    | 9    | THR  | 2.7  |
| 27  | C0    | 19   | LYS  | 2.7  |
| 40  | CM    | 73   | ILE  | 2.7  |
| 45  | CR    | 78   | LYS  | 2.7  |
| 29  | CC    | 86   | ASN  | 2.7  |
| 30  | CD    | 32   | ASN  | 2.7  |
| 7   | BG    | 10   | ARG  | 2.7  |
| 2   | AB    | 114  | LEU  | 2.7  |
| 31  | CA    | 640  | C    | 2.7  |
| 31  | CA    | 953  | G    | 2.7  |
| 31  | CA    | 1117 | C    | 2.7  |
| 31  | CA    | 1251 | C    | 2.7  |
| 27  | C0    | 36   | VAL  | 2.7  |
| 35  | CG    | 71   | LEU  | 2.7  |
| 36  | DH    | 117  | LEU  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | CO    | 106  | ASP  | 2.7  |
| 2   | AB    | 142  | GLU  | 2.7  |
| 1   | AA    | 1035 | A    | 2.7  |
| 8   | BH    | 123  | GLY  | 2.7  |
| 10  | BJ    | 29   | ALA  | 2.7  |
| 16  | BP    | 27   | ALA  | 2.7  |
| 20  | BT    | 7    | ALA  | 2.7  |
| 31  | CA    | 1070 | A    | 2.7  |
| 10  | BJ    | 54   | SER  | 2.7  |
| 27  | C0    | 52   | SER  | 2.7  |
| 29  | CC    | 6    | CYS  | 2.7  |
| 33  | CE    | 107  | SER  | 2.7  |
| 43  | CP    | 85   | LYS  | 2.7  |
| 45  | CR    | 75   | SER  | 2.7  |
| 9   | BI    | 65   | ILE  | 2.7  |
| 20  | BT    | 29   | ARG  | 2.7  |
| 31  | CA    | 72   | U    | 2.7  |
| 31  | CA    | 102  | U    | 2.7  |
| 31  | CA    | 1183 | U    | 2.7  |
| 13  | AM    | 8    | ASN  | 2.7  |
| 14  | BN    | 38   | ASP  | 2.7  |
| 27  | C0    | 51   | VAL  | 2.7  |
| 29  | CC    | 3    | VAL  | 2.7  |
| 31  | CA    | 277  | G    | 2.7  |
| 31  | CA    | 1137 | G    | 2.7  |
| 31  | CA    | 1193 | G    | 2.7  |
| 30  | CD    | 87   | GLY  | 2.7  |
| 11  | BK    | 44   | TRP  | 2.7  |
| 33  | CE    | 161  | ALA  | 2.7  |
| 48  | CU    | 9    | LYS  | 2.7  |
| 1   | BA    | 1213 | A    | 2.7  |
| 31  | CA    | 1635 | A    | 2.7  |
| 40  | CM    | 68   | SER  | 2.7  |
| 14  | AN    | 53   | ARG  | 2.7  |
| 39  | CL    | 1    | MET  | 2.7  |
| 42  | CO    | 30   | ARG  | 2.7  |
| 45  | CR    | 28   | ARG  | 2.7  |
| 1   | AA    | 1126 | U    | 2.7  |
| 1   | BA    | 992  | U    | 2.7  |
| 16  | BP    | 4    | ILE  | 2.7  |
| 31  | CA    | 932  | U    | 2.7  |
| 31  | CA    | 2166 | U    | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | CM    | 103  | ILE  | 2.7  |
| 3   | BC    | 110  | GLU  | 2.7  |
| 2   | BB    | 163  | VAL  | 2.7  |
| 8   | BH    | 99   | LEU  | 2.7  |
| 38  | CK    | 3    | THR  | 2.7  |
| 44  | DQ    | 115  | ASN  | 2.7  |
| 45  | CR    | 66   | ASN  | 2.7  |
| 14  | AN    | 3    | LYS  | 2.7  |
| 15  | AO    | 27   | VAL  | 2.7  |
| 23  | C2    | 42   | VAL  | 2.7  |
| 48  | CU    | 50   | LEU  | 2.7  |
| 31  | CA    | 269  | C    | 2.7  |
| 40  | CM    | 22   | GLY  | 2.7  |
| 3   | AC    | 50   | ALA  | 2.7  |
| 35  | CG    | 97   | ALA  | 2.7  |
| 39  | CL    | 16   | ALA  | 2.7  |
| 11  | AK    | 61   | PHE  | 2.6  |
| 29  | CC    | 203  | ARG  | 2.7  |
| 1   | BA    | 845  | A    | 2.6  |
| 1   | BA    | 1357 | A    | 2.6  |
| 4   | AD    | 178  | MET  | 2.6  |
| 36  | CH    | 131  | SER  | 2.6  |
| 20  | BT    | 57   | ILE  | 2.6  |
| 29  | CC    | 74   | ILE  | 2.6  |
| 31  | CA    | 216  | A    | 2.6  |
| 31  | CA    | 1272 | A    | 2.6  |
| 54  | DI    | 118  | ILE  | 2.6  |
| 55  | DA    | 2173 | A    | 2.6  |
| 3   | BC    | 105  | GLU  | 2.6  |
| 31  | CA    | 511  | U    | 2.6  |
| 14  | BN    | 28   | LYS  | 2.6  |
| 3   | BC    | 31   | ASP  | 2.6  |
| 16  | BP    | 6    | LEU  | 2.6  |
| 18  | AR    | 24   | LYS  | 2.6  |
| 44  | CQ    | 94   | LYS  | 2.6  |
| 3   | BC    | 91   | VAL  | 2.6  |
| 18  | AR    | 47   | THR  | 2.6  |
| 38  | CK    | 50   | THR  | 2.6  |
| 39  | CL    | 84   | CYS  | 2.6  |
| 48  | CU    | 86   | THR  | 2.6  |
| 50  | CW    | 20   | LEU  | 2.6  |
| 29  | CC    | 228  | VAL  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | BN    | 95   | GLY  | 2.6  |
| 31  | CA    | 237  | C    | 2.6  |
| 10  | AJ    | 9    | ARG  | 2.6  |
| 11  | BK    | 13   | ARG  | 2.6  |
| 24  | C3    | 3    | ARG  | 2.6  |
| 29  | CC    | 266  | PHE  | 2.6  |
| 46  | CS    | 77   | PHE  | 2.6  |
| 1   | BA    | 92   | U    | 2.6  |
| 20  | AT    | 76   | LYS  | 2.6  |
| 31  | CA    | 841  | G    | 2.6  |
| 31  | CA    | 1715 | G    | 2.6  |
| 31  | CA    | 2859 | G    | 2.6  |
| 55  | DA    | 1731 | G    | 2.6  |
| 1   | AA    | 1171 | A    | 2.6  |
| 1   | BA    | 1257 | A    | 2.6  |
| 3   | BC    | 168  | TYR  | 2.6  |
| 31  | CA    | 2743 | U    | 2.6  |
| 55  | DA    | 895  | U    | 2.6  |
| 31  | CA    | 1134 | A    | 2.6  |
| 34  | DF    | 117  | LEU  | 2.6  |
| 8   | AH    | 110  | VAL  | 2.6  |
| 9   | AI    | 47   | VAL  | 2.6  |
| 16  | BP    | 30   | GLY  | 2.6  |
| 29  | CC    | 246  | THR  | 2.6  |
| 29  | CC    | 257  | THR  | 2.6  |
| 41  | CN    | 15   | GLY  | 2.6  |
| 42  | CO    | 8    | ARG  | 2.6  |
| 46  | CS    | 80   | ARG  | 2.6  |
| 29  | CC    | 2    | ALA  | 2.6  |
| 34  | CF    | 54   | ALA  | 2.6  |
| 42  | CO    | 68   | ALA  | 2.6  |
| 43  | CP    | 57   | ALA  | 2.6  |
| 43  | CP    | 71   | ALA  | 2.6  |
| 55  | DA    | 1072 | C    | 2.6  |
| 43  | CP    | 76   | LYS  | 2.6  |
| 50  | CW    | 44   | HIS  | 2.6  |
| 6   | AF    | 88   | MET  | 2.6  |
| 1   | BA    | 252  | U    | 2.6  |
| 8   | BH    | 36   | ILE  | 2.6  |
| 17  | BQ    | 20   | SER  | 2.6  |
| 31  | CA    | 2871 | U    | 2.6  |
| 10  | AJ    | 71   | LEU  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | BP    | 74   | LEU  | 2.6  |
| 31  | CA    | 583  | G    | 2.6  |
| 31  | CA    | 1179 | G    | 2.6  |
| 4   | AD    | 174  | ASP  | 2.6  |
| 19  | AS    | 32   | ARG  | 2.6  |
| 31  | CA    | 10   | A    | 2.6  |
| 31  | CA    | 608  | A    | 2.6  |
| 31  | CA    | 631  | A    | 2.6  |
| 31  | CA    | 633  | A    | 2.6  |
| 31  | CA    | 1021 | A    | 2.6  |
| 31  | CA    | 1614 | A    | 2.6  |
| 31  | CA    | 2003 | A    | 2.6  |
| 33  | CE    | 79   | ARG  | 2.6  |
| 35  | CG    | 53   | GLY  | 2.6  |
| 42  | CO    | 72   | ASP  | 2.6  |
| 9   | AI    | 66   | THR  | 2.6  |
| 33  | CE    | 65   | THR  | 2.6  |
| 3   | AC    | 133  | ALA  | 2.6  |
| 44  | CQ    | 18   | PRO  | 2.6  |
| 35  | CG    | 18   | LYS  | 2.6  |
| 37  | CJ    | 10   | LYS  | 2.6  |
| 45  | CR    | 85   | LYS  | 2.6  |
| 11  | AK    | 70   | CYS  | 2.6  |
| 29  | CC    | 180  | GLU  | 2.6  |
| 31  | CA    | 610  | C    | 2.6  |
| 31  | CA    | 1323 | C    | 2.6  |
| 50  | CW    | 35   | GLU  | 2.6  |
| 3   | BC    | 75   | ILE  | 2.6  |
| 23  | D2    | 5    | ILE  | 2.6  |
| 36  | DH    | 72   | ILE  | 2.6  |
| 1   | BA    | 103  | U    | 2.6  |
| 1   | BA    | 1121 | U    | 2.6  |
| 1   | BA    | 1189 | U    | 2.6  |
| 1   | BA    | 1301 | U    | 2.6  |
| 43  | CP    | 19   | GLN  | 2.6  |
| 5   | AE    | 115  | LEU  | 2.6  |
| 9   | AI    | 98   | LEU  | 2.6  |
| 52  | CY    | 39   | TRP  | 2.6  |
| 2   | AB    | 17   | GLY  | 2.6  |
| 2   | AB    | 65   | GLY  | 2.6  |
| 10  | BJ    | 57   | VAL  | 2.6  |
| 13  | BM    | 68   | ASP  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | AS    | 67   | VAL  | 2.6  |
| 30  | CD    | 198  | GLY  | 2.6  |
| 1   | BA    | 609  | A    | 2.6  |
| 28  | CB    | 116  | G    | 2.6  |
| 36  | CH    | 41   | LYS  | 2.6  |
| 42  | CO    | 40   | LYS  | 2.6  |
| 9   | AI    | 23   | PRO  | 2.6  |
| 11  | AK    | 30   | THR  | 2.6  |
| 16  | BP    | 3    | THR  | 2.6  |
| 43  | CP    | 6    | ALA  | 2.6  |
| 51  | CX    | 17   | GLU  | 2.6  |
| 1   | BA    | 1223 | C    | 2.6  |
| 31  | CA    | 2275 | C    | 2.6  |
| 31  | CA    | 667  | U    | 2.6  |
| 31  | CA    | 1141 | U    | 2.6  |
| 31  | CA    | 2690 | U    | 2.6  |
| 37  | DJ    | 17   | MET  | 2.6  |
| 7   | AG    | 30   | LEU  | 2.6  |
| 29  | CC    | 12   | GLY  | 2.6  |
| 29  | CC    | 98   | ASP  | 2.6  |
| 50  | CW    | 60   | VAL  | 2.6  |
| 17  | BQ    | 82   | ALA  | 2.6  |
| 29  | CC    | 194  | GLU  | 2.6  |
| 48  | CU    | 14   | PRO  | 2.6  |
| 1   | AA    | 1166 | G    | 2.6  |
| 1   | BA    | 1146 | A    | 2.6  |
| 19  | AS    | 74   | PHE  | 2.6  |
| 31  | CA    | 528  | A    | 2.6  |
| 31  | CA    | 1276 | A    | 2.6  |
| 31  | CA    | 1354 | A    | 2.6  |
| 31  | CA    | 1867 | G    | 2.6  |
| 31  | CA    | 2857 | G    | 2.6  |
| 53  | CZ    | 16   | THR  | 2.6  |
| 55  | DA    | 2154 | A    | 2.6  |
| 3   | AC    | 64   | ILE  | 2.6  |
| 3   | AC    | 107  | ARG  | 2.6  |
| 13  | AM    | 3    | ARG  | 2.6  |
| 17  | BQ    | 47   | HIS  | 2.6  |
| 31  | CA    | 1454 | C    | 2.6  |
| 50  | CW    | 4    | ILE  | 2.6  |
| 55  | DA    | 2143 | C    | 2.6  |
| 23  | C2    | 38   | LYS  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | BB    | 205  | ASP  | 2.6  |
| 6   | BF    | 96   | VAL  | 2.6  |
| 10  | AJ    | 60   | ASP  | 2.6  |
| 29  | DC    | 272  | SER  | 2.6  |
| 33  | CE    | 116  | ASP  | 2.6  |
| 9   | BI    | 42   | GLU  | 2.6  |
| 13  | AM    | 41   | GLU  | 2.6  |
| 33  | CE    | 198  | GLU  | 2.6  |
| 48  | CU    | 54   | GLU  | 2.6  |
| 3   | BC    | 7    | PRO  | 2.6  |
| 10  | AJ    | 58   | ASN  | 2.6  |
| 37  | DJ    | 44   | ALA  | 2.6  |
| 5   | BE    | 112  | ARG  | 2.6  |
| 27  | C0    | 31   | ARG  | 2.6  |
| 1   | AA    | 1347 | G    | 2.6  |
| 1   | BA    | 107  | G    | 2.6  |
| 1   | BA    | 139  | A    | 2.6  |
| 1   | BA    | 148  | G    | 2.6  |
| 11  | AK    | 107  | ILE  | 2.6  |
| 24  | C3    | 29   | GLN  | 2.6  |
| 28  | CB    | 2    | G    | 2.6  |
| 31  | CA    | 68   | G    | 2.6  |
| 31  | CA    | 389  | G    | 2.6  |
| 36  | CH    | 80   | ILE  | 2.6  |
| 1   | BA    | 84   | U    | 2.6  |
| 13  | AM    | 111  | GLY  | 2.6  |
| 31  | CA    | 624  | C    | 2.6  |
| 31  | CA    | 906  | U    | 2.6  |
| 31  | CA    | 1053 | C    | 2.6  |
| 31  | CA    | 1615 | C    | 2.6  |
| 40  | CM    | 53   | GLY  | 2.6  |
| 55  | DA    | 898  | C    | 2.6  |
| 7   | AG    | 87   | VAL  | 2.6  |
| 30  | CD    | 89   | GLU  | 2.6  |
| 30  | CD    | 113  | SER  | 2.6  |
| 34  | CF    | 89   | VAL  | 2.6  |
| 4   | AD    | 170  | TRP  | 2.6  |
| 7   | BG    | 36   | LYS  | 2.6  |
| 23  | C2    | 41   | PRO  | 2.6  |
| 33  | CE    | 61   | ARG  | 2.6  |
| 35  | CG    | 149  | ARG  | 2.6  |
| 38  | CK    | 63   | ALA  | 2.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 41         | CN           | 14         | LYS         | 2.6         |
| 8          | BH           | 120        | GLY         | 2.6         |
| 19         | AS           | 54         | GLY         | 2.6         |
| 31         | CA           | 1443       | U           | 2.6         |
| 31         | CA           | 2046       | G           | 2.6         |
| 31         | CA           | 2151       | U           | 2.6         |
| 41         | CN           | 124        | LEU         | 2.6         |
| 1          | BA           | 187        | G           | 2.6         |
| 1          | BA           | 351        | G           | 2.6         |
| 1          | BA           | 1255       | G           | 2.6         |
| 31         | CA           | 2791       | G           | 2.6         |
| 12         | BL           | 107        | VAL         | 2.6         |
| 35         | CG           | 137        | ASP         | 2.6         |
| 14         | BN           | 80         | SER         | 2.6         |
| 22         | C1           | 29         | SER         | 2.6         |
| 26         | C5           | 24         | ARG         | 2.6         |
| 34         | CF           | 162        | SER         | 2.6         |
| 35         | CG           | 170        | ARG         | 2.6         |
| 44         | CQ           | 19         | SER         | 2.6         |
| 46         | CS           | 2          | TYR         | 2.6         |
| 41         | CN           | 71         | LYS         | 2.6         |
| 48         | CU           | 49         | LYS         | 2.6         |
| 7          | AG           | 99         | LEU         | 2.5         |
| 17         | BQ           | 54         | GLY         | 2.5         |
| 30         | CD           | 120        | GLY         | 2.5         |
| 30         | CD           | 158        | GLY         | 2.5         |
| 36         | CH           | 5          | LEU         | 2.5         |
| 7          | AG           | 75         | VAL         | 2.5         |
| 10         | BJ           | 62         | ARG         | 2.5         |
| 16         | AP           | 78         | VAL         | 2.5         |
| 20         | BT           | 85         | LYS         | 2.5         |
| 29         | CC           | 250        | VAL         | 2.5         |
| 31         | CA           | 374        | A           | 2.5         |
| 31         | CA           | 246        | C           | 2.5         |
| 31         | CA           | 838        | C           | 2.5         |
| 31         | CA           | 1208       | C           | 2.5         |
| 31         | CA           | 1270       | C           | 2.5         |
| 34         | CF           | 78         | LYS         | 2.5         |
| 31         | CA           | 1          | G           | 2.5         |
| 31         | CA           | 27         | G           | 2.5         |
| 31         | CA           | 386        | G           | 2.5         |
| 31         | CA           | 776        | G           | 2.5         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 1124 | G    | 2.5  |
| 31  | CA    | 2242 | G    | 2.5  |
| 31  | CA    | 2844 | G    | 2.5  |
| 40  | CM    | 60   | ARG  | 2.5  |
| 2   | BB    | 191  | SER  | 2.5  |
| 8   | BH    | 86   | TYR  | 2.5  |
| 24  | C3    | 45   | SER  | 2.5  |
| 25  | C4    | 48   | ALA  | 2.5  |
| 47  | CT    | 10   | ALA  | 2.5  |
| 50  | CW    | 23   | ALA  | 2.5  |
| 52  | CY    | 73   | ALA  | 2.5  |
| 17  | BQ    | 66   | PRO  | 2.5  |
| 14  | AN    | 4    | GLN  | 2.5  |
| 29  | DC    | 241  | GLY  | 2.5  |
| 31  | CA    | 1058 | U    | 2.5  |
| 34  | CF    | 159  | THR  | 2.5  |
| 34  | DF    | 152  | LEU  | 2.5  |
| 37  | CJ    | 141  | GLU  | 2.5  |
| 44  | CQ    | 114  | LEU  | 2.5  |
| 29  | CC    | 181  | MET  | 2.5  |
| 36  | CH    | 22   | LYS  | 2.5  |
| 39  | CL    | 108  | ARG  | 2.5  |
| 42  | CO    | 22   | ARG  | 2.5  |
| 1   | BA    | 135  | C    | 2.5  |
| 1   | BA    | 1441 | A    | 2.5  |
| 31  | CA    | 975  | A    | 2.5  |
| 31  | CA    | 2054 | A    | 2.5  |
| 31  | CA    | 2212 | A    | 2.5  |
| 31  | CA    | 2374 | C    | 2.5  |
| 14  | AN    | 55   | SER  | 2.5  |
| 29  | CC    | 259  | SER  | 2.5  |
| 1   | AA    | 1260 | G    | 2.5  |
| 1   | BA    | 380  | G    | 2.5  |
| 1   | BA    | 1190 | G    | 2.5  |
| 31  | CA    | 489  | G    | 2.5  |
| 31  | CA    | 1361 | G    | 2.5  |
| 31  | CA    | 1811 | G    | 2.5  |
| 31  | CA    | 2053 | G    | 2.5  |
| 36  | DH    | 84   | ALA  | 2.5  |
| 50  | CW    | 16   | ALA  | 2.5  |
| 55  | DA    | 1071 | G    | 2.5  |
| 7   | BG    | 19   | GLY  | 2.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 9          | AI           | 8          | GLY         | 2.5         |
| 10         | BJ           | 66         | GLU         | 2.5         |
| 34         | CF           | 140        | GLU         | 2.5         |
| 47         | CT           | 15         | GLN         | 2.5         |
| 13         | AM           | 62         | LYS         | 2.5         |
| 23         | C2           | 48         | ILE         | 2.5         |
| 8          | AH           | 32         | LEU         | 2.5         |
| 5          | AE           | 120        | VAL         | 2.5         |
| 23         | D2           | 42         | VAL         | 2.5         |
| 29         | DC           | 252        | THR         | 2.5         |
| 1          | BA           | 379        | C           | 2.5         |
| 1          | BA           | 935        | A           | 2.5         |
| 1          | BA           | 1045       | C           | 2.5         |
| 31         | CA           | 198        | C           | 2.5         |
| 31         | CA           | 581        | C           | 2.5         |
| 31         | CA           | 1008       | A           | 2.5         |
| 36         | CH           | 102        | ALA         | 2.5         |
| 55         | DA           | 2179       | C           | 2.5         |
| 14         | BN           | 100        | SER         | 2.5         |
| 9          | BI           | 13         | LYS         | 2.5         |
| 20         | BT           | 82         | GLN         | 2.5         |
| 26         | C5           | 35         | GLN         | 2.5         |
| 38         | CK           | 129        | GLU         | 2.5         |
| 40         | CM           | 51         | GLU         | 2.5         |
| 1          | BA           | 251        | G           | 2.5         |
| 1          | BA           | 326        | G           | 2.5         |
| 31         | CA           | 467        | G           | 2.5         |
| 31         | CA           | 537        | G           | 2.5         |
| 31         | CA           | 1543       | G           | 2.5         |
| 40         | CM           | 49         | GLY         | 2.5         |
| 48         | CU           | 77         | ARG         | 2.5         |
| 2          | AB           | 212        | LEU         | 2.5         |
| 19         | AS           | 5          | LEU         | 2.5         |
| 34         | CF           | 50         | LEU         | 2.5         |
| 1          | BA           | 467        | U           | 2.5         |
| 3          | BC           | 128        | VAL         | 2.5         |
| 55         | DA           | 2130       | U           | 2.5         |
| 52         | CY           | 36         | HIS         | 2.5         |
| 44         | CQ           | 20         | PHE         | 2.5         |
| 11         | AK           | 75         | LYS         | 2.5         |
| 1          | AA           | 1128       | C           | 2.5         |
| 14         | AN           | 22         | ALA         | 2.5         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2527 | C    | 2.5  |
| 37  | DJ    | 15   | ALA  | 2.5  |
| 1   | AA    | 205  | A    | 2.5  |
| 1   | AA    | 1016 | A    | 2.5  |
| 1   | BA    | 461  | A    | 2.5  |
| 1   | BA    | 1311 | A    | 2.5  |
| 5   | AE    | 92   | SER  | 2.5  |
| 31  | CA    | 429  | A    | 2.5  |
| 31  | CA    | 482  | A    | 2.5  |
| 31  | CA    | 800  | A    | 2.5  |
| 31  | CA    | 1722 | A    | 2.5  |
| 31  | CA    | 2274 | A    | 2.5  |
| 33  | CE    | 170  | ARG  | 2.5  |
| 36  | CH    | 92   | GLY  | 2.5  |
| 39  | CL    | 75   | SER  | 2.5  |
| 2   | AB    | 67   | ILE  | 2.5  |
| 13  | AM    | 22   | ILE  | 2.5  |
| 29  | CC    | 49   | ILE  | 2.5  |
| 2   | BB    | 57   | LEU  | 2.5  |
| 31  | CA    | 48   | G    | 2.5  |
| 31  | CA    | 1038 | G    | 2.5  |
| 31  | CA    | 1619 | G    | 2.5  |
| 31  | CA    | 2321 | U    | 2.5  |
| 55  | DA    | 2138 | G    | 2.5  |
| 5   | BE    | 114  | VAL  | 2.5  |
| 44  | CQ    | 47   | VAL  | 2.5  |
| 2   | BB    | 64   | LYS  | 2.5  |
| 12  | BL    | 72   | HIS  | 2.5  |
| 13  | AM    | 58   | ASP  | 2.5  |
| 15  | AO    | 22   | THR  | 2.5  |
| 30  | CD    | 103  | ASP  | 2.5  |
| 7   | BG    | 92   | ARG  | 2.5  |
| 9   | BI    | 108  | ALA  | 2.5  |
| 11  | BK    | 71   | ALA  | 2.5  |
| 1   | AA    | 1140 | C    | 2.5  |
| 1   | BA    | 381  | C    | 2.5  |
| 1   | BA    | 1112 | C    | 2.5  |
| 28  | CB    | 62   | C    | 2.5  |
| 31  | CA    | 1170 | C    | 2.5  |
| 31  | CA    | 2427 | C    | 2.5  |
| 37  | CJ    | 105  | GLN  | 2.5  |
| 35  | CG    | 89   | LEU  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AA    | 4    | U    | 2.5  |
| 3   | BC    | 84   | VAL  | 2.5  |
| 30  | CD    | 104  | VAL  | 2.5  |
| 30  | CD    | 122  | VAL  | 2.5  |
| 51  | CX    | 24   | LYS  | 2.5  |
| 1   | AA    | 971  | G    | 2.5  |
| 13  | BM    | 59   | GLU  | 2.5  |
| 28  | CB    | 79   | G    | 2.5  |
| 19  | BS    | 36   | ARG  | 2.5  |
| 30  | CD    | 99   | GLU  | 2.5  |
| 31  | CA    | 1055 | G    | 2.5  |
| 31  | CA    | 1296 | G    | 2.5  |
| 55  | DA    | 2152 | G    | 2.5  |
| 30  | CD    | 52   | THR  | 2.5  |
| 38  | CK    | 120  | ARG  | 2.5  |
| 48  | CU    | 39   | THR  | 2.5  |
| 49  | CV    | 16   | GLY  | 2.5  |
| 2   | AB    | 43   | LEU  | 2.5  |
| 2   | BB    | 129  | LEU  | 2.5  |
| 3   | BC    | 207  | ILE  | 2.5  |
| 9   | AI    | 125  | PRO  | 2.5  |
| 31  | CA    | 645  | C    | 2.5  |
| 42  | CO    | 98   | LEU  | 2.5  |
| 46  | CS    | 73   | LYS  | 2.5  |
| 48  | CU    | 93   | LEU  | 2.5  |
| 53  | CZ    | 34   | SER  | 2.5  |
| 34  | CF    | 145  | LYS  | 2.5  |
| 37  | CJ    | 40   | LYS  | 2.5  |
| 31  | CA    | 104  | A    | 2.5  |
| 31  | CA    | 342  | A    | 2.5  |
| 31  | CA    | 1039 | A    | 2.5  |
| 31  | CA    | 1522 | A    | 2.5  |
| 31  | CA    | 1654 | A    | 2.5  |
| 31  | CA    | 2287 | A    | 2.5  |
| 54  | DI    | 4    | ASN  | 2.5  |
| 8   | BH    | 91   | GLU  | 2.5  |
| 38  | CK    | 48   | VAL  | 2.5  |
| 39  | CL    | 57   | VAL  | 2.5  |
| 27  | C0    | 30   | ARG  | 2.5  |
| 30  | CD    | 33   | ARG  | 2.5  |
| 14  | BN    | 101  | TRP  | 2.5  |
| 2   | BB    | 189  | THR  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | BB    | 216  | ALA  | 2.5  |
| 3   | AC    | 71   | ALA  | 2.5  |
| 23  | C2    | 16   | GLY  | 2.5  |
| 31  | CA    | 54   | G    | 2.5  |
| 31  | CA    | 242  | G    | 2.5  |
| 31  | CA    | 491  | G    | 2.5  |
| 31  | CA    | 618  | G    | 2.5  |
| 31  | CA    | 1182 | G    | 2.5  |
| 31  | CA    | 1645 | G    | 2.5  |
| 31  | CA    | 2414 | G    | 2.5  |
| 33  | CE    | 84   | THR  | 2.5  |
| 34  | CF    | 116  | GLY  | 2.5  |
| 1   | BA    | 215  | C    | 2.5  |
| 30  | CD    | 40   | LEU  | 2.5  |
| 37  | DJ    | 122  | ILE  | 2.5  |
| 31  | CA    | 2462 | C    | 2.5  |
| 53  | DZ    | 28   | LEU  | 2.5  |
| 16  | BP    | 29   | ASN  | 2.5  |
| 21  | BU    | 9    | ASN  | 2.5  |
| 2   | AB    | 187  | VAL  | 2.5  |
| 33  | CE    | 187  | VAL  | 2.5  |
| 36  | DH    | 76   | GLU  | 2.5  |
| 40  | CM    | 33   | ARG  | 2.5  |
| 1   | AA    | 1368 | A    | 2.5  |
| 28  | CB    | 45   | A    | 2.5  |
| 31  | CA    | 190  | A    | 2.5  |
| 31  | CA    | 294  | A    | 2.5  |
| 31  | CA    | 1165 | A    | 2.5  |
| 31  | CA    | 2837 | A    | 2.5  |
| 2   | AB    | 39   | HIS  | 2.5  |
| 10  | AJ    | 11   | LYS  | 2.5  |
| 14  | AN    | 8    | ALA  | 2.5  |
| 43  | CP    | 72   | ALA  | 2.5  |
| 51  | CX    | 65   | GLY  | 2.5  |
| 15  | BO    | 79   | THR  | 2.5  |
| 38  | CK    | 24   | THR  | 2.5  |
| 12  | BL    | 80   | ILE  | 2.5  |
| 2   | BB    | 182  | PRO  | 2.4  |
| 17  | BQ    | 75   | LEU  | 2.5  |
| 31  | CA    | 1131 | G    | 2.5  |
| 31  | CA    | 2623 | G    | 2.5  |
| 52  | CY    | 64   | ILE  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | AD    | 172  | GLU  | 2.4  |
| 37  | DJ    | 26   | PRO  | 2.4  |
| 48  | CU    | 18   | GLU  | 2.4  |
| 55  | DA    | 1727 | C    | 2.4  |
| 2   | AB    | 50   | PHE  | 2.4  |
| 28  | CB    | 82   | U    | 2.4  |
| 33  | CE    | 169  | VAL  | 2.4  |
| 55  | DA    | 2137 | U    | 2.4  |
| 1   | AA    | 1169 | A    | 2.4  |
| 29  | CC    | 59   | LYS  | 2.4  |
| 31  | CA    | 432  | A    | 2.4  |
| 31  | CA    | 2298 | A    | 2.4  |
| 35  | CG    | 165  | ALA  | 2.4  |
| 44  | CQ    | 41   | GLN  | 2.4  |
| 34  | CF    | 111  | ILE  | 2.4  |
| 47  | CT    | 100  | THR  | 2.4  |
| 10  | BJ    | 17   | LEU  | 2.4  |
| 2   | BB    | 29   | PRO  | 2.4  |
| 1   | AA    | 1138 | G    | 2.4  |
| 8   | BH    | 71   | VAL  | 2.4  |
| 8   | AH    | 111  | MET  | 2.4  |
| 10  | BJ    | 49   | PHE  | 2.4  |
| 16  | AP    | 80   | LYS  | 2.4  |
| 31  | CA    | 112  | U    | 2.4  |
| 31  | CA    | 358  | U    | 2.4  |
| 31  | CA    | 1779 | U    | 2.4  |
| 31  | CA    | 2347 | C    | 2.4  |
| 31  | CA    | 2473 | U    | 2.4  |
| 42  | CO    | 99   | LYS  | 2.4  |
| 55  | DA    | 2151 | U    | 2.4  |
| 10  | BJ    | 60   | ASP  | 2.4  |
| 50  | CW    | 33   | GLY  | 2.4  |
| 1   | BA    | 55   | A    | 2.4  |
| 1   | BA    | 459  | A    | 2.4  |
| 31  | CA    | 1302 | A    | 2.4  |
| 31  | CA    | 1359 | A    | 2.4  |
| 8   | BH    | 59   | LEU  | 2.4  |
| 15  | BO    | 14   | GLU  | 2.4  |
| 23  | C2    | 32   | GLU  | 2.4  |
| 34  | CF    | 103  | LEU  | 2.4  |
| 36  | CH    | 76   | GLU  | 2.4  |
| 44  | CQ    | 76   | THR  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | CT    | 19   | LEU  | 2.4  |
| 50  | CW    | 59   | GLU  | 2.4  |
| 22  | C1    | 49   | TYR  | 2.4  |
| 9   | BI    | 114  | LYS  | 2.4  |
| 39  | CL    | 120  | PRO  | 2.4  |
| 44  | CQ    | 14   | LYS  | 2.4  |
| 45  | CR    | 54   | LYS  | 2.4  |
| 30  | CD    | 142  | VAL  | 2.4  |
| 31  | CA    | 2296 | U    | 2.4  |
| 38  | CK    | 73   | VAL  | 2.4  |
| 46  | CS    | 47   | VAL  | 2.4  |
| 52  | CY    | 51   | VAL  | 2.4  |
| 1   | AA    | 413  | G    | 2.4  |
| 3   | BC    | 8    | ASN  | 2.4  |
| 7   | BG    | 34   | GLY  | 2.4  |
| 28  | CB    | 3    | C    | 2.4  |
| 31  | CA    | 433  | C    | 2.4  |
| 31  | CA    | 435  | C    | 2.4  |
| 31  | CA    | 1540 | G    | 2.4  |
| 31  | CA    | 2318 | G    | 2.4  |
| 39  | CL    | 7    | MET  | 2.4  |
| 9   | AI    | 126  | GLN  | 2.4  |
| 20  | BT    | 55   | GLN  | 2.4  |
| 20  | BT    | 65   | GLY  | 2.4  |
| 54  | DI    | 122  | GLN  | 2.4  |
| 19  | AS    | 3    | ARG  | 2.4  |
| 13  | AM    | 47   | GLU  | 2.4  |
| 44  | CQ    | 44   | GLU  | 2.4  |
| 31  | CA    | 2820 | A    | 2.4  |
| 31  | CA    | 2882 | A    | 2.4  |
| 36  | DH    | 5    | LEU  | 2.4  |
| 50  | CW    | 34   | LYS  | 2.4  |
| 3   | BC    | 151  | VAL  | 2.4  |
| 4   | AD    | 182  | PHE  | 2.4  |
| 35  | CG    | 11   | VAL  | 2.4  |
| 37  | DJ    | 9    | VAL  | 2.4  |
| 1   | BA    | 1202 | U    | 2.4  |
| 28  | CB    | 74   | U    | 2.4  |
| 31  | CA    | 686  | U    | 2.4  |
| 25  | C4    | 54   | ASP  | 2.4  |
| 1   | BA    | 67   | C    | 2.4  |
| 30  | CD    | 124  | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 853  | C    | 2.4  |
| 33  | CE    | 90   | GLN  | 2.4  |
| 54  | DI    | 31   | ARG  | 2.4  |
| 2   | BB    | 76   | ALA  | 2.4  |
| 31  | CA    | 1091 | G    | 2.4  |
| 31  | CA    | 1358 | G    | 2.4  |
| 31  | CA    | 2391 | G    | 2.4  |
| 31  | CA    | 2742 | G    | 2.4  |
| 37  | DJ    | 120  | ALA  | 2.4  |
| 35  | DG    | 177  | LYS  | 2.4  |
| 29  | CC    | 33   | LEU  | 2.4  |
| 42  | CO    | 97   | ILE  | 2.4  |
| 14  | BN    | 42   | TRP  | 2.4  |
| 17  | BQ    | 7    | THR  | 2.4  |
| 30  | CD    | 129  | THR  | 2.4  |
| 31  | CA    | 575  | A    | 2.4  |
| 31  | CA    | 675  | A    | 2.4  |
| 31  | CA    | 1284 | A    | 2.4  |
| 31  | CA    | 2868 | A    | 2.4  |
| 45  | CR    | 32   | TYR  | 2.4  |
| 39  | CL    | 62   | VAL  | 2.4  |
| 47  | CT    | 20   | VAL  | 2.4  |
| 50  | CW    | 65   | VAL  | 2.4  |
| 9   | BI    | 80   | ARG  | 2.4  |
| 9   | BI    | 82   | GLY  | 2.4  |
| 55  | DA    | 139  | U    | 2.4  |
| 55  | DA    | 1729 | U    | 2.4  |
| 30  | CD    | 161  | MET  | 2.4  |
| 2   | AB    | 45   | LYS  | 2.4  |
| 2   | AB    | 64   | LYS  | 2.4  |
| 16  | BP    | 13   | LYS  | 2.4  |
| 19  | BS    | 17   | LYS  | 2.4  |
| 35  | CG    | 101  | ASN  | 2.4  |
| 47  | CT    | 90   | LYS  | 2.4  |
| 52  | CY    | 17   | ASN  | 2.4  |
| 1   | BA    | 848  | C    | 2.4  |
| 8   | BH    | 116  | ALA  | 2.4  |
| 31  | CA    | 115  | C    | 2.4  |
| 31  | CA    | 1102 | C    | 2.4  |
| 43  | CP    | 23   | ALA  | 2.4  |
| 1   | BA    | 76   | G    | 2.4  |
| 26  | C5    | 23   | ILE  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | DF    | 85   | ILE  | 2.4  |
| 1   | AA    | 1236 | A    | 2.4  |
| 4   | AD    | 38   | PRO  | 2.4  |
| 19  | AS    | 77   | THR  | 2.4  |
| 31  | CA    | 1254 | A    | 2.4  |
| 31  | CA    | 1477 | A    | 2.4  |
| 31  | CA    | 1528 | A    | 2.4  |
| 31  | CA    | 2602 | A    | 2.4  |
| 33  | CE    | 53   | THR  | 2.4  |
| 48  | CU    | 51   | PHE  | 2.4  |
| 54  | DI    | 12   | VAL  | 2.4  |
| 24  | C3    | 25   | LYS  | 2.4  |
| 28  | CB    | 32   | U    | 2.4  |
| 29  | CC    | 248  | TRP  | 2.4  |
| 3   | BC    | 187  | SER  | 2.4  |
| 29  | CC    | 100  | GLU  | 2.4  |
| 51  | CX    | 78   | LYS  | 2.4  |
| 49  | CV    | 74   | ASN  | 2.4  |
| 49  | CV    | 99   | ASN  | 2.4  |
| 30  | CD    | 209  | ALA  | 2.4  |
| 31  | CA    | 2795 | C    | 2.4  |
| 30  | CD    | 79   | LEU  | 2.4  |
| 33  | CE    | 108  | ILE  | 2.4  |
| 18  | BR    | 74   | HIS  | 2.4  |
| 2   | BB    | 162  | PHE  | 2.4  |
| 13  | AM    | 113  | ARG  | 2.4  |
| 31  | CA    | 496  | G    | 2.4  |
| 31  | CA    | 1355 | G    | 2.4  |
| 31  | CA    | 2250 | G    | 2.4  |
| 31  | CA    | 2744 | G    | 2.4  |
| 31  | CA    | 2838 | G    | 2.4  |
| 3   | BC    | 60   | PRO  | 2.4  |
| 38  | CK    | 8    | PRO  | 2.4  |
| 1   | BA    | 224  | U    | 2.4  |
| 31  | CA    | 1487 | U    | 2.4  |
| 31  | CA    | 1709 | U    | 2.4  |
| 1   | BA    | 1042 | A    | 2.4  |
| 1   | BA    | 1046 | A    | 2.4  |
| 2   | BB    | 136  | MET  | 2.4  |
| 31  | CA    | 167  | A    | 2.4  |
| 31  | CA    | 1144 | A    | 2.4  |
| 31  | CA    | 1385 | A    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | DA    | 1073 | A    | 2.4  |
| 7   | AG    | 45   | SER  | 2.4  |
| 14  | AN    | 2    | ALA  | 2.4  |
| 16  | AP    | 79   | ASN  | 2.4  |
| 20  | BT    | 47   | ALA  | 2.4  |
| 22  | C1    | 21   | ALA  | 2.4  |
| 43  | CP    | 45   | SER  | 2.4  |
| 1   | AA    | 470  | C    | 2.4  |
| 3   | BC    | 115  | LEU  | 2.4  |
| 6   | BF    | 74   | LEU  | 2.4  |
| 23  | C2    | 34   | LEU  | 2.4  |
| 29  | CC    | 104  | ILE  | 2.4  |
| 29  | CC    | 135  | ILE  | 2.4  |
| 31  | CA    | 179  | C    | 2.4  |
| 44  | CQ    | 48   | ILE  | 2.4  |
| 2   | AB    | 137  | ARG  | 2.4  |
| 30  | CD    | 159  | LYS  | 2.4  |
| 33  | CE    | 29   | HIS  | 2.4  |
| 48  | DU    | 70   | HIS  | 2.4  |
| 3   | AC    | 151  | VAL  | 2.4  |
| 3   | BC    | 173  | VAL  | 2.4  |
| 13  | BM    | 72   | GLU  | 2.4  |
| 53  | CZ    | 26   | PHE  | 2.4  |
| 15  | AO    | 16   | GLY  | 2.4  |
| 16  | BP    | 61   | VAL  | 2.4  |
| 53  | CZ    | 46   | VAL  | 2.4  |
| 1   | AA    | 1185 | G    | 2.4  |
| 28  | CB    | 64   | G    | 2.4  |
| 31  | CA    | 674  | G    | 2.4  |
| 31  | CA    | 1396 | U    | 2.4  |
| 27  | C0    | 47   | MET  | 2.4  |
| 28  | CB    | 52   | A    | 2.4  |
| 28  | CB    | 99   | A    | 2.4  |
| 31  | CA    | 829  | A    | 2.4  |
| 31  | CA    | 1129 | A    | 2.4  |
| 31  | CA    | 1735 | A    | 2.4  |
| 31  | CA    | 1810 | A    | 2.4  |
| 33  | CE    | 86   | ALA  | 2.4  |
| 2   | BB    | 74   | ARG  | 2.4  |
| 2   | BB    | 111  | ILE  | 2.4  |
| 3   | AC    | 77   | ILE  | 2.4  |
| 3   | BC    | 136  | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | C4    | 5    | LYS  | 2.4  |
| 44  | CQ    | 6    | LYS  | 2.4  |
| 47  | CT    | 36   | LEU  | 2.4  |
| 52  | CY    | 3    | ARG  | 2.4  |
| 1   | AA    | 1237 | C    | 2.4  |
| 31  | CA    | 16   | C    | 2.4  |
| 31  | CA    | 2368 | C    | 2.4  |
| 46  | CS    | 16   | GLU  | 2.3  |
| 35  | CG    | 118  | PRO  | 2.3  |
| 54  | DI    | 6    | GLN  | 2.3  |
| 1   | BA    | 1453 | G    | 2.3  |
| 24  | C3    | 2    | LYS  | 2.3  |
| 28  | CB    | 67   | G    | 2.3  |
| 29  | CC    | 265  | LYS  | 2.3  |
| 5   | BE    | 92   | SER  | 2.3  |
| 7   | AG    | 3    | ARG  | 2.3  |
| 31  | CA    | 1546 | G    | 2.3  |
| 31  | CA    | 1651 | G    | 2.3  |
| 31  | CA    | 1861 | G    | 2.3  |
| 33  | CE    | 40   | ARG  | 2.3  |
| 41  | CN    | 8    | LYS  | 2.3  |
| 10  | AJ    | 54   | SER  | 2.3  |
| 33  | CE    | 78   | TRP  | 2.3  |
| 1   | BA    | 143  | A    | 2.3  |
| 1   | BA    | 151  | A    | 2.3  |
| 6   | AF    | 6    | ILE  | 2.3  |
| 31  | CA    | 788  | A    | 2.3  |
| 31  | CA    | 1650 | A    | 2.3  |
| 33  | CE    | 105  | LEU  | 2.3  |
| 48  | CU    | 11   | LEU  | 2.3  |
| 52  | CY    | 16   | ASN  | 2.3  |
| 31  | CA    | 503  | A    | 2.3  |
| 31  | CA    | 547  | A    | 2.3  |
| 47  | CT    | 52   | GLU  | 2.3  |
| 1   | BA    | 110  | C    | 2.3  |
| 20  | AT    | 20   | HIS  | 2.3  |
| 28  | CB    | 28   | C    | 2.3  |
| 4   | AD    | 40   | GLN  | 2.3  |
| 17  | BQ    | 22   | VAL  | 2.3  |
| 29  | CC    | 19   | VAL  | 2.3  |
| 1   | BA    | 1183 | U    | 2.3  |
| 31  | CA    | 1184 | U    | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | CG    | 134  | LYS  | 2.3  |
| 6   | AF    | 38   | ARG  | 2.3  |
| 36  | CH    | 69   | ALA  | 2.3  |
| 3   | BC    | 14   | ILE  | 2.3  |
| 9   | BI    | 87   | LEU  | 2.3  |
| 31  | CA    | 2599 | G    | 2.3  |
| 50  | CW    | 24   | ASN  | 2.3  |
| 6   | AF    | 8    | PHE  | 2.3  |
| 31  | CA    | 1439 | A    | 2.3  |
| 31  | CA    | 2883 | A    | 2.3  |
| 38  | CK    | 38   | GLY  | 2.3  |
| 38  | CK    | 83   | GLY  | 2.3  |
| 8   | BH    | 104  | VAL  | 2.3  |
| 31  | CA    | 393  | C    | 2.3  |
| 31  | CA    | 1646 | C    | 2.3  |
| 31  | CA    | 2215 | C    | 2.3  |
| 31  | CA    | 2863 | C    | 2.3  |
| 54  | DI    | 105  | LYS  | 2.3  |
| 1   | BA    | 843  | U    | 2.3  |
| 38  | CK    | 49   | ASP  | 2.3  |
| 54  | DI    | 102  | ALA  | 2.3  |
| 18  | AR    | 21   | ILE  | 2.3  |
| 22  | C1    | 9    | THR  | 2.3  |
| 29  | CC    | 95   | LEU  | 2.3  |
| 37  | DJ    | 141  | GLU  | 2.3  |
| 40  | DM    | 95   | LEU  | 2.3  |
| 44  | DQ    | 114  | LEU  | 2.3  |
| 49  | CV    | 37   | GLU  | 2.3  |
| 36  | CH    | 119  | ASN  | 2.3  |
| 35  | CG    | 61   | GLY  | 2.3  |
| 1   | AA    | 1003 | G    | 2.3  |
| 1   | BA    | 75   | G    | 2.3  |
| 1   | BA    | 1360 | A    | 2.3  |
| 31  | CA    | 1116 | G    | 2.3  |
| 31  | CA    | 1136 | G    | 2.3  |
| 31  | CA    | 1163 | G    | 2.3  |
| 31  | CA    | 1449 | G    | 2.3  |
| 31  | CA    | 2822 | G    | 2.3  |
| 5   | BE    | 82   | GLN  | 2.3  |
| 11  | AK    | 38   | GLN  | 2.3  |
| 1   | BA    | 221  | C    | 2.3  |
| 17  | BQ    | 40   | ARG  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | CF    | 63   | GLN  | 2.3  |
| 52  | CY    | 40   | VAL  | 2.3  |
| 28  | CB    | 90   | C    | 2.3  |
| 31  | CA    | 957  | C    | 2.3  |
| 9   | AI    | 91   | ASP  | 2.3  |
| 31  | CA    | 395  | U    | 2.3  |
| 12  | BL    | 38   | TYR  | 2.3  |
| 18  | AR    | 32   | TYR  | 2.3  |
| 35  | CG    | 164  | TYR  | 2.3  |
| 36  | CH    | 56   | ALA  | 2.3  |
| 36  | DH    | 59   | ALA  | 2.3  |
| 43  | CP    | 80   | GLU  | 2.3  |
| 5   | BE    | 81   | LEU  | 2.3  |
| 11  | BK    | 23   | ILE  | 2.3  |
| 11  | BK    | 100  | LEU  | 2.3  |
| 5   | BE    | 135  | ASN  | 2.3  |
| 11  | BK    | 29   | ASN  | 2.3  |
| 19  | AS    | 21   | LYS  | 2.3  |
| 20  | AT    | 85   | LYS  | 2.3  |
| 35  | DG    | 101  | ASN  | 2.3  |
| 47  | CT    | 42   | LYS  | 2.3  |
| 14  | BN    | 81   | ARG  | 2.3  |
| 29  | CC    | 52   | ARG  | 2.3  |
| 4   | AD    | 25   | VAL  | 2.3  |
| 1   | AA    | 90   | C    | 2.3  |
| 1   | AA    | 201  | G    | 2.3  |
| 1   | AA    | 468  | A    | 2.3  |
| 1   | AA    | 1188 | A    | 2.3  |
| 1   | BA    | 1365 | G    | 2.3  |
| 3   | AC    | 176  | HIS  | 2.3  |
| 31  | CA    | 254  | G    | 2.3  |
| 31  | CA    | 466  | A    | 2.3  |
| 31  | CA    | 577  | G    | 2.3  |
| 31  | CA    | 671  | C    | 2.3  |
| 31  | CA    | 1040 | A    | 2.3  |
| 31  | CA    | 1455 | G    | 2.3  |
| 31  | CA    | 1655 | A    | 2.3  |
| 31  | CA    | 1721 | G    | 2.3  |
| 31  | CA    | 2671 | G    | 2.3  |
| 1   | BA    | 1232 | U    | 2.3  |
| 3   | BC    | 28   | GLU  | 2.3  |
| 48  | CU    | 5    | GLU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | AF    | 9    | MET  | 2.3  |
| 6   | AF    | 90   | MET  | 2.3  |
| 3   | BC    | 175  | LEU  | 2.3  |
| 34  | CF    | 2    | ALA  | 2.3  |
| 35  | CG    | 29   | LYS  | 2.3  |
| 44  | CQ    | 63   | LYS  | 2.3  |
| 45  | CR    | 22   | LYS  | 2.3  |
| 9   | BI    | 72   | ILE  | 2.3  |
| 2   | BB    | 90   | PHE  | 2.3  |
| 3   | BC    | 29   | PHE  | 2.3  |
| 6   | BF    | 92   | THR  | 2.3  |
| 40  | DM    | 102  | GLY  | 2.3  |
| 41  | CN    | 7    | THR  | 2.3  |
| 42  | CO    | 13   | ASN  | 2.3  |
| 42  | CO    | 27   | SER  | 2.3  |
| 45  | CR    | 72   | ASN  | 2.3  |
| 9   | AI    | 53   | GLU  | 2.3  |
| 12  | BL    | 109  | ASP  | 2.3  |
| 14  | AN    | 28   | LYS  | 2.3  |
| 31  | CA    | 865  | C    | 2.3  |
| 31  | CA    | 2784 | U    | 2.3  |
| 31  | CA    | 2154 | A    | 2.3  |
| 33  | CE    | 74   | LYS  | 2.3  |
| 55  | DA    | 2797 | U    | 2.3  |
| 1   | BA    | 973  | G    | 2.3  |
| 31  | CA    | 125  | A    | 2.3  |
| 31  | CA    | 324  | A    | 2.3  |
| 3   | BC    | 146  | ALA  | 2.3  |
| 6   | BF    | 66   | ALA  | 2.3  |
| 20  | BT    | 54   | MET  | 2.3  |
| 31  | CA    | 446  | G    | 2.3  |
| 31  | CA    | 2230 | G    | 2.3  |
| 31  | CA    | 2488 | G    | 2.3  |
| 31  | CA    | 2753 | A    | 2.3  |
| 31  | CA    | 2894 | G    | 2.3  |
| 36  | CH    | 64   | ALA  | 2.3  |
| 45  | CR    | 21   | ALA  | 2.3  |
| 2   | BB    | 202  | GLY  | 2.3  |
| 11  | BK    | 107  | ILE  | 2.3  |
| 38  | CK    | 115  | GLY  | 2.3  |
| 14  | AN    | 35   | ASN  | 2.3  |
| 29  | CC    | 50   | THR  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | CD    | 58   | ASN  | 2.3  |
| 11  | BK    | 20   | VAL  | 2.3  |
| 36  | CH    | 31   | VAL  | 2.3  |
| 36  | CH    | 103  | VAL  | 2.3  |
| 40  | CM    | 46   | VAL  | 2.3  |
| 19  | BS    | 70   | LYS  | 2.3  |
| 30  | CD    | 23   | PRO  | 2.3  |
| 31  | CA    | 2818 | U    | 2.3  |
| 36  | DH    | 98   | ASP  | 2.3  |
| 1   | BA    | 322  | C    | 2.3  |
| 10  | AJ    | 72   | ARG  | 2.3  |
| 11  | BK    | 62   | ALA  | 2.3  |
| 19  | AS    | 22   | ALA  | 2.3  |
| 19  | BS    | 15   | LEU  | 2.3  |
| 31  | CA    | 677  | A    | 2.3  |
| 31  | CA    | 1156 | A    | 2.3  |
| 31  | CA    | 1469 | A    | 2.3  |
| 31  | CA    | 2317 | A    | 2.3  |
| 36  | DH    | 68   | ARG  | 2.3  |
| 47  | CT    | 88   | ARG  | 2.3  |
| 54  | DI    | 100  | ALA  | 2.3  |
| 29  | CC    | 64   | ILE  | 2.3  |
| 30  | CD    | 93   | GLY  | 2.3  |
| 31  | CA    | 2056 | G    | 2.3  |
| 54  | DI    | 90   | GLY  | 2.3  |
| 5   | AE    | 31   | PHE  | 2.3  |
| 11  | BK    | 70   | CYS  | 2.3  |
| 9   | AI    | 27   | LYS  | 2.3  |
| 9   | AI    | 110  | GLN  | 2.3  |
| 12  | BL    | 29   | GLN  | 2.3  |
| 48  | CU    | 19   | LYS  | 2.3  |
| 54  | DI    | 73   | LYS  | 2.3  |
| 35  | CG    | 98   | VAL  | 2.3  |
| 49  | CV    | 68   | SER  | 2.3  |
| 5   | BE    | 157  | ARG  | 2.3  |
| 12  | BL    | 96   | HIS  | 2.3  |
| 31  | CA    | 1865 | U    | 2.3  |
| 31  | CA    | 2585 | U    | 2.3  |
| 31  | CA    | 2615 | U    | 2.3  |
| 33  | CE    | 69   | ARG  | 2.3  |
| 55  | DA    | 2139 | U    | 2.3  |
| 2   | AB    | 68   | LEU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | AE    | 110  | ALA  | 2.3  |
| 7   | AG    | 101  | MET  | 2.3  |
| 9   | AI    | 52   | LEU  | 2.3  |
| 29  | CC    | 93   | LEU  | 2.3  |
| 34  | CF    | 16   | LEU  | 2.3  |
| 38  | CK    | 6    | ALA  | 2.3  |
| 39  | CL    | 107  | LEU  | 2.3  |
| 48  | DU    | 32   | LEU  | 2.3  |
| 1   | BA    | 1366 | C    | 2.3  |
| 31  | CA    | 414  | C    | 2.3  |
| 39  | CL    | 115  | ILE  | 2.3  |
| 1   | BA    | 274  | A    | 2.3  |
| 11  | BK    | 27   | PHE  | 2.3  |
| 31  | CA    | 73   | A    | 2.3  |
| 31  | CA    | 900  | A    | 2.3  |
| 31  | CA    | 1508 | A    | 2.3  |
| 31  | CA    | 2088 | A    | 2.3  |
| 48  | CU    | 88   | LYS  | 2.3  |
| 1   | AA    | 951  | G    | 2.3  |
| 1   | AA    | 1190 | G    | 2.3  |
| 1   | AA    | 1370 | G    | 2.3  |
| 31  | CA    | 1115 | G    | 2.3  |
| 31  | CA    | 1719 | G    | 2.3  |
| 31  | CA    | 2624 | G    | 2.3  |
| 11  | AK    | 113  | VAL  | 2.2  |
| 26  | C5    | 22   | VAL  | 2.2  |
| 33  | CE    | 120  | VAL  | 2.2  |
| 8   | BH    | 107  | SER  | 2.2  |
| 1   | BA    | 249  | U    | 2.2  |
| 1   | BA    | 1315 | U    | 2.2  |
| 31  | CA    | 67   | U    | 2.2  |
| 31  | CA    | 1765 | U    | 2.2  |
| 4   | AD    | 9    | LEU  | 2.2  |
| 2   | AB    | 151  | ILE  | 2.2  |
| 9   | BI    | 71   | GLY  | 2.2  |
| 29  | CC    | 41   | GLY  | 2.2  |
| 33  | DE    | 6    | LYS  | 2.2  |
| 34  | DF    | 72   | LYS  | 2.2  |
| 53  | DZ    | 37   | LEU  | 2.2  |
| 54  | DI    | 52   | MET  | 2.2  |
| 9   | AI    | 7    | TYR  | 2.2  |
| 31  | CA    | 385  | C    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 903  | C    | 2.2  |
| 31  | CA    | 1161 | C    | 2.2  |
| 31  | CA    | 1488 | C    | 2.2  |
| 1   | BA    | 389  | A    | 2.2  |
| 1   | BA    | 1170 | A    | 2.2  |
| 31  | CA    | 149  | A    | 2.2  |
| 31  | CA    | 2060 | A    | 2.2  |
| 31  | CA    | 2077 | A    | 2.2  |
| 55  | DA    | 1084 | A    | 2.2  |
| 1   | BA    | 1385 | G    | 2.2  |
| 31  | CA    | 1248 | G    | 2.2  |
| 31  | CA    | 1401 | G    | 2.2  |
| 31  | CA    | 2294 | G    | 2.2  |
| 55  | DA    | 2112 | G    | 2.2  |
| 2   | BB    | 45   | LYS  | 2.2  |
| 45  | CR    | 41   | LYS  | 2.2  |
| 3   | BC    | 174  | PRO  | 2.2  |
| 14  | AN    | 15   | ALA  | 2.2  |
| 15  | BO    | 67   | LEU  | 2.2  |
| 52  | CY    | 31   | PRO  | 2.2  |
| 54  | DI    | 91   | ALA  | 2.2  |
| 54  | DI    | 92   | ALA  | 2.2  |
| 14  | AN    | 6    | MET  | 2.2  |
| 7   | AG    | 129  | GLU  | 2.2  |
| 16  | BP    | 32   | PHE  | 2.2  |
| 21  | BU    | 37   | PHE  | 2.2  |
| 33  | CE    | 85   | PHE  | 2.2  |
| 33  | CE    | 141  | MET  | 2.2  |
| 31  | CA    | 238  | C    | 2.2  |
| 33  | CE    | 41   | GLN  | 2.2  |
| 46  | CS    | 86   | GLN  | 2.2  |
| 2   | AB    | 217  | VAL  | 2.2  |
| 5   | BE    | 93   | ARG  | 2.2  |
| 5   | BE    | 153  | VAL  | 2.2  |
| 16  | AP    | 14   | ARG  | 2.2  |
| 21  | BU    | 18   | ARG  | 2.2  |
| 1   | BA    | 630  | A    | 2.2  |
| 5   | BE    | 159  | LYS  | 2.2  |
| 9   | BI    | 100  | LYS  | 2.2  |
| 31  | CA    | 2033 | A    | 2.2  |
| 31  | CA    | 2059 | A    | 2.2  |
| 36  | DH    | 73   | ASN  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | CK    | 123  | LYS  | 2.2  |
| 39  | CL    | 82   | ASN  | 2.2  |
| 50  | CW    | 49   | ASN  | 2.2  |
| 55  | DA    | 2101 | A    | 2.2  |
| 13  | AM    | 55   | THR  | 2.2  |
| 1   | BA    | 113  | G    | 2.2  |
| 1   | BA    | 1455 | G    | 2.2  |
| 3   | BC    | 81   | GLY  | 2.2  |
| 10  | BJ    | 52   | LEU  | 2.2  |
| 15  | BO    | 3    | LEU  | 2.2  |
| 19  | AS    | 31   | LEU  | 2.2  |
| 31  | CA    | 185  | G    | 2.2  |
| 31  | CA    | 469  | G    | 2.2  |
| 31  | CA    | 1203 | U    | 2.2  |
| 31  | CA    | 1910 | G    | 2.2  |
| 31  | CA    | 2522 | U    | 2.2  |
| 31  | CA    | 2631 | G    | 2.2  |
| 34  | DF    | 116  | GLY  | 2.2  |
| 46  | CS    | 57   | GLY  | 2.2  |
| 46  | CS    | 67   | GLY  | 2.2  |
| 47  | CT    | 26   | GLY  | 2.2  |
| 3   | AC    | 149  | ILE  | 2.2  |
| 9   | BI    | 112  | GLU  | 2.2  |
| 14  | AN    | 26   | GLU  | 2.2  |
| 19  | AS    | 50   | ALA  | 2.2  |
| 15  | AO    | 43   | PHE  | 2.2  |
| 23  | D2    | 39   | PHE  | 2.2  |
| 42  | CO    | 87   | PHE  | 2.2  |
| 6   | BF    | 4    | TYR  | 2.2  |
| 14  | AN    | 81   | ARG  | 2.2  |
| 43  | CP    | 116  | GLN  | 2.2  |
| 1   | BA    | 214  | C    | 2.2  |
| 1   | BA    | 1203 | C    | 2.2  |
| 1   | BA    | 1452 | C    | 2.2  |
| 31  | CA    | 143  | C    | 2.2  |
| 31  | CA    | 509  | C    | 2.2  |
| 31  | CA    | 672  | C    | 2.2  |
| 41  | CN    | 135  | VAL  | 2.2  |
| 44  | CQ    | 96   | LYS  | 2.2  |
| 1   | BA    | 65   | A    | 2.2  |
| 1   | BA    | 1067 | A    | 2.2  |
| 31  | CA    | 927  | A    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2020 | A    | 2.2  |
| 31  | CA    | 2758 | A    | 2.2  |
| 47  | CT    | 34   | ASP  | 2.2  |
| 3   | BC    | 125  | GLU  | 2.2  |
| 6   | BF    | 32   | ALA  | 2.2  |
| 9   | BI    | 59   | GLU  | 2.2  |
| 34  | CF    | 57   | LEU  | 2.2  |
| 43  | CP    | 112  | GLU  | 2.2  |
| 44  | CQ    | 112  | GLU  | 2.2  |
| 55  | DA    | 653  | U    | 2.2  |
| 14  | AN    | 71   | HIS  | 2.2  |
| 17  | AQ    | 21   | ILE  | 2.2  |
| 20  | BT    | 41   | ALA  | 2.2  |
| 27  | C0    | 18   | PRO  | 2.2  |
| 29  | CC    | 247  | PRO  | 2.2  |
| 30  | CD    | 127  | PHE  | 2.2  |
| 35  | DG    | 111  | HIS  | 2.2  |
| 47  | CT    | 32   | ALA  | 2.2  |
| 48  | CU    | 38   | ALA  | 2.2  |
| 1   | BA    | 350  | G    | 2.2  |
| 1   | BA    | 457  | G    | 2.2  |
| 3   | BC    | 131  | ARG  | 2.2  |
| 31  | CA    | 60   | G    | 2.2  |
| 31  | CA    | 1374 | G    | 2.2  |
| 31  | CA    | 1382 | G    | 2.2  |
| 54  | DI    | 62   | ARG  | 2.2  |
| 42  | DO    | 121  | LYS  | 2.2  |
| 44  | CQ    | 98   | TYR  | 2.2  |
| 50  | CW    | 82   | TYR  | 2.2  |
| 1   | BA    | 995  | C    | 2.2  |
| 7   | AG    | 80   | VAL  | 2.2  |
| 14  | AN    | 11   | VAL  | 2.2  |
| 19  | AS    | 58   | VAL  | 2.2  |
| 31  | CA    | 1005 | C    | 2.2  |
| 6   | AF    | 98   | GLU  | 2.2  |
| 7   | AG    | 112  | GLY  | 2.2  |
| 12  | BL    | 68   | GLY  | 2.2  |
| 1   | BA    | 1012 | A    | 2.2  |
| 1   | BA    | 1332 | A    | 2.2  |
| 10  | AJ    | 40   | ILE  | 2.2  |
| 12  | BL    | 64   | THR  | 2.2  |
| 28  | CB    | 111  | U    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | BM    | 87   | ARG  | 2.2  |
| 31  | CA    | 430  | A    | 2.2  |
| 31  | CA    | 574  | A    | 2.2  |
| 31  | CA    | 1027 | A    | 2.2  |
| 31  | CA    | 2662 | A    | 2.2  |
| 36  | CH    | 54   | LEU  | 2.2  |
| 38  | CK    | 45   | THR  | 2.2  |
| 39  | CL    | 104  | THR  | 2.2  |
| 40  | CM    | 94   | THR  | 2.2  |
| 54  | DI    | 60   | LEU  | 2.2  |
| 40  | CM    | 56   | PRO  | 2.2  |
| 40  | CM    | 69   | ARG  | 2.2  |
| 42  | CO    | 19   | ALA  | 2.2  |
| 49  | CV    | 96   | PHE  | 2.2  |
| 53  | DZ    | 3    | ALA  | 2.2  |
| 55  | DA    | 1095 | A    | 2.2  |
| 24  | D3    | 1    | MET  | 2.2  |
| 45  | CR    | 84   | LYS  | 2.2  |
| 54  | DI    | 8    | LYS  | 2.2  |
| 54  | DI    | 79   | PRO  | 2.2  |
| 1   | BA    | 1134 | G    | 2.2  |
| 31  | CA    | 1206 | G    | 2.2  |
| 31  | CA    | 2209 | G    | 2.2  |
| 31  | CA    | 2532 | G    | 2.2  |
| 55  | DA    | 1733 | G    | 2.2  |
| 20  | AT    | 35   | VAL  | 2.2  |
| 29  | CC    | 78   | VAL  | 2.2  |
| 51  | CX    | 31   | VAL  | 2.2  |
| 1   | BA    | 106  | C    | 2.2  |
| 29  | CC    | 119  | GLY  | 2.2  |
| 31  | CA    | 692  | C    | 2.2  |
| 31  | CA    | 1472 | C    | 2.2  |
| 31  | CA    | 1675 | C    | 2.2  |
| 31  | CA    | 1748 | C    | 2.2  |
| 1   | BA    | 219  | U    | 2.2  |
| 15  | BO    | 56   | LEU  | 2.2  |
| 16  | AP    | 40   | ASN  | 2.2  |
| 27  | C0    | 38   | ARG  | 2.2  |
| 31  | CA    | 1019 | U    | 2.2  |
| 36  | CH    | 86   | ASP  | 2.2  |
| 41  | CN    | 9    | PHE  | 2.2  |
| 55  | DA    | 1083 | U    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | AB    | 200  | ILE  | 2.2  |
| 1   | BA    | 383  | A    | 2.2  |
| 1   | BA    | 1319 | A    | 2.2  |
| 29  | DC    | 247  | PRO  | 2.2  |
| 31  | CA    | 1808 | A    | 2.2  |
| 33  | CE    | 136  | GLN  | 2.2  |
| 36  | DH    | 104  | THR  | 2.2  |
| 31  | CA    | 223  | A    | 2.2  |
| 37  | DJ    | 105  | GLN  | 2.2  |
| 42  | CO    | 110  | MET  | 2.2  |
| 3   | AC    | 153  | VAL  | 2.2  |
| 14  | AN    | 34   | VAL  | 2.2  |
| 19  | AS    | 24   | GLU  | 2.2  |
| 2   | AB    | 124  | GLY  | 2.2  |
| 1   | BA    | 217  | C    | 2.2  |
| 16  | BP    | 8    | ARG  | 2.2  |
| 31  | CA    | 400  | G    | 2.2  |
| 31  | CA    | 625  | G    | 2.2  |
| 31  | CA    | 1519 | G    | 2.2  |
| 31  | CA    | 2389 | G    | 2.2  |
| 31  | CA    | 2661 | G    | 2.2  |
| 31  | CA    | 2828 | G    | 2.2  |
| 33  | CE    | 51   | GLU  | 2.2  |
| 42  | CO    | 32   | GLU  | 2.2  |
| 40  | CM    | 43   | GLY  | 2.2  |
| 55  | DA    | 1171 | G    | 2.2  |
| 31  | CA    | 157  | C    | 2.2  |
| 31  | CA    | 1229 | C    | 2.2  |
| 31  | CA    | 1957 | C    | 2.2  |
| 31  | CA    | 2055 | C    | 2.2  |
| 35  | DG    | 114  | ASP  | 2.2  |
| 55  | DA    | 414  | C    | 2.2  |
| 1   | AA    | 1364 | U    | 2.2  |
| 1   | BA    | 180  | U    | 2.2  |
| 14  | AN    | 64   | CYS  | 2.2  |
| 29  | CC    | 176  | LEU  | 2.2  |
| 31  | CA    | 2493 | U    | 2.2  |
| 2   | BB    | 226  | SER  | 2.2  |
| 8   | BH    | 126  | ILE  | 2.2  |
| 35  | DG    | 13   | ALA  | 2.2  |
| 37  | CJ    | 63   | ALA  | 2.2  |
| 36  | DH    | 93   | SER  | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 43         | CP           | 91         | SER         | 2.2         |
| 1          | BA           | 353        | A           | 2.2         |
| 31         | CA           | 354        | A           | 2.2         |
| 31         | CA           | 1287       | A           | 2.2         |
| 31         | CA           | 1353       | A           | 2.2         |
| 31         | CA           | 2388       | A           | 2.2         |
| 55         | DA           | 2886[A]    | A           | 2.2         |
| 3          | AC           | 80         | LYS         | 2.2         |
| 3          | BC           | 114        | LYS         | 2.2         |
| 29         | CC           | 268        | VAL         | 2.2         |
| 34         | CF           | 48         | LYS         | 2.2         |
| 36         | CH           | 71         | LYS         | 2.2         |
| 37         | DJ           | 139        | VAL         | 2.2         |
| 46         | CS           | 85         | LYS         | 2.2         |
| 2          | BB           | 65         | GLY         | 2.2         |
| 49         | DV           | 57         | GLY         | 2.2         |
| 54         | DI           | 56         | ARG         | 2.2         |
| 1          | AA           | 183        | C           | 2.2         |
| 14         | BN           | 96         | LEU         | 2.2         |
| 1          | AA           | 1321       | U           | 2.2         |
| 1          | BA           | 1051       | C           | 2.2         |
| 1          | BA           | 1335       | U           | 2.2         |
| 1          | BA           | 1448       | C           | 2.2         |
| 28         | CB           | 18         | G           | 2.2         |
| 28         | CB           | 114        | C           | 2.2         |
| 31         | CA           | 33         | C           | 2.2         |
| 31         | CA           | 105        | C           | 2.2         |
| 31         | CA           | 296        | U           | 2.2         |
| 31         | CA           | 518        | G           | 2.2         |
| 31         | CA           | 1812       | U           | 2.2         |
| 31         | CA           | 1992       | G           | 2.2         |
| 31         | CA           | 2016       | U           | 2.2         |
| 31         | CA           | 2144       | G           | 2.2         |
| 31         | CA           | 2408       | U           | 2.2         |
| 31         | CA           | 2583       | G           | 2.2         |
| 40         | CM           | 125        | LEU         | 2.2         |
| 33         | DE           | 11         | ALA         | 2.2         |
| 47         | CT           | 89         | ALA         | 2.2         |
| 54         | DI           | 103        | ASN         | 2.2         |
| 49         | DV           | 50         | PRO         | 2.2         |
| 13         | AM           | 108        | THR         | 2.2         |
| 18         | AR           | 45         | THR         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 54  | DI    | 71   | CYS  | 2.2  |
| 7   | AG    | 76   | LYS  | 2.2  |
| 12  | BL    | 14   | ARG  | 2.2  |
| 29  | CC    | 221  | ARG  | 2.2  |
| 36  | CH    | 35   | LYS  | 2.2  |
| 40  | CM    | 86   | GLU  | 2.2  |
| 1   | AA    | 1346 | A    | 2.2  |
| 1   | BA    | 1446 | A    | 2.2  |
| 31  | CA    | 1307 | A    | 2.2  |
| 31  | CA    | 1854 | A    | 2.2  |
| 31  | CA    | 2377 | A    | 2.2  |
| 31  | CA    | 2406 | A    | 2.2  |
| 31  | CA    | 2435 | A    | 2.2  |
| 53  | CZ    | 50   | VAL  | 2.2  |
| 11  | BK    | 48   | GLY  | 2.1  |
| 23  | D2    | 18   | GLY  | 2.1  |
| 33  | CE    | 174  | GLY  | 2.1  |
| 2   | BB    | 167  | ASP  | 2.1  |
| 2   | AB    | 203  | ASN  | 2.1  |
| 2   | BB    | 146  | ASN  | 2.1  |
| 15  | AO    | 11   | ILE  | 2.1  |
| 31  | CA    | 234  | U    | 2.1  |
| 31  | CA    | 915  | C    | 2.1  |
| 31  | CA    | 1209 | U    | 2.1  |
| 34  | CF    | 52   | ASN  | 2.1  |
| 34  | DF    | 106  | ILE  | 2.1  |
| 1   | AA    | 1371 | G    | 2.1  |
| 1   | BA    | 324  | G    | 2.1  |
| 31  | CA    | 24   | G    | 2.1  |
| 31  | CA    | 1149 | G    | 2.1  |
| 31  | CA    | 2029 | G    | 2.1  |
| 31  | CA    | 2692 | G    | 2.1  |
| 52  | CY    | 62   | LYS  | 2.1  |
| 55  | DA    | 1091 | G    | 2.1  |
| 55  | DA    | 2144 | G    | 2.1  |
| 3   | AC    | 188  | GLU  | 2.1  |
| 3   | BC    | 142  | MET  | 2.1  |
| 8   | BH    | 3    | MET  | 2.1  |
| 16  | BP    | 48   | GLU  | 2.1  |
| 7   | AG    | 38   | THR  | 2.1  |
| 9   | AI    | 11   | ARG  | 2.1  |
| 15  | AO    | 25   | THR  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | C1    | 52   | ARG  | 2.1  |
| 36  | CH    | 45   | GLU  | 2.1  |
| 9   | BI    | 47   | VAL  | 2.1  |
| 25  | C4    | 56   | GLY  | 2.1  |
| 48  | CU    | 53   | VAL  | 2.1  |
| 31  | CA    | 391  | A    | 2.1  |
| 31  | CA    | 1387 | A    | 2.1  |
| 2   | BB    | 188  | ASP  | 2.1  |
| 12  | BL    | 74   | LEU  | 2.1  |
| 25  | C4    | 33   | LEU  | 2.1  |
| 52  | CY    | 29   | PHE  | 2.1  |
| 52  | CY    | 33   | LEU  | 2.1  |
| 1   | BA    | 472  | U    | 2.1  |
| 3   | BC    | 163  | ALA  | 2.1  |
| 31  | CA    | 286  | U    | 2.1  |
| 31  | CA    | 1294 | U    | 2.1  |
| 31  | CA    | 1621 | U    | 2.1  |
| 31  | CA    | 2798 | U    | 2.1  |
| 11  | AK    | 94   | GLU  | 2.1  |
| 31  | CA    | 1006 | C    | 2.1  |
| 31  | CA    | 1150 | C    | 2.1  |
| 35  | DG    | 173  | GLU  | 2.1  |
| 26  | C5    | 31   | PRO  | 2.1  |
| 1   | BA    | 454  | G    | 2.1  |
| 13  | AM    | 12   | HIS  | 2.1  |
| 28  | CB    | 6    | G    | 2.1  |
| 28  | CB    | 100  | G    | 2.1  |
| 31  | CA    | 15   | G    | 2.1  |
| 31  | CA    | 2010 | G    | 2.1  |
| 31  | CA    | 2409 | G    | 2.1  |
| 31  | CA    | 2415 | G    | 2.1  |
| 31  | CA    | 2659 | G    | 2.1  |
| 31  | CA    | 2834 | G    | 2.1  |
| 55  | DA    | 1074 | G    | 2.1  |
| 3   | AC    | 2    | GLY  | 2.1  |
| 3   | BC    | 15   | VAL  | 2.1  |
| 38  | CK    | 30   | THR  | 2.1  |
| 47  | CT    | 50   | VAL  | 2.1  |
| 54  | DI    | 86   | THR  | 2.1  |
| 18  | BR    | 23   | TYR  | 2.1  |
| 13  | BM    | 110  | LYS  | 2.1  |
| 29  | CC    | 255  | LYS  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 34         | DF           | 145        | LYS         | 2.1         |
| 45         | CR           | 60         | LEU         | 2.1         |
| 47         | CT           | 73         | LYS         | 2.1         |
| 31         | CA           | 278        | A           | 2.1         |
| 47         | CT           | 109        | ASP         | 2.1         |
| 8          | AH           | 130        | ALA         | 2.1         |
| 24         | C3           | 19         | ARG         | 2.1         |
| 25         | C4           | 13         | ARG         | 2.1         |
| 31         | CA           | 1372       | U           | 2.1         |
| 33         | CE           | 44         | ARG         | 2.1         |
| 27         | C0           | 49         | ASN         | 2.1         |
| 1          | BA           | 316        | C           | 2.1         |
| 2          | BB           | 96         | TRP         | 2.1         |
| 31         | CA           | 897        | C           | 2.1         |
| 31         | CA           | 2456       | C           | 2.1         |
| 3          | BC           | 153        | VAL         | 2.1         |
| 7          | BG           | 20         | SER         | 2.1         |
| 13         | BM           | 91         | HIS         | 2.1         |
| 19         | BS           | 62         | VAL         | 2.1         |
| 29         | CC           | 94         | VAL         | 2.1         |
| 36         | CH           | 121        | VAL         | 2.1         |
| 1          | AA           | 838        | G           | 2.1         |
| 2          | AB           | 11         | LYS         | 2.1         |
| 3          | BC           | 67         | THR         | 2.1         |
| 8          | AH           | 55         | THR         | 2.1         |
| 31         | CA           | 604        | G           | 2.1         |
| 31         | CA           | 1601       | G           | 2.1         |
| 31         | CA           | 2027       | G           | 2.1         |
| 31         | CA           | 2349       | G           | 2.1         |
| 31         | CA           | 2494       | G           | 2.1         |
| 2          | AB           | 205        | ASP         | 2.1         |
| 19         | BS           | 64         | ASP         | 2.1         |
| 33         | CE           | 19         | PHE         | 2.1         |
| 31         | CA           | 25         | U           | 2.1         |
| 1          | BA           | 66         | A           | 2.1         |
| 1          | BA           | 253        | A           | 2.1         |
| 2          | AB           | 34         | ALA         | 2.1         |
| 31         | CA           | 1409       | U           | 2.1         |
| 31         | CA           | 1742       | U           | 2.1         |
| 31         | CA           | 2449       | U           | 2.1         |
| 31         | CA           | 2005       | A           | 2.1         |
| 43         | CP           | 113        | ALA         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | BM    | 26   | GLY  | 2.1  |
| 31  | CA    | 351  | C    | 2.1  |
| 31  | CA    | 366  | C    | 2.1  |
| 31  | CA    | 806  | C    | 2.1  |
| 31  | CA    | 898  | C    | 2.1  |
| 48  | CU    | 63   | VAL  | 2.1  |
| 51  | CX    | 27   | GLY  | 2.1  |
| 54  | DI    | 89   | PRO  | 2.1  |
| 55  | DA    | 1728 | C    | 2.1  |
| 55  | DA    | 2150 | C    | 2.1  |
| 2   | BB    | 86   | SER  | 2.1  |
| 10  | AJ    | 24   | GLU  | 2.1  |
| 29  | CC    | 205  | LEU  | 2.1  |
| 52  | CY    | 38   | PHE  | 2.1  |
| 3   | BC    | 3    | GLN  | 2.1  |
| 10  | BJ    | 64   | GLN  | 2.1  |
| 22  | C1    | 31   | ASP  | 2.1  |
| 31  | CA    | 809  | G    | 2.1  |
| 31  | CA    | 855  | G    | 2.1  |
| 31  | CA    | 954  | G    | 2.1  |
| 31  | CA    | 2428 | G    | 2.1  |
| 41  | CN    | 22   | GLN  | 2.1  |
| 55  | DA    | 2136 | G    | 2.1  |
| 9   | AI    | 86   | ALA  | 2.1  |
| 19  | AS    | 40   | ILE  | 2.1  |
| 29  | CC    | 61   | ALA  | 2.1  |
| 31  | CA    | 2155 | U    | 2.1  |
| 42  | CO    | 88   | ALA  | 2.1  |
| 46  | CS    | 65   | ALA  | 2.1  |
| 49  | DV    | 2    | ALA  | 2.1  |
| 1   | BA    | 1246 | A    | 2.1  |
| 1   | BA    | 1251 | A    | 2.1  |
| 31  | CA    | 764  | A    | 2.1  |
| 31  | CA    | 2013 | A    | 2.1  |
| 31  | CA    | 2051 | A    | 2.1  |
| 48  | CU    | 64   | LYS  | 2.1  |
| 49  | CV    | 57   | GLY  | 2.1  |
| 6   | AF    | 64   | VAL  | 2.1  |
| 8   | BH    | 39   | VAL  | 2.1  |
| 20  | AT    | 58   | VAL  | 2.1  |
| 31  | CA    | 1644 | C    | 2.1  |
| 31  | CA    | 2214 | C    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 2755 | C    | 2.1  |
| 31  | CA    | 2824 | C    | 2.1  |
| 55  | DA    | 143  | C    | 2.1  |
| 42  | CO    | 4    | ARG  | 2.1  |
| 7   | BG    | 67   | GLU  | 2.1  |
| 10  | BJ    | 78   | GLU  | 2.1  |
| 19  | BS    | 10   | PHE  | 2.1  |
| 47  | CT    | 59   | GLU  | 2.1  |
| 4   | BD    | 40   | GLN  | 2.1  |
| 47  | CT    | 31   | GLN  | 2.1  |
| 48  | DU    | 91   | GLN  | 2.1  |
| 1   | AA    | 218  | U    | 2.1  |
| 1   | AA    | 961  | U    | 2.1  |
| 26  | C5    | 26   | ILE  | 2.1  |
| 1   | BA    | 184  | G    | 2.1  |
| 1   | BA    | 1064 | G    | 2.1  |
| 1   | BA    | 1386 | G    | 2.1  |
| 3   | BC    | 62   | LYS  | 2.1  |
| 20  | BT    | 19   | LYS  | 2.1  |
| 29  | CC    | 253  | LYS  | 2.1  |
| 29  | CC    | 256  | LYS  | 2.1  |
| 30  | CD    | 85   | ALA  | 2.1  |
| 31  | CA    | 1255 | U    | 2.1  |
| 31  | CA    | 2845 | U    | 2.1  |
| 36  | CH    | 84   | ALA  | 2.1  |
| 31  | CA    | 258  | G    | 2.1  |
| 31  | CA    | 396  | G    | 2.1  |
| 31  | CA    | 585  | G    | 2.1  |
| 31  | CA    | 1555 | G    | 2.1  |
| 31  | CA    | 2304 | G    | 2.1  |
| 31  | CA    | 2351 | G    | 2.1  |
| 31  | CA    | 2674 | G    | 2.1  |
| 31  | CA    | 2825 | G    | 2.1  |
| 14  | AN    | 68   | GLY  | 2.1  |
| 19  | AS    | 46   | GLY  | 2.1  |
| 1   | BA    | 74   | A    | 2.1  |
| 29  | CC    | 220  | VAL  | 2.1  |
| 31  | CA    | 582  | A    | 2.1  |
| 31  | CA    | 632  | A    | 2.1  |
| 31  | CA    | 2433 | A    | 2.1  |
| 31  | CA    | 2670 | A    | 2.1  |
| 1   | AA    | 1096 | C    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | BA    | 970  | C    | 2.1  |
| 8   | AH    | 107  | SER  | 2.1  |
| 31  | CA    | 1656 | C    | 2.1  |
| 31  | CA    | 2888 | C    | 2.1  |
| 25  | C4    | 16   | LYS  | 2.1  |
| 30  | CD    | 12   | THR  | 2.1  |
| 36  | CH    | 79   | THR  | 2.1  |
| 5   | AE    | 141  | ILE  | 2.1  |
| 7   | AG    | 29   | ILE  | 2.1  |
| 33  | CE    | 149  | ILE  | 2.1  |
| 34  | DF    | 128  | TYR  | 2.1  |
| 15  | BO    | 7    | ALA  | 2.1  |
| 16  | BP    | 7    | ALA  | 2.1  |
| 54  | DI    | 83   | ALA  | 2.1  |
| 2   | BB    | 17   | GLY  | 2.1  |
| 29  | CC    | 209  | GLY  | 2.1  |
| 53  | CZ    | 62   | GLY  | 2.1  |
| 1   | AA    | 1186 | G    | 2.1  |
| 1   | BA    | 633  | G    | 2.1  |
| 7   | BG    | 138  | ARG  | 2.1  |
| 10  | BJ    | 58   | ASN  | 2.1  |
| 29  | CC    | 132  | MET  | 2.1  |
| 31  | CA    | 175  | G    | 2.1  |
| 31  | CA    | 664  | G    | 2.1  |
| 31  | CA    | 774  | G    | 2.1  |
| 31  | CA    | 1300 | G    | 2.1  |
| 31  | CA    | 1339 | G    | 2.1  |
| 31  | CA    | 1452 | G    | 2.1  |
| 41  | CN    | 59   | ARG  | 2.1  |
| 31  | CA    | 384  | A    | 2.1  |
| 31  | CA    | 497  | A    | 2.1  |
| 23  | C2    | 13   | SER  | 2.1  |
| 31  | CA    | 795  | C    | 2.1  |
| 31  | CA    | 812  | C    | 2.1  |
| 31  | CA    | 1164 | C    | 2.1  |
| 31  | CA    | 2153 | C    | 2.1  |
| 36  | DH    | 54   | LEU  | 2.1  |
| 36  | DH    | 75   | LEU  | 2.1  |
| 2   | AB    | 75   | ALA  | 2.1  |
| 3   | BC    | 162  | ILE  | 2.1  |
| 5   | BE    | 34   | THR  | 2.1  |
| 23  | C2    | 17   | THR  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 1602 | U    | 2.1  |
| 31  | CA    | 1758 | U    | 2.1  |
| 31  | CA    | 2312 | U    | 2.1  |
| 36  | CH    | 59   | ALA  | 2.1  |
| 42  | CO    | 34   | ILE  | 2.1  |
| 6   | BF    | 91   | ARG  | 2.1  |
| 7   | AG    | 81   | GLY  | 2.1  |
| 9   | BI    | 102  | GLY  | 2.1  |
| 2   | AB    | 201  | PRO  | 2.1  |
| 6   | BF    | 64   | VAL  | 2.1  |
| 14  | AN    | 94   | PRO  | 2.1  |
| 29  | CC    | 216  | VAL  | 2.1  |
| 38  | CK    | 61   | LYS  | 2.1  |
| 39  | CL    | 20   | MET  | 2.1  |
| 48  | CU    | 40   | LYS  | 2.1  |
| 1   | AA    | 200  | G    | 2.1  |
| 1   | BA    | 260  | G    | 2.1  |
| 31  | CA    | 620  | G    | 2.1  |
| 31  | CA    | 926  | G    | 2.1  |
| 31  | CA    | 2048 | G    | 2.1  |
| 5   | AE    | 144  | LEU  | 2.0  |
| 11  | BK    | 22   | HIS  | 2.0  |
| 11  | BK    | 82   | LEU  | 2.0  |
| 15  | BO    | 87   | LEU  | 2.0  |
| 35  | CG    | 87   | LEU  | 2.0  |
| 1   | AA    | 979  | C    | 2.0  |
| 1   | AA    | 983  | A    | 2.0  |
| 1   | BA    | 95   | C    | 2.0  |
| 1   | BA    | 192  | A    | 2.0  |
| 31  | CA    | 910  | A    | 2.0  |
| 31  | CA    | 1908 | C    | 2.0  |
| 31  | CA    | 2143 | C    | 2.0  |
| 31  | CA    | 2160 | C    | 2.0  |
| 31  | CA    | 2682 | A    | 2.0  |
| 31  | CA    | 2712 | C    | 2.0  |
| 31  | CA    | 2850 | A    | 2.0  |
| 55  | DA    | 2104 | C    | 2.0  |
| 3   | AC    | 179  | ARG  | 2.0  |
| 3   | BC    | 61   | ALA  | 2.0  |
| 9   | BI    | 78   | ALA  | 2.0  |
| 11  | AK    | 79   | ILE  | 2.0  |
| 22  | C1    | 43   | ILE  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 1033 | U    | 2.0  |
| 31  | CA    | 1497 | U    | 2.0  |
| 31  | CA    | 2249 | U    | 2.0  |
| 33  | CE    | 87   | ALA  | 2.0  |
| 34  | CF    | 115  | ARG  | 2.0  |
| 35  | DG    | 121  | ILE  | 2.0  |
| 38  | CK    | 101  | ILE  | 2.0  |
| 40  | CM    | 58   | TYR  | 2.0  |
| 45  | CR    | 62   | ILE  | 2.0  |
| 46  | DS    | 26   | ASP  | 2.0  |
| 31  | CA    | 588  | U    | 2.0  |
| 45  | CR    | 15   | LYS  | 2.0  |
| 52  | DY    | 77   | LYS  | 2.0  |
| 5   | BE    | 74   | VAL  | 2.0  |
| 5   | BE    | 85   | VAL  | 2.0  |
| 6   | BF    | 62   | MET  | 2.0  |
| 30  | CD    | 165  | MET  | 2.0  |
| 36  | DH    | 115  | VAL  | 2.0  |
| 45  | CR    | 104  | VAL  | 2.0  |
| 11  | BK    | 52   | PHE  | 2.0  |
| 29  | CC    | 174  | LEU  | 2.0  |
| 35  | CG    | 72   | LEU  | 2.0  |
| 54  | DI    | 95   | LEU  | 2.0  |
| 1   | AA    | 1124 | G    | 2.0  |
| 1   | AA    | 1220 | G    | 2.0  |
| 1   | BA    | 846  | G    | 2.0  |
| 5   | BE    | 72   | ILE  | 2.0  |
| 10  | AJ    | 63   | ASP  | 2.0  |
| 27  | C0    | 11   | ARG  | 2.0  |
| 31  | CA    | 287  | G    | 2.0  |
| 1   | BA    | 1216 | A    | 2.0  |
| 31  | CA    | 560  | C    | 2.0  |
| 31  | CA    | 662  | G    | 2.0  |
| 31  | CA    | 1356 | G    | 2.0  |
| 31  | CA    | 1642 | G    | 2.0  |
| 31  | CA    | 2306 | C    | 2.0  |
| 31  | CA    | 2382 | G    | 2.0  |
| 37  | DJ    | 64   | ASP  | 2.0  |
| 39  | CL    | 14   | SER  | 2.0  |
| 1   | AA    | 91   | U    | 2.0  |
| 14  | BN    | 44   | ALA  | 2.0  |
| 31  | CA    | 118  | A    | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | CA    | 181  | A    | 2.0  |
| 31  | CA    | 804  | A    | 2.0  |
| 31  | CA    | 899  | A    | 2.0  |
| 31  | CA    | 1598 | A    | 2.0  |
| 11  | BK    | 94   | GLU  | 2.0  |
| 13  | BM    | 20   | THR  | 2.0  |
| 17  | BQ    | 43   | LYS  | 2.0  |
| 2   | BB    | 4    | VAL  | 2.0  |
| 9   | AI    | 103  | PHE  | 2.0  |
| 20  | AT    | 56   | PRO  | 2.0  |
| 45  | CR    | 58   | ARG  | 2.0  |
| 8   | BH    | 14   | ILE  | 2.0  |
| 33  | CE    | 181  | ILE  | 2.0  |
| 36  | CH    | 98   | ASP  | 2.0  |
| 15  | BO    | 16   | GLY  | 2.0  |
| 1   | BA    | 70   | U    | 2.0  |
| 1   | BA    | 133  | U    | 2.0  |
| 10  | AJ    | 29   | ALA  | 2.0  |
| 1   | BA    | 259  | G    | 2.0  |
| 28  | CB    | 8    | C    | 2.0  |
| 31  | CA    | 669  | G    | 2.0  |
| 31  | CA    | 1363 | C    | 2.0  |
| 31  | CA    | 1954 | G    | 2.0  |
| 31  | CA    | 2104 | C    | 2.0  |
| 31  | CA    | 2244 | U    | 2.0  |
| 31  | CA    | 2664 | G    | 2.0  |
| 31  | CA    | 2695 | U    | 2.0  |
| 31  | CA    | 2785 | C    | 2.0  |
| 39  | CL    | 60   | ALA  | 2.0  |
| 43  | CP    | 86   | GLY  | 2.0  |
| 28  | CB    | 73   | A    | 2.0  |
| 31  | CA    | 17   | G    | 2.0  |
| 31  | CA    | 58   | G    | 2.0  |
| 31  | CA    | 82   | U    | 2.0  |
| 31  | CA    | 298  | G    | 2.0  |
| 35  | CG    | 34   | THR  | 2.0  |
| 5   | AE    | 74   | VAL  | 2.0  |
| 16  | AP    | 19   | VAL  | 2.0  |
| 3   | AC    | 157  | LEU  | 2.0  |
| 4   | AD    | 168  | PRO  | 2.0  |
| 10  | AJ    | 41   | PRO  | 2.0  |
| 13  | BM    | 92   | ARG  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | AN    | 51   | LEU  | 2.0  |
| 33  | CE    | 9    | GLN  | 2.0  |
| 34  | CF    | 148  | ARG  | 2.0  |
| 38  | CK    | 122  | LEU  | 2.0  |
| 51  | CX    | 50   | ASN  | 2.0  |
| 36  | DH    | 83   | LYS  | 2.0  |
| 8   | BH    | 54   | ASP  | 2.0  |
| 9   | AI    | 81   | HIS  | 2.0  |
| 22  | C1    | 38   | HIS  | 2.0  |
| 7   | AG    | 46   | ALA  | 2.0  |
| 7   | AG    | 145  | ALA  | 2.0  |
| 7   | BG    | 147  | ALA  | 2.0  |
| 24  | C3    | 38   | GLY  | 2.0  |
| 54  | DI    | 82   | ILE  | 2.0  |
| 34  | CF    | 118  | SER  | 2.0  |
| 45  | CR    | 115  | ALA  | 2.0  |
| 1   | BA    | 991  | U    | 2.0  |
| 31  | CA    | 225  | C    | 2.0  |
| 31  | CA    | 416  | U    | 2.0  |
| 31  | CA    | 1461 | C    | 2.0  |
| 31  | CA    | 2551 | C    | 2.0  |
| 31  | CA    | 2779 | U    | 2.0  |
| 1   | AA    | 1274 | A    | 2.0  |
| 1   | BA    | 270  | A    | 2.0  |
| 1   | BA    | 1316 | G    | 2.0  |
| 9   | AI    | 113  | ARG  | 2.0  |
| 16  | AP    | 50   | THR  | 2.0  |
| 17  | AQ    | 58   | VAL  | 2.0  |
| 28  | CB    | 29   | A    | 2.0  |
| 31  | CA    | 916  | G    | 2.0  |
| 31  | CA    | 993  | G    | 2.0  |
| 31  | CA    | 1223 | G    | 2.0  |
| 31  | CA    | 2156 | G    | 2.0  |
| 31  | CA    | 2587 | A    | 2.0  |
| 31  | CA    | 2842 | G    | 2.0  |
| 31  | CA    | 2852 | G    | 2.0  |
| 44  | CQ    | 46   | VAL  | 2.0  |
| 47  | CT    | 106  | VAL  | 2.0  |
| 55  | DA    | 1096 | A    | 2.0  |
| 16  | AP    | 38   | PHE  | 2.0  |
| 47  | DT    | 110  | ARG  | 2.0  |
| 53  | CZ    | 52   | ARG  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | AE    | 81  | LEU  | 2.0  |
| 16  | AP    | 76  | LYS  | 2.0  |
| 40  | CM    | 17  | LYS  | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|------|----------------------------|-------|
| 1   | 5MC  | AA    | 1407   | 21/22 | 0.97 | 0.15 | -    | 60,61,63,64                | 0     |
| 55  | 2MG  | DA    | 2445   | 24/25 | 0.99 | 0.21 | -    | 25,29,33,34                | 0     |
| 12  | D2T  | AL    | 89     | 10/11 | 0.91 | 0.27 | -    | 66,71,78,78                | 0     |
| 1   | 2MG  | BA    | 1207   | 24/25 | 0.80 | 0.29 | -    | 158,161,165,168            | 0     |
| 1   | MA6  | BA    | 1518   | 24/25 | 0.92 | 0.25 | -    | 84,88,95,96                | 0     |
| 31  | PSU  | CA    | 2605   | 20/21 | 0.91 | 0.23 | -    | 82,84,86,87                | 0     |
| 32  | MEQ  | DD    | 150[A] | 10/11 | 0.96 | 0.24 | -    | 14,23,32,32                | 10    |
| 31  | G7M  | CA    | 2069   | 24/25 | 0.87 | 0.26 | -    | 109,112,115,116            | 0     |
| 1   | MA6  | BA    | 1519   | 24/25 | 0.93 | 0.26 | -    | 84,87,91,92                | 0     |
| 55  | 1MG  | DA    | 745    | 24/25 | 0.99 | 0.21 | -    | 28,31,33,38                | 0     |
| 1   | PSU  | AA    | 516    | 20/21 | 0.94 | 0.16 | -    | 88,92,97,97                | 0     |
| 31  | 2MG  | CA    | 1835   | 24/25 | 0.92 | 0.18 | -    | 74,76,78,78                | 0     |
| 31  | PSU  | CA    | 955    | 20/21 | 0.86 | 0.26 | -    | 107,112,115,115            | 0     |
| 1   | 2MG  | AA    | 1207   | 24/25 | 0.91 | 0.16 | -    | 114,118,121,124            | 0     |
| 55  | 6MZ  | DA    | 1618   | 23/24 | 0.99 | 0.20 | -    | 25,30,32,35                | 0     |
| 55  | 2MA  | DA    | 2503   | 23/24 | 0.99 | 0.20 | -    | 33,36,39,43                | 0     |
| 55  | PSU  | DA    | 746    | 20/21 | 0.99 | 0.19 | -    | 28,32,36,38                | 0     |
| 31  | 6MZ  | CA    | 2030   | 23/24 | 0.85 | 0.24 | -    | 108,114,116,117            | 0     |
| 55  | 2MG  | DA    | 1835   | 24/25 | 0.96 | 0.23 | -    | 49,55,56,56                | 0     |
| 1   | MA6  | AA    | 1518   | 24/25 | 0.97 | 0.16 | -    | 60,61,62,64                | 0     |
| 1   | 2MG  | BA    | 966    | 24/25 | 0.75 | 0.36 | -    | 153,160,171,171            | 0     |
| 41  | 4D4  | CN    | 81     | 12/13 | 0.90 | 0.34 | -    | 112,122,143,143            | 0     |
| 1   | UR3  | AA    | 1498   | 21/22 | 0.95 | 0.19 | -    | 64,68,72,73                | 0     |
| 31  | 3TD  | CA    | 1915   | 21/22 | 0.86 | 0.28 | -    | 150,155,157,157            | 0     |
| 55  | 5MU  | DA    | 1939   | 21/22 | 0.98 | 0.23 | -    | 35,38,40,43                | 0     |
| 55  | PSU  | DA    | 2604   | 20/21 | 0.97 | 0.19 | -    | 37,42,54,55                | 0     |
| 31  | 6MZ  | CA    | 1618   | 23/24 | 0.91 | 0.30 | -    | 136,143,148,149            | 0     |
| 1   | 2MG  | AA    | 966    | 24/25 | 0.91 | 0.19 | -    | 95,98,107,108              | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|------|----------------------------|-------|
| 31  | 2MA  | CA    | 2503   | 23/24 | 0.84 | 0.26 | -    | 110,115,118,118            | 0     |
| 1   | 2MG  | AA    | 1516   | 24/25 | 0.96 | 0.17 | -    | 58,61,62,63                | 0     |
| 31  | 5MC  | CA    | 1962   | 21/22 | 0.93 | 0.16 | -    | 72,78,79,82                | 0     |
| 55  | 5MC  | DA    | 1962   | 21/22 | 0.96 | 0.23 | -    | 43,46,50,52                | 0     |
| 55  | PSU  | DA    | 2580   | 20/21 | 0.99 | 0.21 | -    | 25,30,33,35                | 0     |
| 31  | 2MG  | CA    | 2445   | 24/25 | 0.87 | 0.31 | -    | 105,110,112,113            | 0     |
| 55  | OMU  | DA    | 2552   | 21/22 | 0.98 | 0.22 | -    | 33,37,39,43                | 0     |
| 55  | 6MZ  | DA    | 2030   | 23/24 | 0.99 | 0.22 | -    | 24,28,32,39                | 0     |
| 31  | 1MG  | CA    | 745    | 24/25 | 0.90 | 0.25 | -    | 106,113,118,121            | 0     |
| 31  | PSU  | CA    | 2580   | 20/21 | 0.87 | 0.22 | -    | 102,105,109,109            | 0     |
| 55  | PSU  | DA    | 1917   | 20/21 | 0.94 | 0.17 | -    | 74,82,90,90                | 0     |
| 1   | 5MC  | BA    | 967    | 21/22 | 0.67 | 0.39 | -    | 153,164,167,167            | 0     |
| 55  | G7M  | DA    | 2069   | 24/25 | 0.99 | 0.20 | -    | 26,35,36,37                | 0     |
| 55  | OMG  | DA    | 2251   | 24/25 | 0.98 | 0.21 | -    | 29,33,35,39                | 0     |
| 31  | PSU  | CA    | 1917   | 20/21 | 0.81 | 0.21 | -    | 119,125,134,135            | 0     |
| 1   | PSU  | BA    | 516    | 20/21 | 0.85 | 0.16 | -    | 88,99,102,104              | 0     |
| 1   | G7M  | BA    | 527    | 24/25 | 0.96 | 0.15 | -    | 75,80,83,84                | 0     |
| 1   | 4OC  | BA    | 1402   | 22/23 | 0.93 | 0.17 | -    | 78,81,84,85                | 0     |
| 1   | MA6  | AA    | 1519   | 24/25 | 0.96 | 0.19 | -    | 61,62,70,71                | 0     |
| 1   | 2MG  | BA    | 1516   | 24/25 | 0.89 | 0.21 | -    | 82,90,99,100               | 0     |
| 31  | PSU  | CA    | 2504   | 20/21 | 0.86 | 0.25 | -    | 98,108,110,111             | 0     |
| 31  | OMU  | CA    | 2552   | 21/22 | 0.85 | 0.45 | -    | 91,96,100,101              | 0     |
| 41  | 4D4  | DN    | 81[A]  | 12/13 | 0.96 | 0.24 | -    | 33,38,53,55                | 9     |
| 31  | OMG  | CA    | 2251   | 24/25 | 0.89 | 0.26 | -    | 90,95,100,101              | 0     |
| 41  | 4D4  | DN    | 81[B]  | 12/13 | 0.96 | 0.24 | -    | 27,32,34,35                | 9     |
| 1   | G7M  | AA    | 527    | 24/25 | 0.96 | 0.17 | -    | 63,67,73,74                | 0     |
| 31  | PSU  | CA    | 2457   | 20/21 | 0.89 | 0.26 | -    | 106,107,108,109            | 0     |
| 31  | PSU  | CA    | 1911   | 20/21 | 0.86 | 0.24 | -    | 123,137,138,139            | 0     |
| 55  | PSU  | DA    | 2504   | 20/21 | 0.98 | 0.21 | -    | 33,41,49,52                | 0     |
| 32  | MEQ  | DD    | 150[B] | 10/11 | 0.96 | 0.24 | -    | 27,32,45,50                | 10    |
| 1   | 5MC  | AA    | 967    | 21/22 | 0.88 | 0.20 | -    | 90,106,107,108             | 0     |
| 1   | 4OC  | AA    | 1402   | 22/23 | 0.96 | 0.18 | -    | 61,68,72,73                | 0     |
| 1   | UR3  | BA    | 1498   | 21/22 | 0.92 | 0.18 | -    | 89,93,97,98                | 0     |
| 55  | PSU  | DA    | 955    | 20/21 | 0.99 | 0.21 | -    | 27,28,32,35                | 0     |
| 31  | 5MU  | CA    | 1939   | 21/22 | 0.93 | 0.19 | -    | 75,79,81,82                | 0     |
| 55  | OMC  | DA    | 2498   | 21/22 | 0.99 | 0.21 | -    | 20,27,31,37                | 0     |
| 12  | D2T  | BL    | 89     | 10/11 | 0.91 | 0.28 | -    | 86,88,94,95                | 0     |
| 31  | PSU  | CA    | 746    | 20/21 | 0.87 | 0.25 | -    | 120,123,126,127            | 0     |
| 55  | H2U  | DA    | 2449   | 20/21 | 0.99 | 0.22 | -    | 27,30,36,39                | 0     |
| 1   | 5MC  | BA    | 1407   | 21/22 | 0.89 | 0.21 | -    | 100,109,114,117            | 0     |
| 31  | OMC  | CA    | 2498   | 21/22 | 0.92 | 0.28 | -    | 97,102,104,106             | 0     |
| 55  | PSU  | DA    | 1911   | 20/21 | 0.91 | 0.18 | -    | 78,88,91,91                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 55  | 3TD  | DA    | 1915 | 21/22 | 0.91 | 0.22 | -    | 103,106,112,113             | 0     |
| 55  | 5MU  | DA    | 747  | 21/22 | 0.99 | 0.20 | -    | 28,31,37,38                 | 0     |
| 55  | PSU  | DA    | 2605 | 20/21 | 0.98 | 0.19 | -    | 35,41,43,44                 | 0     |
| 31  | 5MU  | CA    | 747  | 21/22 | 0.87 | 0.28 | -    | 126,128,130,131             | 0     |
| 55  | PSU  | DA    | 2457 | 20/21 | 0.99 | 0.19 | -    | 25,29,31,35                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 62  | PEG  | DA    | 3217 | 7/7   | 0.71 | 0.55 | 81.63 | 89,93,98,99                 | 0     |
| 59  | PUT  | AA    | 1674 | 6/6   | 0.72 | 0.73 | 51.76 | 98,99,100,100               | 0     |
| 64  | PGE  | DA    | 3213 | 10/10 | 0.85 | 0.49 | 46.52 | 84,86,90,90                 | 0     |
| 58  | MPD  | DA    | 3203 | 8/8   | 0.76 | 0.75 | 40.62 | 96,99,102,104               | 0     |
| 56  | MG   | DA    | 3182 | 1/1   | 0.58 | 0.54 | 36.79 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3128 | 1/1   | 0.85 | 0.48 | 29.33 | 78,78,78,78                 | 0     |
| 56  | MG   | CA    | 3003 | 1/1   | 0.35 | 2.63 | 28.75 | 284,284,284,284             | 0     |
| 59  | PUT  | DA    | 3195 | 6/6   | 0.82 | 0.54 | 25.62 | 51,53,62,65                 | 0     |
| 58  | MPD  | AA    | 1676 | 8/8   | 0.90 | 0.57 | 23.98 | 97,100,100,102              | 0     |
| 56  | MG   | DA    | 3123 | 1/1   | 0.83 | 0.51 | 21.97 | 77,77,77,77                 | 0     |
| 56  | MG   | CA    | 3133 | 1/1   | 0.45 | 0.63 | 21.66 | 140,140,140,140             | 0     |
| 59  | PUT  | DA    | 3212 | 6/6   | 0.83 | 0.45 | 21.58 | 55,57,64,66                 | 0     |
| 62  | PEG  | D3    | 102  | 7/7   | 0.75 | 1.24 | 20.87 | 72,74,83,84                 | 0     |
| 62  | PEG  | DA    | 3200 | 7/7   | 0.80 | 0.51 | 19.94 | 55,58,65,65                 | 0     |
| 56  | MG   | AA    | 1612 | 1/1   | 0.65 | 0.73 | 19.55 | 81,81,81,81                 | 0     |
| 56  | MG   | AA    | 1607 | 1/1   | 0.90 | 0.61 | 18.99 | 92,92,92,92                 | 0     |
| 65  | SPD  | DA    | 3183 | 10/10 | 0.85 | 0.44 | 18.67 | 57,63,66,66                 | 0     |
| 59  | PUT  | DA    | 3218 | 6/6   | 0.77 | 0.42 | 17.18 | 75,77,80,81                 | 0     |
| 57  | PG4  | DA    | 3193 | 13/13 | 0.85 | 0.87 | 16.43 | 63,65,76,77                 | 0     |
| 62  | PEG  | DQ    | 201  | 7/7   | 0.48 | 1.03 | 16.15 | 107,109,110,110             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 67  | ACY  | DA    | 3201 | 4/4   | 0.84 | 0.33 | 15.61 | 60,64,64,66                 | 0     |
| 64  | PGE  | D3    | 101  | 10/10 | 0.76 | 0.67 | 15.40 | 87,88,88,88                 | 0     |
| 59  | PUT  | AA    | 1673 | 6/6   | 0.78 | 0.48 | 14.85 | 125,126,127,128             | 0     |
| 56  | MG   | DA    | 3127 | 1/1   | 0.95 | 0.43 | 14.37 | 62,62,62,62                 | 0     |
| 65  | SPD  | DA    | 3205 | 10/10 | 0.70 | 0.38 | 13.65 | 75,81,84,85                 | 0     |
| 59  | PUT  | DA    | 3220 | 6/6   | 0.85 | 0.36 | 13.55 | 92,92,94,95                 | 0     |
| 66  | 1PE  | DA    | 3202 | 16/16 | 0.84 | 0.37 | 13.21 | 60,63,65,65                 | 0     |
| 57  | PG4  | DA    | 3215 | 13/13 | 0.76 | 0.43 | 13.14 | 95,103,104,104              | 0     |
| 59  | PUT  | AA    | 1672 | 6/6   | 0.73 | 0.66 | 12.49 | 110,112,114,114             | 0     |
| 56  | MG   | CA    | 3026 | 1/1   | 0.79 | 1.03 | 12.12 | 197,197,197,197             | 0     |
| 63  | EDO  | DA    | 3001 | 4/4   | 0.87 | 0.37 | 11.63 | 72,73,75,77                 | 0     |
| 58  | MPD  | DA    | 3192 | 8/8   | 0.89 | 0.59 | 11.46 | 79,79,82,83                 | 0     |
| 56  | MG   | DA    | 3163 | 1/1   | 0.50 | 0.36 | 11.19 | 84,84,84,84                 | 0     |
| 58  | MPD  | DE    | 302  | 8/8   | 0.76 | 0.57 | 10.95 | 96,97,98,98                 | 0     |
| 56  | MG   | CA    | 3131 | 1/1   | 0.59 | 0.58 | 10.93 | 111,111,111,111             | 0     |
| 64  | PGE  | D1    | 102  | 10/10 | 0.70 | 0.59 | 10.87 | 95,96,100,100               | 0     |
| 59  | PUT  | DA    | 3189 | 6/6   | 0.81 | 0.38 | 10.80 | 47,48,49,49                 | 0     |
| 56  | MG   | DA    | 3125 | 1/1   | 0.71 | 0.42 | 10.14 | 83,83,83,83                 | 0     |
| 62  | PEG  | D1    | 103  | 7/7   | 0.77 | 0.47 | 9.65  | 56,60,61,62                 | 0     |
| 56  | MG   | AA    | 1642 | 1/1   | 0.26 | 0.51 | 9.64  | 165,165,165,165             | 0     |
| 66  | 1PE  | DA    | 3185 | 16/16 | 0.89 | 0.31 | 9.41  | 44,53,71,72                 | 0     |
| 59  | PUT  | DA    | 3221 | 6/6   | 0.89 | 0.33 | 9.07  | 44,48,50,50                 | 0     |
| 58  | MPD  | DA    | 3206 | 8/8   | 0.79 | 0.51 | 9.04  | 89,93,94,94                 | 0     |
| 56  | MG   | DA    | 3172 | 1/1   | 0.84 | 0.38 | 8.66  | 89,89,89,89                 | 0     |
| 59  | PUT  | DA    | 3204 | 6/6   | 0.82 | 0.43 | 8.66  | 66,66,70,71                 | 0     |
| 56  | MG   | CA    | 3147 | 1/1   | 0.80 | 0.40 | 8.63  | 91,91,91,91                 | 1     |
| 56  | MG   | CA    | 3110 | 1/1   | 0.35 | 0.83 | 8.42  | 188,188,188,188             | 0     |
| 56  | MG   | DA    | 3133 | 1/1   | 0.83 | 0.41 | 8.17  | 78,78,78,78                 | 0     |
| 64  | PGE  | DD    | 301  | 10/10 | 0.87 | 0.37 | 7.61  | 63,67,72,73                 | 0     |
| 63  | EDO  | DA    | 3198 | 4/4   | 0.92 | 0.35 | 7.45  | 56,57,58,59                 | 0     |
| 56  | MG   | CA    | 3137 | 1/1   | 0.72 | 0.59 | 7.32  | 168,168,168,168             | 0     |
| 59  | PUT  | DA    | 3211 | 6/6   | 0.79 | 0.34 | 6.45  | 65,66,72,74                 | 0     |
| 57  | PG4  | BA    | 1642 | 13/13 | 0.81 | 0.43 | 6.37  | 96,102,107,107              | 0     |
| 65  | SPD  | DA    | 3223 | 10/10 | 0.91 | 0.26 | 6.28  | 40,44,54,55                 | 0     |
| 64  | PGE  | DU    | 101  | 10/10 | 0.87 | 0.50 | 6.16  | 64,72,83,83                 | 0     |
| 62  | PEG  | AL    | 201  | 7/7   | 0.85 | 0.39 | 5.91  | 74,78,85,85                 | 0     |
| 68  | GUN  | DA    | 3210 | 11/11 | 0.77 | 0.38 | 5.76  | 71,73,74,74                 | 0     |
| 56  | MG   | DA    | 3148 | 1/1   | 0.86 | 0.24 | 5.76  | 115,115,115,115             | 0     |
| 56  | MG   | AA    | 1633 | 1/1   | 0.94 | 0.29 | 5.71  | 101,101,101,101             | 0     |
| 63  | EDO  | D1    | 101  | 4/4   | 0.84 | 0.35 | 5.69  | 67,67,68,68                 | 0     |
| 64  | PGE  | DA    | 3224 | 10/10 | 0.78 | 0.33 | 5.46  | 74,81,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-------|-----------------------------|-------|
| 57  | PG4  | AA    | 1670 | 13/13 | 0.77  | 0.30 | 5.28  | 80,92,101,102               | 0     |
| 63  | EDO  | DA    | 3197 | 4/4   | 0.91  | 0.26 | 4.95  | 68,68,69,69                 | 0     |
| 58  | MPD  | DE    | 301  | 8/8   | 0.80  | 0.61 | 4.94  | 102,104,107,109             | 0     |
| 57  | PG4  | DS    | 202  | 13/13 | 0.87  | 0.34 | 4.33  | 43,51,59,61                 | 0     |
| 56  | MG   | CA    | 3151 | 1/1   | 0.76  | 0.36 | 3.80  | 84,84,84,84                 | 0     |
| 56  | MG   | BA    | 1612 | 1/1   | 0.84  | 0.26 | 3.75  | 137,137,137,137             | 0     |
| 62  | PEG  | DL    | 201  | 7/7   | 0.88  | 0.28 | 3.46  | 65,69,76,78                 | 0     |
| 58  | MPD  | AA    | 1671 | 8/8   | 0.92  | 0.53 | 3.40  | 101,103,104,106             | 0     |
| 56  | MG   | DA    | 3038 | 1/1   | 0.93  | 0.22 | 3.04  | 29,29,29,29                 | 0     |
| 56  | MG   | CA    | 3100 | 1/1   | 0.91  | 0.31 | 2.99  | 110,110,110,110             | 0     |
| 56  | MG   | BA    | 1626 | 1/1   | 0.71  | 0.32 | 2.94  | 111,111,111,111             | 0     |
| 56  | MG   | CA    | 3022 | 1/1   | 0.83  | 0.71 | 2.82  | 188,188,188,188             | 0     |
| 65  | SPD  | DA    | 3187 | 10/10 | 0.94  | 0.24 | 2.10  | 38,40,48,50                 | 0     |
| 56  | MG   | AA    | 1661 | 1/1   | 0.63  | 0.33 | 2.09  | 190,190,190,190             | 0     |
| 56  | MG   | AA    | 1657 | 1/1   | 0.85  | 0.48 | 2.01  | 162,162,162,162             | 0     |
| 64  | PGE  | DA    | 3186 | 10/10 | 0.92  | 0.22 | 1.93  | 39,46,49,50                 | 0     |
| 64  | PGE  | DS    | 201  | 10/10 | 0.84  | 0.37 | 1.90  | 56,66,68,69                 | 0     |
| 56  | MG   | CA    | 3037 | 1/1   | 0.96  | 0.42 | 1.85  | 235,235,235,235             | 0     |
| 57  | PG4  | DQ    | 202  | 13/13 | 0.83  | 0.30 | 1.74  | 64,66,71,72                 | 0     |
| 56  | MG   | CA    | 3032 | 1/1   | 0.73  | 0.53 | 1.71  | 269,269,269,269             | 0     |
| 60  | T1C  | AA    | 1677 | 42/42 | 0.92  | 0.25 | 1.35  | 89,96,109,110               | 0     |
| 56  | MG   | DA    | 3023 | 1/1   | 0.98  | 0.21 | 1.31  | 34,34,34,34                 | 0     |
| 56  | MG   | CA    | 3136 | 1/1   | 0.91  | 0.34 | 0.95  | 105,105,105,105             | 0     |
| 59  | PUT  | DA    | 3002 | 6/6   | 0.92  | 0.24 | 0.88  | 45,52,54,55                 | 0     |
| 56  | MG   | DA    | 3032 | 1/1   | 0.98  | 0.23 | 0.88  | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3018 | 1/1   | 0.97  | 0.25 | 0.87  | 29,29,29,29                 | 0     |
| 56  | MG   | CA    | 3105 | 1/1   | 0.69  | 0.40 | 0.78  | 254,254,254,254             | 0     |
| 56  | MG   | AA    | 1611 | 1/1   | 0.71  | 0.26 | 0.77  | 113,113,113,113             | 0     |
| 56  | MG   | DA    | 3014 | 1/1   | 0.99  | 0.25 | 0.43  | 19,19,19,19                 | 0     |
| 56  | MG   | DA    | 3025 | 1/1   | 0.99  | 0.23 | 0.17  | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 1614 | 1/1   | 0.75  | 0.17 | 0.13  | 147,147,147,147             | 0     |
| 56  | MG   | DA    | 3091 | 1/1   | 0.96  | 0.23 | 0.10  | 55,55,55,55                 | 0     |
| 61  | ZN   | AB    | 301  | 1/1   | 0.92  | 0.30 | -0.10 | 209,209,209,209             | 0     |
| 56  | MG   | CA    | 3033 | 1/1   | -0.13 | 0.30 | -0.14 | 200,200,200,200             | 0     |
| 56  | MG   | DA    | 3094 | 1/1   | 0.93  | 0.21 | -0.22 | 35,35,35,35                 | 0     |
| 60  | T1C  | BA    | 1643 | 42/42 | 0.78  | 0.23 | -0.25 | 169,175,185,185             | 0     |
| 56  | MG   | CA    | 3102 | 1/1   | 0.93  | 0.27 | -0.48 | 114,114,114,114             | 0     |
| 56  | MG   | CA    | 3054 | 1/1   | 0.59  | 0.21 | -0.49 | 140,140,140,140             | 0     |
| 56  | MG   | BA    | 1601 | 1/1   | 0.85  | 0.17 | -0.58 | 95,95,95,95                 | 0     |
| 56  | MG   | AA    | 1662 | 1/1   | 0.98  | 0.22 | -0.72 | 110,110,110,110             | 0     |
| 56  | MG   | CA    | 3061 | 1/1   | 0.20  | 0.21 | -0.88 | 274,274,274,274             | 0     |
| 56  | MG   | CA    | 3153 | 1/1   | 0.88  | 0.22 | -0.94 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | BA    | 1624 | 1/1   | 0.67 | 0.26 | -0.97 | 275,275,275,275             | 0     |
| 56  | MG   | CA    | 3011 | 1/1   | 0.92 | 0.28 | -1.02 | 117,117,117,117             | 0     |
| 56  | MG   | AA    | 1679 | 1/1   | 0.74 | 0.25 | -1.04 | 189,189,189,189             | 0     |
| 56  | MG   | DA    | 3067 | 1/1   | 0.98 | 0.19 | -1.04 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3089 | 1/1   | 0.91 | 0.22 | -1.06 | 95,95,95,95                 | 0     |
| 58  | MPD  | DS    | 203  | 8/8   | 0.98 | 0.21 | -1.18 | 37,40,44,47                 | 0     |
| 61  | ZN   | D5    | 101  | 1/1   | 0.95 | 0.15 | -1.29 | 60,60,60,60                 | 0     |
| 56  | MG   | CA    | 3095 | 1/1   | 0.91 | 0.18 | -1.32 | 81,81,81,81                 | 0     |
| 56  | MG   | BA    | 1620 | 1/1   | 0.97 | 0.17 | -1.33 | 97,97,97,97                 | 0     |
| 56  | MG   | DA    | 3024 | 1/1   | 0.99 | 0.20 | -1.35 | 32,32,32,32                 | 0     |
| 56  | MG   | CA    | 3018 | 1/1   | 0.65 | 0.16 | -1.45 | 133,133,133,133             | 0     |
| 56  | MG   | DA    | 3011 | 1/1   | 1.00 | 0.17 | -1.48 | 28,28,28,28                 | 0     |
| 56  | MG   | CA    | 3099 | 1/1   | 0.72 | 0.28 | -1.53 | 235,235,235,235             | 0     |
| 61  | ZN   | C5    | 101  | 1/1   | 0.82 | 0.06 | -1.57 | 148,148,148,148             | 0     |
| 56  | MG   | DA    | 3177 | 1/1   | 0.95 | 0.18 | -1.58 | 68,68,68,68                 | 0     |
| 56  | MG   | CA    | 3103 | 1/1   | 0.91 | 0.15 | -1.65 | 120,120,120,120             | 0     |
| 56  | MG   | DA    | 3113 | 1/1   | 1.00 | 0.22 | -1.91 | 18,18,18,18                 | 0     |
| 56  | MG   | CA    | 3094 | 1/1   | 0.86 | 0.26 | -1.91 | 159,159,159,159             | 0     |
| 56  | MG   | AA    | 1647 | 1/1   | 0.90 | 0.13 | -1.95 | 202,202,202,202             | 0     |
| 56  | MG   | CA    | 3019 | 1/1   | 0.89 | 0.10 | -1.99 | 79,79,79,79                 | 0     |
| 56  | MG   | CA    | 3063 | 1/1   | 0.79 | 0.24 | -2.03 | 207,207,207,207             | 0     |
| 56  | MG   | CA    | 3031 | 1/1   | 0.67 | 0.23 | -2.23 | 127,127,127,127             | 0     |
| 56  | MG   | CA    | 3052 | 1/1   | 0.88 | 0.13 | -2.28 | 97,97,97,97                 | 0     |
| 56  | MG   | BA    | 1622 | 1/1   | 0.82 | 0.12 | -2.41 | 95,95,95,95                 | 0     |
| 56  | MG   | CB    | 201  | 1/1   | 0.78 | 0.10 | -2.48 | 166,166,166,166             | 0     |
| 56  | MG   | CA    | 3079 | 1/1   | 0.65 | 0.16 | -2.49 | 143,143,143,143             | 0     |
| 56  | MG   | CA    | 3009 | 1/1   | 0.81 | 0.16 | -2.52 | 248,248,248,248             | 0     |
| 56  | MG   | DA    | 3010 | 1/1   | 0.98 | 0.14 | -2.53 | 34,34,34,34                 | 0     |
| 56  | MG   | AA    | 1663 | 1/1   | 0.77 | 0.19 | -2.60 | 110,110,110,110             | 0     |
| 56  | MG   | DA    | 3095 | 1/1   | 0.88 | 0.17 | -2.72 | 33,33,33,33                 | 0     |
| 56  | MG   | AA    | 1644 | 1/1   | 0.82 | 0.14 | -2.73 | 94,94,94,94                 | 0     |
| 56  | MG   | BA    | 1617 | 1/1   | 0.90 | 0.14 | -2.81 | 126,126,126,126             | 0     |
| 56  | MG   | DA    | 3047 | 1/1   | 0.99 | 0.19 | -2.86 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 1613 | 1/1   | 0.95 | 0.18 | -2.86 | 78,78,78,78                 | 0     |
| 56  | MG   | CA    | 3006 | 1/1   | 0.78 | 0.19 | -2.97 | 227,227,227,227             | 0     |
| 56  | MG   | DB    | 201  | 1/1   | 0.94 | 0.14 | -3.02 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3065 | 1/1   | 0.85 | 0.17 | -3.04 | 71,71,71,71                 | 0     |
| 56  | MG   | AA    | 1637 | 1/1   | 0.97 | 0.08 | -3.08 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 1610 | 1/1   | 0.84 | 0.08 | -3.23 | 109,109,109,109             | 0     |
| 56  | MG   | CA    | 3051 | 1/1   | 0.85 | 0.13 | -3.28 | 109,109,109,109             | 0     |
| 56  | MG   | CA    | 3101 | 1/1   | 0.90 | 0.11 | -3.29 | 149,149,149,149             | 0     |
| 56  | MG   | CA    | 3024 | 1/1   | 0.97 | 0.17 | -3.33 | 141,141,141,141             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | AA    | 1656 | 1/1   | 0.90 | 0.16 | -3.37 | 149,149,149,149             | 0     |
| 56  | MG   | DA    | 3007 | 1/1   | 0.85 | 0.12 | -3.40 | 112,112,112,112             | 0     |
| 56  | MG   | CA    | 3144 | 1/1   | 0.90 | 0.13 | -3.45 | 83,83,83,83                 | 0     |
| 56  | MG   | BA    | 1632 | 1/1   | 0.91 | 0.12 | -3.64 | 72,72,72,72                 | 0     |
| 56  | MG   | AA    | 1659 | 1/1   | 0.83 | 0.09 | -3.67 | 97,97,97,97                 | 0     |
| 56  | MG   | DA    | 3027 | 1/1   | 0.98 | 0.15 | -3.67 | 71,71,71,71                 | 0     |
| 56  | MG   | CA    | 3044 | 1/1   | 0.81 | 0.18 | -3.70 | 84,84,84,84                 | 0     |
| 56  | MG   | CA    | 3020 | 1/1   | 0.87 | 0.11 | -3.72 | 103,103,103,103             | 0     |
| 56  | MG   | CA    | 3088 | 1/1   | 0.87 | 0.10 | -3.78 | 88,88,88,88                 | 0     |
| 56  | MG   | BA    | 1615 | 1/1   | 0.94 | 0.08 | -3.78 | 76,76,76,76                 | 0     |
| 56  | MG   | AA    | 1629 | 1/1   | 0.96 | 0.14 | -3.84 | 83,83,83,83                 | 0     |
| 56  | MG   | DA    | 3085 | 1/1   | 0.98 | 0.14 | -3.89 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 1608 | 1/1   | 0.73 | 0.13 | -3.92 | 122,122,122,122             | 0     |
| 56  | MG   | DA    | 3098 | 1/1   | 0.96 | 0.09 | -4.12 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3059 | 1/1   | 1.00 | 0.15 | -4.14 | 37,37,37,37                 | 0     |
| 56  | MG   | DD    | 302  | 1/1   | 0.97 | 0.13 | -4.21 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3015 | 1/1   | 0.98 | 0.18 | -4.25 | 18,18,18,18                 | 0     |
| 56  | MG   | CA    | 3040 | 1/1   | 0.85 | 0.09 | -4.41 | 126,126,126,126             | 0     |
| 56  | MG   | CA    | 3086 | 1/1   | 0.86 | 0.17 | -4.41 | 97,97,97,97                 | 0     |
| 56  | MG   | DA    | 3111 | 1/1   | 0.98 | 0.15 | -4.52 | 32,32,32,32                 | 0     |
| 56  | MG   | AA    | 1668 | 1/1   | 0.99 | 0.11 | -4.92 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3030 | 1/1   | 0.99 | 0.14 | -4.93 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3136 | 1/1   | 0.76 | 0.12 | -5.01 | 92,92,92,92                 | 0     |
| 56  | MG   | DA    | 3104 | 1/1   | 0.99 | 0.09 | -5.06 | 42,42,42,42                 | 0     |
| 56  | MG   | AA    | 1631 | 1/1   | 0.98 | 0.06 | -5.12 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3048 | 1/1   | 0.99 | 0.13 | -5.29 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3096 | 1/1   | 0.99 | 0.11 | -5.38 | 61,61,61,61                 | 0     |
| 56  | MG   | CA    | 3013 | 1/1   | 0.70 | 0.18 | -5.57 | 135,135,135,135             | 0     |
| 56  | MG   | BA    | 1605 | 1/1   | 0.97 | 0.09 | -5.59 | 125,125,125,125             | 0     |
| 56  | MG   | DA    | 3060 | 1/1   | 0.99 | 0.11 | -5.72 | 16,16,16,16                 | 0     |
| 56  | MG   | DA    | 3019 | 1/1   | 0.99 | 0.10 | -5.76 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3005 | 1/1   | 0.94 | 0.10 | -5.87 | 81,81,81,81                 | 0     |
| 56  | MG   | DA    | 3151 | 1/1   | 0.84 | 0.10 | -6.17 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 1602 | 1/1   | 0.88 | 0.07 | -6.25 | 100,100,100,100             | 0     |
| 56  | MG   | DA    | 3044 | 1/1   | 0.93 | 0.15 | -6.29 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3072 | 1/1   | 0.99 | 0.09 | -6.59 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 1639 | 1/1   | 0.85 | 0.09 | -6.74 | 132,132,132,132             | 0     |
| 56  | MG   | DA    | 3227 | 1/1   | 0.96 | 0.14 | -6.87 | 45,45,45,45                 | 0     |
| 56  | MG   | AA    | 1643 | 1/1   | 0.94 | 0.14 | -7.22 | 78,78,78,78                 | 0     |
| 56  | MG   | DA    | 3036 | 1/1   | 0.98 | 0.16 | -7.67 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3051 | 1/1   | 1.00 | 0.14 | -7.71 | 17,17,17,17                 | 0     |
| 56  | MG   | DA    | 3064 | 1/1   | 0.99 | 0.08 | -7.81 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56  | MG   | AA    | 1648 | 1/1   | 0.99 | 0.09 | -7.98  | 76,76,76,76                 | 0     |
| 56  | MG   | DA    | 3028 | 1/1   | 0.97 | 0.14 | -8.06  | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3093 | 1/1   | 0.98 | 0.14 | -8.49  | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3100 | 1/1   | 0.97 | 0.14 | -9.26  | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3102 | 1/1   | 0.97 | 0.14 | -9.67  | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3008 | 1/1   | 0.96 | 0.05 | -11.27 | 82,82,82,82                 | 0     |
| 56  | MG   | AA    | 1653 | 1/1   | 0.95 | 0.04 | -12.82 | 75,75,75,75                 | 0     |
| 56  | MG   | DA    | 3103 | 1/1   | 0.91 | 0.12 | -14.10 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 1646 | 1/1   | 0.98 | 0.08 | -17.66 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3110 | 1/1   | 0.99 | 0.19 | -18.38 | 19,19,19,19                 | 0     |
| 56  | MG   | CA    | 3129 | 1/1   | 0.69 | 0.23 | -      | 141,141,141,141             | 0     |
| 56  | MG   | DA    | 3147 | 1/1   | 0.60 | 0.42 | -      | 89,89,89,89                 | 0     |
| 56  | MG   | DA    | 3022 | 1/1   | 0.96 | 0.15 | -      | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3171 | 1/1   | 0.79 | 0.57 | -      | 82,82,82,82                 | 0     |
| 56  | MG   | AA    | 1652 | 1/1   | 0.97 | 0.28 | -      | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3145 | 1/1   | 0.40 | 0.75 | -      | 101,101,101,101             | 0     |
| 56  | MG   | CA    | 3075 | 1/1   | 0.56 | 1.37 | -      | 253,253,253,253             | 0     |
| 56  | MG   | DA    | 3118 | 1/1   | 0.93 | 0.34 | -      | 76,76,76,76                 | 0     |
| 56  | MG   | AA    | 1620 | 1/1   | 0.76 | 0.44 | -      | 83,83,83,83                 | 0     |
| 56  | MG   | AA    | 1613 | 1/1   | 0.71 | 1.50 | -      | 85,85,85,85                 | 0     |
| 63  | EDO  | DA    | 3207 | 4/4   | 0.88 | 0.26 | -      | 58,60,62,63                 | 0     |
| 58  | MPD  | DT    | 202  | 8/8   | 0.73 | 0.41 | -      | 87,88,89,91                 | 0     |
| 56  | MG   | CA    | 3039 | 1/1   | 0.53 | 0.36 | -      | 153,153,153,153             | 0     |
| 56  | MG   | AA    | 1624 | 1/1   | 0.63 | 0.79 | -      | 93,93,93,93                 | 0     |
| 56  | MG   | CA    | 3036 | 1/1   | 0.88 | 0.33 | -      | 203,203,203,203             | 0     |
| 56  | MG   | CA    | 3078 | 1/1   | 0.66 | 0.19 | -      | 195,195,195,195             | 0     |
| 56  | MG   | DA    | 3078 | 1/1   | 0.97 | 0.10 | -      | 38,38,38,38                 | 0     |
| 56  | MG   | AA    | 1627 | 1/1   | 0.62 | 0.56 | -      | 99,99,99,99                 | 0     |
| 56  | MG   | AA    | 1669 | 1/1   | 0.93 | 0.41 | -      | 118,118,118,118             | 0     |
| 58  | MPD  | DT    | 201  | 8/8   | 0.71 | 0.41 | -      | 73,82,84,86                 | 0     |
| 56  | MG   | DA    | 3057 | 1/1   | 0.98 | 0.23 | -      | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 1604 | 1/1   | 0.70 | 0.19 | -      | 182,182,182,182             | 0     |
| 56  | MG   | DA    | 3161 | 1/1   | 0.73 | 0.43 | -      | 78,78,78,78                 | 0     |
| 56  | MG   | DA    | 3043 | 1/1   | 0.96 | 0.08 | -      | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3099 | 1/1   | 0.96 | 0.13 | -      | 78,78,78,78                 | 0     |
| 56  | MG   | DA    | 3026 | 1/1   | 0.98 | 0.10 | -      | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 1606 | 1/1   | 0.72 | 0.21 | -      | 251,251,251,251             | 0     |
| 56  | MG   | CA    | 3087 | 1/1   | 0.93 | 0.07 | -      | 97,97,97,97                 | 0     |
| 56  | MG   | DR    | 203  | 1/1   | 0.92 | 0.42 | -      | 111,111,111,111             | 0     |
| 56  | MG   | DA    | 3135 | 1/1   | 0.95 | 0.27 | -      | 72,72,72,72                 | 0     |
| 56  | MG   | CA    | 3055 | 1/1   | 0.73 | 0.10 | -      | 195,195,195,195             | 0     |
| 56  | MG   | CA    | 3139 | 1/1   | 0.19 | 1.22 | -      | 139,139,139,139             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | AA    | 1616 | 1/1   | 0.51 | 0.93 | -    | 88,88,88,88                 | 0     |
| 56  | MG   | DM    | 201  | 1/1   | 0.96 | 0.06 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3040 | 1/1   | 0.98 | 0.14 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | CA    | 3126 | 1/1   | 0.61 | 0.39 | -    | 136,136,136,136             | 0     |
| 56  | MG   | DA    | 3142 | 1/1   | 0.90 | 0.28 | -    | 79,79,79,79                 | 0     |
| 56  | MG   | CA    | 3021 | 1/1   | 0.87 | 1.09 | -    | 278,278,278,278             | 0     |
| 56  | MG   | DA    | 3071 | 1/1   | 0.98 | 0.06 | -    | 91,91,91,91                 | 0     |
| 56  | MG   | DA    | 3157 | 1/1   | 0.69 | 0.53 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3120 | 1/1   | 0.90 | 0.36 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | AA    | 1625 | 1/1   | 0.81 | 0.31 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | CA    | 3007 | 1/1   | 0.66 | 0.46 | -    | 257,257,257,257             | 0     |
| 56  | MG   | CA    | 3074 | 1/1   | 0.93 | 0.27 | -    | 206,206,206,206             | 0     |
| 56  | MG   | AA    | 1610 | 1/1   | 0.89 | 0.40 | -    | 99,99,99,99                 | 0     |
| 56  | MG   | CA    | 3010 | 1/1   | 0.77 | 0.52 | -    | 231,231,231,231             | 0     |
| 56  | MG   | DA    | 3088 | 1/1   | 0.96 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | CA    | 3005 | 1/1   | 0.44 | 1.14 | -    | 253,253,253,253             | 0     |
| 56  | MG   | CA    | 3071 | 1/1   | 0.62 | 0.20 | -    | 207,207,207,207             | 0     |
| 56  | MG   | CA    | 3085 | 1/1   | 0.95 | 0.12 | -    | 89,89,89,89                 | 0     |
| 56  | MG   | CA    | 3117 | 1/1   | 0.90 | 0.77 | -    | 109,109,109,109             | 0     |
| 56  | MG   | DA    | 3124 | 1/1   | 0.84 | 0.39 | -    | 114,114,114,114             | 0     |
| 56  | MG   | DA    | 3069 | 1/1   | 0.95 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 1630 | 1/1   | 0.92 | 0.15 | -    | 134,134,134,134             | 0     |
| 56  | MG   | CA    | 3145 | 1/1   | 0.79 | 0.38 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | BA    | 1619 | 1/1   | 0.95 | 0.19 | -    | 107,107,107,107             | 0     |
| 56  | MG   | CA    | 3135 | 1/1   | 0.65 | 0.54 | -    | 104,104,104,104             | 0     |
| 56  | MG   | CA    | 3069 | 1/1   | 0.80 | 0.21 | -    | 115,115,115,115             | 0     |
| 56  | MG   | CA    | 3143 | 1/1   | 0.87 | 0.50 | -    | 107,107,107,107             | 0     |
| 56  | MG   | AA    | 1649 | 1/1   | 0.88 | 0.12 | -    | 77,77,77,77                 | 0     |
| 56  | MG   | CA    | 3106 | 1/1   | 0.73 | 0.60 | -    | 103,103,103,103             | 0     |
| 63  | EDO  | DA    | 3208 | 4/4   | 0.75 | 0.48 | -    | 98,99,100,101               | 0     |
| 56  | MG   | CA    | 3148 | 1/1   | 0.77 | 0.79 | -    | 86,86,86,86                 | 1     |
| 56  | MG   | DA    | 3041 | 1/1   | 0.98 | 0.10 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3080 | 1/1   | 0.94 | 0.10 | -    | 109,109,109,109             | 0     |
| 56  | MG   | DA    | 3165 | 1/1   | 0.86 | 0.45 | -    | 69,69,69,69                 | 0     |
| 58  | MPD  | DA    | 3190 | 8/8   | 0.85 | 0.34 | -    | 91,92,93,94                 | 0     |
| 56  | MG   | DA    | 3159 | 1/1   | 0.75 | 0.44 | -    | 80,80,80,80                 | 0     |
| 56  | MG   | BA    | 1645 | 1/1   | 0.92 | 0.05 | -    | 98,98,98,98                 | 0     |
| 56  | MG   | CA    | 3059 | 1/1   | 0.84 | 0.36 | -    | 147,147,147,147             | 0     |
| 56  | MG   | DA    | 3152 | 1/1   | 0.94 | 0.23 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3128 | 1/1   | 0.79 | 0.42 | -    | 87,87,87,87                 | 0     |
| 56  | MG   | DA    | 3101 | 1/1   | 0.98 | 0.22 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | AA    | 1654 | 1/1   | 0.82 | 0.47 | -    | 252,252,252,252             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3073 | 1/1   | 0.95 | 0.28 | -    | 260,260,260,260             | 0     |
| 56  | MG   | DA    | 3049 | 1/1   | 0.96 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | AA    | 1608 | 1/1   | 0.66 | 0.50 | -    | 119,119,119,119             | 0     |
| 56  | MG   | DA    | 3029 | 1/1   | 0.96 | 0.14 | -    | 61,61,61,61                 | 0     |
| 63  | EDO  | DB    | 210  | 4/4   | 0.78 | 0.43 | -    | 85,85,85,86                 | 0     |
| 59  | PUT  | DA    | 3222 | 6/6   | 0.94 | 0.24 | -    | 50,54,55,55                 | 0     |
| 56  | MG   | AA    | 1665 | 1/1   | 0.86 | 0.43 | -    | 168,168,168,168             | 0     |
| 56  | MG   | DA    | 3162 | 1/1   | 0.89 | 0.25 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | CA    | 3034 | 1/1   | 0.62 | 0.17 | -    | 256,256,256,256             | 0     |
| 56  | MG   | AA    | 1678 | 1/1   | 0.95 | 0.16 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | DA    | 3106 | 1/1   | 0.98 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | CA    | 3053 | 1/1   | 0.87 | 0.22 | -    | 108,108,108,108             | 0     |
| 56  | MG   | AA    | 1609 | 1/1   | 0.86 | 0.38 | -    | 107,107,107,107             | 0     |
| 56  | MG   | CA    | 3121 | 1/1   | 0.73 | 0.51 | -    | 101,101,101,101             | 0     |
| 56  | MG   | AA    | 1635 | 1/1   | 0.91 | 0.10 | -    | 100,100,100,100             | 0     |
| 56  | MG   | CA    | 3111 | 1/1   | 0.75 | 1.00 | -    | 159,159,159,159             | 0     |
| 62  | PEG  | DA    | 3199 | 7/7   | 0.87 | 0.44 | -    | 60,64,69,70                 | 0     |
| 56  | MG   | AA    | 1604 | 1/1   | 0.26 | 0.85 | -    | 82,82,82,82                 | 0     |
| 56  | MG   | BA    | 1637 | 1/1   | 0.65 | 0.59 | -    | 93,93,93,93                 | 0     |
| 56  | MG   | AA    | 1650 | 1/1   | 0.95 | 0.09 | -    | 87,87,87,87                 | 0     |
| 56  | MG   | CB    | 202  | 1/1   | 0.85 | 0.12 | -    | 139,139,139,139             | 0     |
| 56  | MG   | CA    | 3154 | 1/1   | 0.57 | 0.44 | -    | 155,155,155,155             | 0     |
| 56  | MG   | DA    | 3070 | 1/1   | 0.95 | 0.15 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | DD    | 303  | 1/1   | 0.85 | 0.36 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | CA    | 3120 | 1/1   | 0.78 | 0.25 | -    | 195,195,195,195             | 0     |
| 56  | MG   | CA    | 3096 | 1/1   | 0.86 | 0.13 | -    | 116,116,116,116             | 0     |
| 56  | MG   | CA    | 3118 | 1/1   | 0.92 | 0.45 | -    | 90,90,90,90                 | 0     |
| 56  | MG   | DA    | 3006 | 1/1   | 0.96 | 0.11 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | AA    | 1628 | 1/1   | 0.30 | 0.96 | -    | 142,142,142,142             | 0     |
| 56  | MG   | DA    | 3166 | 1/1   | 0.90 | 0.86 | -    | 90,90,90,90                 | 0     |
| 56  | MG   | DA    | 3082 | 1/1   | 0.95 | 0.08 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3173 | 1/1   | 0.79 | 0.56 | -    | 81,81,81,81                 | 0     |
| 56  | MG   | CA    | 3004 | 1/1   | 0.87 | 0.23 | -    | 223,223,223,223             | 0     |
| 56  | MG   | DA    | 3138 | 1/1   | 0.33 | 0.39 | -    | 89,89,89,89                 | 0     |
| 56  | MG   | DA    | 3116 | 1/1   | 0.98 | 0.13 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | DA    | 3084 | 1/1   | 0.94 | 0.08 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | CA    | 3119 | 1/1   | 0.82 | 0.73 | -    | 134,134,134,134             | 0     |
| 56  | MG   | DA    | 3146 | 1/1   | 0.95 | 0.16 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | CA    | 3049 | 1/1   | 0.74 | 0.24 | -    | 100,100,100,100             | 0     |
| 56  | MG   | DA    | 3132 | 1/1   | 0.94 | 0.53 | -    | 77,77,77,77                 | 0     |
| 56  | MG   | CA    | 3012 | 1/1   | 0.86 | 0.27 | -    | 130,130,130,130             | 0     |
| 56  | MG   | AA    | 1660 | 1/1   | 0.88 | 0.29 | -    | 286,286,286,286             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3138 | 1/1   | 0.94  | 0.16 | -    | 103,103,103,103             | 0     |
| 56  | MG   | CA    | 3065 | 1/1   | 0.80  | 0.25 | -    | 122,122,122,122             | 0     |
| 56  | MG   | DA    | 3230 | 1/1   | 0.97  | 0.35 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3130 | 1/1   | 0.53  | 0.36 | -    | 87,87,87,87                 | 0     |
| 62  | PEG  | DP    | 201  | 7/7   | 0.78  | 0.53 | -    | 94,94,99,100                | 0     |
| 63  | EDO  | DA    | 3214 | 4/4   | 0.85  | 0.32 | -    | 77,78,79,79                 | 0     |
| 59  | PUT  | AA    | 1675 | 6/6   | 0.64  | 0.61 | -    | 90,92,93,93                 | 0     |
| 56  | MG   | AA    | 1621 | 1/1   | 0.66  | 0.44 | -    | 83,83,83,83                 | 0     |
| 56  | MG   | CA    | 3109 | 1/1   | 0.77  | 0.58 | -    | 93,93,93,93                 | 0     |
| 56  | MG   | AA    | 1618 | 1/1   | 0.74  | 0.83 | -    | 91,91,91,91                 | 0     |
| 56  | MG   | DA    | 3140 | 1/1   | 0.95  | 0.19 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 1639 | 1/1   | 0.62  | 0.63 | -    | 106,106,106,106             | 0     |
| 56  | MG   | DA    | 3083 | 1/1   | 0.97  | 0.09 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | CA    | 3050 | 1/1   | 0.86  | 0.13 | -    | 91,91,91,91                 | 0     |
| 56  | MG   | CA    | 3123 | 1/1   | -0.04 | 0.98 | -    | 188,188,188,188             | 0     |
| 56  | MG   | DA    | 3121 | 1/1   | 0.94  | 0.37 | -    | 91,91,91,91                 | 0     |
| 56  | MG   | DA    | 3079 | 1/1   | 0.97  | 0.07 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 1640 | 1/1   | 0.91  | 0.82 | -    | 156,156,156,156             | 0     |
| 56  | MG   | AA    | 1606 | 1/1   | 0.46  | 0.49 | -    | 120,120,120,120             | 0     |
| 56  | MG   | DA    | 3045 | 1/1   | 0.89  | 0.09 | -    | 85,85,85,85                 | 0     |
| 56  | MG   | BA    | 1609 | 1/1   | 0.91  | 0.16 | -    | 194,194,194,194             | 0     |
| 58  | MPD  | DN    | 201  | 8/8   | 0.83  | 0.41 | -    | 87,89,92,93                 | 0     |
| 56  | MG   | AA    | 1623 | 1/1   | 0.88  | 0.36 | -    | 85,85,85,85                 | 0     |
| 56  | MG   | AA    | 1640 | 1/1   | 0.84  | 0.13 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | CA    | 3081 | 1/1   | 0.93  | 0.17 | -    | 134,134,134,134             | 0     |
| 56  | MG   | CA    | 3107 | 1/1   | 0.80  | 0.72 | -    | 106,106,106,106             | 0     |
| 56  | MG   | CA    | 3015 | 1/1   | 0.93  | 0.26 | -    | 83,83,83,83                 | 0     |
| 56  | MG   | DA    | 3081 | 1/1   | 0.95  | 0.17 | -    | 94,94,94,94                 | 0     |
| 56  | MG   | DA    | 3168 | 1/1   | 0.27  | 0.48 | -    | 108,108,108,108             | 0     |
| 56  | MG   | DA    | 3228 | 1/1   | 0.98  | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3143 | 1/1   | 0.80  | 0.46 | -    | 95,95,95,95                 | 0     |
| 56  | MG   | CA    | 3038 | 1/1   | -0.04 | 0.22 | -    | 268,268,268,268             | 0     |
| 56  | MG   | CA    | 3060 | 1/1   | 0.75  | 0.38 | -    | 242,242,242,242             | 0     |
| 56  | MG   | DA    | 3075 | 1/1   | 0.97  | 0.07 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3141 | 1/1   | 0.98  | 0.22 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | DA    | 3126 | 1/1   | 0.78  | 0.37 | -    | 76,76,76,76                 | 0     |
| 56  | MG   | AA    | 1651 | 1/1   | 0.93  | 0.13 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | CA    | 3014 | 1/1   | 0.72  | 0.18 | -    | 262,262,262,262             | 0     |
| 56  | MG   | DA    | 3108 | 1/1   | 0.95  | 0.18 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3178 | 1/1   | 0.55  | 0.68 | -    | 101,101,101,101             | 0     |
| 64  | PGE  | DA    | 3216 | 10/10 | 0.87  | 0.39 | -    | 62,64,65,65                 | 0     |
| 56  | MG   | DA    | 3061 | 1/1   | 0.99  | 0.15 | -    | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3001 | 1/1   | 0.77  | 0.38 | -    | 299,299,299,299             | 0     |
| 56  | MG   | CA    | 3017 | 1/1   | 0.86  | 0.10 | -    | 106,106,106,106             | 0     |
| 56  | MG   | CA    | 3083 | 1/1   | 0.81  | 0.34 | -    | 241,241,241,241             | 0     |
| 56  | MG   | AA    | 1636 | 1/1   | 0.91  | 0.28 | -    | 97,97,97,97                 | 0     |
| 56  | MG   | CA    | 3149 | 1/1   | 0.09  | 1.21 | -    | 92,92,92,92                 | 0     |
| 56  | MG   | DA    | 3087 | 1/1   | 0.99  | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3097 | 1/1   | 0.95  | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | DR    | 201  | 1/1   | 0.92  | 0.60 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3020 | 1/1   | 0.96  | 0.32 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | CA    | 3070 | 1/1   | 0.93  | 0.08 | -    | 112,112,112,112             | 0     |
| 56  | MG   | CA    | 3084 | 1/1   | 0.91  | 0.34 | -    | 208,208,208,208             | 0     |
| 56  | MG   | CA    | 3098 | 1/1   | 0.85  | 0.13 | -    | 110,110,110,110             | 0     |
| 56  | MG   | DA    | 3034 | 1/1   | 0.98  | 0.17 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | CA    | 3091 | 1/1   | 0.94  | 0.10 | -    | 96,96,96,96                 | 0     |
| 56  | MG   | BA    | 1623 | 1/1   | 0.67  | 1.43 | -    | 235,235,235,235             | 0     |
| 56  | MG   | DA    | 3164 | 1/1   | 0.94  | 0.32 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | CA    | 3155 | 1/1   | 0.82  | 0.31 | -    | 204,204,204,204             | 0     |
| 56  | MG   | CA    | 3048 | 1/1   | 0.83  | 0.17 | -    | 107,107,107,107             | 0     |
| 56  | MG   | AA    | 1645 | 1/1   | 0.98  | 0.12 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | DB    | 202  | 1/1   | 0.97  | 0.13 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | CA    | 3132 | 1/1   | 0.62  | 0.75 | -    | 152,152,152,152             | 0     |
| 56  | MG   | DA    | 3174 | 1/1   | 0.86  | 0.30 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | DA    | 3180 | 1/1   | 0.14  | 1.25 | -    | 97,97,97,97                 | 0     |
| 56  | MG   | AA    | 1622 | 1/1   | -0.16 | 1.84 | -    | 130,130,130,130             | 0     |
| 56  | MG   | DA    | 3139 | 1/1   | 0.95  | 0.40 | -    | 64,64,64,64                 | 1     |
| 56  | MG   | DA    | 3056 | 1/1   | 0.99  | 0.17 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | AA    | 1601 | 1/1   | 0.87  | 1.44 | -    | 104,104,104,104             | 0     |
| 56  | MG   | CA    | 3097 | 1/1   | 0.54  | 0.16 | -    | 125,125,125,125             | 0     |
| 56  | MG   | DA    | 3129 | 1/1   | 0.88  | 1.13 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3077 | 1/1   | 0.97  | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | DB    | 207  | 1/1   | 0.47  | 0.77 | -    | 105,105,105,105             | 0     |
| 56  | MG   | DA    | 3131 | 1/1   | 0.32  | 0.76 | -    | 87,87,87,87                 | 0     |
| 59  | PUT  | DA    | 3188 | 6/6   | 0.94  | 0.22 | -    | 32,35,40,41                 | 0     |
| 56  | MG   | CA    | 3064 | 1/1   | 0.87  | 0.57 | -    | 267,267,267,267             | 0     |
| 56  | MG   | DA    | 3016 | 1/1   | 0.93  | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | CA    | 3029 | 1/1   | 0.90  | 0.36 | -    | 177,177,177,177             | 0     |
| 56  | MG   | CA    | 3067 | 1/1   | 0.82  | 0.45 | -    | 289,289,289,289             | 0     |
| 63  | EDO  | DA    | 3003 | 4/4   | 0.88  | 0.52 | -    | 64,64,66,67                 | 0     |
| 56  | MG   | DA    | 3137 | 1/1   | 0.96  | 0.26 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 1635 | 1/1   | 0.92  | 0.10 | -    | 111,111,111,111             | 0     |
| 56  | MG   | CA    | 3104 | 1/1   | 0.13  | 0.32 | -    | 263,263,263,263             | 0     |
| 56  | MG   | BA    | 1636 | 1/1   | 0.88  | 0.64 | -    | 172,172,172,172             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3023 | 1/1   | 0.82 | 0.14 | -    | 150,150,150,150             | 0     |
| 56  | MG   | AA    | 1638 | 1/1   | 0.97 | 0.09 | -    | 103,103,103,103             | 0     |
| 56  | MG   | CA    | 3035 | 1/1   | 0.89 | 0.26 | -    | 158,158,158,158             | 0     |
| 56  | MG   | DA    | 3117 | 1/1   | 0.96 | 0.11 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | CA    | 3008 | 1/1   | 0.82 | 0.10 | -    | 179,179,179,179             | 0     |
| 56  | MG   | CA    | 3076 | 1/1   | 0.69 | 0.22 | -    | 213,213,213,213             | 0     |
| 56  | MG   | CA    | 3141 | 1/1   | 0.20 | 0.60 | -    | 109,109,109,109             | 0     |
| 59  | PUT  | DA    | 3184 | 6/6   | 0.85 | 0.37 | -    | 42,48,50,51                 | 0     |
| 56  | MG   | CA    | 3130 | 1/1   | 0.18 | 1.11 | -    | 141,141,141,141             | 0     |
| 56  | MG   | AA    | 1615 | 1/1   | 0.67 | 0.55 | -    | 90,90,90,90                 | 0     |
| 56  | MG   | DA    | 3050 | 1/1   | 0.96 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 1638 | 1/1   | 0.59 | 0.93 | -    | 110,110,110,110             | 0     |
| 56  | MG   | CA    | 3142 | 1/1   | 0.03 | 0.56 | -    | 133,133,133,133             | 0     |
| 56  | MG   | DA    | 3089 | 1/1   | 0.98 | 0.08 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | CA    | 3152 | 1/1   | 0.88 | 0.45 | -    | 215,215,215,215             | 0     |
| 56  | MG   | CA    | 3057 | 1/1   | 0.81 | 0.16 | -    | 132,132,132,132             | 0     |
| 56  | MG   | DA    | 3176 | 1/1   | 0.83 | 0.32 | -    | 93,93,93,93                 | 0     |
| 63  | EDO  | DA    | 3194 | 4/4   | 0.84 | 0.30 | -    | 51,56,59,60                 | 0     |
| 56  | MG   | CA    | 3066 | 1/1   | 0.82 | 0.14 | -    | 125,125,125,125             | 0     |
| 56  | MG   | CA    | 3116 | 1/1   | 0.90 | 0.81 | -    | 89,89,89,89                 | 0     |
| 56  | MG   | DA    | 3033 | 1/1   | 0.99 | 0.19 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3021 | 1/1   | 0.94 | 0.07 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3066 | 1/1   | 0.98 | 0.19 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 1616 | 1/1   | 0.97 | 0.17 | -    | 149,149,149,149             | 0     |
| 56  | MG   | DA    | 3122 | 1/1   | 0.92 | 0.32 | -    | 80,80,80,80                 | 0     |
| 56  | MG   | BA    | 1607 | 1/1   | 0.86 | 0.38 | -    | 162,162,162,162             | 0     |
| 56  | MG   | AA    | 1664 | 1/1   | 0.87 | 0.35 | -    | 186,186,186,186             | 0     |
| 63  | EDO  | DA    | 3004 | 4/4   | 0.76 | 0.46 | -    | 107,107,108,109             | 0     |
| 56  | MG   | DA    | 3107 | 1/1   | 0.98 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3154 | 1/1   | 0.87 | 0.46 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | DB    | 209  | 1/1   | 0.96 | 0.49 | -    | 80,80,80,80                 | 0     |
| 56  | MG   | CA    | 3043 | 1/1   | 0.92 | 0.15 | -    | 101,101,101,101             | 0     |
| 56  | MG   | DA    | 3119 | 1/1   | 0.94 | 0.11 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | AA    | 1603 | 1/1   | 0.20 | 1.10 | -    | 119,119,119,119             | 0     |
| 56  | MG   | DA    | 3068 | 1/1   | 0.98 | 0.11 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3052 | 1/1   | 0.99 | 0.15 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | CA    | 3125 | 1/1   | 0.85 | 0.27 | -    | 141,141,141,141             | 0     |
| 56  | MG   | DA    | 3170 | 1/1   | 0.76 | 0.40 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | AA    | 1619 | 1/1   | 0.90 | 0.27 | -    | 92,92,92,92                 | 0     |
| 56  | MG   | CA    | 3068 | 1/1   | 0.53 | 0.43 | -    | 253,253,253,253             | 0     |
| 56  | MG   | BA    | 1633 | 1/1   | 0.90 | 0.27 | -    | 235,235,235,235             | 0     |
| 56  | MG   | BA    | 1630 | 1/1   | 0.29 | 0.15 | -    | 221,221,221,221             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 1634 | 1/1   | 0.90 | 0.07 | -    | 116,116,116,116             | 0     |
| 56  | MG   | CA    | 3058 | 1/1   | 0.85 | 0.40 | -    | 135,135,135,135             | 0     |
| 56  | MG   | DA    | 3013 | 1/1   | 0.96 | 0.13 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | DA    | 3105 | 1/1   | 0.96 | 0.19 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3156 | 1/1   | 0.89 | 0.34 | -    | 74,74,74,74                 | 0     |
| 67  | ACY  | DA    | 3191 | 4/4   | 0.95 | 0.27 | -    | 56,57,58,59                 | 0     |
| 56  | MG   | CA    | 3127 | 1/1   | 0.90 | 0.12 | -    | 85,85,85,85                 | 0     |
| 56  | MG   | DA    | 3179 | 1/1   | 0.35 | 0.48 | -    | 102,102,102,102             | 0     |
| 56  | MG   | DB    | 203  | 1/1   | 0.97 | 0.05 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | DB    | 204  | 1/1   | 0.99 | 0.15 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3062 | 1/1   | 0.98 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | CA    | 3134 | 1/1   | 0.54 | 0.52 | -    | 204,204,204,204             | 0     |
| 56  | MG   | DA    | 3158 | 1/1   | 0.96 | 0.17 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | CA    | 3093 | 1/1   | 0.79 | 0.23 | -    | 123,123,123,123             | 0     |
| 56  | MG   | CA    | 3115 | 1/1   | 0.64 | 0.46 | -    | 108,108,108,108             | 0     |
| 56  | MG   | CA    | 3112 | 1/1   | 0.82 | 0.33 | -    | 110,110,110,110             | 0     |
| 62  | PEG  | DA    | 3225 | 7/7   | 0.76 | 0.39 | -    | 62,65,70,70                 | 0     |
| 56  | MG   | CA    | 3113 | 1/1   | 0.30 | 0.78 | -    | 94,94,94,94                 | 0     |
| 56  | MG   | DA    | 3167 | 1/1   | 0.72 | 0.40 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | DA    | 3169 | 1/1   | 0.85 | 0.33 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | AA    | 1617 | 1/1   | 0.68 | 0.36 | -    | 98,98,98,98                 | 0     |
| 56  | MG   | DA    | 3155 | 1/1   | 0.73 | 0.58 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | CA    | 3122 | 1/1   | 0.61 | 0.78 | -    | 136,136,136,136             | 0     |
| 56  | MG   | CA    | 3077 | 1/1   | 0.00 | 0.48 | -    | 252,252,252,252             | 0     |
| 56  | MG   | DA    | 3031 | 1/1   | 0.97 | 0.21 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3153 | 1/1   | 0.82 | 0.33 | -    | 100,100,100,100             | 0     |
| 56  | MG   | BA    | 1631 | 1/1   | 0.80 | 0.07 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | DA    | 3175 | 1/1   | 0.87 | 0.50 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | DA    | 3160 | 1/1   | 0.93 | 0.12 | -    | 72,72,72,72                 | 0     |
| 57  | PG4  | DR    | 202  | 13/13 | 0.84 | 0.46 | -    | 61,63,75,75                 | 0     |
| 56  | MG   | AA    | 1667 | 1/1   | 0.97 | 0.12 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 1666 | 1/1   | 0.96 | 0.05 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | CA    | 3042 | 1/1   | 0.93 | 0.12 | -    | 91,91,91,91                 | 0     |
| 56  | MG   | DA    | 3181 | 1/1   | 0.83 | 0.71 | -    | 91,91,91,91                 | 0     |
| 56  | MG   | CA    | 3027 | 1/1   | 0.63 | 0.31 | -    | 137,137,137,137             | 0     |
| 56  | MG   | DA    | 3012 | 1/1   | 1.00 | 0.09 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3144 | 1/1   | 0.95 | 0.37 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | CA    | 3072 | 1/1   | 0.82 | 0.87 | -    | 272,272,272,272             | 0     |
| 56  | MG   | CA    | 3062 | 1/1   | 0.87 | 0.19 | -    | 237,237,237,237             | 0     |
| 56  | MG   | AA    | 1655 | 1/1   | 0.81 | 0.16 | -    | 115,115,115,115             | 0     |
| 56  | MG   | DA    | 3053 | 1/1   | 0.93 | 0.12 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | DA    | 3086 | 1/1   | 0.98 | 0.12 | -    | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3090 | 1/1   | 0.96  | 0.18 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | AA    | 1626 | 1/1   | 0.04  | 1.41 | -    | 111,111,111,111             | 0     |
| 56  | MG   | CA    | 3002 | 1/1   | 0.38  | 0.31 | -    | 259,259,259,259             | 0     |
| 56  | MG   | AA    | 1614 | 1/1   | 0.34  | 0.20 | -    | 131,131,131,131             | 0     |
| 56  | MG   | BA    | 1618 | 1/1   | 0.82  | 0.19 | -    | 106,106,106,106             | 0     |
| 56  | MG   | AA    | 1658 | 1/1   | 0.93  | 0.10 | -    | 100,100,100,100             | 0     |
| 56  | MG   | BA    | 1621 | 1/1   | 0.95  | 0.20 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3156 | 1/1   | 0.09  | 0.18 | -    | 246,246,246,246             | 0     |
| 58  | MPD  | DA    | 3209 | 8/8   | 0.88  | 0.31 | -    | 68,70,70,71                 | 0     |
| 56  | MG   | CA    | 3140 | 1/1   | -0.34 | 0.60 | -    | 147,147,147,147             | 0     |
| 56  | MG   | DA    | 3134 | 1/1   | 0.62  | 0.37 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | DA    | 3076 | 1/1   | 0.95  | 0.19 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3039 | 1/1   | 0.98  | 0.12 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | BA    | 1641 | 1/1   | 0.59  | 0.95 | -    | 140,140,140,140             | 0     |
| 56  | MG   | CA    | 3030 | 1/1   | 0.87  | 0.15 | -    | 124,124,124,124             | 0     |
| 56  | MG   | DA    | 3150 | 1/1   | 0.95  | 0.18 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | CA    | 3090 | 1/1   | 0.59  | 0.57 | -    | 215,215,215,215             | 0     |
| 56  | MG   | BA    | 1603 | 1/1   | 0.81  | 0.69 | -    | 261,261,261,261             | 0     |
| 56  | MG   | CA    | 3092 | 1/1   | 0.50  | 0.23 | -    | 202,202,202,202             | 0     |
| 56  | MG   | BA    | 1644 | 1/1   | 0.91  | 0.12 | -    | 97,97,97,97                 | 0     |
| 56  | MG   | DB    | 208  | 1/1   | 0.95  | 0.26 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | AA    | 1632 | 1/1   | 0.63  | 0.08 | -    | 124,124,124,124             | 0     |
| 56  | MG   | CA    | 3108 | 1/1   | 0.68  | 0.52 | -    | 109,109,109,109             | 0     |
| 56  | MG   | DA    | 3112 | 1/1   | 0.84  | 0.44 | -    | 293,293,293,293             | 0     |
| 56  | MG   | CA    | 3041 | 1/1   | 0.94  | 0.19 | -    | 71,71,71,71                 | 0     |
| 62  | PEG  | DA    | 3226 | 7/7   | 0.86  | 0.33 | -    | 58,59,65,67                 | 0     |
| 56  | MG   | AA    | 1605 | 1/1   | 0.58  | 0.71 | -    | 99,99,99,99                 | 0     |
| 56  | MG   | CA    | 3025 | 1/1   | 0.98  | 0.28 | -    | 105,105,105,105             | 0     |
| 56  | MG   | DA    | 3017 | 1/1   | 0.97  | 0.13 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3028 | 1/1   | 0.14  | 0.75 | -    | 283,283,283,283             | 0     |
| 56  | MG   | CB    | 203  | 1/1   | 0.70  | 0.10 | -    | 155,155,155,155             | 0     |
| 56  | MG   | DB    | 205  | 1/1   | 0.95  | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3114 | 1/1   | 0.95  | 0.47 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3114 | 1/1   | 0.97  | 0.11 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3149 | 1/1   | 0.89  | 0.28 | -    | 77,77,77,77                 | 0     |
| 56  | MG   | BA    | 1628 | 1/1   | 0.92  | 0.18 | -    | 111,111,111,111             | 0     |
| 56  | MG   | DA    | 3229 | 1/1   | 0.94  | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3054 | 1/1   | 0.98  | 0.09 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | CA    | 3150 | 1/1   | 0.90  | 0.50 | -    | 82,82,82,82                 | 0     |
| 63  | EDO  | DB    | 211  | 4/4   | 0.90  | 0.23 | -    | 73,73,74,75                 | 0     |
| 56  | MG   | BA    | 1627 | 1/1   | 0.84  | 0.77 | -    | 129,129,129,129             | 0     |
| 56  | MG   | DA    | 3074 | 1/1   | 0.98  | 0.15 | -    | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3092 | 1/1   | 0.99 | 0.17 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3055 | 1/1   | 0.98 | 0.08 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3009 | 1/1   | 0.95 | 0.12 | -    | 102,102,102,102             | 0     |
| 69  | TRS  | DA    | 3219 | 8/8   | 0.76 | 0.55 | -    | 98,99,102,104               | 0     |
| 56  | MG   | CA    | 3056 | 1/1   | 0.35 | 0.72 | -    | 100,100,100,100             | 0     |
| 56  | MG   | AA    | 1641 | 1/1   | 0.96 | 0.08 | -    | 92,92,92,92                 | 0     |
| 56  | MG   | CA    | 3045 | 1/1   | 0.90 | 0.07 | -    | 93,93,93,93                 | 0     |
| 56  | MG   | DA    | 3035 | 1/1   | 1.00 | 0.18 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | BA    | 1611 | 1/1   | 0.98 | 0.11 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | CA    | 3016 | 1/1   | 0.74 | 0.34 | -    | 148,148,148,148             | 0     |
| 56  | MG   | CA    | 3082 | 1/1   | 0.78 | 0.45 | -    | 160,160,160,160             | 0     |
| 56  | MG   | CA    | 3124 | 1/1   | 0.35 | 0.53 | -    | 202,202,202,202             | 0     |
| 58  | MPD  | DK    | 201  | 8/8   | 0.81 | 0.27 | -    | 93,94,95,95                 | 0     |
| 56  | MG   | CA    | 3146 | 1/1   | 0.26 | 0.37 | -    | 247,247,247,247             | 0     |
| 56  | MG   | DB    | 206  | 1/1   | 0.56 | 0.47 | -    | 102,102,102,102             | 0     |
| 56  | MG   | DA    | 3046 | 1/1   | 0.97 | 0.08 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 1629 | 1/1   | 0.52 | 0.58 | -    | 157,157,157,157             | 0     |
| 56  | MG   | DA    | 3063 | 1/1   | 0.85 | 0.13 | -    | 222,222,222,222             | 0     |
| 56  | MG   | DA    | 3058 | 1/1   | 0.99 | 0.08 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3109 | 1/1   | 0.97 | 0.10 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3073 | 1/1   | 0.98 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3115 | 1/1   | 0.96 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3080 | 1/1   | 0.85 | 0.34 | -    | 186,186,186,186             | 0     |
| 56  | MG   | DA    | 3042 | 1/1   | 0.99 | 0.16 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | AA    | 1634 | 1/1   | 0.91 | 0.19 | -    | 108,108,108,108             | 0     |
| 67  | ACY  | DA    | 3196 | 4/4   | 0.77 | 0.32 | -    | 75,79,79,80                 | 0     |
| 56  | MG   | DA    | 3037 | 1/1   | 0.98 | 0.23 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 1625 | 1/1   | 0.76 | 0.39 | -    | 274,274,274,274             | 0     |
| 56  | MG   | AA    | 1602 | 1/1   | 0.64 | 0.55 | -    | 88,88,88,88                 | 0     |
| 56  | MG   | CA    | 3046 | 1/1   | 0.97 | 0.14 | -    | 143,143,143,143             | 0     |
| 56  | MG   | CA    | 3047 | 1/1   | 0.59 | 1.51 | -    | 240,240,240,240             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.