



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:50 PM UTC

PDB ID : 6ORD / pdb\_00006ord  
Title : Crystal structure of tRNA<sup>Ala</sup>(GGC) U32-A38 bound to cognate 70S A site  
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.  
Deposited on : 2019-04-30  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

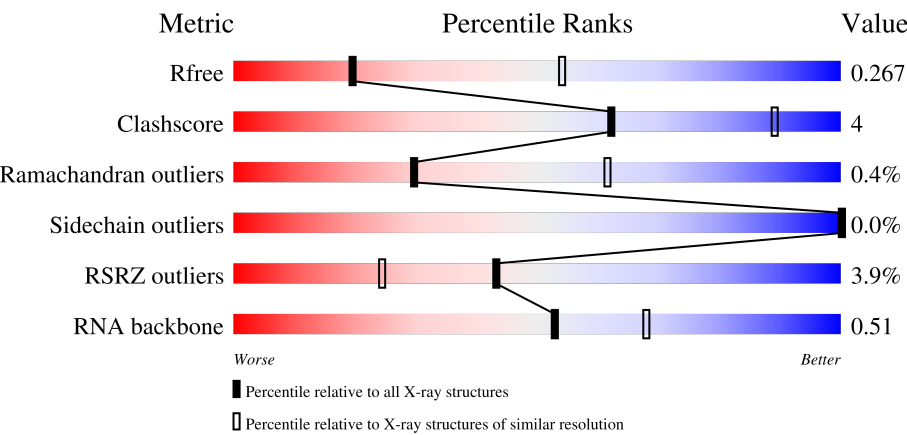
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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 <sub>free</sub>     | 180053                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |
| RNA backbone          | 3983                        | 1022 (3.32-2.88)                                      |

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

| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|-----------------------------------------------|
| 1   | QA    | 1522   | <div><div>5%</div><div>70%25%..</div></div>   |
| 1   | XA    | 1522   | <div><div>5%</div><div>70%26%..</div></div>   |
| 2   | QB    | 256    | <div><div>5%</div><div>68%20%•10%</div></div> |
| 2   | XB    | 256    | <div><div>3%</div><div>73%17%•10%</div></div> |

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | XO    | 89     |                  |
| 16  | QP    | 88     |                  |
| 16  | XP    | 88     |                  |
| 17  | QQ    | 105    |                  |
| 17  | XQ    | 105    |                  |
| 18  | QR    | 88     |                  |
| 18  | XR    | 88     |                  |
| 19  | QS    | 93     |                  |
| 19  | XS    | 93     |                  |
| 20  | QT    | 106    |                  |
| 20  | XT    | 106    |                  |
| 21  | QU    | 27     |                  |
| 21  | XU    | 27     |                  |
| 22  | QV    | 77     |                  |
| 22  | XV    | 77     |                  |
| 23  | QX    | 19     |                  |
| 23  | XX    | 19     |                  |
| 24  | QY    | 76     |                  |
| 24  | XY    | 76     |                  |
| 25  | R0    | 85     |                  |
| 25  | Y0    | 85     |                  |
| 26  | R1    | 98     |                  |
| 26  | Y1    | 98     |                  |
| 27  | R2    | 72     |                  |
| 27  | Y2    | 72     |                  |

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| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 28  | R3    | 60     | <div> <div>5%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>                 |
| 28  | Y3    | 60     | <div> <div>7%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>                 |
| 29  | R4    | 71     | <div> <div>%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>                  |
| 29  | Y4    | 71     | <div> <div>13%</div> <div>65%</div> <div>25%</div> <div>6%</div> <div>..</div> </div> |
| 30  | R5    | 60     | <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div>                   |
| 30  | Y5    | 60     | <div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>                 |
| 31  | R6    | 54     | <div> <div>2%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>                  |
| 31  | Y6    | 54     | <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div>                   |
| 32  | R7    | 49     | <div> <div>8%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>                 |
| 32  | Y7    | 49     | <div> <div>6%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>                 |
| 33  | R8    | 65     | <div> <div>9%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>                 |
| 33  | Y8    | 65     | <div> <div>9%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>                 |
| 34  | R9    | 37     | <div> <div>14%</div> <div>78%</div> <div>22%</div> <div></div> </div>                 |
| 34  | Y9    | 37     | <div> <div>3%</div> <div>70%</div> <div>30%</div> <div></div> </div>                  |
| 35  | RA    | 2915   | <div> <div>2%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>                |
| 35  | YA    | 2915   | <div> <div>2%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>                |
| 36  | RB    | 122    | <div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>                  |
| 36  | YB    | 122    | <div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>                  |
| 37  | RD    | 276    | <div> <div>5%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>                 |
| 37  | YD    | 276    | <div> <div>2%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>                 |
| 38  | RE    | 206    | <div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>                 |
| 38  | YE    | 206    | <div> <div>3%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>                 |
| 39  | RF    | 210    | <div> <div>2%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>                 |
| 39  | YF    | 210    | <div> <div>%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>                  |
| 40  | RG    | 182    | <div> <div>4%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>                |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | YG    | 182    |                  |
| 41  | RH    | 180    |                  |
| 41  | YH    | 180    |                  |
| 42  | RI    | 148    |                  |
| 42  | YI    | 148    |                  |
| 43  | RN    | 140    |                  |
| 43  | YN    | 140    |                  |
| 44  | RO    | 122    |                  |
| 44  | YO    | 122    |                  |
| 45  | RP    | 150    |                  |
| 45  | YP    | 150    |                  |
| 46  | RQ    | 141    |                  |
| 46  | YQ    | 141    |                  |
| 47  | RR    | 118    |                  |
| 47  | YR    | 118    |                  |
| 48  | RS    | 112    |                  |
| 48  | YS    | 112    |                  |
| 49  | RT    | 146    |                  |
| 49  | YT    | 146    |                  |
| 50  | RU    | 118    |                  |
| 50  | YU    | 118    |                  |
| 51  | RV    | 101    |                  |
| 51  | YV    | 101    |                  |
| 52  | RW    | 113    |                  |
| 52  | YW    | 113    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | RX    | 96     |                  |
| 53  | YX    | 96     |                  |
| 54  | RY    | 110    |                  |
| 54  | YY    | 110    |                  |
| 55  | RZ    | 206    |                  |
| 55  | YZ    | 206    |                  |

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   | QA    | 1703 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1795 | -         | -        | -       | X                |
| 56  | MG   | QO    | 101  | -         | -        | -       | X                |
| 56  | MG   | RA    | 3011 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3027 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3053 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3063 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3069 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3072 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3080 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3104 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3152 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3153 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3159 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3173 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3175 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3192 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3201 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3205 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3221 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3256 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3269 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3311 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3322 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3350 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3363 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3381 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | RA    | 3383 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3395 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3401 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3416 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3417 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3424 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3450 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3460 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3469 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3482 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3499 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3511 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3514 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3526 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3591 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3641 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3647 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3654 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3673 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1718 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1778 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3066 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3119 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3201 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3400 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3412 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3478 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3499 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3512 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3547 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3697 | -         | -        | -       | X                |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293819 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | QA    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14358 | 5975 | 10413 | 1500 |         |         |       |
| 1   | XA    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32331 | 14396 | 5990 | 10441 | 1504 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | QB    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1842  | 1175 | 330 | 332 | 5 |         |         |       |
| 2   | XB    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1167 | 326 | 327 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | QC    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1558  | 979 | 305 | 273 | 1 |         |         |       |
| 3   | XC    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1542  | 968 | 300 | 273 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | QD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1665  | 1043 | 329 | 286 | 7 |         |         |       |
| 4   | XD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1047 | 330 | 284 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | QE    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |
| 5   | XE    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | QF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 814   | 516 | 144 | 151 | 3 |         |         |       |
| 6   | XF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | QG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |
| 7   | XG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1229  | 766 | 241 | 216 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | QH    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1098  | 694 | 210 | 192 | 2 |         |         |       |
| 8   | XH    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | QI    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 986   | 625 | 193 | 168 |  |         |         |       |
| 9   | XI    | 126      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 966   | 613 | 186 | 167 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 10  | QJ    | 97       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 719   | 446 | 142 | 131 |  |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10  | XJ    | 96       | Total | C   | N   | O   |         |         |       |
|     |       |          | 710   | 442 | 137 | 131 | 0       | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 11  | QK    | 114      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 834   | 520 | 156 | 155 | 3       | 0       | 0     |
| 11  | XK    | 114      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 833   | 519 | 156 | 155 | 3       | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12  | QL    | 122      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 932   | 586 | 185 | 159 | 2       | 0       | 0     |
| 12  | XL    | 122      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 932   | 586 | 185 | 159 | 2       | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 13  | QM    | 116      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 914   | 564 | 189 | 159 | 2       | 0       | 0     |
| 13  | XM    | 114      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 895   | 550 | 186 | 157 | 2       | 0       | 0     |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15  | QO    | 88       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 728   | 456 | 144 | 126 | 2       | 0       | 0     |
| 15  | XO    | 88       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 728   | 456 | 144 | 126 | 2       | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | QP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 433 | 134 | 113 | 1 |         |         |       |
| 16  | XP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 677   | 430 | 133 | 113 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | QQ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |
| 17  | XQ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | QR    | 68       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |         |         |       |
| 18  | XR    | 68       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | QS    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 415 | 120 | 111 | 2 |         |         |       |
| 19  | XS    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 410 | 118 | 115 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | QT    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 732   | 449 | 157 | 124 | 2 |         |         |       |
| 20  | XT    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 451 | 154 | 126 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | QU    | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |
| 21  | XU    | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |

- Molecule 22 is a RNA chain called P-site tRNA<sup>fMet</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | QV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | XV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |

- Molecule 23 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 23  | QX    | 18       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 394   | 176 | 80 | 120 | 18 |         |         |       |
| 23  | XX    | 18       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 394   | 176 | 80 | 120 | 18 |         |         |       |

- Molecule 24 is a RNA chain called A-site tRNA<sup>Ala</sup>(GGC) U32-A38.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 24  | QY    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1625  | 724 | 293 | 532 | 76 |         |         |       |
| 24  | XY    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1625  | 724 | 293 | 532 | 76 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | R0    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |
| 25  | Y0    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | R1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 475 | 148 | 130 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | Y1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 149 | 131 | 1 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | R2    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 27  | Y2    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 592   | 368 | 119 | 103 | 2 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 28  | R3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 28  | Y3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 464   | 296 | 90 | 78 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | R4    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 546   | 346 | 96 | 99 | 5 |         |         |       |
| 29  | Y4    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 536   | 342 | 98 | 91 | 5 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | R5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 30  | Y5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | R6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 31  | Y6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 279 | 91 | 75 | 4 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32  | R7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 32  | Y7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | R8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 33  | Y8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 34  | R9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 34  | Y9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 35 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 35  | RA    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61758 | 27491 | 11552 | 19850 | 2865 |         |         |       |
| 35  | YA    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61758 | 27491 | 11552 | 19850 | 2865 |         |         |       |

- Molecule 36 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 36  | RB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2572  | 1145 | 476 | 832 | 119 |         |         |       |
| 36  | YB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 37  | RD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2131  | 1346 | 422 | 360 | 3 |         |         |       |
| 37  | YD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | RE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |
| 38  | YE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39  | RF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1583  | 1009 | 297 | 275 | 2 |         |         |       |
| 39  | YF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1579  | 1007 | 296 | 274 | 2 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | RG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 916 | 253 | 253 | 4 |         |         |       |
| 40  | YG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 912 | 259 | 249 | 4 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | RH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 41  | YH    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 842 | 247 | 234 | 1 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | RI    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 699 | 191 | 203 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | YI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 687 | 186 | 202 | 1 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | RN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 722 | 208 | 187 | 4 |         |         |       |
| 43  | YN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | RO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 44  | YO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | RP    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |
| 45  | YP    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | RQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 46  | YQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | RR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 47  | YR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 48  | RS    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |         |         |       |
| 48  | YS    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | RT    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1091  | 680 | 225 | 185 | 1 |         |         |       |
| 49  | YT    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 675 | 224 | 183 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | RU    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |
| 50  | YU    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | RV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 498 | 141 | 135 | 1 |         |         |       |
| 51  | YV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | RW    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |
| 52  | YW    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | RX    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |
| 53  | YX    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | RY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 520 | 153 | 131 | 6 |         |         |       |
| 54  | YY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | RZ    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 898 | 253 | 253 | 2 |         |         |       |
| 55  | YZ    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1381  | 885 | 246 | 248 | 2 |         |         |       |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56  | QA    | 221      | Total | Mg  | 0       | 0       |
|     |       |          | 221   | 221 |         |         |
| 56  | QB    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | QD    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 56  | QE    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 56  | QF    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 56  | QG    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 56  | QH    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 56  | QI    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | QK    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | QL    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | QN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | QO    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | QP    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | QT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | QV    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | R0    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | R1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | R3    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | R5    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | R6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | R7    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | R9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RA    | 709      | Total<br>709 | Mg<br>709 | 0       | 0       |
| 56  | RB    | 17       | Total<br>17  | Mg<br>17  | 0       | 0       |
| 56  | RD    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 56  | RE    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | RF    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | RG    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | RH    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | RN    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

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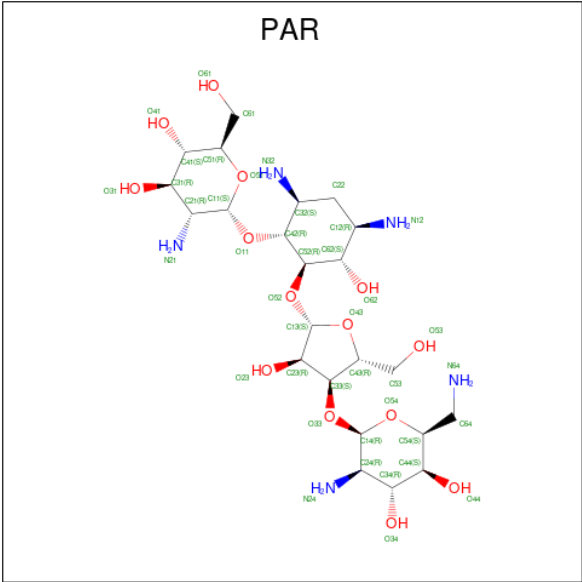
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | RO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RP    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | RQ    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | RR    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | RT    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | RU    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | RV    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | RW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RZ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XA    | 193      | Total<br>193 | Mg<br>193 | 0       | 0       |
| 56  | XE    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | XF    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | XJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XL    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | XR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XV    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | XY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y1    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | Y3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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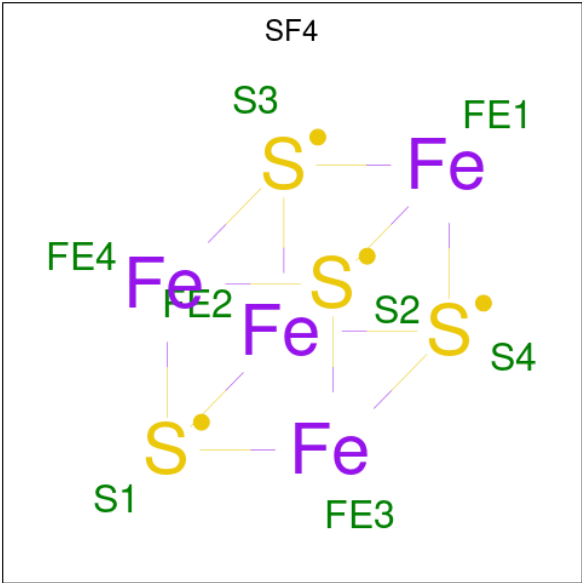
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | Y5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y7    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | Y8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YA    | 707      | Total<br>707 | Mg<br>707 | 0       | 0       |
| 56  | YB    | 20       | Total<br>20  | Mg<br>20  | 0       | 0       |
| 56  | YD    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 56  | YE    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | YF    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | YG    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | YI    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YP    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | YQ    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | YR    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | YT    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | YV    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YW    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 57  | QA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |
| 57  | XA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 58  | QD    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 58  | XD    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

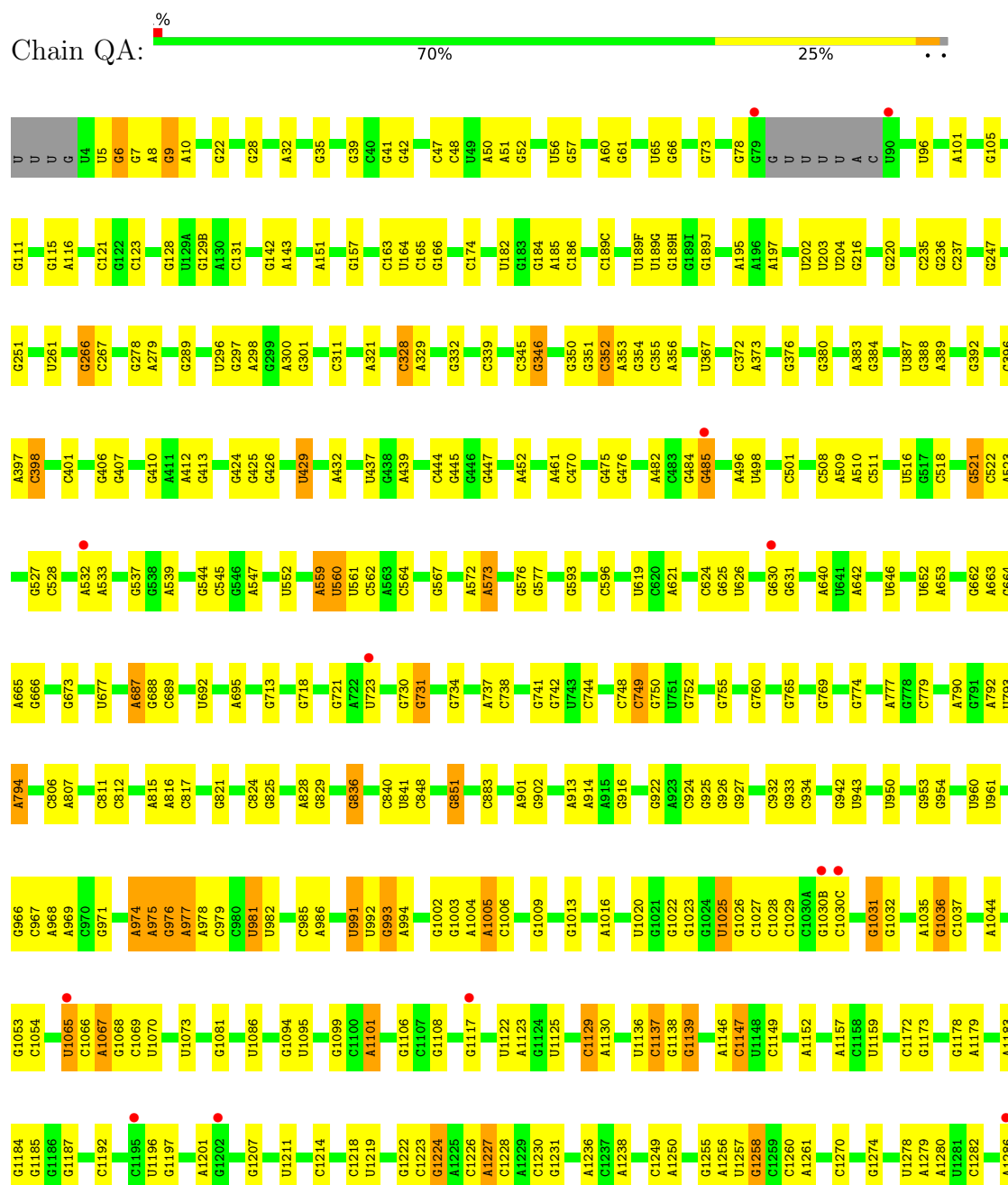
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

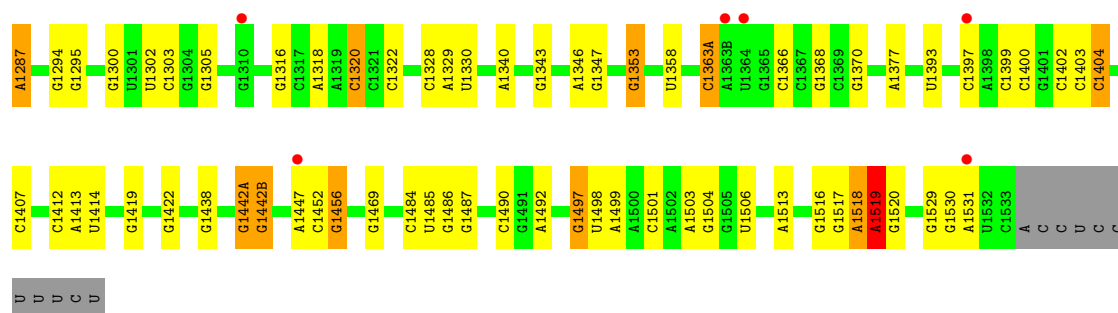
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59  | QN    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | R4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | R5    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | R6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | R9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | RY    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | XN    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | Y4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | Y5    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | Y6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | Y9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | YY    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

### 3 Residue-property plots

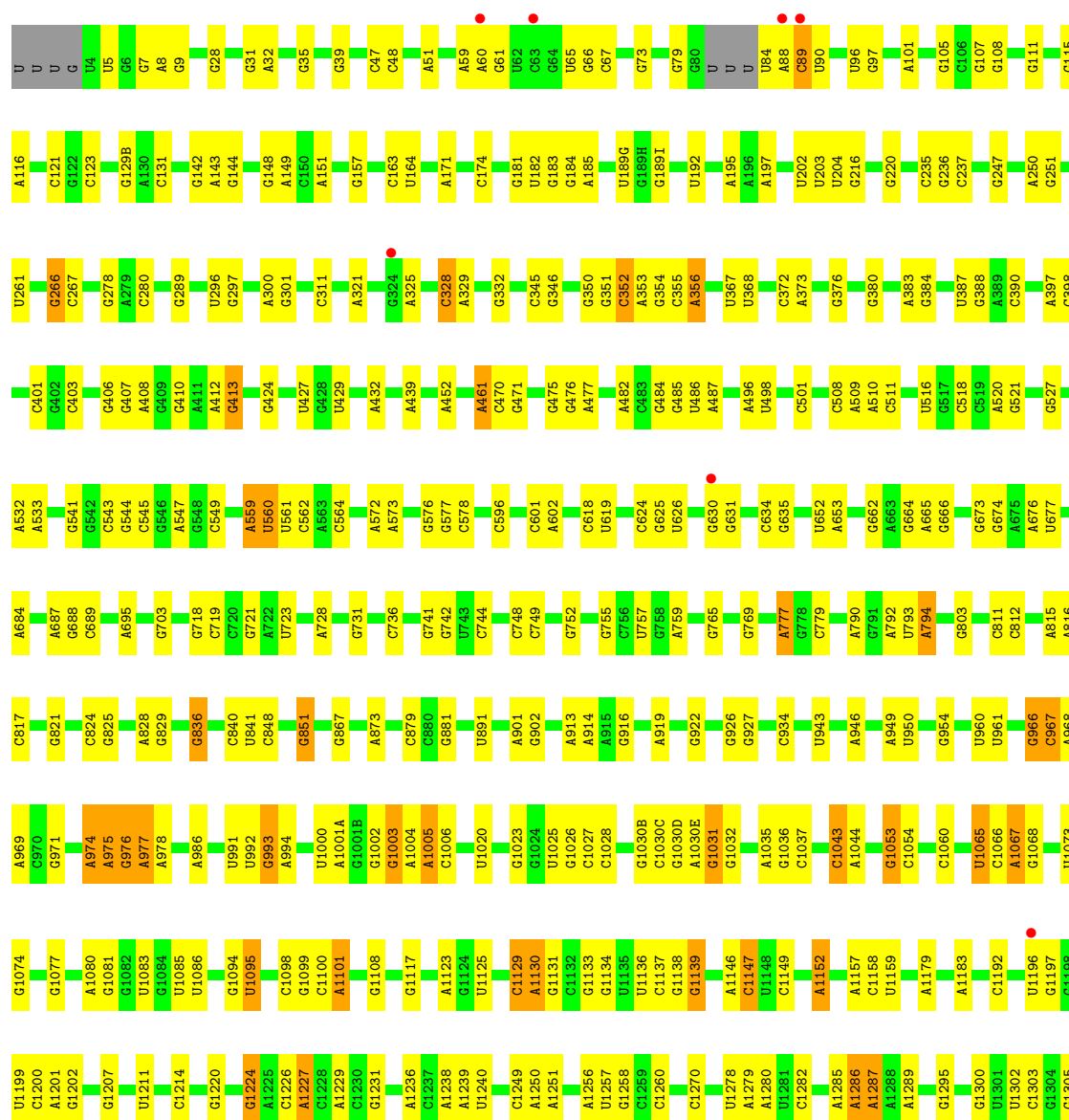
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

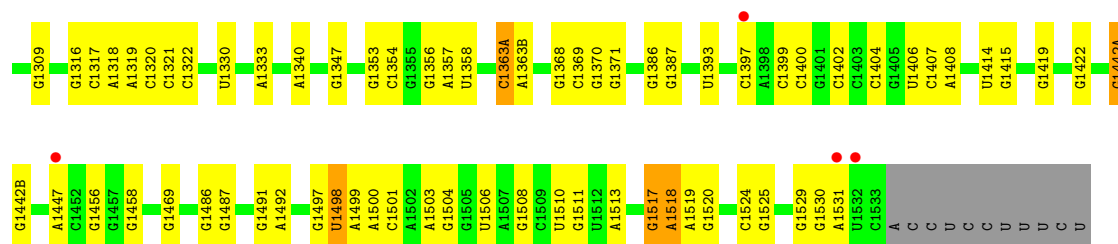
#### • Molecule 1: 16S rRNA



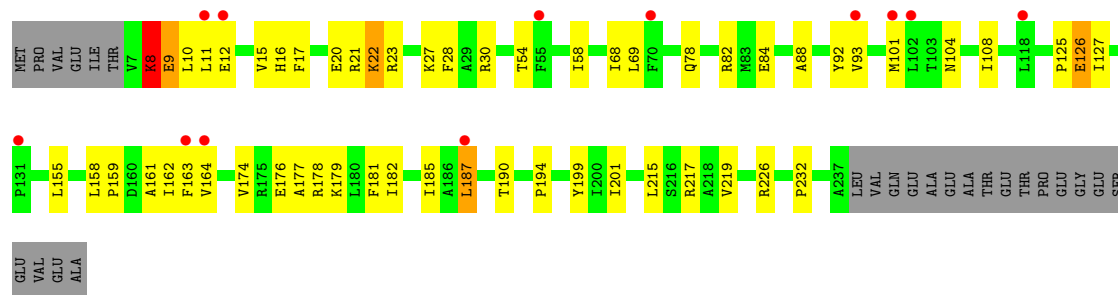


- Molecule 1: 16S rRNA

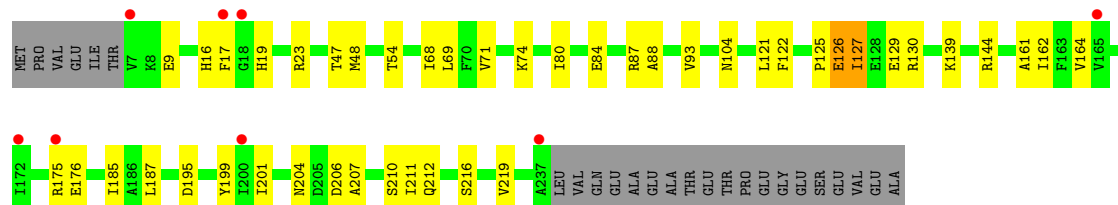
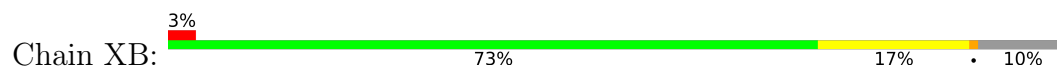




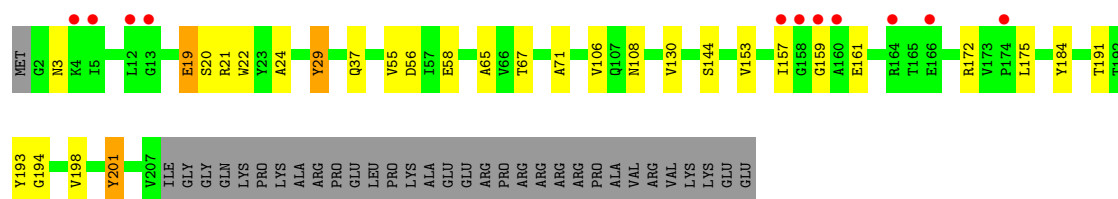
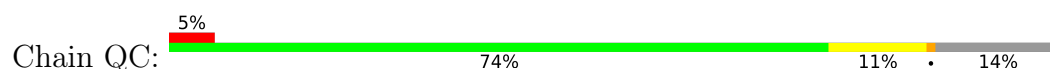
• Molecule 2: 30S ribosomal protein S2



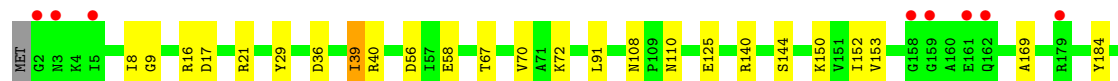
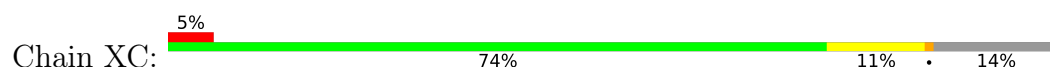
• Molecule 2: 30S ribosomal protein S2

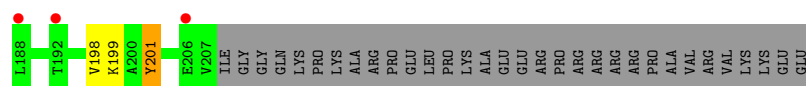


• Molecule 3: 30S ribosomal protein S3

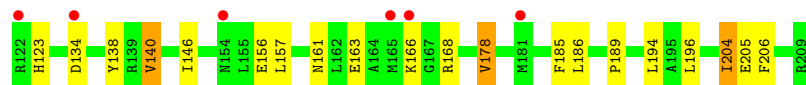
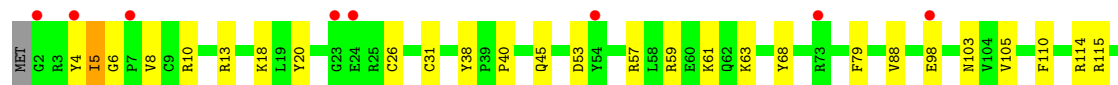
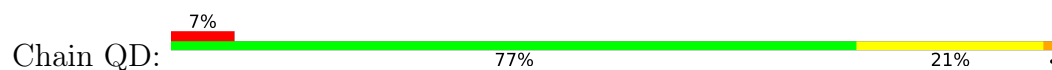


• Molecule 3: 30S ribosomal protein S3

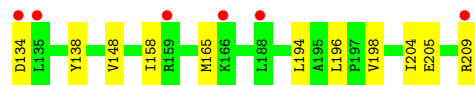
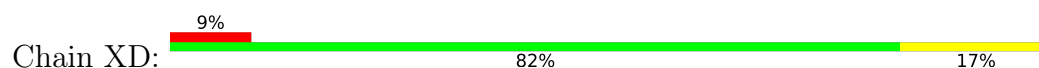




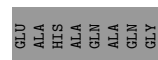
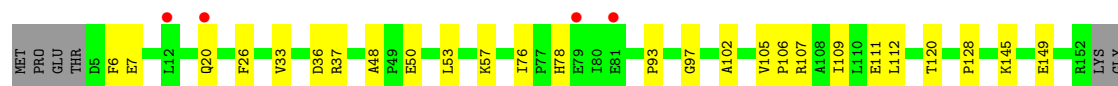
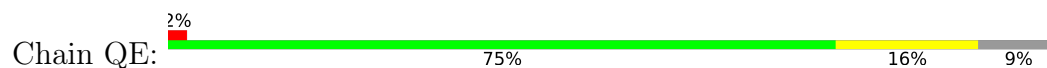
- Molecule 4: 30S ribosomal protein S4



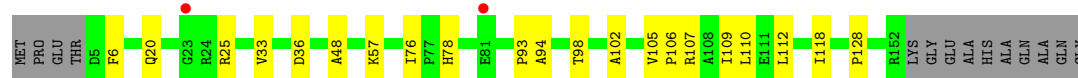
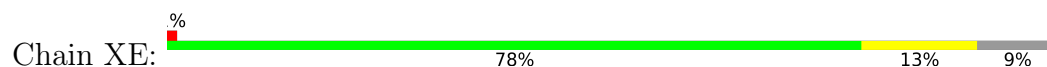
- Molecule 4: 30S ribosomal protein S4



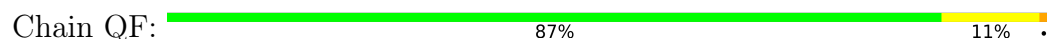
- Molecule 5: 30S ribosomal protein S5



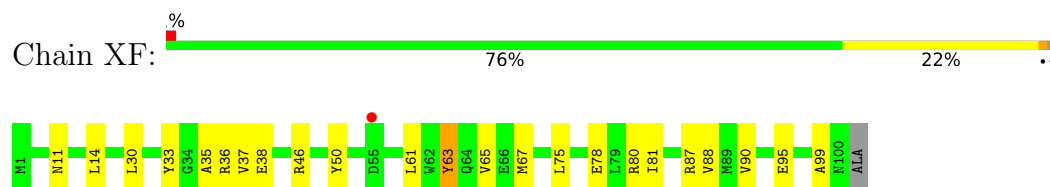
- Molecule 5: 30S ribosomal protein S5



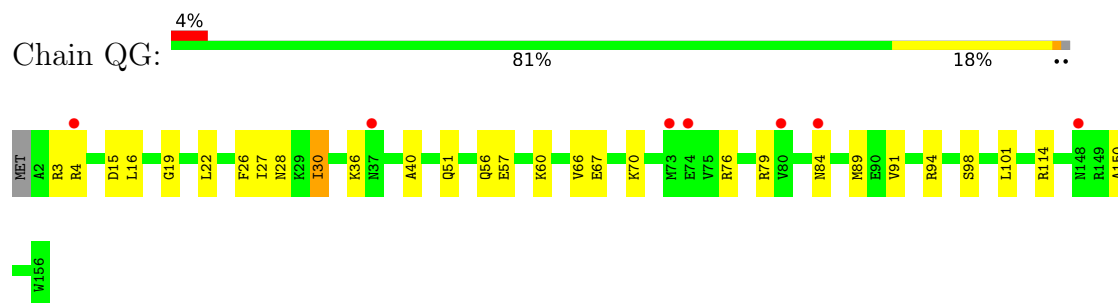
- Molecule 6: 30S ribosomal protein S6



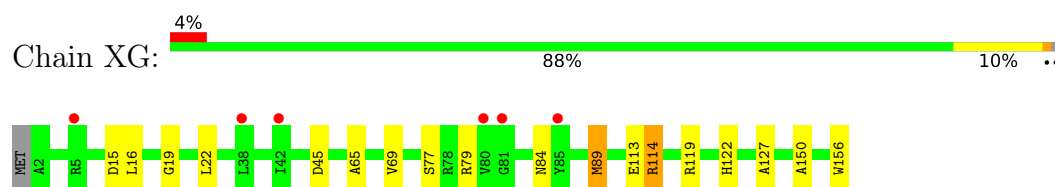
- Molecule 6: 30S ribosomal protein S6



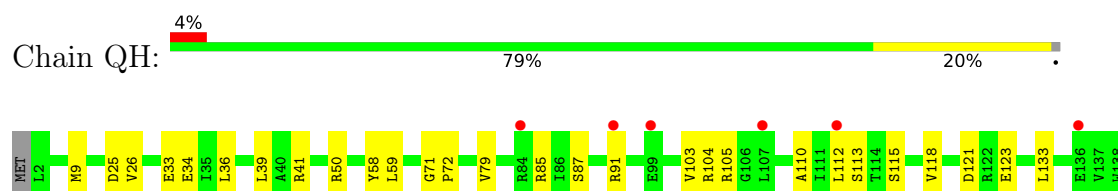
- Molecule 7: 30S ribosomal protein S7



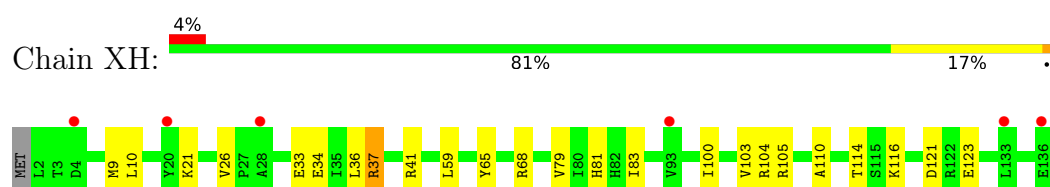
- Molecule 7: 30S ribosomal protein S7



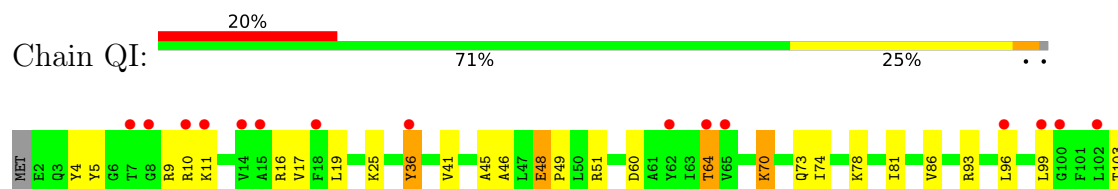
- Molecule 8: 30S ribosomal protein S8

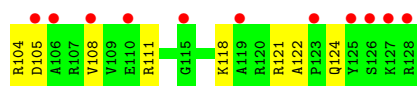


- Molecule 8: 30S ribosomal protein S8

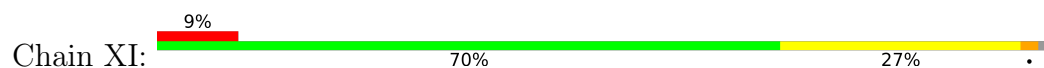


- Molecule 9: 30S ribosomal protein S9

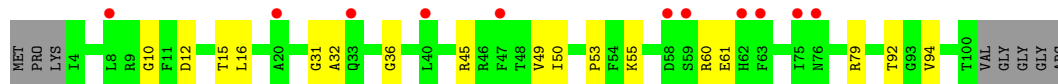
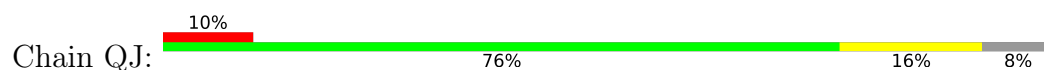




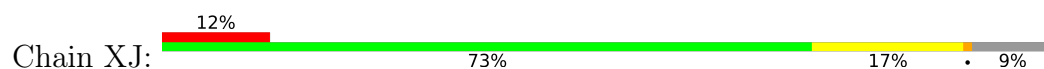
- Molecule 9: 30S ribosomal protein S9



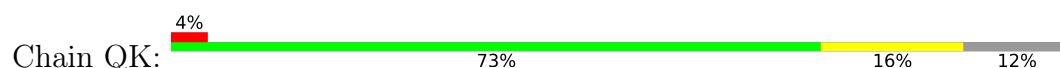
- Molecule 10: 30S ribosomal protein S10



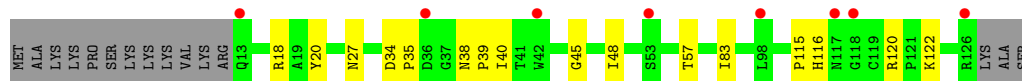
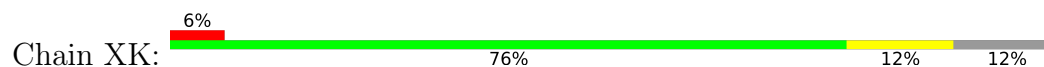
- Molecule 10: 30S ribosomal protein S10



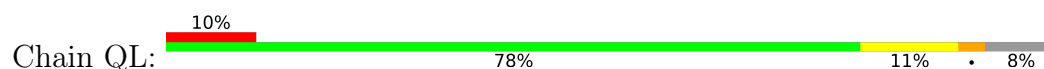
- Molecule 11: 30S ribosomal protein S11

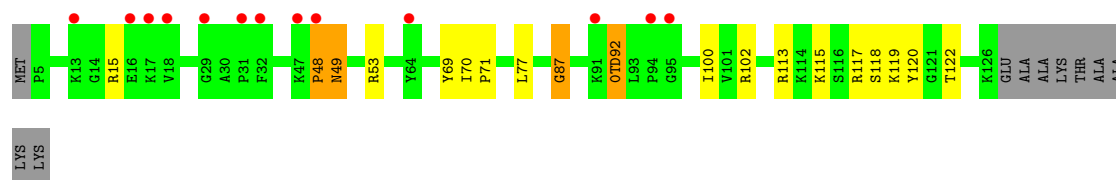


- Molecule 11: 30S ribosomal protein S11

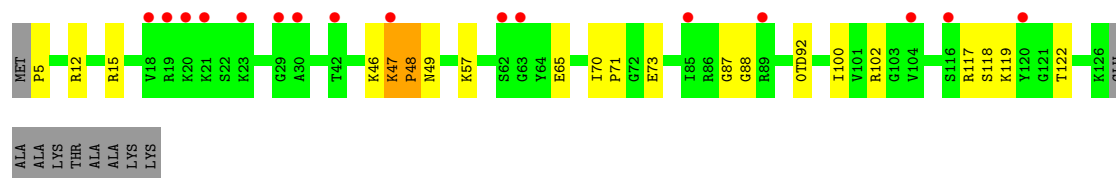
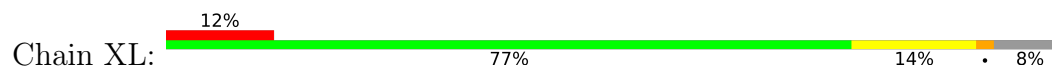


- Molecule 12: 30S ribosomal protein S12

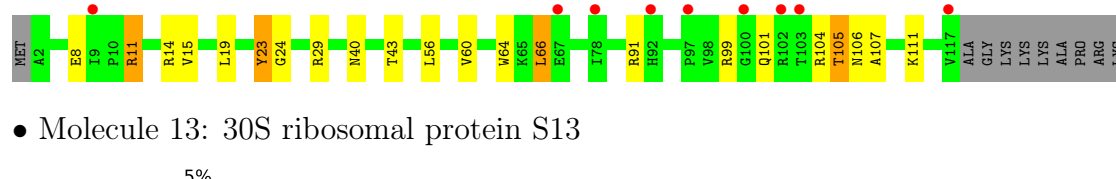
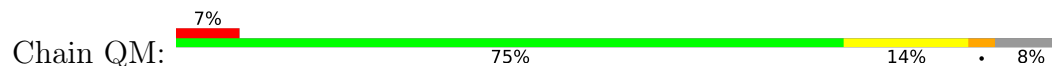




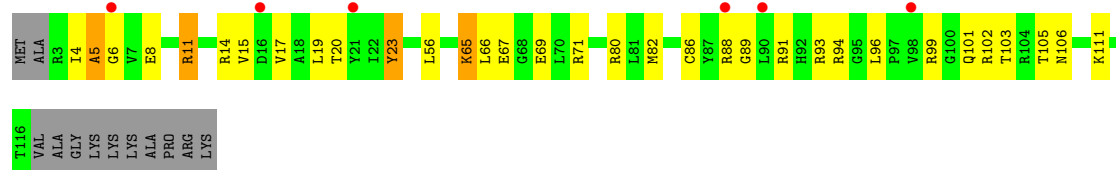
- Molecule 12: 30S ribosomal protein S12



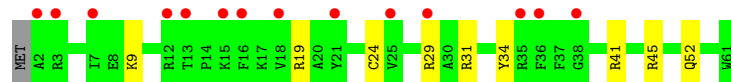
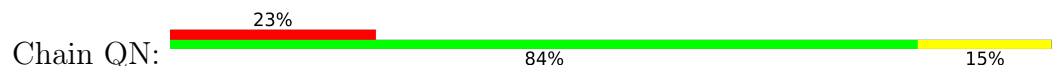
- Molecule 13: 30S ribosomal protein S13



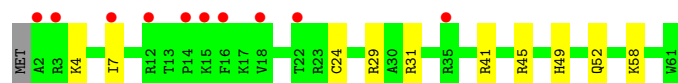
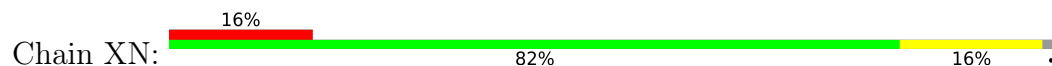
- Molecule 13: 30S ribosomal protein S13



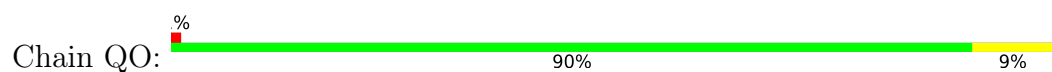
- Molecule 14: 30S ribosomal protein S14 type Z



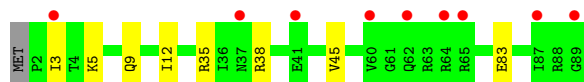
- Molecule 14: 30S ribosomal protein S14 type Z



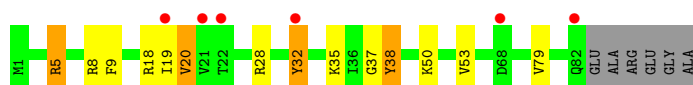
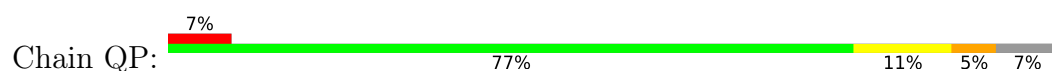
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



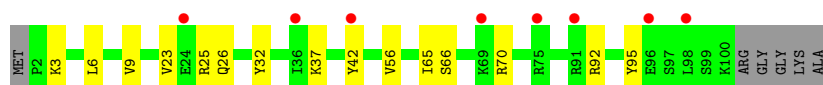
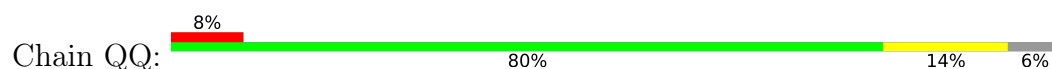
- Molecule 16: 30S ribosomal protein S16



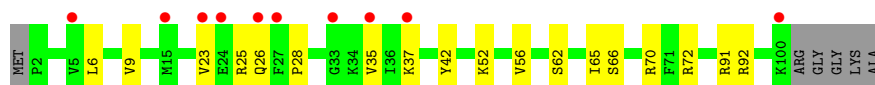
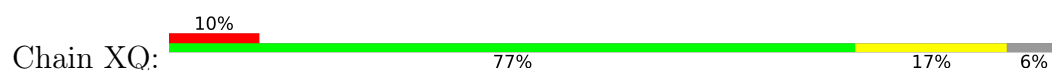
- Molecule 16: 30S ribosomal protein S16



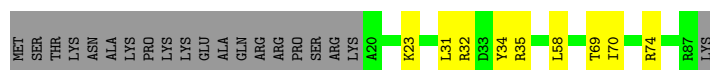
- Molecule 17: 30S ribosomal protein S17



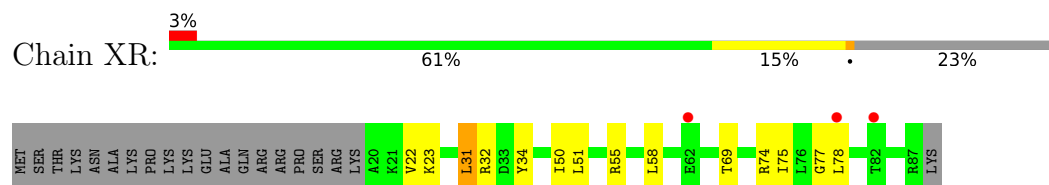
- Molecule 17: 30S ribosomal protein S17



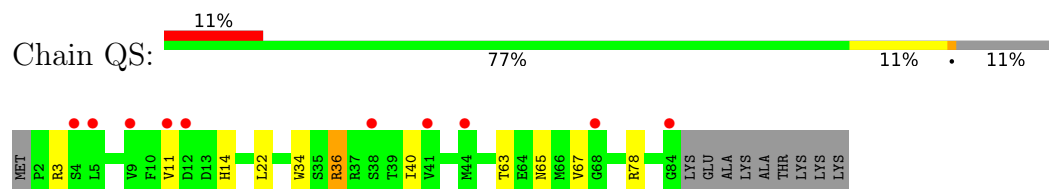
- Molecule 18: 30S ribosomal protein S18



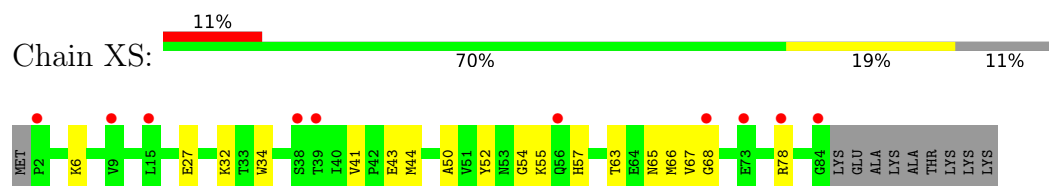
- Molecule 18: 30S ribosomal protein S18



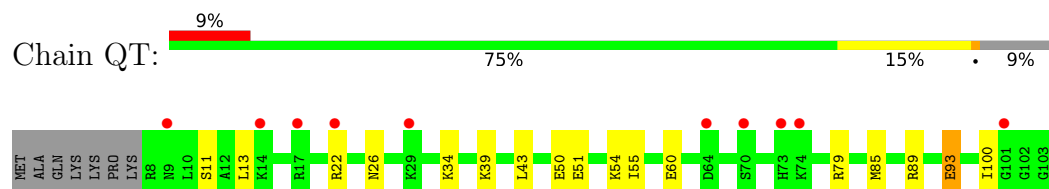
- Molecule 19: 30S ribosomal protein S19



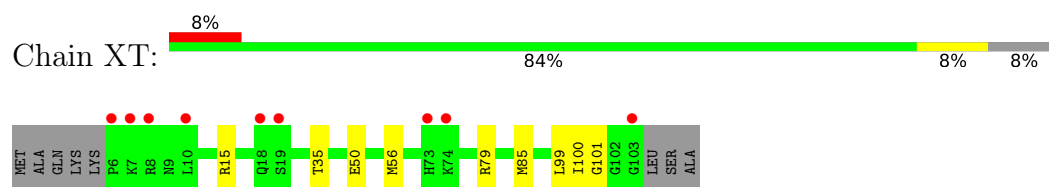
- Molecule 19: 30S ribosomal protein S19



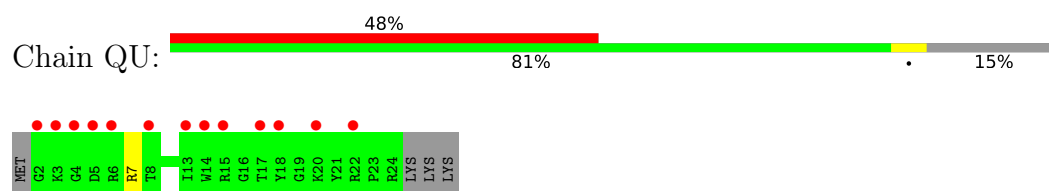
- Molecule 20: 30S ribosomal protein S20



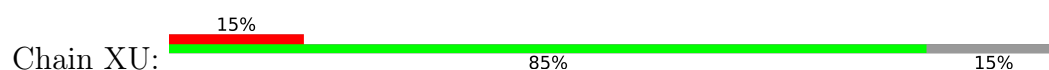
- Molecule 20: 30S ribosomal protein S20

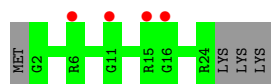


- Molecule 21: 30S ribosomal protein Thx

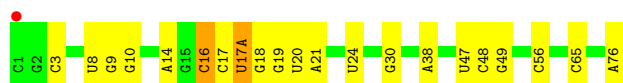
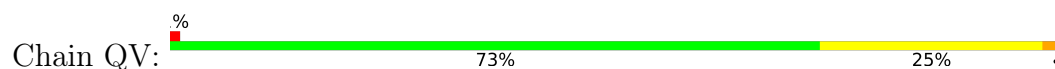


- Molecule 21: 30S ribosomal protein Thx

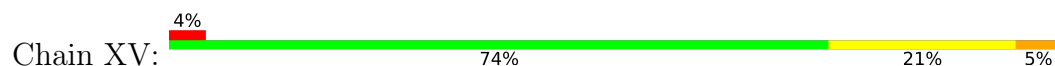




- Molecule 22: P-site tRNAfMet



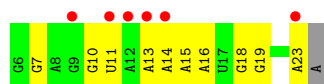
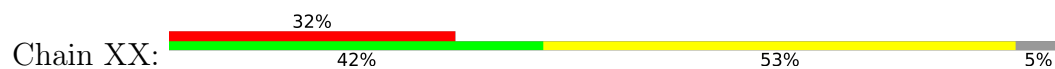
- Molecule 22: P-site tRNAfMet



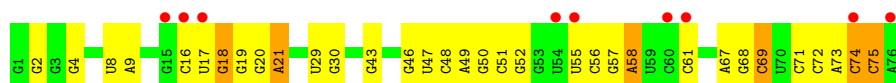
- Molecule 23: mRNA



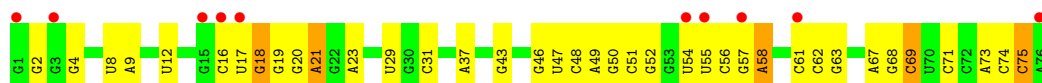
- Molecule 23: mRNA



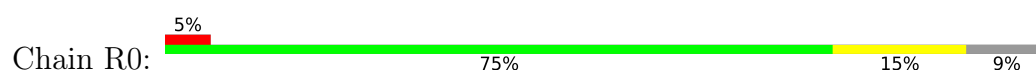
- Molecule 24: A-site tRNAAla(GGC) U32-A38



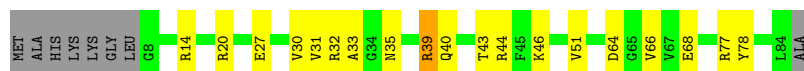
- Molecule 24: A-site tRNAAla(GGC) U32-A38



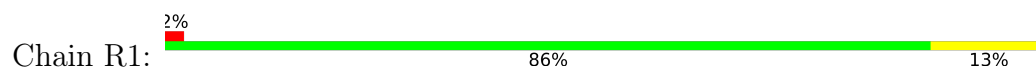
- Molecule 25: 50S ribosomal protein L27



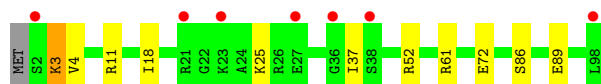
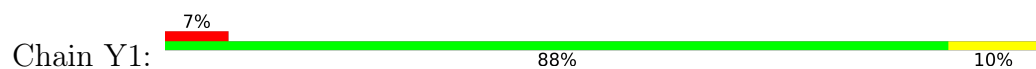
- Molecule 25: 50S ribosomal protein L27



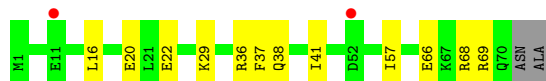
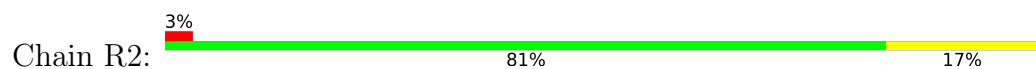
- Molecule 26: 50S ribosomal protein L28



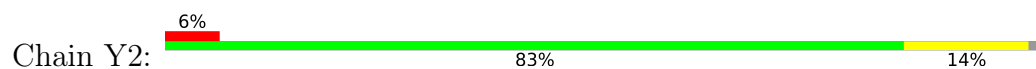
- Molecule 26: 50S ribosomal protein L28



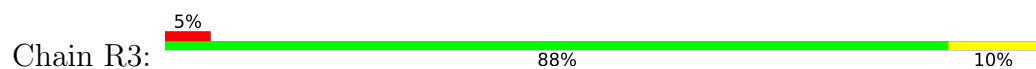
- Molecule 27: 50S ribosomal protein L29



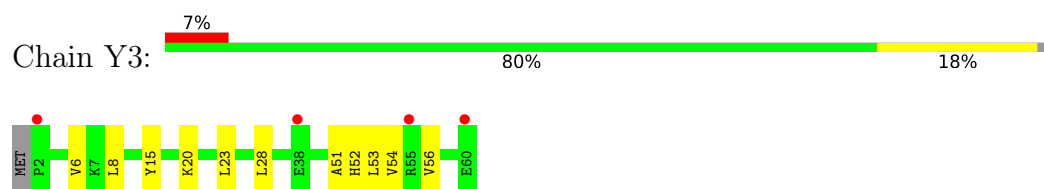
- Molecule 27: 50S ribosomal protein L29



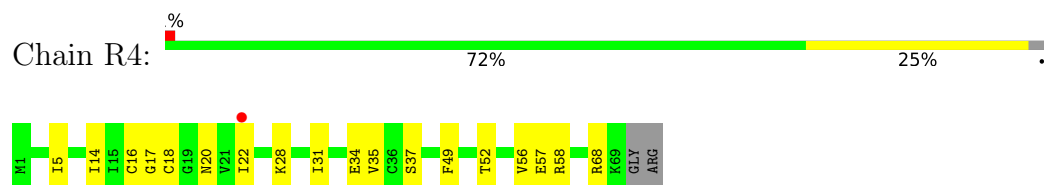
- Molecule 28: 50S ribosomal protein L30



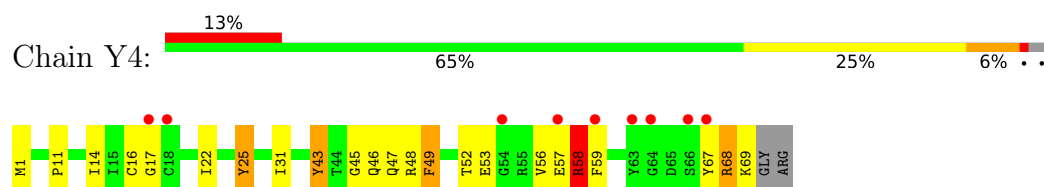
- Molecule 28: 50S ribosomal protein L30



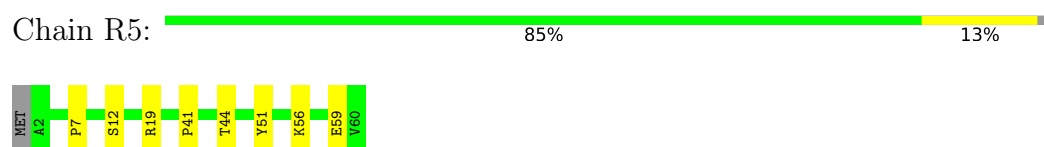
- Molecule 29: 50S ribosomal protein L31



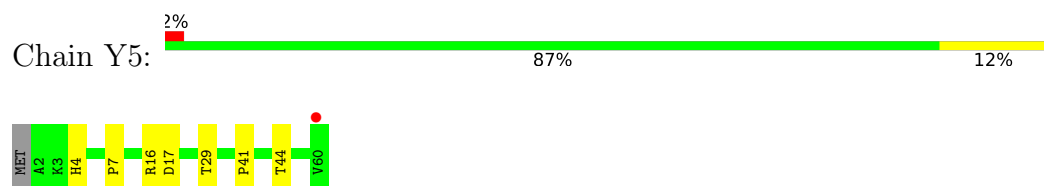
- Molecule 29: 50S ribosomal protein L31



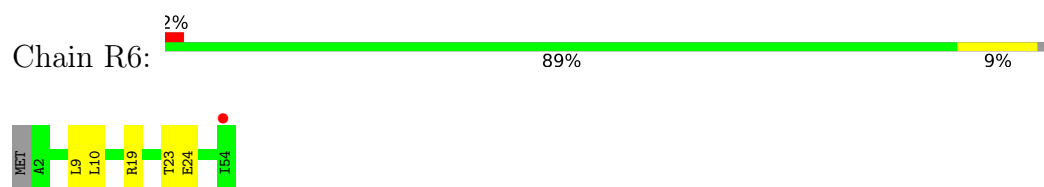
- Molecule 30: 50S ribosomal protein L32



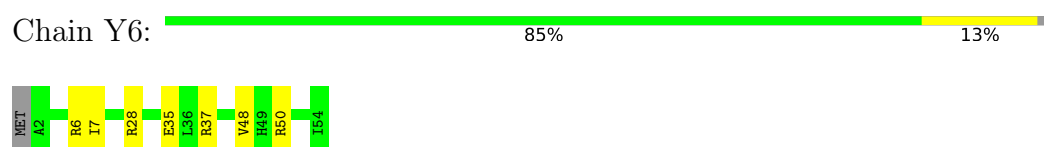
- Molecule 30: 50S ribosomal protein L32



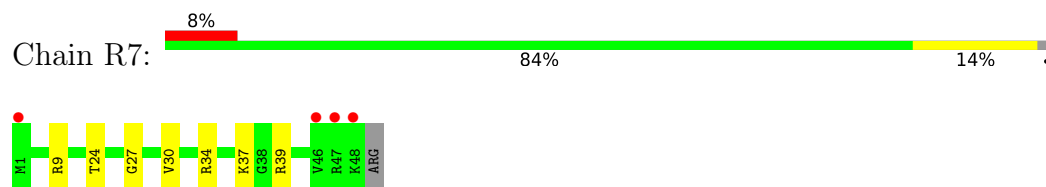
- Molecule 31: 50S ribosomal protein L33



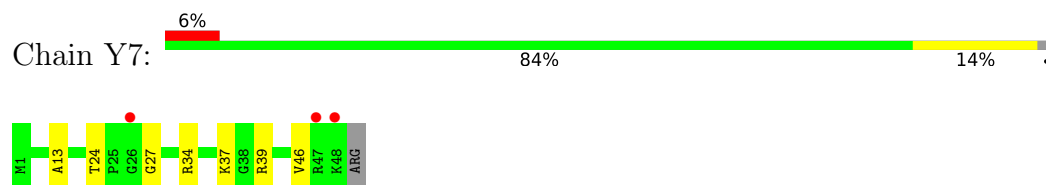
- Molecule 31: 50S ribosomal protein L33



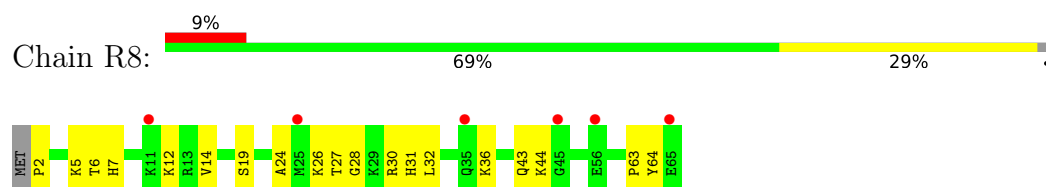
- Molecule 32: 50S ribosomal protein L34



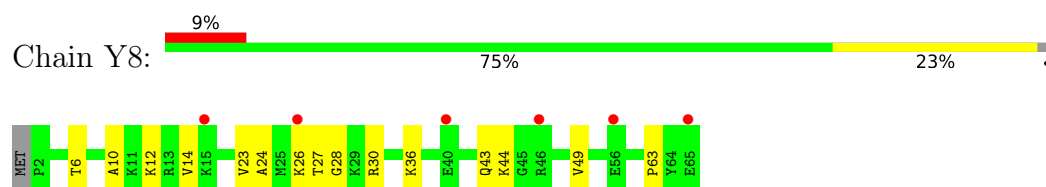
- Molecule 32: 50S ribosomal protein L34



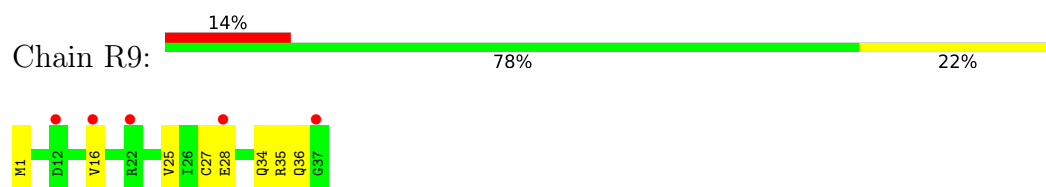
- Molecule 33: 50S ribosomal protein L35



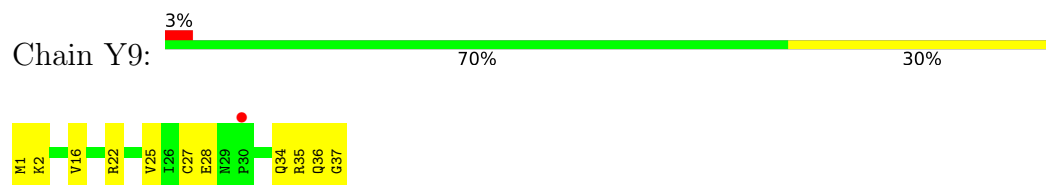
- Molecule 33: 50S ribosomal protein L35



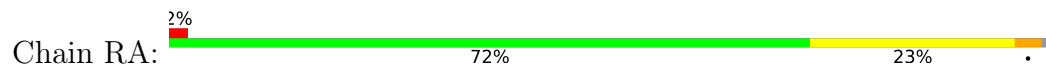
- Molecule 34: 50S ribosomal protein L36

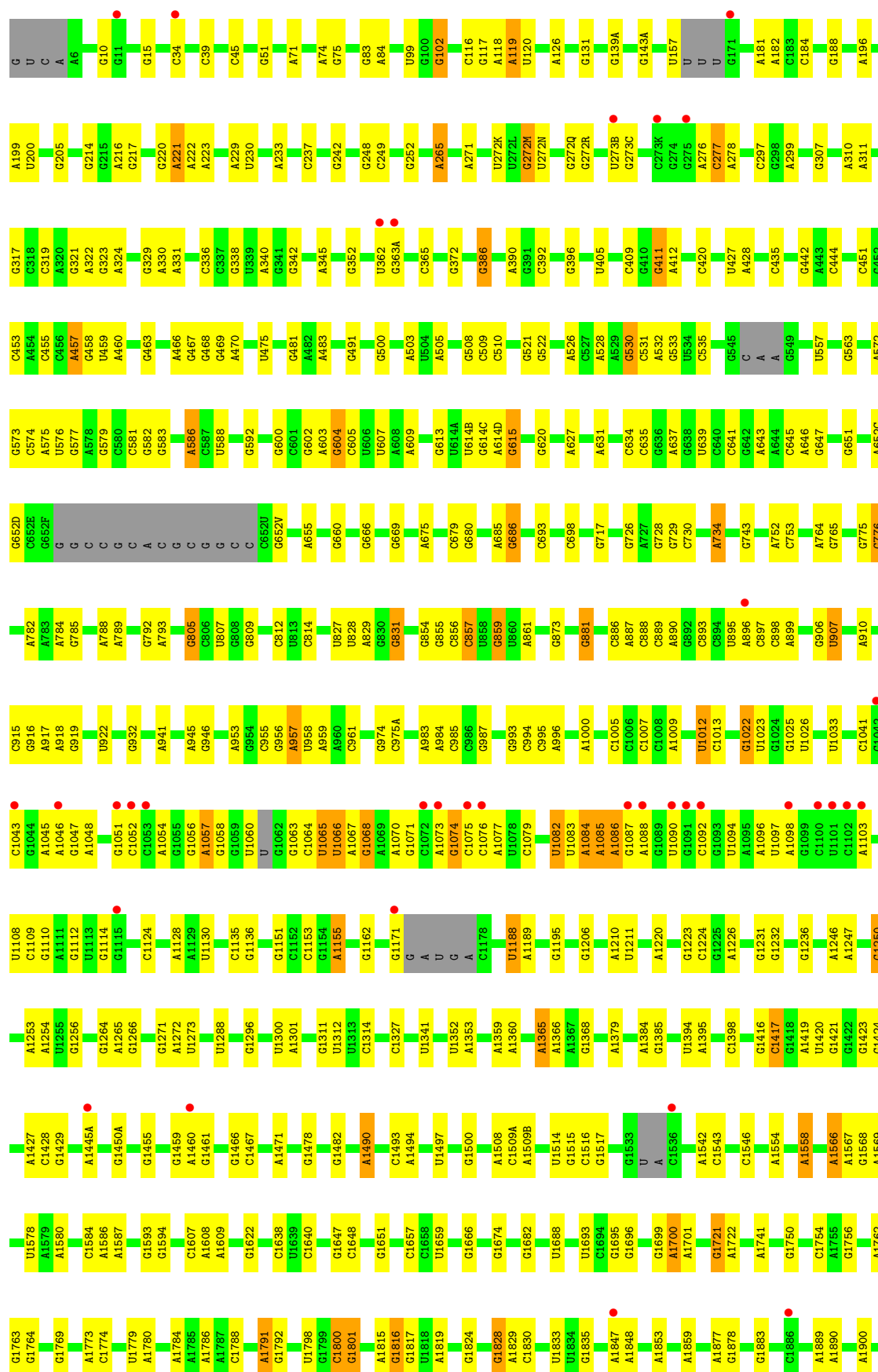


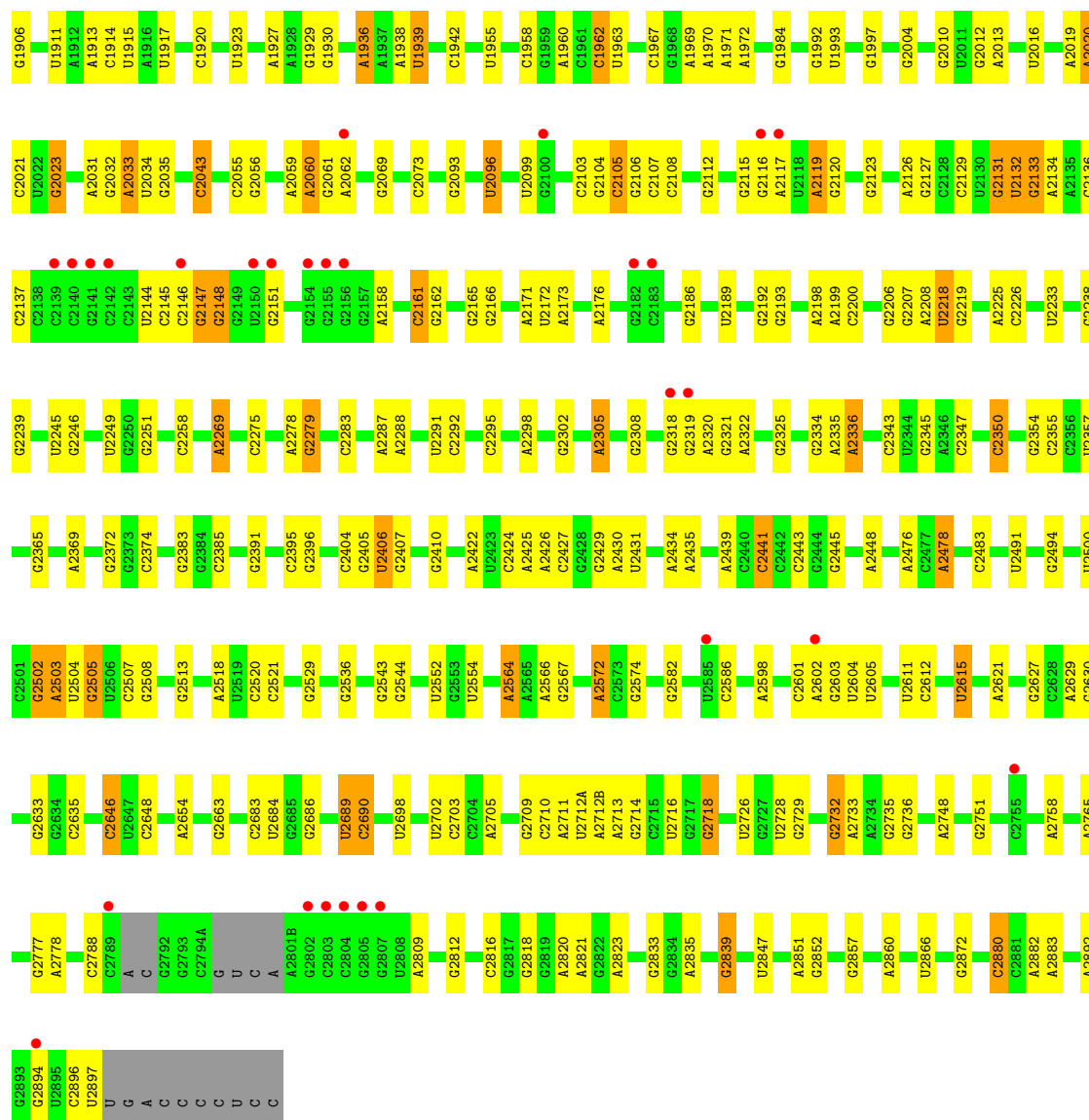
- Molecule 34: 50S ribosomal protein L36

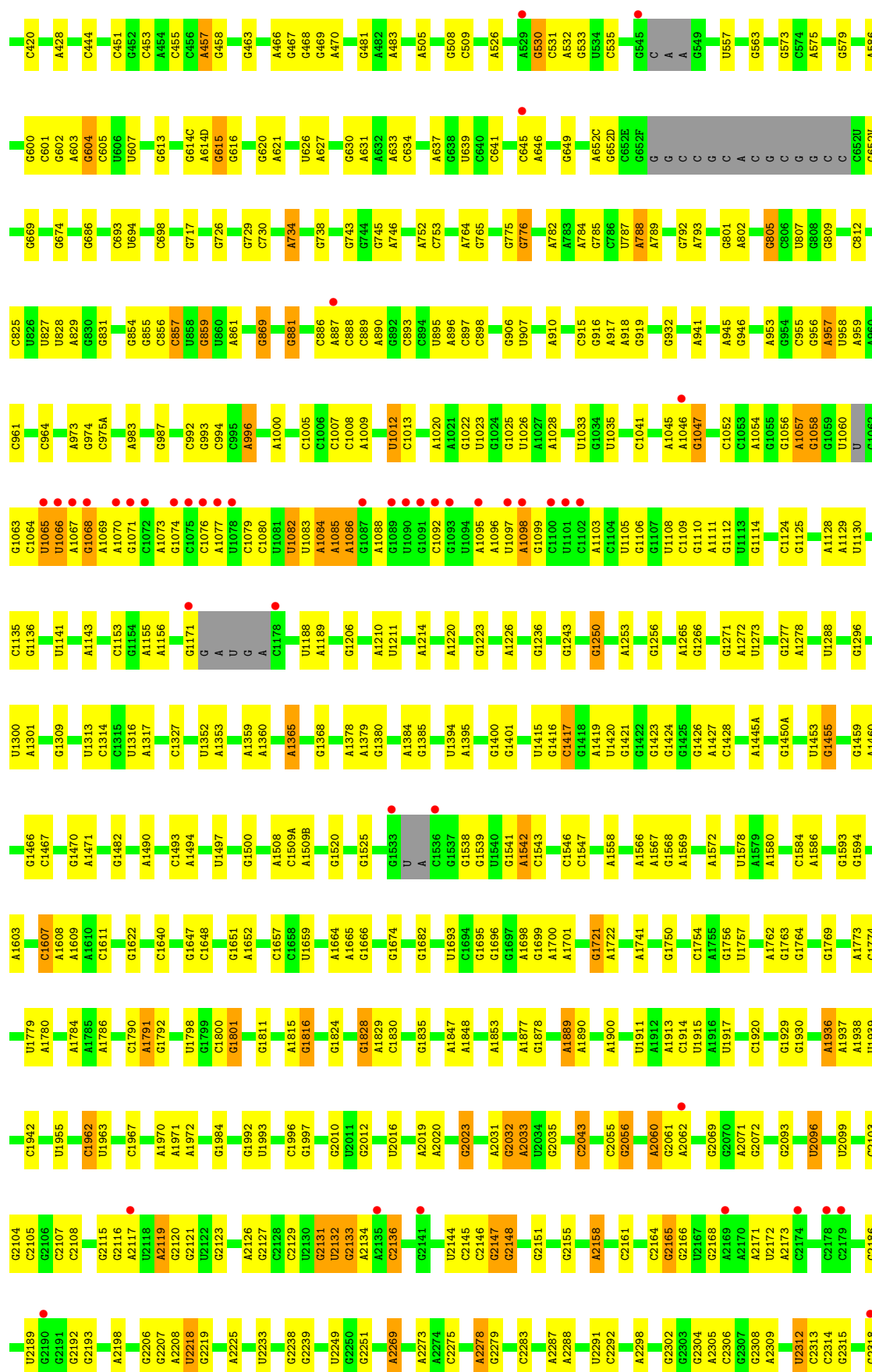


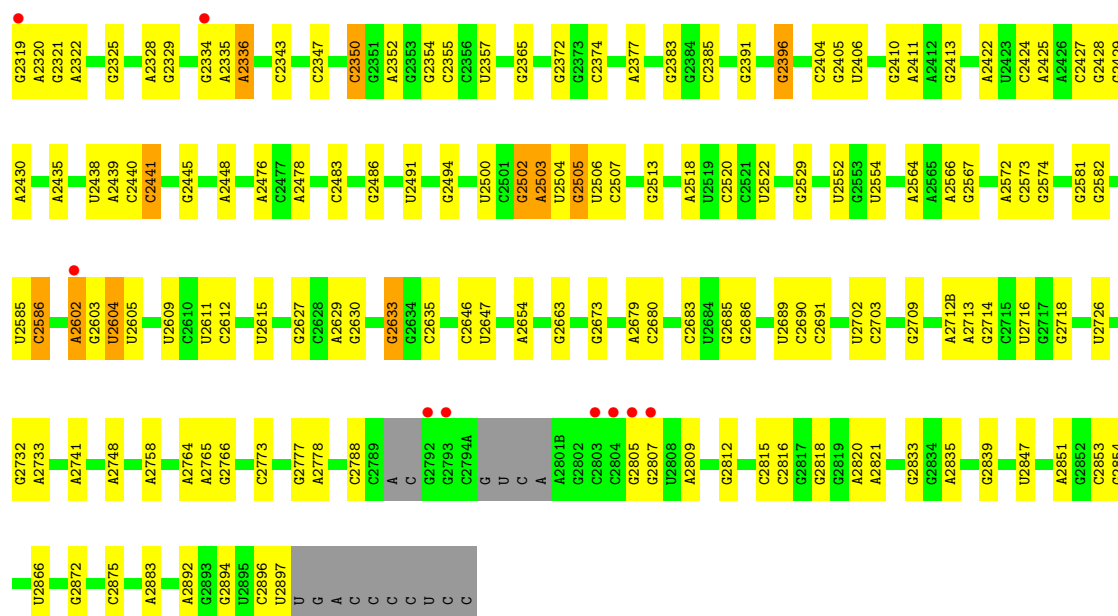
- Molecule 35: 23S rRNA



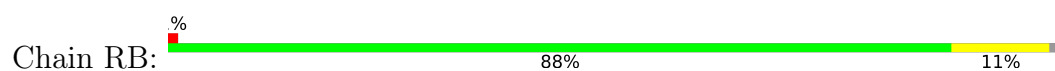




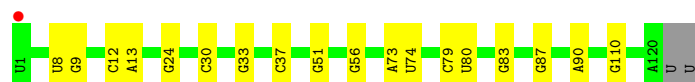
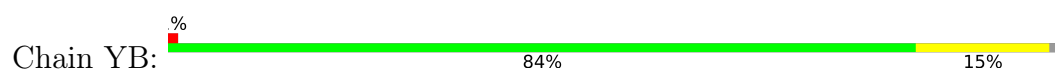




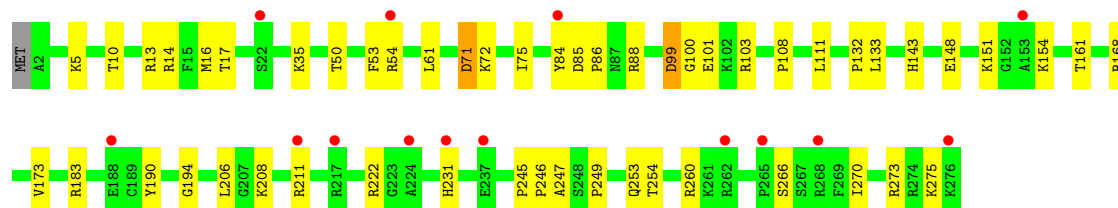
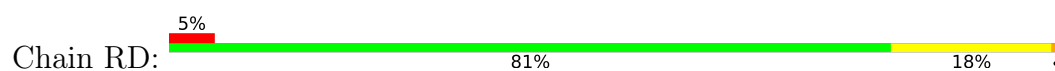
• Molecule 36: 5S rRNA



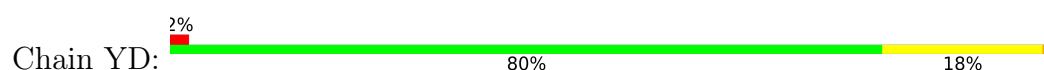
• Molecule 36: 5S rRNA

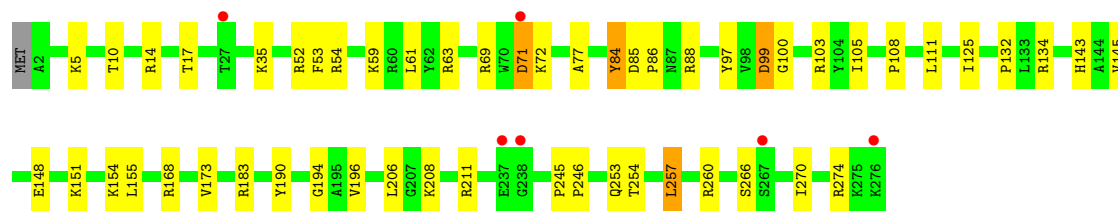


• Molecule 37: 50S ribosomal protein L2

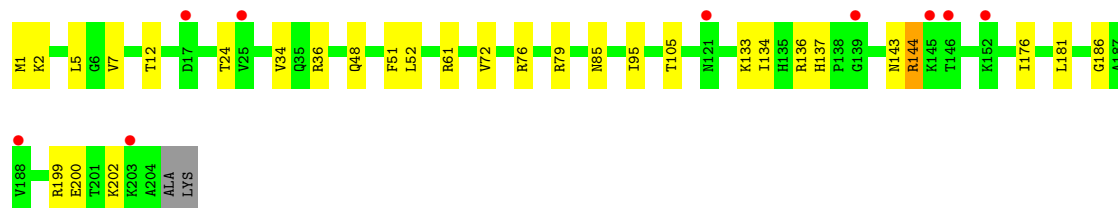
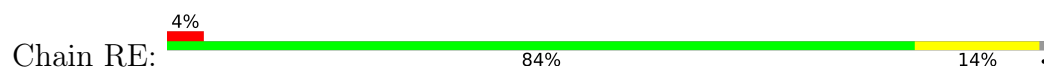


• Molecule 37: 50S ribosomal protein L2

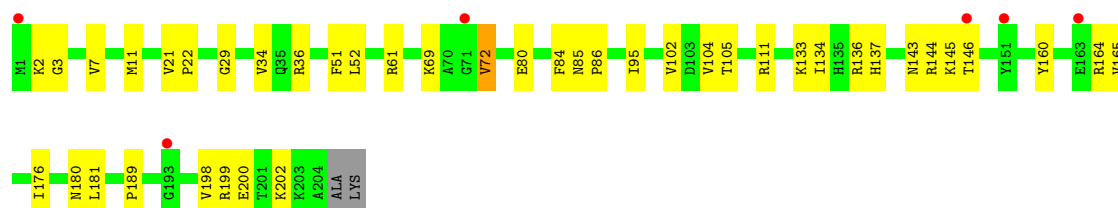
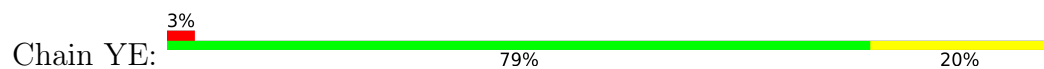




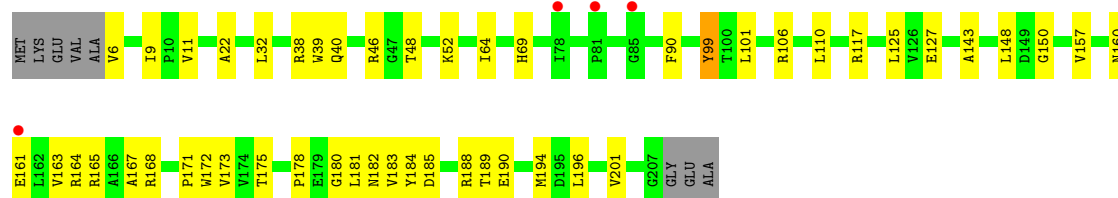
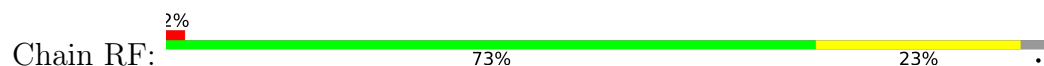
• Molecule 38: 50S ribosomal protein L3



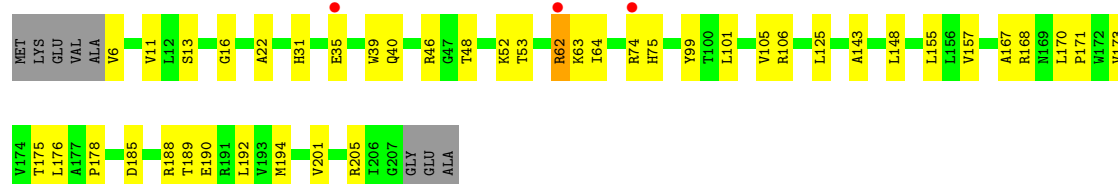
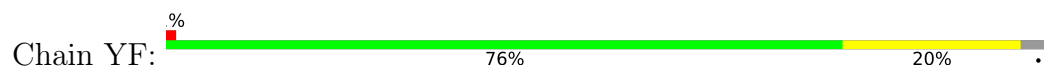
• Molecule 38: 50S ribosomal protein L3



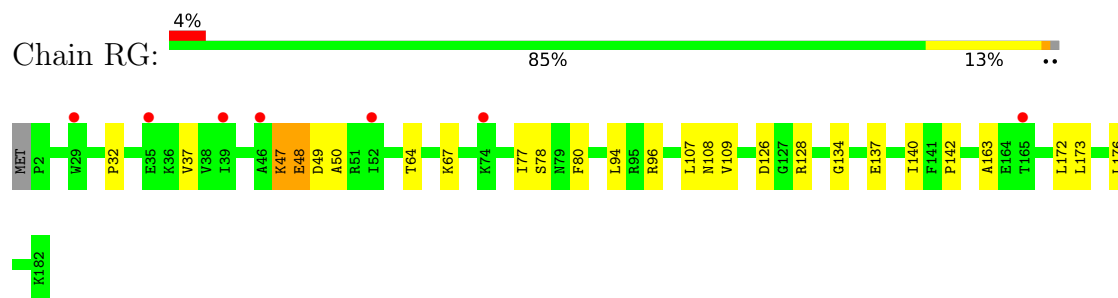
• Molecule 39: 50S ribosomal protein L4



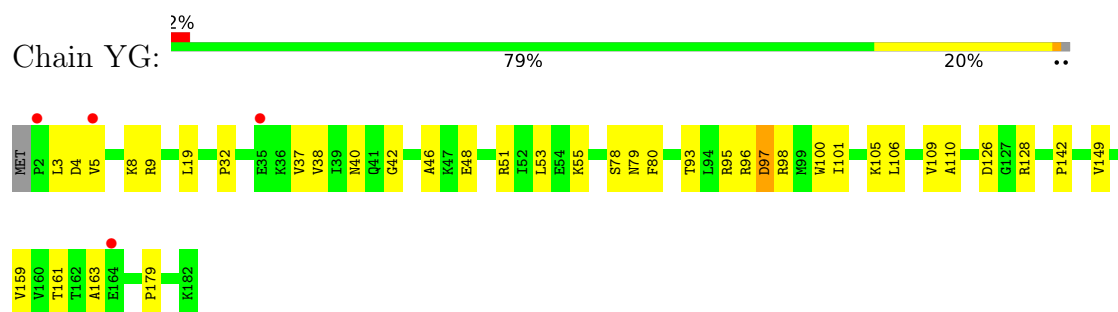
• Molecule 39: 50S ribosomal protein L4



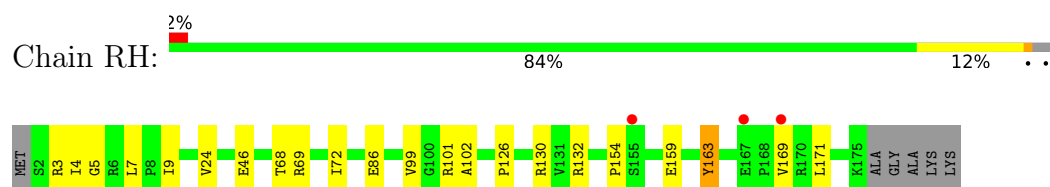
- Molecule 40: 50S ribosomal protein L5



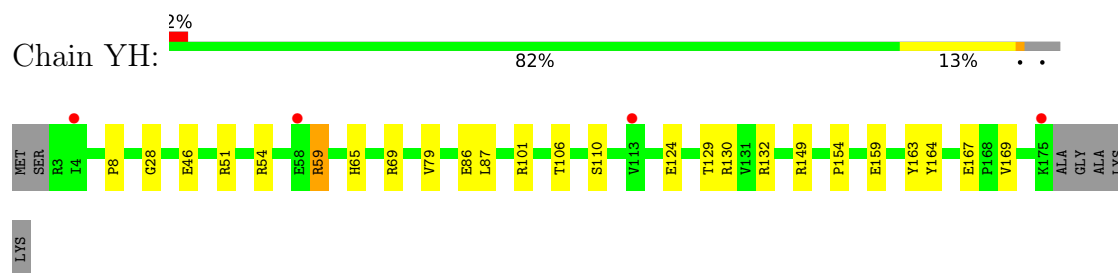
- Molecule 40: 50S ribosomal protein L5



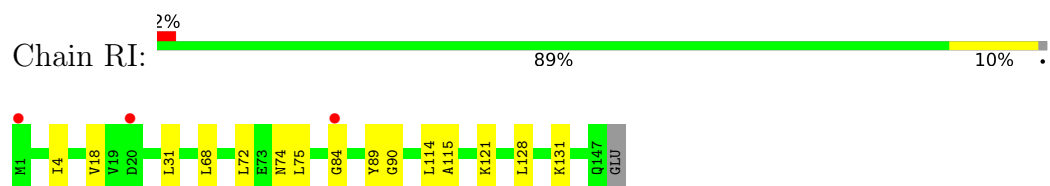
- Molecule 41: 50S ribosomal protein L6



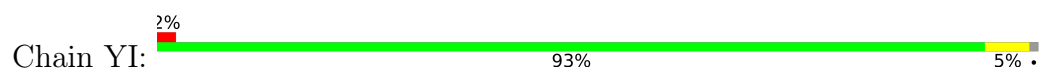
- Molecule 41: 50S ribosomal protein L6



- Molecule 42: 50S ribosomal protein L9

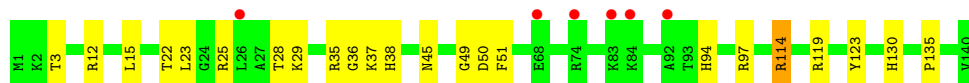
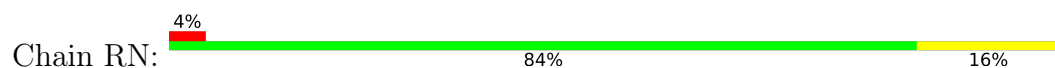


- Molecule 42: 50S ribosomal protein L9

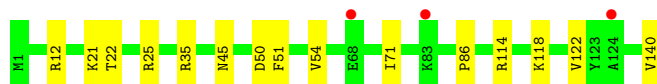
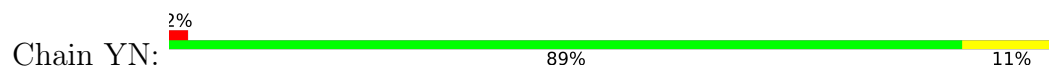




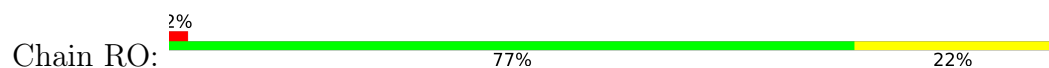
- Molecule 43: 50S ribosomal protein L13



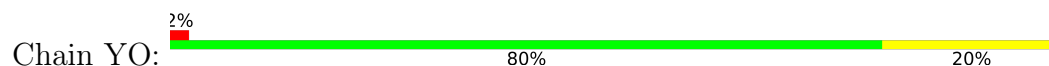
- Molecule 43: 50S ribosomal protein L13



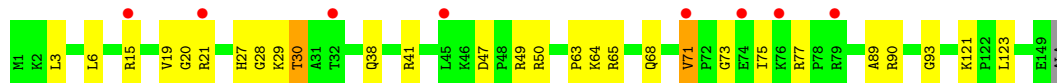
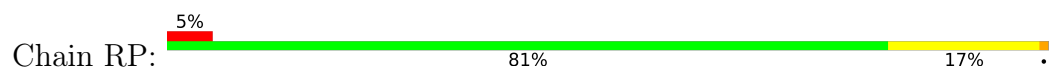
- Molecule 44: 50S ribosomal protein L14



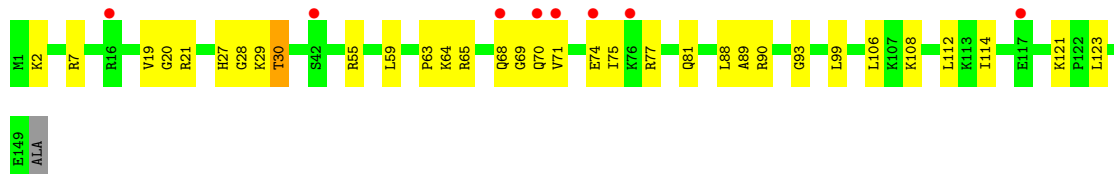
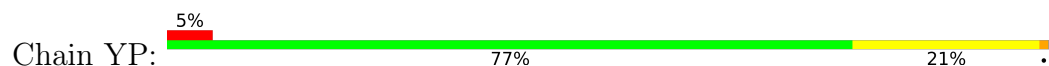
- Molecule 44: 50S ribosomal protein L14



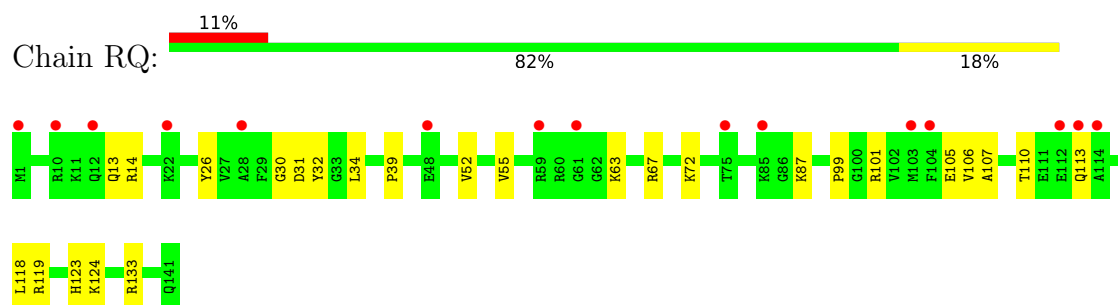
- Molecule 45: 50S ribosomal protein L15



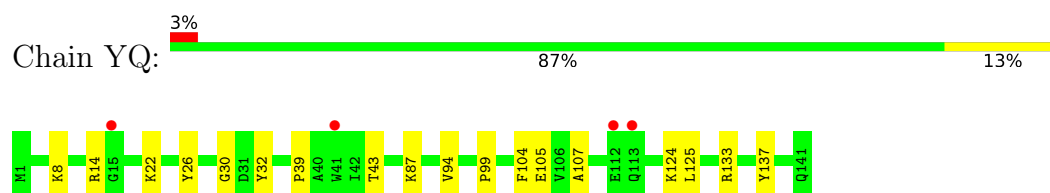
- Molecule 45: 50S ribosomal protein L15



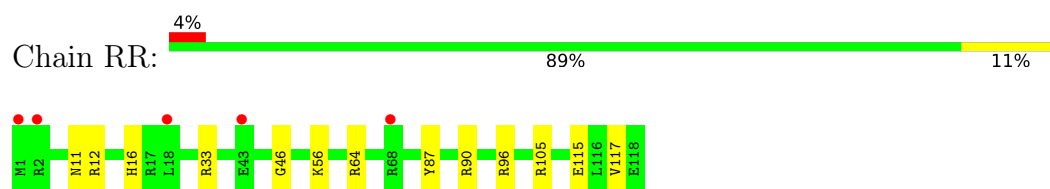
- Molecule 46: 50S ribosomal protein L16



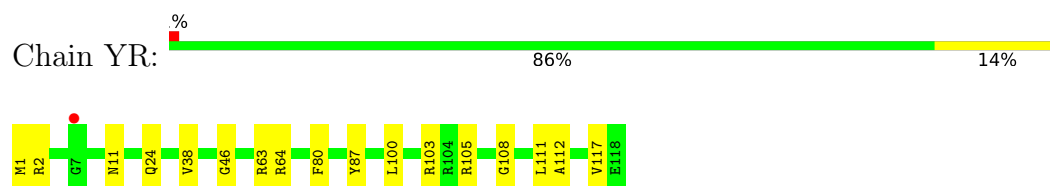
- Molecule 46: 50S ribosomal protein L16



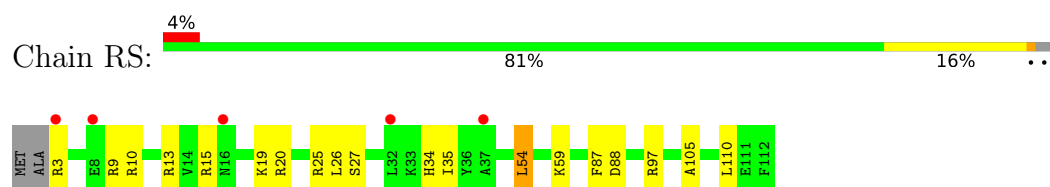
- Molecule 47: 50S ribosomal protein L17



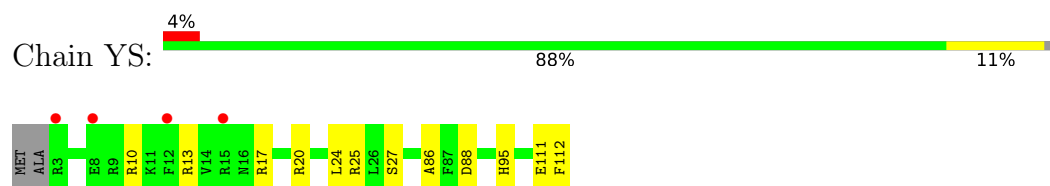
- Molecule 47: 50S ribosomal protein L17



- Molecule 48: 50S ribosomal protein L18

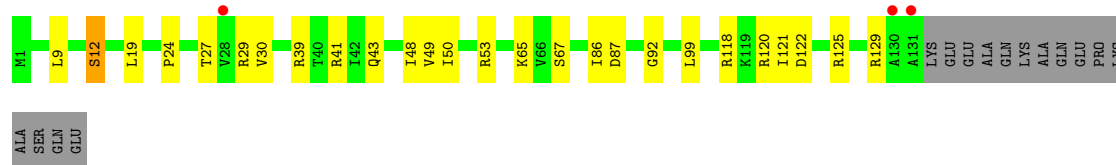


- Molecule 48: 50S ribosomal protein L18



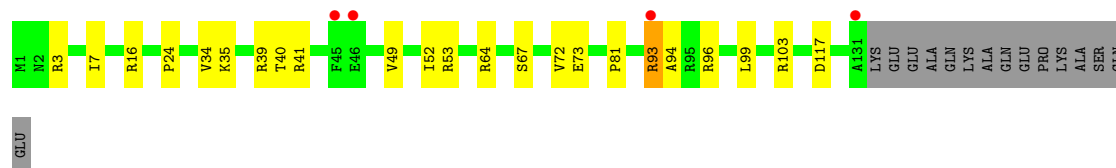
- Molecule 49: 50S ribosomal protein L19

Chain RT:  2% 72% 17% 10%



- Molecule 49: 50S ribosomal protein L19

Chain YT:  3% 74% 15% 10%



- Molecule 50: 50S ribosomal protein L20

Chain RU:  3% 82% 15% 2%



- Molecule 50: 50S ribosomal protein L20

Chain YU:  0% 86% 11% 3%

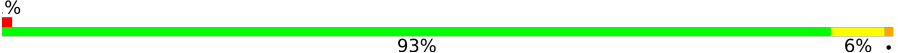


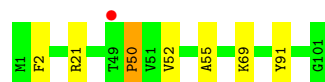
- Molecule 51: 50S ribosomal protein L21

Chain RV:  4% 78% 19% 1%

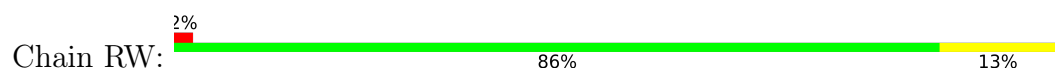


- Molecule 51: 50S ribosomal protein L21

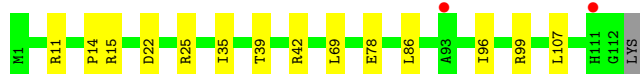
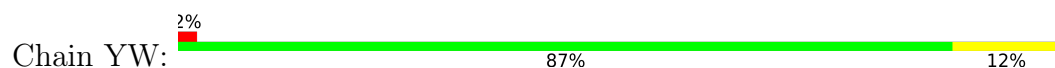
Chain YV:  0% 93% 6% 1%



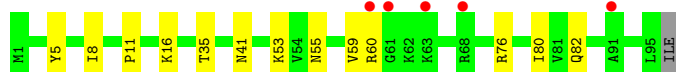
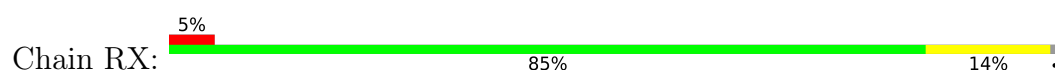
- Molecule 52: 50S ribosomal protein L22



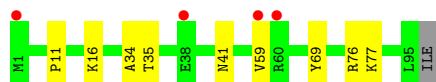
- Molecule 52: 50S ribosomal protein L22



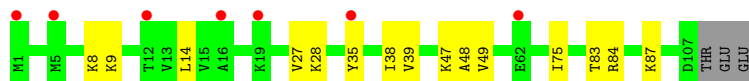
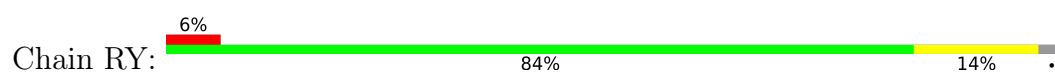
- Molecule 53: 50S ribosomal protein L23



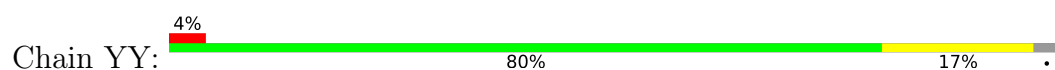
- Molecule 53: 50S ribosomal protein L23



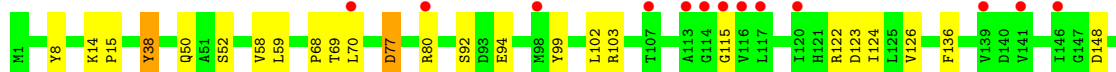
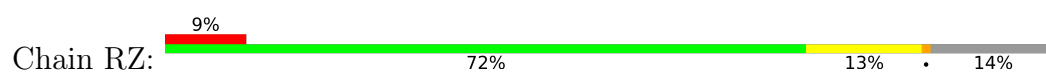
- Molecule 54: 50S ribosomal protein L24

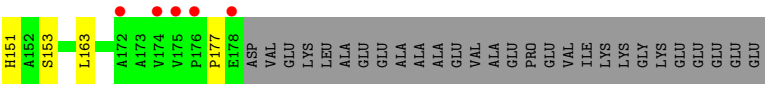


- Molecule 54: 50S ribosomal protein L24

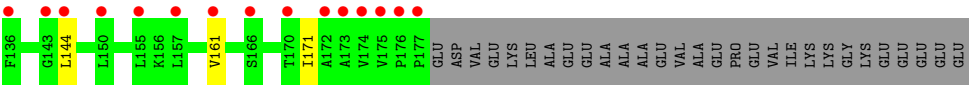
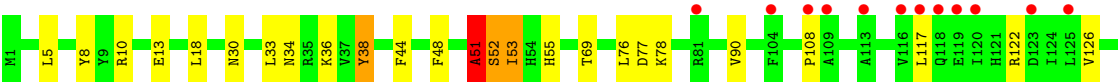
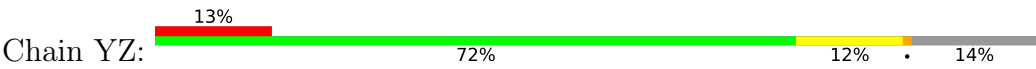


- Molecule 55: 50S ribosomal protein L25





● Molecule 55: 50S ribosomal protein L25



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.38Å 445.83Å 616.03Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.00 – 3.10<br>50.00 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.2 (50.00-3.10)<br>95.2 (50.00-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.20                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.06 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.15_3459                                            | Depositor        |
| R, $R_{free}$                                                           | 0.231 , 0.268<br>0.231 , 0.267                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 48817 reflections (4.49%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.273                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 59.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 293819                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 91.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: SF4, PAR, 4OC, UR3, 2MA, G7M, OMG, OMC, PSU, M2G, 5MC, 5MU, OMU, ZN, 2MG, 0TD, MG, MA6

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | QA    | 0.37         | 0/35795     | 0.38        | 7/55864 (0.0%) |
| 1   | XA    | 0.39         | 0/35890     | 0.39        | 5/56012 (0.0%) |
| 2   | QB    | 0.41         | 0/1876      | 1.14        | 20/2533 (0.8%) |
| 2   | XB    | 0.40         | 0/1860      | 1.03        | 11/2518 (0.4%) |
| 3   | QC    | 0.35         | 0/1582      | 0.81        | 4/2137 (0.2%)  |
| 3   | XC    | 0.42         | 0/1566      | 0.89        | 7/2119 (0.3%)  |
| 4   | QD    | 0.48         | 0/1695      | 1.01        | 13/2274 (0.6%) |
| 4   | XD    | 0.43         | 0/1698      | 0.89        | 4/2277 (0.2%)  |
| 5   | QE    | 0.36         | 0/1149      | 0.76        | 2/1548 (0.1%)  |
| 5   | XE    | 0.38         | 0/1149      | 0.77        | 0/1548         |
| 6   | QF    | 0.45         | 0/827       | 0.80        | 2/1120 (0.2%)  |
| 6   | XF    | 0.45         | 0/829       | 0.80        | 1/1123 (0.1%)  |
| 7   | QG    | 0.37         | 0/1254      | 0.86        | 3/1683 (0.2%)  |
| 7   | XG    | 0.42         | 0/1248      | 0.87        | 6/1676 (0.4%)  |
| 8   | QH    | 0.40         | 0/1118      | 0.85        | 2/1506 (0.1%)  |
| 8   | XH    | 0.40         | 0/1108      | 0.84        | 4/1494 (0.3%)  |
| 9   | QI    | 0.36         | 0/1005      | 0.97        | 7/1351 (0.5%)  |
| 9   | XI    | 0.36         | 0/985       | 0.93        | 4/1329 (0.3%)  |
| 10  | QJ    | 0.40         | 0/732       | 0.96        | 3/993 (0.3%)   |
| 10  | XJ    | 0.43         | 0/723       | 0.85        | 2/984 (0.2%)   |
| 11  | QK    | 0.38         | 0/849       | 0.79        | 2/1150 (0.2%)  |
| 11  | XK    | 0.38         | 0/848       | 0.80        | 3/1149 (0.3%)  |
| 12  | QL    | 0.49         | 0/937       | 1.03        | 4/1260 (0.3%)  |
| 12  | XL    | 0.52         | 0/937       | 1.02        | 3/1260 (0.2%)  |
| 13  | QM    | 0.38         | 0/924       | 1.03        | 9/1242 (0.7%)  |
| 13  | XM    | 0.42         | 0/905       | 1.05        | 7/1217 (0.6%)  |
| 14  | QN    | 0.37         | 0/501       | 0.80        | 0/664          |
| 14  | XN    | 0.39         | 0/501       | 0.79        | 0/664          |
| 15  | QO    | 0.41         | 0/739       | 0.91        | 4/985 (0.4%)   |
| 15  | XO    | 0.40         | 0/739       | 0.90        | 3/985 (0.3%)   |
| 16  | QP    | 0.41         | 0/697       | 0.99        | 5/939 (0.5%)   |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 16  | XP    | 0.43         | 0/693   | 0.97        | 6/935 (0.6%)    |
| 17  | QQ    | 0.42         | 0/836   | 0.82        | 1/1117 (0.1%)   |
| 17  | XQ    | 0.40         | 0/836   | 0.85        | 2/1117 (0.2%)   |
| 18  | QR    | 0.38         | 0/560   | 0.78        | 2/746 (0.3%)    |
| 18  | XR    | 0.42         | 0/560   | 0.79        | 2/746 (0.3%)    |
| 19  | QS    | 0.40         | 0/663   | 0.97        | 4/895 (0.4%)    |
| 19  | XS    | 0.38         | 0/660   | 0.97        | 4/893 (0.4%)    |
| 20  | QT    | 0.36         | 0/734   | 0.84        | 4/969 (0.4%)    |
| 20  | XT    | 0.36         | 0/736   | 0.75        | 0/976           |
| 21  | QU    | 0.32         | 0/203   | 0.67        | 0/266           |
| 21  | XU    | 0.36         | 0/203   | 0.73        | 0/266           |
| 22  | QV    | 0.33         | 0/1832  | 0.35        | 0/2855          |
| 22  | XV    | 0.38         | 0/1832  | 0.38        | 0/2855          |
| 23  | QX    | 0.31         | 0/443   | 0.51        | 0/690           |
| 23  | XX    | 0.31         | 0/443   | 0.53        | 0/690           |
| 24  | QY    | 0.28         | 0/1816  | 0.39        | 0/2830          |
| 24  | XY    | 0.33         | 0/1816  | 0.42        | 0/2830          |
| 25  | R0    | 0.44         | 0/616   | 0.93        | 2/821 (0.2%)    |
| 25  | Y0    | 0.48         | 0/616   | 0.97        | 3/821 (0.4%)    |
| 26  | R1    | 0.44         | 0/761   | 0.76        | 0/1013          |
| 26  | Y1    | 0.47         | 0/766   | 0.78        | 2/1018 (0.2%)   |
| 27  | R2    | 0.43         | 0/590   | 0.81        | 0/781           |
| 27  | Y2    | 0.48         | 0/594   | 0.95        | 2/785 (0.3%)    |
| 28  | R3    | 0.43         | 0/474   | 0.91        | 2/635 (0.3%)    |
| 28  | Y3    | 0.48         | 0/469   | 0.90        | 1/630 (0.2%)    |
| 29  | R4    | 0.46         | 0/559   | 1.22        | 6/754 (0.8%)    |
| 29  | Y4    | 0.48         | 0/549   | 1.28        | 13/741 (1.8%)   |
| 30  | R5    | 0.48         | 0/473   | 0.86        | 1/639 (0.2%)    |
| 30  | Y5    | 0.48         | 0/469   | 0.78        | 0/635           |
| 31  | R6    | 0.48         | 0/460   | 0.91        | 1/613 (0.2%)    |
| 31  | Y6    | 0.50         | 0/456   | 0.89        | 2/608 (0.3%)    |
| 32  | R7    | 0.49         | 0/426   | 0.92        | 1/561 (0.2%)    |
| 32  | Y7    | 0.49         | 0/426   | 0.90        | 0/561           |
| 33  | R8    | 0.46         | 0/525   | 0.76        | 0/691           |
| 33  | Y8    | 0.50         | 0/525   | 0.75        | 0/691           |
| 34  | R9    | 0.45         | 0/310   | 0.79        | 0/407           |
| 34  | Y9    | 0.52         | 0/310   | 0.79        | 0/407           |
| 35  | RA    | 0.42         | 0/68903 | 0.40        | 3/107552 (0.0%) |
| 35  | YA    | 0.47         | 0/68903 | 0.41        | 3/107552 (0.0%) |
| 36  | RB    | 0.37         | 0/2876  | 0.36        | 0/4486          |
| 36  | YB    | 0.43         | 0/2878  | 0.38        | 0/4490          |
| 37  | RD    | 0.49         | 0/2181  | 0.87        | 6/2940 (0.2%)   |
| 37  | YD    | 0.52         | 0/2186  | 0.85        | 6/2944 (0.2%)   |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 38  | RE    | 0.44         | 0/1592   | 0.89        | 3/2149 (0.1%)     |
| 38  | YE    | 0.51         | 0/1592   | 0.91        | 5/2149 (0.2%)     |
| 39  | RF    | 0.50         | 0/1618   | 0.94        | 8/2191 (0.4%)     |
| 39  | YF    | 0.49         | 0/1614   | 0.91        | 3/2186 (0.1%)     |
| 40  | RG    | 0.41         | 0/1451   | 0.92        | 8/1961 (0.4%)     |
| 40  | YG    | 0.44         | 0/1449   | 0.87        | 5/1957 (0.3%)     |
| 41  | RH    | 0.40         | 0/1356   | 0.86        | 4/1834 (0.2%)     |
| 41  | YH    | 0.45         | 0/1350   | 0.78        | 4/1826 (0.2%)     |
| 42  | RI    | 0.39         | 0/1109   | 0.90        | 6/1512 (0.4%)     |
| 42  | YI    | 0.42         | 0/1091   | 0.80        | 1/1490 (0.1%)     |
| 43  | RN    | 0.44         | 0/1148   | 0.78        | 3/1547 (0.2%)     |
| 43  | YN    | 0.48         | 0/1144   | 0.80        | 1/1543 (0.1%)     |
| 44  | RO    | 0.47         | 0/943    | 0.84        | 3/1269 (0.2%)     |
| 44  | YO    | 0.51         | 0/943    | 0.82        | 0/1269            |
| 45  | RP    | 0.45         | 0/1152   | 0.88        | 3/1533 (0.2%)     |
| 45  | YP    | 0.51         | 0/1152   | 0.88        | 4/1533 (0.3%)     |
| 46  | RQ    | 0.39         | 0/1143   | 0.77        | 0/1527            |
| 46  | YQ    | 0.45         | 0/1143   | 0.80        | 0/1527            |
| 47  | RR    | 0.45         | 0/982    | 0.84        | 0/1312            |
| 47  | YR    | 0.48         | 0/982    | 0.85        | 1/1312 (0.1%)     |
| 48  | RS    | 0.40         | 0/887    | 0.91        | 4/1180 (0.3%)     |
| 48  | YS    | 0.44         | 0/880    | 0.84        | 1/1172 (0.1%)     |
| 49  | RT    | 0.42         | 0/1105   | 0.81        | 2/1477 (0.1%)     |
| 49  | YT    | 0.43         | 0/1097   | 0.83        | 2/1468 (0.1%)     |
| 50  | RU    | 0.44         | 0/977    | 0.88        | 5/1301 (0.4%)     |
| 50  | YU    | 0.49         | 0/977    | 0.92        | 7/1301 (0.5%)     |
| 51  | RV    | 0.50         | 0/786    | 1.02        | 4/1053 (0.4%)     |
| 51  | YV    | 0.49         | 0/782    | 0.88        | 3/1049 (0.3%)     |
| 52  | RW    | 0.43         | 0/897    | 0.77        | 1/1205 (0.1%)     |
| 52  | YW    | 0.47         | 0/897    | 0.75        | 1/1205 (0.1%)     |
| 53  | RX    | 0.43         | 0/764    | 0.81        | 0/1025            |
| 53  | YX    | 0.45         | 0/764    | 0.81        | 1/1025 (0.1%)     |
| 54  | RY    | 0.41         | 0/823    | 0.85        | 0/1099            |
| 54  | YY    | 0.48         | 0/823    | 0.89        | 0/1100            |
| 55  | RZ    | 0.39         | 0/1438   | 0.95        | 6/1955 (0.3%)     |
| 55  | YZ    | 0.43         | 0/1413   | 1.00        | 8/1924 (0.4%)     |
| All | All   | 0.43         | 0/316097 | 0.57        | 333/473222 (0.1%) |

There are no bond length outliers.

All (333) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 51  | RV    | 49  | THR  | N-CA-C   | -13.80 | 90.09       | 110.24   |
| 55  | RZ    | 38  | TYR  | CA-CB-CG | 11.45  | 134.50      | 113.90   |
| 2   | QB    | 232 | PRO  | CA-C-N   | 11.02  | 152.25      | 120.97   |
| 2   | QB    | 232 | PRO  | C-N-CA   | 11.02  | 152.25      | 120.97   |
| 13  | XM    | 80  | ARG  | N-CA-C   | -10.71 | 98.52       | 111.69   |
| 41  | RH    | 101 | ARG  | N-CA-C   | -10.62 | 100.45      | 113.41   |
| 2   | QB    | 23  | ARG  | N-CA-C   | -10.60 | 98.47       | 114.16   |
| 12  | QL    | 119 | LYS  | N-CA-C   | -10.42 | 93.73       | 110.20   |
| 13  | QM    | 23  | TYR  | CA-CB-CG | 10.26  | 132.37      | 113.90   |
| 50  | YU    | 52  | ARG  | CG-CD-NE | 10.05  | 134.11      | 112.00   |
| 29  | Y4    | 68  | ARG  | N-CA-C   | 9.99   | 122.17      | 111.28   |
| 29  | R4    | 52  | THR  | N-CA-C   | -9.88  | 97.17       | 111.30   |
| 16  | QP    | 38  | TYR  | CA-CB-CG | 9.78   | 131.50      | 113.90   |
| 12  | XL    | 119 | LYS  | N-CA-C   | -9.70  | 93.66       | 109.96   |
| 37  | YD    | 84  | TYR  | CA-CB-CG | 9.65   | 131.27      | 113.90   |
| 8   | XH    | 79  | VAL  | N-CA-C   | -9.60  | 101.41      | 111.58   |
| 55  | YZ    | 38  | TYR  | CA-CB-CG | 9.58   | 131.15      | 113.90   |
| 50  | RU    | 52  | ARG  | CG-CD-NE | 9.39   | 132.66      | 112.00   |
| 50  | YU    | 9   | VAL  | N-CA-C   | 9.26   | 119.86      | 110.23   |
| 2   | QB    | 10  | LEU  | N-CA-C   | -9.16  | 102.49      | 114.31   |
| 55  | RZ    | 122 | ARG  | N-CA-C   | -8.97  | 102.05      | 113.72   |
| 37  | RD    | 84  | TYR  | CA-CB-CG | 8.92   | 129.96      | 113.90   |
| 39  | YF    | 64  | ILE  | N-CA-C   | 8.78   | 120.62      | 110.62   |
| 3   | XC    | 39  | ILE  | N-CA-C   | -8.69  | 101.94      | 110.72   |
| 13  | XM    | 23  | TYR  | CA-CB-CG | 8.59   | 129.36      | 113.90   |
| 16  | XP    | 38  | TYR  | CA-CB-CG | 8.32   | 128.87      | 113.90   |
| 25  | R0    | 44  | ARG  | N-CA-C   | -8.28  | 101.80      | 112.23   |
| 39  | RF    | 99  | TYR  | CA-CB-CG | 8.23   | 128.71      | 113.90   |
| 17  | XQ    | 65  | ILE  | N-CA-C   | -8.18  | 105.28      | 111.90   |
| 3   | XC    | 125 | GLU  | N-CA-C   | -7.99  | 103.67      | 113.50   |
| 50  | RU    | 9   | VAL  | N-CA-C   | 7.98   | 118.53      | 110.23   |
| 8   | QH    | 79  | VAL  | N-CA-C   | -7.97  | 101.12      | 112.35   |
| 38  | YE    | 69  | LYS  | N-CA-C   | -7.83  | 102.82      | 111.36   |
| 13  | XM    | 66  | LEU  | N-CA-C   | 7.70   | 122.81      | 111.34   |
| 40  | RG    | 48  | GLU  | CA-C-N   | 7.64   | 136.13      | 121.54   |
| 40  | RG    | 48  | GLU  | C-N-CA   | 7.64   | 136.13      | 121.54   |
| 2   | XB    | 19  | HIS  | N-CA-C   | 7.49   | 120.30      | 107.93   |
| 4   | QD    | 8   | VAL  | N-CA-C   | 7.49   | 121.59      | 113.43   |
| 39  | RF    | 64  | ILE  | N-CA-C   | 7.35   | 119.00      | 110.62   |
| 2   | QB    | 126 | GLU  | CA-C-N   | 7.32   | 135.15      | 121.97   |
| 2   | QB    | 126 | GLU  | C-N-CA   | 7.32   | 135.15      | 121.97   |
| 9   | QI    | 36  | TYR  | CA-CB-CG | 7.29   | 127.03      | 113.90   |
| 12  | QL    | 48  | PRO  | CA-C-N   | 7.29   | 135.46      | 121.54   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 12  | QL    | 48  | PRO  | C-N-CA    | 7.29  | 135.46      | 121.54   |
| 45  | RP    | 73  | GLY  | N-CA-C    | 7.27  | 118.90      | 111.56   |
| 39  | YF    | 62  | ARG  | N-CA-C    | -7.25 | 98.75       | 110.20   |
| 2   | QB    | 190 | THR  | N-CA-C    | 7.21  | 120.01      | 111.71   |
| 45  | RP    | 30  | THR  | N-CA-C    | -7.21 | 105.67      | 114.75   |
| 19  | QS    | 14  | HIS  | N-CA-C    | -7.19 | 103.48      | 112.90   |
| 11  | XK    | 116 | HIS  | CA-C-N    | 7.16  | 135.21      | 121.54   |
| 11  | XK    | 116 | HIS  | C-N-CA    | 7.16  | 135.21      | 121.54   |
| 4   | QD    | 196 | LEU  | N-CA-C    | -7.15 | 100.78      | 110.36   |
| 45  | YP    | 99  | LEU  | N-CA-C    | -7.14 | 102.90      | 111.69   |
| 2   | XB    | 23  | ARG  | N-CA-C    | -7.13 | 101.82      | 111.87   |
| 9   | QI    | 99  | LEU  | N-CA-C    | -7.11 | 104.64      | 113.38   |
| 13  | QM    | 11  | ARG  | N-CA-C    | -7.10 | 101.37      | 110.53   |
| 9   | XI    | 96  | LEU  | N-CA-C    | -7.09 | 105.25      | 114.04   |
| 3   | XC    | 21  | ARG  | N-CA-C    | 7.05  | 120.40      | 107.99   |
| 2   | QB    | 8   | LYS  | CA-C-N    | 7.01  | 134.93      | 121.54   |
| 2   | QB    | 8   | LYS  | C-N-CA    | 7.01  | 134.93      | 121.54   |
| 12  | QL    | 87  | GLY  | N-CA-C    | 7.00  | 129.76      | 113.18   |
| 12  | XL    | 48  | PRO  | N-CA-C    | 6.99  | 126.87      | 112.47   |
| 19  | QS    | 34  | TRP  | N-CA-C    | -6.92 | 103.23      | 113.61   |
| 42  | RI    | 74  | ASN  | N-CA-C    | -6.91 | 101.41      | 111.30   |
| 13  | QM    | 15  | VAL  | N-CA-C    | 6.91  | 117.67      | 110.62   |
| 1   | QA    | 266 | G    | P-O3'-C3' | 6.89  | 130.54      | 120.20   |
| 9   | QI    | 96  | LEU  | N-CA-C    | -6.85 | 104.07      | 113.18   |
| 39  | RF    | 32  | LEU  | N-CA-C    | -6.84 | 103.91      | 111.36   |
| 29  | Y4    | 58  | ARG  | N-CA-CB   | 6.83  | 122.03      | 110.49   |
| 41  | RH    | 9   | ILE  | N-CA-C    | 6.81  | 113.75      | 107.56   |
| 3   | XC    | 29  | TYR  | CA-CB-CG  | 6.80  | 126.14      | 113.90   |
| 51  | RV    | 12  | TYR  | CA-CB-CG  | 6.78  | 126.10      | 113.90   |
| 4   | XD    | 8   | VAL  | N-CA-C    | 6.77  | 117.38      | 111.90   |
| 45  | YP    | 71  | VAL  | N-CA-C    | 6.74  | 122.38      | 112.61   |
| 3   | QC    | 19  | GLU  | N-CA-C    | -6.72 | 105.09      | 113.28   |
| 55  | YZ    | 51  | ALA  | CA-C-N    | 6.71  | 134.36      | 121.54   |
| 55  | YZ    | 51  | ALA  | C-N-CA    | 6.71  | 134.36      | 121.54   |
| 17  | QQ    | 65  | ILE  | N-CA-C    | -6.70 | 106.26      | 112.96   |
| 15  | XO    | 12  | ILE  | N-CA-C    | -6.68 | 103.97      | 110.72   |
| 29  | Y4    | 57  | GLU  | CA-C-N    | 6.64  | 134.23      | 121.54   |
| 29  | Y4    | 57  | GLU  | C-N-CA    | 6.64  | 134.23      | 121.54   |
| 26  | Y1    | 3   | LYS  | N-CA-C    | 6.64  | 118.74      | 109.31   |
| 55  | YZ    | 171 | ILE  | N-CA-C    | 6.64  | 119.60      | 112.96   |
| 11  | XK    | 40  | ILE  | N-CA-C    | -6.59 | 106.41      | 111.62   |
| 1   | XA    | 266 | G    | P-O3'-C3' | 6.58  | 130.08      | 120.20   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 43  | RN    | 114     | ARG  | N-CA-C      | -6.58 | 105.07      | 113.23   |
| 38  | RE    | 144     | ARG  | N-CA-CB     | 6.58  | 116.22      | 109.51   |
| 2   | XB    | 19      | HIS  | CA-C-N      | 6.57  | 134.09      | 121.54   |
| 2   | XB    | 19      | HIS  | C-N-CA      | 6.57  | 134.09      | 121.54   |
| 1   | QA    | 266     | G    | C2'-C3'-O3' | 6.49  | 119.24      | 109.50   |
| 41  | RH    | 46      | GLU  | N-CA-C      | -6.49 | 100.27      | 108.45   |
| 40  | RG    | 47      | LYS  | CA-C-N      | 6.49  | 133.93      | 121.54   |
| 40  | RG    | 47      | LYS  | C-N-CA      | 6.49  | 133.93      | 121.54   |
| 30  | R5    | 59      | GLU  | N-CA-C      | -6.48 | 98.71       | 109.46   |
| 19  | XS    | 27      | GLU  | N-CA-C      | 6.46  | 119.27      | 108.73   |
| 29  | R4    | 57      | GLU  | CA-C-N      | 6.46  | 133.87      | 121.54   |
| 29  | R4    | 57      | GLU  | C-N-CA      | 6.46  | 133.87      | 121.54   |
| 12  | XL    | 87      | GLY  | N-CA-C      | 6.43  | 128.42      | 113.18   |
| 16  | XP    | 5       | ARG  | N-CA-C      | 6.41  | 116.74      | 108.34   |
| 55  | YZ    | 122     | ARG  | N-CA-C      | -6.39 | 105.30      | 113.23   |
| 50  | YU    | 52      | ARG  | CD-NE-CZ    | 6.39  | 133.34      | 124.40   |
| 15  | QO    | 12      | ILE  | N-CA-C      | -6.38 | 104.28      | 110.72   |
| 3   | QC    | 29      | TYR  | CA-CB-CG    | 6.37  | 125.37      | 113.90   |
| 15  | QO    | 65      | ARG  | N-CA-C      | -6.37 | 104.41      | 111.36   |
| 1   | XA    | 266     | G    | C2'-C3'-O3' | 6.37  | 119.05      | 109.50   |
| 45  | YP    | 69      | GLY  | N-CA-C      | 6.34  | 117.97      | 111.95   |
| 19  | XS    | 67      | VAL  | N-CA-C      | 6.33  | 116.96      | 110.82   |
| 9   | QI    | 41      | VAL  | N-CA-C      | -6.32 | 103.74      | 113.16   |
| 4   | QD    | 185     | PHE  | CA-CB-CG    | 6.30  | 120.10      | 113.80   |
| 35  | YA    | 272(M)  | G    | P-O3'-C3'   | 6.30  | 127.26      | 119.70   |
| 2   | QB    | 23      | ARG  | CA-C-N      | 6.29  | 132.15      | 120.95   |
| 2   | QB    | 23      | ARG  | C-N-CA      | 6.29  | 132.15      | 120.95   |
| 13  | XM    | 11      | ARG  | N-CA-C      | 6.29  | 118.94      | 111.71   |
| 7   | XG    | 69      | VAL  | N-CA-C      | -6.29 | 107.12      | 113.47   |
| 1   | QA    | 1442(A) | G    | P-O3'-C3'   | 6.28  | 127.24      | 119.70   |
| 45  | RP    | 71      | VAL  | N-CA-C      | 6.25  | 119.85      | 112.35   |
| 48  | RS    | 20      | ARG  | N-CA-C      | 6.25  | 118.09      | 111.28   |
| 37  | YD    | 71      | ASP  | N-CA-C      | -6.24 | 104.02      | 111.69   |
| 3   | XC    | 36      | ASP  | N-CA-C      | -6.23 | 104.57      | 111.36   |
| 41  | YH    | 101     | ARG  | N-CA-C      | -6.23 | 106.00      | 113.97   |
| 10  | QJ    | 31      | GLY  | CA-C-N      | 6.22  | 133.42      | 121.54   |
| 10  | QJ    | 31      | GLY  | C-N-CA      | 6.22  | 133.42      | 121.54   |
| 35  | RA    | 272(M)  | G    | P-O3'-C3'   | 6.20  | 127.14      | 119.70   |
| 25  | Y0    | 44      | ARG  | N-CA-C      | -6.20 | 104.42      | 112.23   |
| 40  | YG    | 80      | PHE  | N-CA-C      | -6.19 | 99.19       | 109.46   |
| 7   | XG    | 77      | SER  | N-CA-C      | 6.18  | 118.76      | 110.35   |
| 6   | QF    | 63      | TYR  | CA-CB-CG    | 6.18  | 125.03      | 113.90   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 39  | YF    | 105     | VAL  | N-CA-C    | -6.17 | 104.28      | 111.00   |
| 45  | YP    | 30      | THR  | N-CA-C    | -6.17 | 106.98      | 114.75   |
| 27  | Y2    | 20      | GLU  | N-CA-C    | -6.17 | 104.82      | 112.90   |
| 42  | RI    | 84      | GLY  | CA-C-N    | 6.16  | 133.31      | 121.54   |
| 42  | RI    | 84      | GLY  | C-N-CA    | 6.16  | 133.31      | 121.54   |
| 3   | XC    | 201     | TYR  | CA-CB-CG  | 6.16  | 124.99      | 113.90   |
| 4   | QD    | 5       | ILE  | N-CA-C    | 6.16  | 122.14      | 109.34   |
| 4   | XD    | 204     | ILE  | N-CA-C    | -6.14 | 104.52      | 110.72   |
| 2   | QB    | 15      | VAL  | CA-C-N    | 6.13  | 133.26      | 121.54   |
| 2   | QB    | 15      | VAL  | C-N-CA    | 6.13  | 133.26      | 121.54   |
| 35  | RA    | 272(M)  | G    | OP1-P-O3' | 6.13  | 118.68      | 105.20   |
| 37  | RD    | 71      | ASP  | N-CA-C    | -6.12 | 104.16      | 111.69   |
| 20  | QT    | 11      | SER  | N-CA-C    | -6.12 | 105.58      | 113.16   |
| 49  | YT    | 93      | ARG  | N-CA-C    | 6.08  | 118.63      | 108.73   |
| 1   | XA    | 1442(A) | G    | P-O3'-C3' | 6.07  | 126.99      | 119.70   |
| 7   | XG    | 114     | ARG  | N-CA-C    | 6.04  | 118.77      | 111.40   |
| 19  | QS    | 36      | ARG  | N-CA-C    | -6.03 | 105.92      | 113.28   |
| 2   | XB    | 185     | ILE  | N-CA-C    | -6.03 | 99.73       | 108.71   |
| 37  | RD    | 53      | PHE  | N-CA-C    | 6.02  | 119.94      | 111.52   |
| 35  | YA    | 272(M)  | G    | OP1-P-O3' | 6.02  | 118.44      | 105.20   |
| 18  | QR    | 70      | ILE  | N-CA-C    | -5.99 | 104.67      | 110.72   |
| 2   | QB    | 16      | HIS  | N-CA-C    | 5.97  | 123.53      | 110.80   |
| 51  | RV    | 2       | PHE  | N-CA-CB   | 5.97  | 119.67      | 110.60   |
| 16  | QP    | 20      | VAL  | N-CA-C    | 5.96  | 116.95      | 108.42   |
| 4   | QD    | 138     | TYR  | CA-CB-CG  | 5.95  | 124.61      | 113.90   |
| 29  | Y4    | 45      | GLY  | CA-C-N    | 5.95  | 132.90      | 121.54   |
| 29  | Y4    | 45      | GLY  | C-N-CA    | 5.95  | 132.90      | 121.54   |
| 55  | YZ    | 48      | PHE  | N-CA-C    | 5.92  | 117.74      | 111.28   |
| 7   | XG    | 22      | LEU  | N-CA-C    | -5.92 | 104.78      | 112.23   |
| 9   | XI    | 87      | GLN  | N-CA-C    | -5.90 | 104.79      | 112.23   |
| 48  | RS    | 59      | LYS  | N-CA-C    | 5.90  | 120.27      | 112.72   |
| 7   | XG    | 45      | ASP  | N-CA-C    | -5.86 | 104.84      | 112.23   |
| 40  | YG    | 128     | ARG  | N-CA-C    | -5.86 | 105.78      | 113.17   |
| 50  | RU    | 52      | ARG  | CD-NE-CZ  | 5.85  | 132.59      | 124.40   |
| 50  | YU    | 52      | ARG  | CB-CG-CD  | 5.85  | 124.75      | 111.30   |
| 40  | YG    | 95      | ARG  | CA-C-N    | 5.84  | 132.70      | 121.54   |
| 40  | YG    | 95      | ARG  | C-N-CA    | 5.84  | 132.70      | 121.54   |
| 8   | QH    | 103     | VAL  | N-CA-C    | 5.83  | 116.54      | 108.84   |
| 13  | QM    | 105     | THR  | CA-C-N    | 5.83  | 132.68      | 121.54   |
| 13  | QM    | 105     | THR  | C-N-CA    | 5.83  | 132.68      | 121.54   |
| 29  | Y4    | 43      | TYR  | CA-CB-CG  | 5.82  | 124.38      | 113.90   |
| 4   | QD    | 186     | LEU  | N-CA-C    | 5.82  | 117.49      | 111.03   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 15  | QO    | 6    | GLU  | N-CA-C    | 5.81  | 117.29      | 111.07   |
| 4   | QD    | 63   | LYS  | N-CA-C    | -5.80 | 104.59      | 111.03   |
| 29  | Y4    | 52   | THR  | N-CA-C    | -5.79 | 106.22      | 113.28   |
| 7   | QG    | 91   | VAL  | N-CA-C    | 5.79  | 117.04      | 109.58   |
| 44  | RO    | 94   | ARG  | N-CA-C    | -5.78 | 106.23      | 113.28   |
| 6   | XF    | 63   | TYR  | CA-CB-CG  | 5.77  | 124.28      | 113.90   |
| 50  | YU    | 50   | ARG  | N-CA-C    | -5.77 | 104.96      | 112.23   |
| 19  | XS    | 6    | LYS  | N-CA-C    | -5.76 | 105.08      | 111.36   |
| 7   | QG    | 30   | ILE  | N-CA-C    | -5.75 | 103.73      | 111.44   |
| 3   | QC    | 201  | TYR  | CA-CB-CG  | 5.75  | 124.25      | 113.90   |
| 29  | R4    | 58   | ARG  | N-CA-C    | 5.73  | 123.01      | 110.80   |
| 2   | XB    | 17   | PHE  | N-CA-C    | 5.72  | 119.08      | 111.75   |
| 39  | RF    | 9    | ILE  | N-CA-C    | 5.72  | 114.12      | 107.89   |
| 39  | RF    | 196  | LEU  | N-CA-C    | -5.71 | 105.03      | 112.23   |
| 13  | XM    | 15   | VAL  | N-CA-C    | 5.69  | 118.17      | 111.05   |
| 43  | YN    | 51   | PHE  | N-CA-C    | -5.68 | 99.97       | 109.24   |
| 40  | RG    | 128  | ARG  | N-CA-C    | -5.66 | 106.42      | 113.38   |
| 50  | RU    | 51   | LYS  | N-CA-C    | -5.66 | 104.58      | 112.45   |
| 27  | Y2    | 9    | GLN  | N-CA-C    | -5.65 | 105.20      | 111.36   |
| 52  | RW    | 99   | ARG  | N-CA-C    | 5.65  | 117.99      | 110.53   |
| 31  | Y6    | 7    | ILE  | N-CA-C    | 5.64  | 116.20      | 110.05   |
| 48  | YS    | 111  | GLU  | N-CA-C    | 5.64  | 117.97      | 107.99   |
| 40  | YG    | 95   | ARG  | N-CA-C    | -5.64 | 100.22      | 109.80   |
| 35  | YA    | 1065 | U    | P-O3'-C3' | 5.63  | 128.65      | 120.20   |
| 41  | YH    | 59   | ARG  | N-CA-C    | 5.63  | 117.42      | 111.28   |
| 15  | XO    | 45   | VAL  | N-CA-C    | -5.63 | 106.21      | 111.45   |
| 20  | QT    | 13   | LEU  | N-CA-C    | -5.63 | 105.23      | 111.36   |
| 40  | RG    | 96   | ARG  | N-CA-C    | 5.63  | 122.79      | 110.80   |
| 49  | RT    | 121  | ILE  | N-CA-C    | -5.63 | 104.86      | 111.00   |
| 15  | XO    | 83   | GLU  | N-CA-C    | -5.62 | 104.77      | 111.69   |
| 38  | YE    | 72   | VAL  | N-CA-C    | 5.62  | 117.77      | 108.99   |
| 37  | YD    | 10   | THR  | N-CA-C    | -5.62 | 99.78       | 108.55   |
| 43  | RN    | 51   | PHE  | N-CA-C    | -5.61 | 101.33      | 110.20   |
| 4   | QD    | 178  | VAL  | CA-C-N    | 5.59  | 132.22      | 121.54   |
| 4   | QD    | 178  | VAL  | C-N-CA    | 5.59  | 132.22      | 121.54   |
| 4   | QD    | 156  | GLU  | N-CA-C    | 5.58  | 117.37      | 111.28   |
| 38  | RE    | 76   | ARG  | N-CA-C    | 5.57  | 118.19      | 111.40   |
| 16  | XP    | 33   | ILE  | N-CA-C    | 5.54  | 115.63      | 110.42   |
| 16  | QP    | 5    | ARG  | N-CA-C    | 5.54  | 115.59      | 108.34   |
| 49  | YT    | 7    | ILE  | N-CA-C    | -5.53 | 105.46      | 110.82   |
| 4   | QD    | 163  | GLU  | N-CA-C    | -5.52 | 105.28      | 112.23   |
| 18  | QR    | 31   | LEU  | N-CA-C    | -5.52 | 105.28      | 112.23   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37  | YD    | 257  | LEU  | N-CA-C    | 5.51  | 117.08      | 109.15   |
| 16  | XP    | 20   | VAL  | N-CA-C    | 5.50  | 116.28      | 108.42   |
| 16  | XP    | 27   | LYS  | N-CA-C    | -5.47 | 103.16      | 110.55   |
| 41  | YH    | 129  | THR  | N-CA-C    | -5.47 | 107.15      | 113.88   |
| 26  | Y1    | 72   | GLU  | N-CA-C    | -5.47 | 105.40      | 111.36   |
| 35  | RA    | 1065 | U    | P-O3'-C3' | 5.47  | 128.40      | 120.20   |
| 39  | RF    | 183  | VAL  | N-CA-C    | 5.47  | 116.19      | 110.62   |
| 29  | R4    | 49   | PHE  | CB-CA-C   | -5.46 | 101.77      | 110.84   |
| 51  | YV    | 50   | PRO  | CA-C-N    | 5.45  | 129.26      | 121.96   |
| 51  | YV    | 50   | PRO  | C-N-CA    | 5.45  | 129.26      | 121.96   |
| 37  | RD    | 50   | THR  | N-CA-C    | -5.44 | 106.32      | 113.12   |
| 10  | QJ    | 92   | THR  | N-CA-C    | 5.44  | 117.02      | 111.14   |
| 5   | QE    | 26   | PHE  | N-CA-C    | 5.42  | 117.87      | 110.55   |
| 25  | Y0    | 40   | GLN  | N-CA-C    | 5.42  | 116.51      | 108.60   |
| 29  | Y4    | 67   | TYR  | CA-CB-CG  | 5.42  | 123.65      | 113.90   |
| 43  | RN    | 23   | LEU  | N-CA-C    | 5.42  | 116.87      | 110.97   |
| 2   | QB    | 78   | GLN  | N-CA-C    | 5.41  | 117.18      | 111.28   |
| 8   | XH    | 37   | ARG  | N-CA-C    | -5.41 | 105.42      | 112.23   |
| 42  | RI    | 31   | LEU  | N-CA-C    | 5.41  | 120.84      | 113.16   |
| 50  | RU    | 40   | PHE  | N-CA-C    | -5.40 | 105.47      | 111.36   |
| 37  | YD    | 99   | ASP  | N-CA-C    | -5.40 | 106.19      | 112.89   |
| 2   | QB    | 187  | LEU  | N-CA-C    | -5.39 | 100.38      | 108.96   |
| 28  | R3    | 31   | LEU  | N-CA-C    | -5.37 | 102.53      | 110.48   |
| 29  | Y4    | 46   | GLN  | CA-C-N    | 5.37  | 131.80      | 121.54   |
| 29  | Y4    | 46   | GLN  | C-N-CA    | 5.37  | 131.80      | 121.54   |
| 37  | YD    | 53   | PHE  | N-CA-C    | 5.36  | 118.64      | 111.24   |
| 7   | QG    | 114  | ARG  | N-CA-C    | 5.36  | 117.20      | 111.36   |
| 55  | RZ    | 50   | GLN  | N-CA-C    | -5.36 | 107.40      | 114.31   |
| 1   | QA    | 1067 | A    | P-O3'-C3' | 5.36  | 128.23      | 120.20   |
| 3   | XC    | 17   | ASP  | N-CA-C    | -5.36 | 102.53      | 110.46   |
| 9   | XI    | 70   | LYS  | N-CA-C    | 5.36  | 120.15      | 111.37   |
| 37  | RD    | 99   | ASP  | N-CA-C    | -5.35 | 106.25      | 112.89   |
| 47  | YR    | 2    | ARG  | N-CA-C    | -5.35 | 105.03      | 112.03   |
| 52  | YW    | 99   | ARG  | N-CA-C    | 5.34  | 117.43      | 110.43   |
| 17  | XQ    | 42   | TYR  | CA-CB-CG  | 5.34  | 123.51      | 113.90   |
| 11  | QK    | 40   | ILE  | N-CA-C    | -5.33 | 106.98      | 111.56   |
| 13  | QM    | 66   | LEU  | N-CA-C    | 5.33  | 116.88      | 109.31   |
| 44  | RO    | 9    | GLU  | N-CA-C    | -5.33 | 103.36      | 110.55   |
| 55  | RZ    | 148  | ASP  | N-CA-C    | -5.32 | 102.87      | 110.59   |
| 1   | XA    | 1067 | A    | P-O3'-C3' | 5.32  | 128.19      | 120.20   |
| 41  | RH    | 163  | TYR  | CA-CB-CG  | 5.32  | 123.48      | 113.90   |
| 3   | QC    | 161  | GLU  | N-CA-C    | -5.31 | 105.66      | 111.82   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 50  | YU    | 40  | PHE  | N-CA-C   | -5.31 | 105.58      | 111.36   |
| 4   | QD    | 140 | VAL  | N-CA-C   | -5.31 | 101.99      | 109.21   |
| 9   | QI    | 48  | GLU  | N-CA-C   | 5.30  | 120.89      | 113.57   |
| 39  | RF    | 190 | GLU  | N-CA-C   | -5.30 | 106.65      | 113.23   |
| 32  | R7    | 30  | VAL  | N-CA-C   | -5.30 | 105.55      | 110.53   |
| 9   | QI    | 64  | THR  | N-CA-C   | -5.29 | 101.54      | 109.95   |
| 16  | QP    | 32  | TYR  | CA-CB-CG | 5.27  | 123.39      | 113.90   |
| 2   | QB    | 22  | LYS  | CA-C-N   | 5.27  | 129.29      | 120.70   |
| 2   | QB    | 22  | LYS  | C-N-CA   | 5.27  | 129.29      | 120.70   |
| 50  | YU    | 29  | SER  | N-CA-C   | -5.27 | 107.51      | 114.31   |
| 37  | RD    | 10  | THR  | N-CA-C   | -5.26 | 100.34      | 108.55   |
| 20  | QT    | 55  | ILE  | N-CA-C   | -5.25 | 105.41      | 110.72   |
| 51  | RV    | 46  | VAL  | N-CA-C   | 5.25  | 115.42      | 107.80   |
| 41  | YH    | 110 | SER  | N-CA-C   | -5.25 | 106.46      | 112.92   |
| 4   | XD    | 116 | GLN  | N-CA-C   | -5.25 | 105.23      | 111.69   |
| 18  | XR    | 31  | LEU  | N-CA-C   | -5.24 | 106.73      | 113.23   |
| 40  | RG    | 109 | VAL  | N-CA-C   | 5.23  | 116.06      | 111.56   |
| 53  | YX    | 69  | TYR  | N-CA-C   | 5.23  | 116.78      | 108.67   |
| 5   | QE    | 111 | GLU  | N-CA-C   | -5.22 | 105.27      | 111.69   |
| 2   | QB    | 20  | GLU  | N-CA-C   | 5.22  | 121.91      | 110.80   |
| 29  | R4    | 68  | ARG  | N-CA-C   | 5.21  | 118.31      | 109.76   |
| 42  | RI    | 89  | TYR  | N-CA-C   | -5.21 | 105.51      | 111.14   |
| 28  | Y3    | 56  | VAL  | N-CA-C   | 5.21  | 115.46      | 108.17   |
| 55  | YZ    | 77  | ASP  | N-CA-C   | -5.20 | 101.66      | 109.15   |
| 2   | XB    | 129 | GLU  | CA-C-N   | 5.20  | 138.47      | 122.71   |
| 2   | XB    | 129 | GLU  | C-N-CA   | 5.20  | 138.47      | 122.71   |
| 19  | XS    | 34  | TRP  | N-CA-C   | -5.20 | 105.61      | 112.94   |
| 42  | RI    | 68  | LEU  | N-CA-C   | -5.20 | 105.69      | 112.23   |
| 51  | YV    | 2   | PHE  | N-CA-C   | -5.19 | 101.53      | 109.41   |
| 10  | XJ    | 34  | VAL  | N-CA-C   | 5.18  | 115.56      | 107.99   |
| 15  | QO    | 45  | VAL  | N-CA-C   | -5.18 | 106.03      | 110.74   |
| 39  | RF    | 127 | GLU  | N-CA-C   | -5.17 | 105.26      | 112.45   |
| 55  | RZ    | 59  | LEU  | N-CA-C   | 5.17  | 117.18      | 108.96   |
| 19  | QS    | 11  | VAL  | N-CA-C   | -5.17 | 100.80      | 108.45   |
| 25  | R0    | 40  | GLN  | N-CA-C   | 5.17  | 116.66      | 108.96   |
| 48  | RS    | 34  | HIS  | N-CA-C   | 5.15  | 117.10      | 109.69   |
| 29  | Y4    | 25  | TYR  | CA-CB-CG | 5.14  | 123.16      | 113.90   |
| 2   | QB    | 12  | GLU  | N-CA-C   | -5.14 | 106.25      | 112.88   |
| 13  | XM    | 65  | LYS  | N-CA-C   | -5.14 | 102.08      | 110.20   |
| 38  | RE    | 12  | THR  | N-CA-C   | -5.14 | 101.97      | 108.45   |
| 13  | XM    | 5   | ALA  | N-CA-C   | 5.14  | 121.74      | 110.80   |
| 11  | QK    | 102 | GLY  | N-CA-C   | -5.13 | 107.59      | 116.01   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 31  | Y6    | 28   | ARG  | N-CA-C    | -5.13 | 105.38      | 111.69   |
| 44  | RO    | 113  | LYS  | N-CA-C    | -5.12 | 105.77      | 111.36   |
| 1   | QA    | 1065 | U    | P-O3'-C3' | 5.11  | 127.87      | 120.20   |
| 9   | QI    | 70   | LYS  | N-CA-C    | 5.11  | 117.24      | 111.11   |
| 1   | QA    | 991  | U    | P-O3'-C3' | 5.11  | 127.86      | 120.20   |
| 9   | XI    | 51   | ARG  | N-CA-C    | -5.10 | 106.90      | 113.23   |
| 25  | Y0    | 39   | ARG  | N-CA-C    | -5.10 | 100.42      | 108.73   |
| 55  | YZ    | 53   | ILE  | N-CA-C    | -5.10 | 106.61      | 112.98   |
| 1   | XA    | 1065 | U    | P-O3'-C3' | 5.10  | 127.85      | 120.20   |
| 18  | XR    | 22   | VAL  | N-CA-C    | -5.09 | 105.57      | 113.16   |
| 4   | QD    | 204  | ILE  | N-CA-C    | -5.09 | 105.58      | 110.72   |
| 42  | YI    | 126  | TYR  | CA-CB-CG  | 5.09  | 123.06      | 113.90   |
| 29  | Y4    | 49   | PHE  | N-CA-C    | 5.09  | 121.64      | 110.80   |
| 16  | XP    | 53   | VAL  | N-CA-C    | 5.08  | 117.44      | 111.09   |
| 31  | R6    | 9    | LEU  | N-CA-C    | 5.08  | 115.75      | 108.74   |
| 1   | QA    | 687  | A    | P-O3'-C3' | 5.07  | 127.81      | 120.20   |
| 38  | YE    | 61   | ARG  | N-CA-C    | 5.07  | 120.50      | 113.45   |
| 28  | R3    | 54   | VAL  | N-CA-C    | 5.06  | 115.20      | 108.11   |
| 13  | QM    | 66   | LEU  | CA-C-N    | 5.06  | 129.24      | 121.19   |
| 13  | QM    | 66   | LEU  | C-N-CA    | 5.06  | 129.24      | 121.19   |
| 49  | RT    | 12   | SER  | N-CA-C    | 5.05  | 117.52      | 111.71   |
| 4   | XD    | 38   | TYR  | CA-CB-CG  | 5.05  | 122.99      | 113.90   |
| 55  | RZ    | 77   | ASP  | N-CA-C    | -5.05 | 100.85      | 108.67   |
| 6   | QF    | 65   | VAL  | N-CA-C    | 5.04  | 116.12      | 108.96   |
| 20  | QT    | 93   | GLU  | N-CA-C    | -5.04 | 105.97      | 111.82   |
| 8   | XH    | 100  | ILE  | N-CA-C    | -5.04 | 104.01      | 108.95   |
| 13  | QM    | 23   | TYR  | CB-CA-C   | 5.04  | 117.42      | 110.16   |
| 2   | XB    | 127  | ILE  | CA-C-N    | 5.04  | 131.16      | 121.54   |
| 2   | XB    | 127  | ILE  | C-N-CA    | 5.04  | 131.16      | 121.54   |
| 38  | YE    | 202  | LYS  | N-CA-C    | -5.03 | 106.56      | 113.30   |
| 8   | XH    | 103  | VAL  | N-CA-C    | 5.03  | 115.48      | 108.84   |
| 38  | YE    | 102  | VAL  | N-CA-C    | 5.02  | 117.23      | 108.95   |
| 2   | XB    | 87   | ARG  | N-CA-C    | -5.02 | 106.00      | 111.82   |
| 10  | XJ    | 50   | ILE  | N-CA-C    | -5.02 | 103.02      | 109.30   |
| 16  | QP    | 9    | PHE  | N-CA-C    | -5.02 | 102.13      | 109.81   |
| 40  | RG    | 107  | LEU  | N-CA-C    | 5.01  | 117.48      | 111.71   |
| 48  | RS    | 54   | LEU  | N-CA-C    | -5.01 | 105.53      | 111.69   |
| 7   | XG    | 89   | MET  | N-CA-C    | 5.01  | 117.57      | 109.40   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | QA    | 32246 | 0        | 16295    | 176     | 0            |
| 1   | XA    | 32331 | 0        | 16337    | 186     | 0            |
| 2   | QB    | 1842  | 0        | 1861     | 27      | 0            |
| 2   | XB    | 1825  | 0        | 1828     | 23      | 0            |
| 3   | QC    | 1558  | 0        | 1557     | 29      | 0            |
| 3   | XC    | 1542  | 0        | 1517     | 16      | 0            |
| 4   | QD    | 1665  | 0        | 1691     | 35      | 0            |
| 4   | XD    | 1668  | 0        | 1707     | 26      | 0            |
| 5   | QE    | 1133  | 0        | 1191     | 16      | 0            |
| 5   | XE    | 1133  | 0        | 1191     | 14      | 0            |
| 6   | QF    | 814   | 0        | 808      | 8       | 0            |
| 6   | XF    | 816   | 0        | 808      | 20      | 0            |
| 7   | QG    | 1235  | 0        | 1249     | 17      | 0            |
| 7   | XG    | 1229  | 0        | 1238     | 11      | 0            |
| 8   | QH    | 1098  | 0        | 1143     | 18      | 0            |
| 8   | XH    | 1088  | 0        | 1126     | 14      | 0            |
| 9   | QI    | 986   | 0        | 990      | 25      | 0            |
| 9   | XI    | 966   | 0        | 953      | 25      | 0            |
| 10  | QJ    | 719   | 0        | 672      | 10      | 0            |
| 10  | XJ    | 710   | 0        | 661      | 15      | 0            |
| 11  | QK    | 834   | 0        | 838      | 12      | 0            |
| 11  | XK    | 833   | 0        | 836      | 12      | 0            |
| 12  | QL    | 932   | 0        | 981      | 17      | 0            |
| 12  | XL    | 932   | 0        | 981      | 11      | 0            |
| 13  | QM    | 914   | 0        | 954      | 14      | 0            |
| 13  | XM    | 895   | 0        | 920      | 23      | 0            |
| 14  | QN    | 492   | 0        | 529      | 11      | 0            |
| 14  | XN    | 492   | 0        | 529      | 11      | 0            |
| 15  | QO    | 728   | 0        | 760      | 2       | 0            |
| 15  | XO    | 728   | 0        | 760      | 3       | 0            |
| 16  | QP    | 681   | 0        | 697      | 20      | 0            |
| 16  | XP    | 677   | 0        | 686      | 22      | 0            |
| 17  | QQ    | 823   | 0        | 891      | 10      | 0            |
| 17  | XQ    | 823   | 0        | 891      | 10      | 0            |
| 18  | QR    | 555   | 0        | 618      | 5       | 0            |
| 18  | XR    | 555   | 0        | 618      | 12      | 0            |
| 19  | QS    | 648   | 0        | 658      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | XS    | 645   | 0        | 635      | 17      | 0            |
| 20  | QT    | 732   | 0        | 809      | 9       | 0            |
| 20  | XT    | 733   | 0        | 795      | 9       | 0            |
| 21  | QU    | 199   | 0        | 208      | 1       | 0            |
| 21  | XU    | 199   | 0        | 208      | 0       | 0            |
| 22  | QV    | 1640  | 0        | 837      | 6       | 0            |
| 22  | XV    | 1640  | 0        | 837      | 7       | 0            |
| 23  | QX    | 394   | 0        | 197      | 1       | 0            |
| 23  | XX    | 394   | 0        | 197      | 1       | 0            |
| 24  | QY    | 1625  | 0        | 822      | 5       | 0            |
| 24  | XY    | 1625  | 0        | 822      | 7       | 0            |
| 25  | R0    | 608   | 0        | 622      | 8       | 0            |
| 25  | Y0    | 608   | 0        | 622      | 12      | 0            |
| 26  | R1    | 754   | 0        | 823      | 10      | 0            |
| 26  | Y1    | 759   | 0        | 837      | 7       | 0            |
| 27  | R2    | 588   | 0        | 643      | 8       | 0            |
| 27  | Y2    | 592   | 0        | 654      | 6       | 0            |
| 28  | R3    | 469   | 0        | 518      | 2       | 0            |
| 28  | Y3    | 464   | 0        | 514      | 8       | 0            |
| 29  | R4    | 546   | 0        | 522      | 9       | 0            |
| 29  | Y4    | 536   | 0        | 514      | 12      | 0            |
| 30  | R5    | 459   | 0        | 476      | 8       | 0            |
| 30  | Y5    | 455   | 0        | 465      | 6       | 0            |
| 31  | R6    | 453   | 0        | 473      | 2       | 0            |
| 31  | Y6    | 449   | 0        | 469      | 3       | 0            |
| 32  | R7    | 418   | 0        | 466      | 5       | 0            |
| 32  | Y7    | 418   | 0        | 466      | 4       | 0            |
| 33  | R8    | 517   | 0        | 582      | 16      | 0            |
| 33  | Y8    | 517   | 0        | 582      | 12      | 0            |
| 34  | R9    | 307   | 0        | 335      | 5       | 0            |
| 34  | Y9    | 307   | 0        | 335      | 8       | 0            |
| 35  | RA    | 61758 | 0        | 31137    | 286     | 0            |
| 35  | YA    | 61758 | 0        | 31138    | 275     | 0            |
| 36  | RB    | 2572  | 0        | 1304     | 3       | 0            |
| 36  | YB    | 2573  | 0        | 1306     | 7       | 0            |
| 37  | RD    | 2131  | 0        | 2205     | 41      | 0            |
| 37  | YD    | 2136  | 0        | 2217     | 44      | 0            |
| 38  | RE    | 1559  | 0        | 1618     | 21      | 0            |
| 38  | YE    | 1559  | 0        | 1618     | 35      | 0            |
| 39  | RF    | 1583  | 0        | 1624     | 43      | 0            |
| 39  | YF    | 1579  | 0        | 1618     | 29      | 0            |
| 40  | RG    | 1426  | 0        | 1445     | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40  | YG    | 1424  | 0        | 1441     | 22      | 0            |
| 41  | RH    | 1330  | 0        | 1407     | 16      | 0            |
| 41  | YH    | 1324  | 0        | 1402     | 14      | 0            |
| 42  | RI    | 1094  | 0        | 1127     | 5       | 0            |
| 42  | YI    | 1076  | 0        | 1094     | 4       | 0            |
| 43  | RN    | 1121  | 0        | 1195     | 16      | 0            |
| 43  | YN    | 1117  | 0        | 1184     | 9       | 0            |
| 44  | RO    | 933   | 0        | 996      | 19      | 0            |
| 44  | YO    | 933   | 0        | 996      | 18      | 0            |
| 45  | RP    | 1135  | 0        | 1212     | 22      | 0            |
| 45  | YP    | 1135  | 0        | 1212     | 24      | 0            |
| 46  | RQ    | 1122  | 0        | 1179     | 18      | 0            |
| 46  | YQ    | 1122  | 0        | 1179     | 14      | 0            |
| 47  | RR    | 968   | 0        | 1033     | 10      | 0            |
| 47  | YR    | 968   | 0        | 1033     | 12      | 0            |
| 48  | RS    | 877   | 0        | 938      | 10      | 0            |
| 48  | YS    | 870   | 0        | 923      | 8       | 0            |
| 49  | RT    | 1091  | 0        | 1151     | 17      | 0            |
| 49  | YT    | 1083  | 0        | 1136     | 15      | 0            |
| 50  | RU    | 959   | 0        | 1019     | 15      | 0            |
| 50  | YU    | 959   | 0        | 1019     | 11      | 0            |
| 51  | RV    | 775   | 0        | 841      | 15      | 0            |
| 51  | YV    | 771   | 0        | 830      | 8       | 0            |
| 52  | RW    | 886   | 0        | 940      | 9       | 0            |
| 52  | YW    | 886   | 0        | 940      | 9       | 0            |
| 53  | RX    | 750   | 0        | 814      | 11      | 0            |
| 53  | YX    | 750   | 0        | 814      | 6       | 0            |
| 54  | RY    | 810   | 0        | 892      | 10      | 0            |
| 54  | YY    | 810   | 0        | 887      | 14      | 0            |
| 55  | RZ    | 1406  | 0        | 1418     | 17      | 0            |
| 55  | YZ    | 1381  | 0        | 1386     | 15      | 0            |
| 56  | QA    | 221   | 0        | 0        | 0       | 0            |
| 56  | QB    | 1     | 0        | 0        | 0       | 0            |
| 56  | QD    | 4     | 0        | 0        | 0       | 0            |
| 56  | QE    | 4     | 0        | 0        | 0       | 0            |
| 56  | QF    | 2     | 0        | 0        | 0       | 0            |
| 56  | QG    | 2     | 0        | 0        | 0       | 0            |
| 56  | QH    | 2     | 0        | 0        | 0       | 0            |
| 56  | QI    | 1     | 0        | 0        | 0       | 0            |
| 56  | QK    | 1     | 0        | 0        | 0       | 0            |
| 56  | QL    | 3     | 0        | 0        | 0       | 0            |
| 56  | QN    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | QO    | 2     | 0        | 0        | 0       | 0            |
| 56  | QP    | 1     | 0        | 0        | 0       | 0            |
| 56  | QT    | 1     | 0        | 0        | 0       | 0            |
| 56  | QV    | 5     | 0        | 0        | 0       | 0            |
| 56  | R0    | 3     | 0        | 0        | 0       | 0            |
| 56  | R1    | 1     | 0        | 0        | 0       | 0            |
| 56  | R3    | 3     | 0        | 0        | 0       | 0            |
| 56  | R5    | 2     | 0        | 0        | 0       | 0            |
| 56  | R6    | 1     | 0        | 0        | 0       | 0            |
| 56  | R7    | 3     | 0        | 0        | 0       | 0            |
| 56  | R9    | 1     | 0        | 0        | 0       | 0            |
| 56  | RA    | 709   | 0        | 0        | 0       | 0            |
| 56  | RB    | 17    | 0        | 0        | 0       | 0            |
| 56  | RD    | 8     | 0        | 0        | 0       | 0            |
| 56  | RE    | 4     | 0        | 0        | 0       | 0            |
| 56  | RF    | 4     | 0        | 0        | 0       | 0            |
| 56  | RG    | 4     | 0        | 0        | 0       | 0            |
| 56  | RH    | 2     | 0        | 0        | 0       | 0            |
| 56  | RN    | 2     | 0        | 0        | 0       | 0            |
| 56  | RO    | 1     | 0        | 0        | 0       | 0            |
| 56  | RP    | 3     | 0        | 0        | 0       | 0            |
| 56  | RQ    | 4     | 0        | 0        | 0       | 0            |
| 56  | RR    | 2     | 0        | 0        | 0       | 0            |
| 56  | RT    | 4     | 0        | 0        | 0       | 0            |
| 56  | RU    | 2     | 0        | 0        | 0       | 0            |
| 56  | RV    | 3     | 0        | 0        | 0       | 0            |
| 56  | RW    | 1     | 0        | 0        | 0       | 0            |
| 56  | RZ    | 1     | 0        | 0        | 0       | 0            |
| 56  | XA    | 193   | 0        | 0        | 0       | 0            |
| 56  | XE    | 2     | 0        | 0        | 0       | 0            |
| 56  | XF    | 2     | 0        | 0        | 0       | 0            |
| 56  | XJ    | 1     | 0        | 0        | 0       | 0            |
| 56  | XL    | 2     | 0        | 0        | 0       | 0            |
| 56  | XR    | 1     | 0        | 0        | 0       | 0            |
| 56  | XT    | 1     | 0        | 0        | 0       | 0            |
| 56  | XV    | 3     | 0        | 0        | 0       | 0            |
| 56  | XY    | 1     | 0        | 0        | 0       | 0            |
| 56  | Y0    | 1     | 0        | 0        | 0       | 0            |
| 56  | Y1    | 2     | 0        | 0        | 0       | 0            |
| 56  | Y3    | 1     | 0        | 0        | 0       | 0            |
| 56  | Y5    | 1     | 0        | 0        | 0       | 0            |
| 56  | Y6    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56  | Y7    | 2      | 0        | 0        | 0       | 0            |
| 56  | Y8    | 1      | 0        | 0        | 0       | 0            |
| 56  | YA    | 707    | 0        | 0        | 0       | 0            |
| 56  | YB    | 20     | 0        | 0        | 0       | 0            |
| 56  | YD    | 7      | 0        | 0        | 0       | 0            |
| 56  | YE    | 5      | 0        | 0        | 0       | 0            |
| 56  | YF    | 3      | 0        | 0        | 0       | 0            |
| 56  | YG    | 3      | 0        | 0        | 0       | 0            |
| 56  | YI    | 1      | 0        | 0        | 0       | 0            |
| 56  | YN    | 1      | 0        | 0        | 0       | 0            |
| 56  | YO    | 1      | 0        | 0        | 0       | 0            |
| 56  | YP    | 2      | 0        | 0        | 0       | 0            |
| 56  | YQ    | 2      | 0        | 0        | 0       | 0            |
| 56  | YR    | 2      | 0        | 0        | 0       | 0            |
| 56  | YT    | 3      | 0        | 0        | 0       | 0            |
| 56  | YV    | 1      | 0        | 0        | 0       | 0            |
| 56  | YW    | 2      | 0        | 0        | 0       | 0            |
| 57  | QA    | 42     | 0        | 45       | 1       | 0            |
| 57  | XA    | 42     | 0        | 45       | 2       | 0            |
| 58  | QD    | 8      | 0        | 0        | 0       | 0            |
| 58  | XD    | 8      | 0        | 0        | 1       | 0            |
| 59  | QN    | 1      | 0        | 0        | 0       | 0            |
| 59  | R4    | 1      | 0        | 0        | 0       | 0            |
| 59  | R5    | 1      | 0        | 0        | 0       | 0            |
| 59  | R6    | 1      | 0        | 0        | 0       | 0            |
| 59  | R9    | 1      | 0        | 0        | 0       | 0            |
| 59  | RY    | 1      | 0        | 0        | 0       | 0            |
| 59  | XN    | 1      | 0        | 0        | 0       | 0            |
| 59  | Y4    | 1      | 0        | 0        | 0       | 0            |
| 59  | Y5    | 1      | 0        | 0        | 0       | 0            |
| 59  | Y6    | 1      | 0        | 0        | 0       | 0            |
| 59  | Y9    | 1      | 0        | 0        | 0       | 0            |
| 59  | YY    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 293819 | 0        | 196213   | 1818    | 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 4.

All (1818) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:RZ:8:TYR:HB2   | 55:RZ:38:TYR:CE1   | 1.78                     | 1.17              |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:HD2   | 1.09                     | 1.13              |
| 55:RZ:8:TYR:HB2   | 55:RZ:38:TYR:CD1   | 1.90                     | 1.07              |
| 35:RA:660:G:H5'   | 39:RF:99:TYR:CE2   | 1.94                     | 1.03              |
| 16:QP:20:VAL:HG21 | 16:QP:32:TYR:CD2   | 1.94                     | 1.02              |
| 4:QD:38:TYR:HE2   | 4:QD:45:GLN:HG2    | 1.26                     | 1.00              |
| 16:XP:20:VAL:HG21 | 16:XP:32:TYR:CD2   | 1.96                     | 0.99              |
| 3:QC:159:GLY:N    | 3:QC:193:TYR:HE2   | 1.60                     | 0.99              |
| 35:RA:660:G:C5'   | 39:RF:99:TYR:CE2   | 2.47                     | 0.97              |
| 35:RA:660:G:C5'   | 39:RF:99:TYR:HE2   | 1.78                     | 0.95              |
| 35:YA:2604:U:H5'' | 35:YA:2604:U:H6    | 1.31                     | 0.94              |
| 16:XP:20:VAL:HG21 | 16:XP:32:TYR:HD2   | 1.30                     | 0.94              |
| 16:QP:38:TYR:CD1  | 16:QP:50:LYS:HB3   | 2.04                     | 0.91              |
| 55:RZ:8:TYR:CB    | 55:RZ:38:TYR:CE1   | 2.56                     | 0.87              |
| 35:YA:1567:A:C5   | 37:YD:84:TYR:HE2   | 1.92                     | 0.87              |
| 35:RA:528:A:H2    | 43:RN:114:ARG:NH2  | 1.72                     | 0.86              |
| 16:QP:38:TYR:CE1  | 16:QP:50:LYS:HB3   | 2.12                     | 0.85              |
| 3:QC:159:GLY:HA2  | 3:QC:193:TYR:CE2   | 2.11                     | 0.85              |
| 38:YE:84:PHE:CD2  | 38:YE:86:PRO:HD3   | 2.11                     | 0.84              |
| 19:XS:41:VAL:CG2  | 19:XS:43:GLU:OE1   | 2.25                     | 0.84              |
| 35:RA:528:A:H2    | 43:RN:114:ARG:HH21 | 1.21                     | 0.83              |
| 35:YA:1567:A:C5   | 37:YD:84:TYR:CE2   | 2.68                     | 0.82              |
| 19:XS:41:VAL:HB   | 19:XS:43:GLU:OE1   | 1.80                     | 0.82              |
| 3:QC:159:GLY:CA   | 3:QC:193:TYR:HE2   | 1.92                     | 0.81              |
| 35:RA:660:G:H4'   | 39:RF:99:TYR:HE2   | 1.45                     | 0.80              |
| 35:RA:660:G:H5'   | 39:RF:99:TYR:CD2   | 2.17                     | 0.79              |
| 19:XS:41:VAL:HG23 | 19:XS:43:GLU:OE1   | 1.80                     | 0.79              |
| 3:QC:159:GLY:HA2  | 3:QC:193:TYR:CD2   | 2.18                     | 0.79              |
| 35:YA:1567:A:N7   | 37:YD:84:TYR:HE2   | 1.80                     | 0.79              |
| 1:QA:1422:G:H5''  | 44:RO:48:PRO:HB3   | 1.65                     | 0.79              |
| 4:QD:98:GLU:OE1   | 4:QD:189:PRO:CG    | 2.30                     | 0.78              |
| 39:RF:39:TRP:HA   | 39:RF:99:TYR:HE1   | 1.48                     | 0.78              |
| 1:XA:1330:U:H4'   | 13:XM:23:TYR:CD1   | 2.17                     | 0.78              |
| 4:QD:38:TYR:CE2   | 4:QD:45:GLN:HG2    | 2.15                     | 0.78              |
| 1:QA:1330:U:H4'   | 13:QM:23:TYR:CD1   | 2.18                     | 0.77              |
| 50:RU:49:HIS:HA   | 50:RU:52:ARG:HB3   | 1.66                     | 0.77              |
| 4:QD:98:GLU:OE2   | 4:QD:194:LEU:HD23  | 1.83                     | 0.77              |
| 55:RZ:8:TYR:CB    | 55:RZ:38:TYR:HE1   | 1.97                     | 0.77              |
| 1:QA:626:U:H4'    | 16:QP:38:TYR:CE2   | 2.20                     | 0.76              |
| 16:QP:38:TYR:CE1  | 16:QP:50:LYS:CB    | 2.69                     | 0.76              |
| 29:Y4:11:PRO:HG3  | 29:Y4:25:TYR:CE2   | 2.21                     | 0.76              |
| 35:YA:2604:U:H5'' | 35:YA:2604:U:C6    | 2.19                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:QC:159:GLY:H    | 3:QC:193:TYR:HE2  | 1.33                     | 0.75              |
| 1:QA:626:U:H4'    | 16:QP:38:TYR:HE2  | 1.51                     | 0.74              |
| 19:XS:43:GLU:OE1  | 19:XS:43:GLU:N    | 2.20                     | 0.74              |
| 3:QC:159:GLY:CA   | 3:QC:193:TYR:CE2  | 2.69                     | 0.74              |
| 19:XS:41:VAL:CB   | 19:XS:43:GLU:OE1  | 2.35                     | 0.74              |
| 35:RA:660:G:C4'   | 39:RF:99:TYR:HE2  | 2.00                     | 0.74              |
| 50:YU:49:HIS:HA   | 50:YU:52:ARG:HB3  | 1.70                     | 0.74              |
| 1:XA:1043:C:OP1   | 1:XA:1043:C:H4'   | 1.87                     | 0.74              |
| 1:QA:1086:U:H3    | 1:QA:1099:G:H22   | 1.36                     | 0.73              |
| 3:QC:184:TYR:HE1  | 3:QC:201:TYR:HE1  | 1.36                     | 0.73              |
| 1:XA:626:U:H4'    | 16:XP:38:TYR:CE2  | 2.24                     | 0.73              |
| 1:XA:501:C:OP1    | 12:XL:117:ARG:NH2 | 2.22                     | 0.72              |
| 4:QD:98:GLU:OE1   | 4:QD:189:PRO:HG3  | 1.90                     | 0.72              |
| 38:YE:84:PHE:CE2  | 38:YE:86:PRO:HD3  | 2.24                     | 0.72              |
| 41:RH:154:PRO:HB3 | 41:RH:163:TYR:CE1 | 2.24                     | 0.72              |
| 1:XA:1422:G:H5''  | 44:YO:48:PRO:HB3  | 1.71                     | 0.71              |
| 1:XA:1393:U:HO2'  | 1:XA:1501:C:HO2'  | 1.39                     | 0.71              |
| 4:QD:68:TYR:HE2   | 4:QD:103:ASN:ND2  | 1.88                     | 0.71              |
| 48:YS:25:ARG:NH1  | 48:YS:88:ASP:OD2  | 2.22                     | 0.71              |
| 3:QC:184:TYR:CE1  | 3:QC:201:TYR:CE1  | 2.79                     | 0.71              |
| 1:XA:1249:C:O2'   | 9:XI:73:GLN:NE2   | 2.24                     | 0.70              |
| 6:XF:50:TYR:HE1   | 18:XR:77:GLY:HA2  | 1.55                     | 0.70              |
| 35:YA:1041:C:H42  | 35:YA:1114:G:H1   | 1.39                     | 0.70              |
| 3:QC:159:GLY:N    | 3:QC:193:TYR:CE2  | 2.53                     | 0.70              |
| 10:QJ:10:GLY:HA3  | 10:QJ:16:LEU:HD21 | 1.72                     | 0.70              |
| 16:QP:38:TYR:HE1  | 16:QP:50:LYS:HB2  | 1.55                     | 0.70              |
| 24:QY:4:G:H1      | 24:QY:69:C:H42    | 1.37                     | 0.70              |
| 35:RA:2131:G:H5'' | 35:RA:2132:U:H5'  | 1.74                     | 0.70              |
| 1:XA:664:G:H22    | 1:XA:741:G:H1     | 1.38                     | 0.69              |
| 1:QA:236:G:H5''   | 17:QQ:42:TYR:OH   | 1.92                     | 0.69              |
| 40:RG:47:LYS:NZ   | 40:RG:80:PHE:O    | 2.25                     | 0.69              |
| 1:QA:559:A:H4'    | 1:QA:560:U:H3'    | 1.72                     | 0.69              |
| 2:QB:185:ILE:HG22 | 2:QB:199:TYR:HB2  | 1.74                     | 0.69              |
| 16:QP:5:ARG:HH12  | 16:QP:28:ARG:HA   | 1.56                     | 0.69              |
| 35:RA:528:A:C2    | 43:RN:114:ARG:NH2 | 2.60                     | 0.69              |
| 35:RA:660:G:C5'   | 39:RF:99:TYR:CD2  | 2.76                     | 0.69              |
| 1:QA:544:G:OP1    | 4:QD:59:ARG:NH2   | 2.25                     | 0.69              |
| 1:XA:544:G:OP1    | 4:XD:59:ARG:NH2   | 2.26                     | 0.69              |
| 35:RA:881:G:H1    | 35:RA:895:U:H3    | 1.39                     | 0.69              |
| 33:Y8:30:ARG:HH21 | 45:YP:63:PRO:HB2  | 1.57                     | 0.69              |
| 35:YA:1056:G:H21  | 35:YA:1103:A:H62  | 1.39                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:XB:122:PHE:HE2   | 2:XB:139:LYS:HD3  | 1.58                     | 0.68              |
| 1:QA:429:U:OP1     | 4:QD:13:ARG:NH1   | 2.27                     | 0.68              |
| 16:QP:38:TYR:HE1   | 16:QP:50:LYS:CB   | 2.07                     | 0.68              |
| 1:XA:1130:A:O2'    | 9:XI:3:GLN:NE2    | 2.26                     | 0.68              |
| 27:R2:66:GLU:HA    | 27:R2:69:ARG:HD3  | 1.76                     | 0.67              |
| 44:RO:35:VAL:HG11  | 44:RO:103:ALA:HB3 | 1.76                     | 0.67              |
| 35:RA:83:G:H1      | 35:RA:102:G:HO2'  | 1.41                     | 0.67              |
| 35:RA:1153:C:OP1   | 50:RU:92:ARG:NH2  | 2.25                     | 0.67              |
| 51:YV:21:ARG:NE    | 51:YV:91:TYR:HE2  | 1.93                     | 0.67              |
| 1:QA:1295:G:O2'    | 13:QM:14:ARG:NH1  | 2.27                     | 0.67              |
| 2:QB:8:LYS:O       | 2:QB:217:ARG:NH2  | 2.28                     | 0.67              |
| 4:QD:98:GLU:OE1    | 4:QD:189:PRO:HG2  | 1.94                     | 0.67              |
| 1:XA:559:A:H4'     | 1:XA:560:U:H3'    | 1.77                     | 0.67              |
| 34:R9:27:CYS:SG    | 34:R9:28:GLU:N    | 2.68                     | 0.66              |
| 5:XE:102:ALA:HB1   | 5:XE:106:PRO:HG2  | 1.77                     | 0.66              |
| 25:Y0:39:ARG:HH21  | 35:YA:2355:C:H1'  | 1.61                     | 0.66              |
| 3:QC:184:TYR:HE1   | 3:QC:201:TYR:CE1  | 2.13                     | 0.66              |
| 52:RW:14:PRO:HG2   | 52:RW:78:GLU:HG2  | 1.76                     | 0.66              |
| 35:RA:958:U:OP2    | 46:RQ:14:ARG:NH1  | 2.29                     | 0.66              |
| 16:QP:38:TYR:HD1   | 16:QP:50:LYS:HB3  | 1.60                     | 0.66              |
| 35:YA:881:G:H1     | 35:YA:895:U:H3    | 1.43                     | 0.66              |
| 35:RA:1041:C:H42   | 35:RA:1114:G:H1   | 1.44                     | 0.66              |
| 20:XT:100:ILE:HG22 | 20:XT:101:GLY:H   | 1.59                     | 0.66              |
| 9:QI:86:VAL:HG21   | 9:QI:93:ARG:HE    | 1.59                     | 0.66              |
| 29:R4:16:CYS:SG    | 29:R4:17:GLY:N    | 2.69                     | 0.66              |
| 55:YZ:51:ALA:HB1   | 55:YZ:55:HIS:HB2  | 1.78                     | 0.66              |
| 8:XH:114:THR:HG23  | 8:XH:116:LYS:H    | 1.61                     | 0.66              |
| 10:XJ:57:LYS:HE2   | 10:XJ:60:ARG:HH22 | 1.60                     | 0.66              |
| 55:YZ:10:ARG:HE    | 55:YZ:36:LYS:HB3  | 1.61                     | 0.65              |
| 1:XA:8:A:N6        | 4:XD:205:GLU:O    | 2.29                     | 0.65              |
| 35:YA:2131:G:H5''  | 35:YA:2132:U:H5'  | 1.77                     | 0.65              |
| 39:RF:157:VAL:HB   | 39:RF:194:MET:HG2 | 1.78                     | 0.65              |
| 35:YA:2506:U:C2    | 35:YA:2585:U:O4   | 2.49                     | 0.65              |
| 35:YA:2298:A:H62   | 35:YA:2318:G:H8   | 1.44                     | 0.65              |
| 1:QA:501:C:OP1     | 12:QL:117:ARG:NH2 | 2.29                     | 0.65              |
| 1:QA:545:C:OP1     | 4:QD:61:LYS:NZ    | 2.29                     | 0.65              |
| 4:XD:98:GLU:HA     | 4:XD:103:ASN:HD22 | 1.62                     | 0.65              |
| 12:XL:47:LYS:O     | 12:XL:49:ASN:N    | 2.30                     | 0.65              |
| 35:YA:483:A:H5''   | 54:YY:50:ARG:HE   | 1.61                     | 0.65              |
| 38:YE:84:PHE:HE2   | 38:YE:86:PRO:HG3  | 1.62                     | 0.65              |
| 2:QB:187:LEU:HA    | 2:QB:201:ILE:HB   | 1.77                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1123:A:H4'   | 10:XJ:36:GLY:HA3   | 1.78                     | 0.65              |
| 6:XF:81:ILE:HD11  | 37:YD:125:ILE:HB   | 1.79                     | 0.65              |
| 51:RV:21:ARG:HH11 | 51:RV:91:TYR:HE2   | 1.45                     | 0.65              |
| 29:Y4:14:ILE:HB   | 29:Y4:22:ILE:HB    | 1.79                     | 0.65              |
| 35:YA:2010:G:H5'' | 52:YW:42:ARG:HB2   | 1.79                     | 0.65              |
| 39:RF:143:ALA:HB1 | 39:RF:148:LEU:HB2  | 1.78                     | 0.64              |
| 13:XM:6:GLY:HA3   | 13:XM:67:GLU:HG3   | 1.78                     | 0.64              |
| 35:YA:1153:C:OP1  | 50:YU:92:ARG:NH2   | 2.29                     | 0.64              |
| 4:QD:4:TYR:O      | 4:QD:6:GLY:N       | 2.31                     | 0.64              |
| 37:RD:85:ASP:OD2  | 37:RD:88:ARG:NH1   | 2.29                     | 0.64              |
| 38:RE:2:LYS:HB2   | 38:RE:95:ILE:HD12  | 1.78                     | 0.64              |
| 17:QQ:26:GLN:HG2  | 17:QQ:37:LYS:HG2   | 1.78                     | 0.64              |
| 35:RA:2010:G:H5'' | 52:RW:42:ARG:HB2   | 1.79                     | 0.64              |
| 6:XF:87:ARG:NH1   | 18:XR:75:ILE:O     | 2.31                     | 0.64              |
| 1:XA:1101:A:N7    | 2:XB:175:ARG:NH2   | 2.46                     | 0.64              |
| 55:RZ:115:GLY:HA2 | 55:RZ:177:PRO:HD3  | 1.79                     | 0.64              |
| 38:YE:84:PHE:HE2  | 38:YE:86:PRO:CG    | 2.10                     | 0.64              |
| 1:QA:664:G:H22    | 1:QA:741:G:H1      | 1.45                     | 0.63              |
| 33:R8:6:THR:HG22  | 33:R8:63:PRO:HD2   | 1.81                     | 0.63              |
| 35:YA:39:C:O2     | 39:YF:46:ARG:NH2   | 2.28                     | 0.63              |
| 9:QI:121:ARG:NH1  | 9:QI:122:ALA:O     | 2.30                     | 0.63              |
| 4:QD:18:LYS:NZ    | 4:QD:31:CYS:SG     | 2.72                     | 0.63              |
| 1:XA:626:U:H4'    | 16:XP:38:TYR:HE2   | 1.61                     | 0.63              |
| 34:Y9:27:CYS:SG   | 34:Y9:28:GLU:N     | 2.71                     | 0.63              |
| 5:QE:102:ALA:HB1  | 5:QE:106:PRO:HG2   | 1.79                     | 0.63              |
| 35:RA:1791:A:H5'  | 37:RD:206:LEU:HD12 | 1.81                     | 0.63              |
| 3:QC:108:ASN:ND2  | 3:QC:144:SER:OG    | 2.32                     | 0.63              |
| 22:QV:9:G:O2'     | 22:QV:10:G:N7      | 2.32                     | 0.63              |
| 29:Y4:16:CYS:SG   | 29:Y4:17:GLY:N     | 2.72                     | 0.63              |
| 35:YA:1824:G:N3   | 37:YD:254:THR:OG1  | 2.32                     | 0.63              |
| 35:YA:2604:U:H6   | 35:YA:2604:U:C5'   | 2.10                     | 0.63              |
| 35:RA:2851:A:O2'  | 47:RR:64:ARG:NH2   | 2.32                     | 0.62              |
| 35:YA:1470:G:N2   | 35:YA:1520:G:OP2   | 2.31                     | 0.62              |
| 35:YA:2032:G:N2   | 38:YE:146:THR:OG1  | 2.32                     | 0.62              |
| 33:R8:30:ARG:HH21 | 45:RP:63:PRO:HB2   | 1.63                     | 0.62              |
| 4:QD:68:TYR:CE2   | 4:QD:103:ASN:ND2   | 2.67                     | 0.62              |
| 12:QL:71:PRO:O    | 12:QL:102:ARG:NH1  | 2.33                     | 0.62              |
| 35:RA:1607:C:N4   | 35:RA:1622:G:OP2   | 2.30                     | 0.62              |
| 49:RT:125:ARG:O   | 49:RT:129:ARG:NH1  | 2.32                     | 0.62              |
| 35:RA:993:G:N3    | 51:RV:89:GLN:NE2   | 2.46                     | 0.62              |
| 48:YS:25:ARG:HD3  | 48:YS:27:SER:HB2   | 1.81                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:R8:28:GLY:O    | 33:R8:36:LYS:NZ    | 2.31                     | 0.62              |
| 43:RN:12:ARG:NH1  | 43:RN:50:ASP:OD2   | 2.32                     | 0.62              |
| 35:YA:1721:G:H8   | 35:YA:1741:A:H62   | 1.46                     | 0.62              |
| 17:QQ:66:SER:O    | 17:QQ:70:ARG:NH1   | 2.33                     | 0.62              |
| 26:R1:51:VAL:HG11 | 26:R1:74:VAL:HG21  | 1.81                     | 0.62              |
| 29:R4:34:GLU:OE1  | 29:R4:35:VAL:HG23  | 2.00                     | 0.62              |
| 38:RE:36:ARG:NH1  | 38:RE:85:ASN:OD1   | 2.33                     | 0.62              |
| 3:XC:56:ASP:HB2   | 3:XC:67:THR:HB     | 1.82                     | 0.62              |
| 37:YD:108:PRO:HD2 | 37:YD:111:LEU:HD22 | 1.80                     | 0.62              |
| 54:YY:9:LYS:NZ    | 54:YY:28:LYS:O     | 2.30                     | 0.62              |
| 1:QA:539:A:OP2    | 12:QL:115:LYS:NZ   | 2.33                     | 0.62              |
| 2:QB:54:THR:HG22  | 2:QB:199:TYR:HB3   | 1.81                     | 0.62              |
| 35:RA:1195:G:OP2  | 45:RP:15:ARG:NH1   | 2.32                     | 0.62              |
| 35:YA:993:G:OP1   | 50:YU:50:ARG:NH2   | 2.31                     | 0.62              |
| 39:YF:157:VAL:HB  | 39:YF:194:MET:HG2  | 1.81                     | 0.62              |
| 35:RA:1695:G:N7   | 37:RD:14:ARG:NH2   | 2.48                     | 0.62              |
| 41:YH:86:GLU:OE2  | 41:YH:130:ARG:NH1  | 2.33                     | 0.62              |
| 17:XQ:26:GLN:HG2  | 17:XQ:37:LYS:HG2   | 1.82                     | 0.61              |
| 37:RD:108:PRO:HD2 | 37:RD:111:LEU:HD22 | 1.82                     | 0.61              |
| 40:YG:48:GLU:O    | 40:YG:51:ARG:NH1   | 2.33                     | 0.61              |
| 1:QA:352:C:O2     | 1:QA:355:C:N4      | 2.32                     | 0.61              |
| 1:QA:626:U:H5''   | 16:QP:38:TYR:HD2   | 1.64                     | 0.61              |
| 3:XC:184:TYR:HE1  | 3:XC:201:TYR:HE1   | 1.48                     | 0.61              |
| 1:QA:1497:G:H1'   | 1:QA:1518:MA6:H2   | 1.82                     | 0.61              |
| 1:QA:1328:C:O2'   | 13:QM:29:ARG:NH2   | 2.34                     | 0.61              |
| 3:QC:56:ASP:HB2   | 3:QC:67:THR:HB     | 1.83                     | 0.61              |
| 1:QA:1137:C:O2    | 1:QA:1138:G:N2     | 2.34                     | 0.61              |
| 51:RV:40:LEU:HB2  | 51:RV:46:VAL:HG22  | 1.82                     | 0.61              |
| 35:YA:83:G:H1     | 35:YA:102:G:HO2'   | 1.45                     | 0.61              |
| 35:RA:807:U:O2'   | 35:RA:2060:A:N1    | 2.33                     | 0.61              |
| 17:XQ:66:SER:O    | 17:XQ:70:ARG:NH1   | 2.34                     | 0.61              |
| 24:XY:18:G:N2     | 24:XY:58:A:OP1     | 2.33                     | 0.61              |
| 35:YA:2413:G:H21  | 45:YP:70:GLN:HE22  | 1.48                     | 0.61              |
| 45:YP:93:GLY:H    | 45:YP:123:LEU:HD22 | 1.66                     | 0.61              |
| 38:YE:84:PHE:CE2  | 38:YE:86:PRO:CD    | 2.84                     | 0.61              |
| 43:YN:22:THR:HB   | 43:YN:25:ARG:HB2   | 1.83                     | 0.61              |
| 35:RA:660:G:H5''  | 39:RF:99:TYR:CE2   | 2.35                     | 0.60              |
| 44:RO:23:ARG:NH2  | 44:RO:28:SER:O     | 2.34                     | 0.60              |
| 35:YA:958:U:OP2   | 46:YQ:14:ARG:NH1   | 2.34                     | 0.60              |
| 35:YA:1567:A:N7   | 37:YD:84:TYR:CE2   | 2.67                     | 0.60              |
| 44:YO:35:VAL:HG11 | 44:YO:103:ALA:HB3  | 1.82                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:737:A:H1'    | 6:QF:73:ASN:HD21   | 1.66                     | 0.60              |
| 25:Y0:20:ARG:HH12 | 35:YA:2357:U:H5'   | 1.66                     | 0.60              |
| 1:QA:8:A:N6       | 4:QD:205:GLU:O     | 2.32                     | 0.60              |
| 9:QI:17:VAL:HG21  | 9:QI:81:ILE:HG22   | 1.84                     | 0.60              |
| 26:Y1:52:ARG:NH1  | 35:YA:2218:U:O2    | 2.35                     | 0.60              |
| 7:QG:150:ALA:HB1  | 11:QK:57:THR:HG21  | 1.83                     | 0.60              |
| 1:XA:974:A:OP2    | 14:XN:41:ARG:NH1   | 2.34                     | 0.60              |
| 8:QH:110:ALA:HB3  | 8:QH:121:ASP:HB3   | 1.82                     | 0.60              |
| 35:RA:613:G:N2    | 35:RA:614(D):A:O2' | 2.35                     | 0.60              |
| 35:YA:2292:C:OP1  | 48:YS:17:ARG:NH2   | 2.34                     | 0.60              |
| 2:QB:69:LEU:HB3   | 2:QB:162:ILE:HG22  | 1.82                     | 0.60              |
| 24:QY:74:C:H42    | 35:RA:2508:G:H5'   | 1.65                     | 0.60              |
| 55:RZ:99:TYR:HB3  | 55:RZ:123:ASP:HB2  | 1.82                     | 0.60              |
| 38:YE:105:THR:OG1 | 38:YE:199:ARG:NH2  | 2.34                     | 0.60              |
| 35:RA:1824:G:N3   | 37:RD:254:THR:OG1  | 2.35                     | 0.60              |
| 3:QC:58:GLU:HB2   | 3:QC:65:ALA:HB3    | 1.84                     | 0.60              |
| 40:RG:64:THR:HB   | 40:RG:94:LEU:HD21  | 1.83                     | 0.60              |
| 49:RT:92:GLY:O    | 49:RT:120:ARG:NH2  | 2.34                     | 0.60              |
| 16:XP:38:TYR:HE1  | 16:XP:50:LYS:CB    | 2.13                     | 0.60              |
| 1:XA:954:G:H21    | 1:XA:1227:A:H62    | 1.48                     | 0.60              |
| 30:Y5:29:THR:HG21 | 35:YA:2815:C:H5'   | 1.83                     | 0.60              |
| 35:YA:674:G:H1'   | 39:YF:74:ARG:HD3   | 1.83                     | 0.60              |
| 37:YD:85:ASP:OD2  | 37:YD:88:ARG:NH1   | 2.32                     | 0.60              |
| 35:YA:301:G:OP2   | 54:YY:84:ARG:NH2   | 2.34                     | 0.60              |
| 35:YA:336:C:O2'   | 54:YY:35:TYR:OH    | 2.20                     | 0.60              |
| 35:RA:987:G:O2'   | 35:RA:1000:A:N3    | 2.34                     | 0.59              |
| 3:XC:110:ASN:OD1  | 3:XC:140:ARG:NH1   | 2.35                     | 0.59              |
| 50:YU:97:ASP:OD1  | 50:YU:101:ARG:NH1  | 2.34                     | 0.59              |
| 37:YD:143:HIS:ND1 | 37:YD:194:GLY:O    | 2.33                     | 0.59              |
| 38:YE:29:GLY:HA2  | 38:YE:180:ASN:HB3  | 1.83                     | 0.59              |
| 1:XA:978:A:H61    | 1:XA:1316:G:H1'    | 1.66                     | 0.59              |
| 1:XA:427:U:OP1    | 4:XD:13:ARG:NH1    | 2.35                     | 0.59              |
| 1:XA:1406:U:O2    | 1:XA:1517:G:N2     | 2.35                     | 0.59              |
| 1:QA:425:G:O3'    | 4:QD:45:GLN:NE2    | 2.35                     | 0.59              |
| 4:QD:20:TYR:CD2   | 4:QD:26:CYS:HB3    | 2.37                     | 0.59              |
| 35:YA:2602:A:H2'  | 35:YA:2602:A:N3    | 2.18                     | 0.59              |
| 1:QA:974:A:OP2    | 14:QN:41:ARG:NH1   | 2.35                     | 0.59              |
| 3:QC:21:ARG:NH2   | 3:QC:58:GLU:OE2    | 2.36                     | 0.59              |
| 35:RA:2096:U:H3   | 35:RA:2193:G:H1    | 1.50                     | 0.59              |
| 16:XP:8:ARG:HB3   | 16:XP:28:ARG:HH12  | 1.66                     | 0.59              |
| 1:QA:111:G:HO2'   | 1:QA:389:A:HO2'    | 1.51                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1330:U:H4'   | 13:QM:23:TYR:CE1   | 2.37                     | 0.59              |
| 35:RA:1815:A:OP2  | 37:RD:54:ARG:NH2   | 2.36                     | 0.59              |
| 2:XB:68:ILE:HG12  | 2:XB:161:ALA:HB3   | 1.84                     | 0.59              |
| 8:XH:10:LEU:HD22  | 8:XH:83:ILE:HD11   | 1.84                     | 0.59              |
| 55:YZ:8:TYR:HB2   | 55:YZ:38:TYR:CE1   | 2.38                     | 0.59              |
| 35:RA:181:A:H1'   | 35:RA:435:C:H5'    | 1.85                     | 0.59              |
| 1:XA:508:C:OP1    | 4:XD:209:ARG:NH2   | 2.35                     | 0.59              |
| 1:XA:1500:A:H5''  | 1:XA:1508:G:H5''   | 1.84                     | 0.59              |
| 10:XJ:17:ASP:OD1  | 10:XJ:70:ARG:NH1   | 2.35                     | 0.59              |
| 1:QA:1013:G:N2    | 1:QA:1016:A:OP2    | 2.36                     | 0.59              |
| 33:R8:14:VAL:HG12 | 33:R8:24:ALA:HB2   | 1.85                     | 0.59              |
| 20:XT:56:MET:HE3  | 20:XT:85:MET:HG2   | 1.85                     | 0.59              |
| 37:YD:260:ARG:NH2 | 37:YD:266:SER:OG   | 2.36                     | 0.59              |
| 40:YG:19:LEU:HD23 | 40:YG:32:PRO:HD2   | 1.85                     | 0.59              |
| 54:YY:15:VAL:HG21 | 54:YY:42:VAL:HG11  | 1.84                     | 0.59              |
| 1:QA:933:G:O6     | 7:QG:3:ARG:NH2     | 2.36                     | 0.58              |
| 46:RQ:13:GLN:O    | 46:RQ:72:LYS:NZ    | 2.33                     | 0.58              |
| 48:RS:105:ALA:HB1 | 48:RS:110:LEU:HD12 | 1.85                     | 0.58              |
| 5:XE:33:VAL:HG21  | 5:XE:109:ILE:HA    | 1.85                     | 0.58              |
| 35:YA:693:C:O2'   | 35:YA:1353:A:N3    | 2.34                     | 0.58              |
| 35:RA:1791:A:H4'  | 37:RD:206:LEU:HB2  | 1.85                     | 0.58              |
| 35:YA:987:G:O2'   | 35:YA:1000:A:N3    | 2.35                     | 0.58              |
| 55:YZ:8:TYR:HB2   | 55:YZ:38:TYR:CD1   | 2.38                     | 0.58              |
| 28:R3:15:TYR:O    | 28:R3:20:LYS:NZ    | 2.37                     | 0.58              |
| 39:RF:101:LEU:O   | 39:RF:106:ARG:NH1  | 2.35                     | 0.58              |
| 41:RH:159:GLU:HG3 | 41:RH:171:LEU:HD11 | 1.85                     | 0.58              |
| 24:XY:4:G:H1      | 24:XY:69:C:H42     | 1.50                     | 0.58              |
| 35:YA:1058:G:N2   | 35:YA:1080:C:O2    | 2.35                     | 0.58              |
| 35:YA:2096:U:H3   | 35:YA:2193:G:H1    | 1.50                     | 0.58              |
| 45:YP:29:LYS:HD3  | 45:YP:30:THR:HG23  | 1.85                     | 0.58              |
| 20:QT:51:GLU:HA   | 20:QT:54:LYS:HE2   | 1.84                     | 0.58              |
| 25:R0:14:ARG:NH1  | 35:RA:2279:G:O6    | 2.36                     | 0.58              |
| 33:R8:30:ARG:NH2  | 45:RP:64:LYS:O     | 2.36                     | 0.58              |
| 35:YA:2604:U:C6   | 35:YA:2604:U:C5'   | 2.85                     | 0.58              |
| 16:XP:18:ARG:NH1  | 16:XP:32:TYR:OH    | 2.36                     | 0.58              |
| 35:RA:2298:A:H62  | 35:RA:2318:G:H8    | 1.51                     | 0.58              |
| 33:Y8:43:GLN:NE2  | 35:YA:2365:G:O6    | 2.30                     | 0.58              |
| 35:YA:526:A:O2'   | 35:YA:2043:C:O2    | 2.21                     | 0.58              |
| 40:YG:55:LYS:HZ1  | 40:YG:149:VAL:HA   | 1.69                     | 0.58              |
| 24:XY:75:C:O2'    | 35:YA:2573:C:N4    | 2.37                     | 0.58              |
| 35:YA:631:A:OP1   | 45:YP:65:ARG:NH1   | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YA:1155:A:OP1   | 50:YU:55:ARG:HG2   | 2.04                     | 0.58              |
| 34:R9:36:GLN:NE2   | 35:RA:1124:C:O2    | 2.36                     | 0.58              |
| 35:RA:956:G:H2'    | 35:RA:957:A:H2'    | 1.86                     | 0.58              |
| 17:QQ:9:VAL:HG22   | 17:QQ:56:VAL:HG22  | 1.85                     | 0.58              |
| 1:XA:1286:A:H2'    | 1:XA:1287:A:H4'    | 1.85                     | 0.58              |
| 24:XY:20:G:N2      | 24:XY:21:A:O2'     | 2.37                     | 0.58              |
| 35:YA:2574:G:N3    | 38:YE:143:ASN:ND2  | 2.52                     | 0.58              |
| 1:QA:779:C:O2'     | 11:QK:120:ARG:NH1  | 2.37                     | 0.58              |
| 1:QA:528:C:N4      | 12:QL:49:ASN:OD1   | 2.34                     | 0.57              |
| 35:RA:39:C:O2      | 39:RF:46:ARG:NH2   | 2.33                     | 0.57              |
| 35:RA:340:A:O2'    | 39:RF:168:ARG:NH2  | 2.37                     | 0.57              |
| 35:RA:1800:C:OP2   | 37:RD:183:ARG:NH2  | 2.37                     | 0.57              |
| 27:Y2:16:LEU:O     | 27:Y2:67:LYS:NZ    | 2.36                     | 0.57              |
| 35:YA:1791:A:H5'   | 37:YD:206:LEU:HD12 | 1.86                     | 0.57              |
| 35:YA:2483:C:N3    | 46:YQ:124:LYS:NZ   | 2.42                     | 0.57              |
| 1:XA:1086:U:H3     | 1:XA:1099:G:H22    | 1.52                     | 0.57              |
| 35:RA:1791:A:N6    | 35:RA:1828:G:O2'   | 2.34                     | 0.57              |
| 35:RA:2627:G:N2    | 35:RA:2777:G:OP2   | 2.36                     | 0.57              |
| 3:XC:40:ARG:HH12   | 14:XN:52:GLN:HG2   | 1.69                     | 0.57              |
| 35:RA:994:C:OP1    | 50:RU:53:ARG:NH2   | 2.37                     | 0.57              |
| 12:XL:70:ILE:HG13  | 12:XL:100:ILE:HD12 | 1.86                     | 0.57              |
| 39:YF:190:GLU:HA   | 45:YP:2:LYS:HE3    | 1.86                     | 0.57              |
| 1:QA:977:A:N6      | 1:QA:1224:G:OP1    | 2.29                     | 0.57              |
| 28:R3:8:LEU:HB2    | 28:R3:28:LEU:HD13  | 1.86                     | 0.57              |
| 35:RA:500:G:N1     | 35:RA:503:A:OP2    | 2.37                     | 0.57              |
| 35:RA:631:A:OP1    | 45:RP:65:ARG:NH1   | 2.37                     | 0.57              |
| 35:RA:1162:G:H4'   | 51:RV:24:LYS:HB3   | 1.87                     | 0.57              |
| 4:XD:18:LYS:HD2    | 58:XD:301:SF4:S2   | 2.44                     | 0.57              |
| 25:R0:20:ARG:HH12  | 35:RA:2357:U:H5'   | 1.69                     | 0.57              |
| 35:RA:143(A):G:H4' | 53:RX:35:THR:HG21  | 1.87                     | 0.57              |
| 37:RD:143:HIS:ND1  | 37:RD:194:GLY:O    | 2.34                     | 0.57              |
| 44:RO:104:ARG:NH2  | 44:RO:121:VAL:O    | 2.38                     | 0.57              |
| 35:YA:859:G:O2'    | 35:YA:916:G:O6     | 2.22                     | 0.57              |
| 13:QM:99:ARG:HB2   | 13:QM:101:GLN:HE22 | 1.69                     | 0.57              |
| 35:RA:615:G:OP1    | 39:RF:40:GLN:NE2   | 2.38                     | 0.57              |
| 41:RH:154:PRO:HG3  | 41:RH:163:TYR:CD1  | 2.40                     | 0.57              |
| 28:Y3:15:TYR:O     | 28:Y3:20:LYS:NZ    | 2.37                     | 0.57              |
| 31:Y6:35:GLU:OE2   | 31:Y6:50:ARG:NH1   | 2.38                     | 0.57              |
| 1:XA:1295:G:O2'    | 13:XM:14:ARG:NH1   | 2.38                     | 0.57              |
| 35:RA:1009:A:OP2   | 43:RN:37:LYS:NZ    | 2.35                     | 0.57              |
| 35:YA:1791:A:N6    | 35:YA:1828:G:O2'   | 2.38                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:RF:11:VAL:HG22  | 39:RF:125:LEU:HB2  | 1.86                     | 0.56              |
| 45:RP:93:GLY:H     | 45:RP:123:LEU:HD22 | 1.70                     | 0.56              |
| 13:XM:8:GLU:OE2    | 13:XM:11:ARG:NH2   | 2.38                     | 0.56              |
| 10:QJ:49:VAL:HG23  | 14:QN:41:ARG:HB2   | 1.86                     | 0.56              |
| 26:R1:52:ARG:NH1   | 35:RA:2218:U:O2    | 2.38                     | 0.56              |
| 35:RA:2839:G:H5'   | 47:RR:46:GLY:HA2   | 1.87                     | 0.56              |
| 33:Y8:28:GLY:O     | 33:Y8:36:LYS:NZ    | 2.36                     | 0.56              |
| 35:YA:1651:G:N7    | 47:YR:11:ASN:ND2   | 2.52                     | 0.56              |
| 47:YR:103:ARG:NH1  | 47:YR:108:GLY:O    | 2.38                     | 0.56              |
| 1:QA:1318:A:OP1    | 19:QS:3:ARG:NH2    | 2.37                     | 0.56              |
| 54:RY:47:LYS:NZ    | 54:RY:48:ALA:O     | 2.39                     | 0.56              |
| 1:XA:545:C:OP1     | 4:XD:61:LYS:NZ     | 2.38                     | 0.56              |
| 1:XA:626:U:H5''    | 16:XP:38:TYR:HD2   | 1.69                     | 0.56              |
| 19:XS:63:THR:HG23  | 19:XS:65:ASN:H     | 1.70                     | 0.56              |
| 35:YA:458:G:O2'    | 35:YA:469:G:O6     | 2.24                     | 0.56              |
| 35:YA:1695:G:N7    | 37:YD:14:ARG:NH2   | 2.54                     | 0.56              |
| 26:R1:3:LYS:NZ     | 35:RA:1366:A:OP1   | 2.38                     | 0.56              |
| 49:RT:122:ASP:OD1  | 49:RT:125:ARG:NH2  | 2.35                     | 0.56              |
| 1:XA:1003:G:H1     | 1:XA:1035:A:H61    | 1.52                     | 0.56              |
| 29:Y4:43:TYR:OH    | 40:YG:179:PRO:HG3  | 2.05                     | 0.56              |
| 40:RG:137:GLU:HG3  | 40:RG:140:ILE:HG12 | 1.88                     | 0.56              |
| 5:QE:7:GLU:OE1     | 5:QE:37:ARG:NE     | 2.35                     | 0.56              |
| 25:Y0:51:VAL:O     | 48:YS:20:ARG:NH2   | 2.39                     | 0.56              |
| 34:Y9:22:ARG:HH12  | 35:YA:2741:A:H5''  | 1.71                     | 0.56              |
| 35:YA:1466:G:HO2'  | 35:YA:1546:C:HO2'  | 1.50                     | 0.56              |
| 1:QA:1226:C:O2'    | 13:QM:111:LYS:NZ   | 2.34                     | 0.56              |
| 35:RA:297:C:OP1    | 54:RY:87:LYS:NZ    | 2.38                     | 0.56              |
| 50:RU:97:ASP:OD1   | 50:RU:101:ARG:NH1  | 2.38                     | 0.56              |
| 55:RZ:126:VAL:HG12 | 55:RZ:163:LEU:HA   | 1.86                     | 0.56              |
| 8:XH:9:MET:HG3     | 8:XH:26:VAL:HG11   | 1.87                     | 0.56              |
| 1:QA:619:U:N3      | 4:QD:134:ASP:OD1   | 2.38                     | 0.56              |
| 1:XA:1321:C:O2'    | 19:XS:78:ARG:NH1   | 2.39                     | 0.56              |
| 19:XS:50:ALA:HB1   | 19:XS:57:HIS:HB3   | 1.88                     | 0.56              |
| 38:YE:84:PHE:CE2   | 38:YE:86:PRO:CG    | 2.88                     | 0.56              |
| 1:QA:7:G:O2'       | 5:QE:120:THR:O     | 2.23                     | 0.56              |
| 1:QA:345:C:OP2     | 49:RT:39:ARG:NH2   | 2.39                     | 0.56              |
| 12:QL:117:ARG:HB2  | 12:QL:122:THR:HB   | 1.86                     | 0.56              |
| 38:RE:105:THR:OG1  | 38:RE:199:ARG:NH2  | 2.38                     | 0.56              |
| 1:XA:1226:C:O2'    | 13:XM:111:LYS:NZ   | 2.37                     | 0.56              |
| 4:QD:157:LEU:O     | 4:QD:161:ASN:ND2   | 2.38                     | 0.56              |
| 1:XA:562:C:H1'     | 12:XL:15:ARG:HB3   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:XB:74:LYS:NZ    | 2:XB:206:ASP:OD1  | 2.37                     | 0.56              |
| 2:XB:187:LEU:HA   | 2:XB:201:ILE:HB   | 1.87                     | 0.56              |
| 29:Y4:53:GLU:HG3  | 29:Y4:56:VAL:HB   | 1.87                     | 0.56              |
| 35:YA:615:G:OP1   | 39:YF:40:GLN:NE2  | 2.39                     | 0.56              |
| 35:YA:2144:U:O2   | 35:YA:2148:G:N1   | 2.34                     | 0.56              |
| 30:R5:19:ARG:NH2  | 35:RA:1264:G:OP1  | 2.38                     | 0.55              |
| 1:XA:352:C:O2     | 1:XA:355:C:N4     | 2.39                     | 0.55              |
| 2:XB:195:ASP:O    | 8:XH:68:ARG:NH2   | 2.39                     | 0.55              |
| 20:XT:50:GLU:HB2  | 20:XT:99:LEU:HD22 | 1.88                     | 0.55              |
| 50:YU:83:LEU:HD13 | 50:YU:88:ILE:HB   | 1.89                     | 0.55              |
| 35:RA:1250:G:OP2  | 45:RP:21:ARG:NH1  | 2.39                     | 0.55              |
| 35:RA:1266:G:O5'  | 52:RW:15:ARG:NH2  | 2.39                     | 0.55              |
| 1:XA:662:G:O2'    | 1:XA:836:G:OP1    | 2.25                     | 0.55              |
| 3:XC:184:TYR:CE1  | 3:XC:201:TYR:CE1  | 2.94                     | 0.55              |
| 12:XL:71:PRO:O    | 12:XL:102:ARG:NH1 | 2.39                     | 0.55              |
| 13:XM:19:LEU:HD11 | 13:XM:56:LEU:HD21 | 1.87                     | 0.55              |
| 37:YD:72:LYS:NZ   | 37:YD:99:ASP:OD2  | 2.40                     | 0.55              |
| 1:QA:1316:G:O2'   | 1:QA:1318:A:N7    | 2.39                     | 0.55              |
| 35:RA:1638:C:O2   | 35:RA:2698:U:O2'  | 2.24                     | 0.55              |
| 35:RA:2635:C:O2'  | 38:RE:48:GLN:NE2  | 2.38                     | 0.55              |
| 51:RV:21:ARG:HD3  | 51:RV:91:TYR:HE2  | 1.72                     | 0.55              |
| 1:XA:1152:A:OP1   | 10:XJ:70:ARG:NH2  | 2.39                     | 0.55              |
| 41:YH:124:GLU:HB2 | 41:YH:132:ARG:HB3 | 1.89                     | 0.55              |
| 1:QA:297:G:N2     | 1:QA:300:A:OP2    | 2.40                     | 0.55              |
| 1:QA:1249:C:O2'   | 9:QI:73:GLN:NE2   | 2.39                     | 0.55              |
| 8:QH:9:MET:HG3    | 8:QH:26:VAL:HG11  | 1.87                     | 0.55              |
| 35:RA:1066:U:O2'  | 35:RA:1068:G:OP2  | 2.21                     | 0.55              |
| 35:RA:1721:G:H8   | 35:RA:1741:A:H62  | 1.53                     | 0.55              |
| 38:RE:7:VAL:HG13  | 38:RE:51:PHE:HE2  | 1.72                     | 0.55              |
| 49:RT:29:ARG:HB3  | 49:RT:87:ASP:HB2  | 1.88                     | 0.55              |
| 39:YF:143:ALA:HB1 | 39:YF:148:LEU:HB2 | 1.87                     | 0.55              |
| 44:YO:104:ARG:NH2 | 44:YO:121:VAL:O   | 2.38                     | 0.55              |
| 24:QY:20:G:N2     | 24:QY:21:A:O2'    | 2.38                     | 0.55              |
| 27:R2:16:LEU:HB3  | 27:R2:20:GLU:HG3  | 1.89                     | 0.55              |
| 35:RA:526:A:O2'   | 35:RA:2043:C:O2   | 2.23                     | 0.55              |
| 41:RH:86:GLU:OE2  | 41:RH:132:ARG:NH2 | 2.37                     | 0.55              |
| 49:RT:65:LYS:HE3  | 49:RT:67:SER:HB2  | 1.89                     | 0.55              |
| 3:XC:70:VAL:HG12  | 3:XC:72:LYS:H     | 1.72                     | 0.55              |
| 11:XK:34:ASP:OD1  | 11:XK:38:ASN:N    | 2.40                     | 0.55              |
| 32:Y7:24:THR:HG23 | 32:Y7:27:GLY:H    | 1.71                     | 0.55              |
| 1:QA:922:G:H4'    | 5:QE:20:GLN:HA    | 1.88                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1320:C:O2    | 19:QS:36:ARG:NH2   | 2.35                     | 0.55              |
| 35:RA:1246:A:OP1  | 39:RF:38:ARG:NH2   | 2.37                     | 0.55              |
| 1:QA:978:A:O2'    | 1:QA:1322:C:N3     | 2.39                     | 0.55              |
| 1:QA:1178:G:OP1   | 9:QI:93:ARG:NH1    | 2.40                     | 0.55              |
| 9:QI:11:LYS:HA    | 9:QI:108:VAL:HG12  | 1.88                     | 0.55              |
| 33:R8:43:GLN:NE2  | 35:RA:2365:G:O6    | 2.38                     | 0.55              |
| 35:RA:919:G:N2    | 35:RA:2269:A:OP2   | 2.40                     | 0.55              |
| 43:RN:123:TYR:OH  | 43:RN:130:HIS:NE2  | 2.37                     | 0.55              |
| 35:RA:604:G:OP2   | 45:RP:90:ARG:NH1   | 2.40                     | 0.55              |
| 35:YA:451:C:OP1   | 39:YF:52:LYS:NZ    | 2.39                     | 0.55              |
| 35:RA:993:G:OP1   | 50:RU:50:ARG:NH2   | 2.39                     | 0.55              |
| 1:XA:1414:U:H3    | 1:XA:1486:G:H1     | 1.54                     | 0.55              |
| 3:XC:184:TYR:HE1  | 3:XC:201:TYR:CE1   | 2.25                     | 0.55              |
| 35:YA:918:A:N3    | 36:YB:80:U:O2'     | 2.40                     | 0.55              |
| 37:YD:168:ARG:HG2 | 37:YD:173:VAL:HG12 | 1.89                     | 0.55              |
| 1:QA:573:A:N3     | 1:QA:883:C:O2'     | 2.36                     | 0.55              |
| 6:QF:41:GLU:OE1   | 18:QR:35:ARG:NH1   | 2.37                     | 0.55              |
| 35:RA:458:G:O2'   | 35:RA:469:G:O6     | 2.24                     | 0.55              |
| 35:RA:2683:C:OP1  | 49:RT:53:ARG:NH2   | 2.34                     | 0.55              |
| 39:RF:40:GLN:HE22 | 39:RF:182:ASN:HB2  | 1.72                     | 0.55              |
| 55:RZ:8:TYR:HB3   | 55:RZ:38:TYR:HE1   | 1.71                     | 0.55              |
| 1:XA:79:G:H1      | 1:XA:90:U:H3       | 1.55                     | 0.55              |
| 8:QH:41:ARG:NH2   | 8:QH:123:GLU:OE1   | 2.40                     | 0.54              |
| 35:YA:604:G:OP2   | 45:YP:90:ARG:NH1   | 2.39                     | 0.54              |
| 35:YA:2291:U:O2'  | 35:YA:2374:C:O2    | 2.24                     | 0.54              |
| 38:YE:84:PHE:CE2  | 38:YE:86:PRO:HB3   | 2.42                     | 0.54              |
| 9:QI:10:ARG:HG3   | 9:QI:11:LYS:H      | 1.72                     | 0.54              |
| 35:RA:237:C:O2    | 35:RA:609:A:O2'    | 2.25                     | 0.54              |
| 25:Y0:30:VAL:HG22 | 25:Y0:66:VAL:HG22  | 1.89                     | 0.54              |
| 4:QD:20:TYR:HD2   | 4:QD:26:CYS:HB3    | 1.72                     | 0.54              |
| 9:QI:49:PRO:HD2   | 9:QI:81:ILE:HD11   | 1.89                     | 0.54              |
| 35:RA:861:A:N3    | 36:RB:79:C:O2'     | 2.40                     | 0.54              |
| 35:YA:613:G:N2    | 35:YA:614(D):A:O2' | 2.40                     | 0.54              |
| 35:YA:807:U:O2'   | 35:YA:2060:A:N1    | 2.41                     | 0.54              |
| 35:YA:2788:C:O2'  | 35:YA:2809:A:N3    | 2.35                     | 0.54              |
| 44:YO:23:ARG:NH2  | 44:YO:28:SER:O     | 2.40                     | 0.54              |
| 1:QA:261:U:OP2    | 20:QT:79:ARG:NH2   | 2.40                     | 0.54              |
| 1:QA:1147:C:HO2'  | 9:QI:5:TYR:HH      | 1.52                     | 0.54              |
| 35:RA:600:G:N2    | 35:RA:605:C:O3'    | 2.40                     | 0.54              |
| 35:RA:907:U:O2'   | 46:RQ:101:ARG:NH2  | 2.38                     | 0.54              |
| 35:RA:2073:C:HO2' | 35:RA:2598:A:HO2'  | 1.55                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:XF:36:ARG:NH2   | 6:XF:38:GLU:OE2   | 2.41                     | 0.54              |
| 1:QA:1003:G:H1    | 1:QA:1035:A:H61   | 1.56                     | 0.54              |
| 1:QA:1484:C:HO2'  | 35:RA:1960:A:HO2' | 1.48                     | 0.54              |
| 35:RA:660:G:H4'   | 39:RF:99:TYR:CE2  | 2.34                     | 0.54              |
| 46:RQ:32:TYR:CE1  | 46:RQ:133:ARG:HG3 | 2.42                     | 0.54              |
| 1:XA:676:A:H1'    | 11:XK:115:PRO:HB3 | 1.89                     | 0.54              |
| 32:Y7:34:ARG:HG3  | 32:Y7:39:ARG:HG3  | 1.90                     | 0.54              |
| 38:YE:36:ARG:NH1  | 38:YE:85:ASN:OD1  | 2.41                     | 0.54              |
| 1:QA:692:U:OP2    | 11:QK:26:ASN:ND2  | 2.37                     | 0.54              |
| 7:QG:94:ARG:NH1   | 7:QG:98:SER:OG    | 2.41                     | 0.54              |
| 35:RA:2115:G:N1   | 35:RA:2119:A:OP2  | 2.36                     | 0.54              |
| 45:RP:29:LYS:HD3  | 45:RP:30:THR:HG23 | 1.89                     | 0.54              |
| 1:XA:1060:C:OP1   | 14:XN:45:ARG:NH2  | 2.41                     | 0.54              |
| 1:XA:1101:A:N6    | 2:XB:176:GLU:OE2  | 2.40                     | 0.54              |
| 36:RB:117:G:H4'   | 48:RS:54:LEU:HD22 | 1.89                     | 0.54              |
| 35:YA:1652:A:N6   | 47:YR:11:ASN:OD1  | 2.34                     | 0.54              |
| 54:YY:47:LYS:NZ   | 54:YY:48:ALA:O    | 2.41                     | 0.54              |
| 35:YA:2683:C:OP1  | 49:YT:53:ARG:NH2  | 2.36                     | 0.54              |
| 46:YQ:137:TYR:HB3 | 55:YZ:76:LEU:HD11 | 1.90                     | 0.54              |
| 37:RD:5:LYS:HG2   | 37:RD:17:THR:HG22 | 1.90                     | 0.54              |
| 55:RZ:92:SER:OG   | 55:RZ:94:GLU:OE1  | 2.25                     | 0.54              |
| 35:YA:307:G:N1    | 35:YA:310:A:OP2   | 2.39                     | 0.54              |
| 1:XA:626:U:C5'    | 16:XP:38:TYR:HD2  | 2.21                     | 0.54              |
| 40:YG:46:ALA:HB2  | 40:YG:53:LEU:HD12 | 1.90                     | 0.54              |
| 2:QB:28:PHE:HD1   | 2:QB:194:PRO:HG3  | 1.73                     | 0.53              |
| 35:RA:2012:G:OP1  | 52:RW:11:ARG:NH2  | 2.41                     | 0.53              |
| 29:Y4:31:ILE:HG21 | 40:YG:142:PRO:HB2 | 1.89                     | 0.53              |
| 35:YA:184:C:O2'   | 35:YA:217:G:N3    | 2.42                     | 0.53              |
| 46:YQ:32:TYR:CE1  | 46:YQ:133:ARG:HG3 | 2.43                     | 0.53              |
| 5:QE:33:VAL:HG21  | 5:QE:109:ILE:HA   | 1.89                     | 0.53              |
| 7:QG:15:ASP:OD1   | 7:QG:19:GLY:N     | 2.42                     | 0.53              |
| 35:RA:2033:A:O2'  | 35:RA:2035:G:OP2  | 2.25                     | 0.53              |
| 38:RE:176:ILE:HB  | 38:RE:181:LEU:HB2 | 1.90                     | 0.53              |
| 44:RO:9:GLU:OE2   | 44:RO:18:LYS:NZ   | 2.39                     | 0.53              |
| 2:XB:47:THR:OG1   | 2:XB:48:MET:N     | 2.39                     | 0.53              |
| 34:Y9:16:VAL:HG22 | 34:Y9:25:VAL:HG22 | 1.90                     | 0.53              |
| 35:YA:1754:C:N3   | 35:YA:2716:U:O2'  | 2.33                     | 0.53              |
| 46:YQ:30:GLY:N    | 46:YQ:105:GLU:OE2 | 2.41                     | 0.53              |
| 1:QA:1368:G:OP1   | 9:QI:111:ARG:NH2  | 2.41                     | 0.53              |
| 35:RA:2245:U:H5'' | 35:RA:2246:G:H5'  | 1.91                     | 0.53              |
| 1:XA:977:A:N6     | 1:XA:1224:G:OP1   | 2.35                     | 0.53              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:XC:152:ILE:HD11 | 3:XC:199:LYS:HD2    | 1.89                     | 0.53              |
| 4:XD:59:ARG:HH21  | 4:XD:62:GLN:HG3     | 1.71                     | 0.53              |
| 20:XT:50:GLU:HG3  | 20:XT:100:ILE:HD11  | 1.90                     | 0.53              |
| 25:Y0:77:ARG:NH2  | 35:YA:857:C:OP2     | 2.40                     | 0.53              |
| 35:YA:1607:C:N4   | 35:YA:1622:G:OP2    | 2.34                     | 0.53              |
| 39:YF:62:ARG:HD2  | 39:YF:63:LYS:C      | 2.33                     | 0.53              |
| 45:YP:89:ALA:O    | 45:YP:121:LYS:NZ    | 2.38                     | 0.53              |
| 35:YA:1066:U:O2'  | 35:YA:1068:G:OP2    | 2.21                     | 0.53              |
| 35:RA:1398:C:OP1  | 53:RX:53:LYS:NZ     | 2.40                     | 0.53              |
| 35:RA:2258:C:O2'  | 35:RA:2427:C:OP2    | 2.26                     | 0.53              |
| 35:RA:2502:G:H5'' | 35:RA:2503:2MA:H5'' | 1.91                     | 0.53              |
| 35:YA:2115:G:N1   | 35:YA:2119:A:OP2    | 2.41                     | 0.53              |
| 39:YF:185:ASP:OD1 | 39:YF:188:ARG:NH1   | 2.41                     | 0.53              |
| 4:QD:168:ARG:HH22 | 37:YD:134:ARG:HH21  | 1.57                     | 0.53              |
| 35:RA:1788:C:OP1  | 37:RD:222:ARG:NH2   | 2.41                     | 0.53              |
| 1:XA:578:C:O2'    | 1:XA:728:A:N3       | 2.38                     | 0.53              |
| 1:XA:811:C:O2'    | 1:XA:901:A:N1       | 2.42                     | 0.53              |
| 35:YA:300:A:OP1   | 54:YY:86:ARG:NH2    | 2.42                     | 0.53              |
| 38:YE:2:LYS:HB2   | 38:YE:95:ILE:HD12   | 1.91                     | 0.53              |
| 35:RA:1801:G:OP2  | 37:RD:154:LYS:NZ    | 2.42                     | 0.53              |
| 39:RF:46:ARG:HG3  | 39:RF:48:THR:HG23   | 1.91                     | 0.53              |
| 6:XF:99:ALA:HB2   | 18:XR:31:LEU:HD11   | 1.91                     | 0.53              |
| 34:Y9:36:GLN:NE2  | 35:YA:1124:C:O2     | 2.42                     | 0.53              |
| 52:YW:22:ASP:OD1  | 52:YW:25:ARG:NH1    | 2.38                     | 0.53              |
| 1:QA:437:U:O2'    | 4:QD:123:HIS:ND1    | 2.39                     | 0.53              |
| 16:QP:53:VAL:HG13 | 16:QP:79:VAL:HG12   | 1.90                     | 0.53              |
| 35:RA:2572:A:OP1  | 35:RA:2574:G:O2'    | 2.25                     | 0.53              |
| 1:XA:765:G:N1     | 1:XA:812:C:O2'      | 2.37                     | 0.53              |
| 1:XA:976:G:OP2    | 1:XA:1358:U:O2'     | 2.27                     | 0.53              |
| 13:XM:99:ARG:HB2  | 13:XM:101:GLN:HE22  | 1.73                     | 0.53              |
| 35:YA:2033:A:O2'  | 35:YA:2035:G:OP2    | 2.24                     | 0.53              |
| 1:QA:662:G:O2'    | 1:QA:836:G:OP1      | 2.27                     | 0.53              |
| 3:QC:191:THR:OG1  | 3:QC:194:GLY:O      | 2.27                     | 0.53              |
| 18:QR:32:ARG:HA   | 18:QR:69:THR:HG21   | 1.91                     | 0.53              |
| 39:RF:117:ARG:NH2 | 39:RF:189:THR:O     | 2.42                     | 0.53              |
| 4:XD:109:GLY:HA3  | 4:XD:165:MET:HG3    | 1.90                     | 0.53              |
| 9:XI:7:THR:OG1    | 9:XI:83:ARG:NH1     | 2.39                     | 0.53              |
| 35:YA:2851:A:O2'  | 47:YR:64:ARG:NH2    | 2.41                     | 0.53              |
| 42:YI:23:PRO:HB3  | 42:YI:27:ARG:HE     | 1.73                     | 0.53              |
| 24:QY:18:G:N2     | 24:QY:58:A:OP1      | 2.41                     | 0.53              |
| 40:RG:32:PRO:HB2  | 40:RG:172:LEU:HD22  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:RU:89:GLU:O     | 51:RV:11:GLN:NE2   | 2.35                     | 0.53              |
| 6:XF:33:TYR:HB2    | 6:XF:75:LEU:HD12   | 1.91                     | 0.53              |
| 35:YA:600:G:N2     | 35:YA:605:C:O3'    | 2.42                     | 0.53              |
| 1:QA:1218:C:OP2    | 14:QN:9:LYS:NZ     | 2.41                     | 0.52              |
| 8:QH:36:LEU:HD23   | 8:QH:39:LEU:HD12   | 1.91                     | 0.52              |
| 16:XP:20:VAL:HG23  | 16:XP:35:LYS:HA    | 1.91                     | 0.52              |
| 35:YA:2404:C:O3'   | 45:YP:77:ARG:NH2   | 2.40                     | 0.52              |
| 1:QA:792:A:O2'     | 1:QA:794:A:N7      | 2.42                     | 0.52              |
| 4:QD:98:GLU:HA     | 4:QD:103:ASN:HD22  | 1.75                     | 0.52              |
| 7:QG:76:ARG:HD3    | 7:QG:89:MET:HG3    | 1.92                     | 0.52              |
| 35:RA:574:C:N4     | 35:RA:2034:U:OP1   | 2.41                     | 0.52              |
| 35:RA:1817:G:OP1   | 37:RD:88:ARG:NH2   | 2.41                     | 0.52              |
| 55:RZ:69:THR:OG1   | 55:RZ:70:LEU:N     | 2.42                     | 0.52              |
| 1:XA:824:C:H2'     | 1:XA:825:G:H8      | 1.73                     | 0.52              |
| 3:XC:39:ILE:HG23   | 3:XC:91:LEU:HD11   | 1.89                     | 0.52              |
| 40:YG:161:THR:HG22 | 40:YG:163:ALA:H    | 1.74                     | 0.52              |
| 35:RA:1693:U:O2'   | 37:RD:14:ARG:NH2   | 2.42                     | 0.52              |
| 1:XA:67:C:O2'      | 1:XA:171:A:N3      | 2.35                     | 0.52              |
| 26:Y1:11:ARG:NH2   | 35:YA:1365:A:O2'   | 2.42                     | 0.52              |
| 42:YI:92:VAL:HG23  | 42:YI:120:ILE:HB   | 1.91                     | 0.52              |
| 1:QA:677:U:H3      | 1:QA:713:G:H22     | 1.58                     | 0.52              |
| 46:RQ:31:ASP:N     | 46:RQ:106:VAL:O    | 2.42                     | 0.52              |
| 30:Y5:16:ARG:NH1   | 30:Y5:17:ASP:OD1   | 2.43                     | 0.52              |
| 1:QA:738:C:OP1     | 6:QF:4:TYR:OH      | 2.24                     | 0.52              |
| 9:QI:48:GLU:HG3    | 9:QI:51:ARG:HH11   | 1.75                     | 0.52              |
| 32:R7:39:ARG:NH2   | 35:RA:468:G:N7     | 2.51                     | 0.52              |
| 47:RR:56:LYS:NZ    | 47:RR:90:ARG:O     | 2.43                     | 0.52              |
| 54:RY:14:LEU:HB2   | 54:RY:75:ILE:HD11  | 1.92                     | 0.52              |
| 1:XA:486:U:H2'     | 1:XA:487:A:H8      | 1.74                     | 0.52              |
| 1:XA:1030(D):G:H2' | 1:XA:1030(E):A:H8  | 1.73                     | 0.52              |
| 44:YO:98:VAL:HG21  | 44:YO:114:ILE:HG23 | 1.92                     | 0.52              |
| 2:QB:88:ALA:HB2    | 2:QB:219:VAL:HG13  | 1.92                     | 0.52              |
| 5:QE:105:VAL:HG21  | 5:QE:128:PRO:HB3   | 1.90                     | 0.52              |
| 35:RA:859:G:O2'    | 35:RA:916:G:O6     | 2.25                     | 0.52              |
| 44:RO:98:VAL:HG21  | 44:RO:114:ILE:HG23 | 1.91                     | 0.52              |
| 1:XA:413:G:N7      | 4:XD:35:ARG:NH1    | 2.57                     | 0.52              |
| 9:XI:121:ARG:NH1   | 9:XI:122:ALA:O     | 2.43                     | 0.52              |
| 19:XS:32:LYS:HA    | 19:XS:50:ALA:HB3   | 1.92                     | 0.52              |
| 35:YA:805:G:N2     | 35:YA:829:A:OP1    | 2.40                     | 0.52              |
| 1:QA:157:G:H1      | 1:QA:164:U:H3      | 1.57                     | 0.52              |
| 1:QA:1003:G:N2     | 1:QA:1025:U:O4     | 2.42                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1286:A:H2'   | 1:QA:1287:A:H4'    | 1.91                     | 0.52              |
| 1:QA:1438:G:OP2   | 20:QT:34:LYS:NZ    | 2.37                     | 0.52              |
| 3:QC:20:SER:OG    | 3:QC:22:TRP:NE1    | 2.43                     | 0.52              |
| 35:RA:99:U:O4     | 54:RY:8:LYS:NZ     | 2.37                     | 0.52              |
| 1:XA:950:U:H3     | 1:XA:1231:G:H1     | 1.58                     | 0.52              |
| 35:YA:86:C:H4'    | 35:YA:104:U:H1'    | 1.92                     | 0.52              |
| 38:YE:2:LYS:HG2   | 38:YE:200:GLU:HB2  | 1.92                     | 0.52              |
| 43:YN:114:ARG:O   | 43:YN:118:LYS:NZ   | 2.37                     | 0.52              |
| 44:YO:87:ILE:HD12 | 44:YO:91:LEU:HA    | 1.91                     | 0.52              |
| 1:QA:954:G:H21    | 1:QA:1227:A:H62    | 1.57                     | 0.52              |
| 2:QB:93:VAL:HG11  | 2:QB:101:MET:HE1   | 1.90                     | 0.52              |
| 31:R6:23:THR:OG1  | 31:R6:24:GLU:N     | 2.41                     | 0.52              |
| 52:YW:69:LEU:HB3  | 52:YW:107:LEU:HD23 | 1.90                     | 0.52              |
| 35:RA:200:U:O2    | 35:RA:386:G:N2     | 2.43                     | 0.52              |
| 35:RA:2646:C:OP2  | 35:RA:2732:G:O2'   | 2.22                     | 0.52              |
| 35:RA:2684:U:O2'  | 44:RO:68:GLU:OE2   | 2.24                     | 0.52              |
| 55:RZ:103:ARG:HE  | 55:RZ:136:PHE:HD2  | 1.58                     | 0.52              |
| 2:XB:88:ALA:HB2   | 2:XB:219:VAL:HG13  | 1.92                     | 0.52              |
| 33:Y8:6:THR:HG22  | 33:Y8:63:PRO:HD2   | 1.92                     | 0.52              |
| 35:YA:641:C:O2'   | 35:YA:2350:C:OP1   | 2.23                     | 0.52              |
| 35:YA:906:G:OP1   | 46:YQ:26:TYR:OH    | 2.22                     | 0.52              |
| 35:YA:2313:C:O4'  | 40:YG:40:ASN:ND2   | 2.43                     | 0.52              |
| 32:Y7:37:LYS:NZ   | 35:YA:468:G:OP2    | 2.42                     | 0.52              |
| 35:YA:24:G:O2'    | 52:YW:78:GLU:O     | 2.26                     | 0.52              |
| 35:YA:2602:A:N3   | 35:YA:2602:A:C2'   | 2.73                     | 0.52              |
| 1:QA:235:C:H2'    | 1:QA:236:G:H8      | 1.74                     | 0.51              |
| 1:QA:742:G:OP2    | 15:QO:35:ARG:NH2   | 2.42                     | 0.51              |
| 8:QH:36:LEU:HD12  | 8:QH:59:LEU:HD23   | 1.92                     | 0.51              |
| 35:RA:1819:A:H5'' | 37:RD:161:THR:HG21 | 1.92                     | 0.51              |
| 1:XA:35:G:N3      | 12:XL:118:SER:OG   | 2.42                     | 0.51              |
| 35:YA:221:A:N1    | 35:YA:265:A:O2'    | 2.41                     | 0.51              |
| 35:YA:2627:G:N2   | 35:YA:2777:G:OP2   | 2.42                     | 0.51              |
| 35:YA:2718:G:O2'  | 35:YA:2847:U:OP1   | 2.26                     | 0.51              |
| 53:YX:34:ALA:O    | 53:YX:77:LYS:NZ    | 2.42                     | 0.51              |
| 1:QA:475:G:H2'    | 1:QA:476:G:H8      | 1.75                     | 0.51              |
| 7:QG:26:PHE:HD1   | 7:QG:101:LEU:HD22  | 1.75                     | 0.51              |
| 1:XA:410:G:H21    | 1:XA:432:A:H62     | 1.59                     | 0.51              |
| 1:XA:922:G:H4'    | 5:XE:20:GLN:HA     | 1.92                     | 0.51              |
| 1:XA:1147:C:O2    | 9:XI:16:ARG:NH1    | 2.43                     | 0.51              |
| 1:XA:1386:G:H2'   | 1:XA:1387:G:H8     | 1.75                     | 0.51              |
| 6:XF:37:VAL:HA    | 6:XF:65:VAL:HG12   | 1.91                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:Y5:29:THR:O    | 30:Y5:29:THR:OG1   | 2.26                     | 0.51              |
| 39:YF:101:LEU:O   | 39:YF:106:ARG:NH1  | 2.42                     | 0.51              |
| 1:QA:950:U:H3     | 1:QA:1231:G:H1     | 1.56                     | 0.51              |
| 26:R1:76:ARG:O    | 35:RA:272(Q):G:O2' | 2.28                     | 0.51              |
| 35:RA:577:G:O2'   | 35:RA:1254:A:OP1   | 2.27                     | 0.51              |
| 35:RA:2133:G:O2'  | 35:RA:2158:A:N1    | 2.43                     | 0.51              |
| 43:RN:49:GLY:O    | 43:RN:119:ARG:NH1  | 2.43                     | 0.51              |
| 35:YA:2306:C:N4   | 40:YG:42:GLY:O     | 2.43                     | 0.51              |
| 47:YR:38:VAL:HG22 | 47:YR:112:ALA:HB2  | 1.91                     | 0.51              |
| 51:YV:21:ARG:CD   | 51:YV:91:TYR:HE2   | 2.24                     | 0.51              |
| 54:RY:83:THR:OG1  | 54:RY:84:ARG:N     | 2.44                     | 0.51              |
| 1:XA:390:C:O3'    | 16:XP:28:ARG:NH2   | 2.42                     | 0.51              |
| 1:XA:1077:G:N2    | 1:XA:1080:A:OP2    | 2.35                     | 0.51              |
| 35:YA:299:A:N1    | 35:YA:322:A:O2'    | 2.41                     | 0.51              |
| 1:QA:339:C:OP2    | 44:RO:97:ARG:NH2   | 2.44                     | 0.51              |
| 35:RA:116:C:O2'   | 35:RA:126:A:N3     | 2.41                     | 0.51              |
| 35:RA:2705:A:O2'  | 35:RA:2852:G:OP1   | 2.27                     | 0.51              |
| 1:XA:73:G:H1      | 1:XA:96:U:H3       | 1.57                     | 0.51              |
| 3:XC:153:VAL:HG22 | 3:XC:198:VAL:HG22  | 1.90                     | 0.51              |
| 29:Y4:68:ARG:NH2  | 29:Y4:69:LYS:O     | 2.44                     | 0.51              |
| 37:YD:148:GLU:HB3 | 37:YD:151:LYS:HD2  | 1.93                     | 0.51              |
| 40:YG:4:ASP:OD2   | 40:YG:9:ARG:NH2    | 2.43                     | 0.51              |
| 35:RA:1666:G:HO2' | 44:RO:6:THR:HG1    | 1.55                     | 0.51              |
| 1:XA:1316:G:O2'   | 1:XA:1318:A:N7     | 2.43                     | 0.51              |
| 8:XH:81:HIS:N     | 8:XH:138:TRP:O     | 2.44                     | 0.51              |
| 27:Y2:48:HIS:ND1  | 35:YA:95:G:O2'     | 2.37                     | 0.51              |
| 33:Y8:26:LYS:HD3  | 33:Y8:44:LYS:HA    | 1.93                     | 0.51              |
| 34:Y9:25:VAL:HB   | 34:Y9:34:GLN:HB2   | 1.93                     | 0.51              |
| 35:YA:1791:A:H4'  | 37:YD:206:LEU:HB2  | 1.92                     | 0.51              |
| 43:YN:54:VAL:HB   | 43:YN:122:VAL:HG22 | 1.91                     | 0.51              |
| 35:RA:2115:G:O2'  | 35:RA:2166:G:N2    | 2.43                     | 0.51              |
| 49:RT:19:LEU:HD13 | 49:RT:86:ILE:HD12  | 1.92                     | 0.51              |
| 9:XI:28:VAL:HG12  | 9:XI:63:ILE:HB     | 1.93                     | 0.51              |
| 35:YA:1266:G:O2'  | 35:YA:2012:G:O6    | 2.27                     | 0.51              |
| 39:YF:63:LYS:NZ   | 39:YF:75:HIS:O     | 2.38                     | 0.51              |
| 1:XA:401:C:OP2    | 4:XD:73:ARG:NH2    | 2.43                     | 0.51              |
| 1:XA:403:C:OP2    | 4:XD:74:GLN:NE2    | 2.44                     | 0.51              |
| 1:XA:993:G:O2'    | 1:XA:994:A:N7      | 2.43                     | 0.51              |
| 1:XA:1525:G:OP1   | 11:XK:120:ARG:NH2  | 2.44                     | 0.51              |
| 7:XG:89:MET:HE1   | 7:XG:156:TRP:H     | 1.75                     | 0.51              |
| 13:XM:65:LYS:HB2  | 13:XM:69:GLU:HB3   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:QE:102:ALA:HB3  | 5:QE:107:ARG:HB2   | 1.93                     | 0.51              |
| 16:QP:19:ILE:HB   | 16:QP:37:GLY:HA3   | 1.92                     | 0.51              |
| 35:RA:453:C:O2    | 35:RA:457:A:O2'    | 2.28                     | 0.51              |
| 35:RA:2144:U:HO2' | 35:RA:2147:G:H1    | 1.57                     | 0.51              |
| 7:XG:113:GLU:HB2  | 7:XG:119:ARG:HG2   | 1.92                     | 0.51              |
| 16:XP:8:ARG:NH2   | 16:XP:11:SER:O     | 2.44                     | 0.51              |
| 35:YA:1266:G:O5'  | 52:YW:15:ARG:NH2   | 2.44                     | 0.51              |
| 40:YG:37:VAL:HG22 | 40:YG:159:VAL:HG12 | 1.93                     | 0.51              |
| 46:YQ:22:LYS:O    | 55:YZ:78:LYS:NZ    | 2.44                     | 0.51              |
| 47:RR:33:ARG:NH2  | 47:RR:115:GLU:OE1  | 2.42                     | 0.51              |
| 55:RZ:77:ASP:OD2  | 55:RZ:80:ARG:NH1   | 2.40                     | 0.51              |
| 1:XA:376:G:H1     | 1:XA:387:U:H3      | 1.59                     | 0.51              |
| 9:XI:53:VAL:HG23  | 9:XI:55:ALA:H      | 1.76                     | 0.51              |
| 1:QA:1123:A:H4'   | 10:QJ:36:GLY:HA3   | 1.93                     | 0.50              |
| 29:R4:5:ILE:HD12  | 40:RG:67:LYS:HE2   | 1.92                     | 0.50              |
| 39:RF:185:ASP:OD1 | 39:RF:188:ARG:NH1  | 2.42                     | 0.50              |
| 8:XH:21:LYS:O     | 8:XH:65:TYR:OH     | 2.29                     | 0.50              |
| 25:Y0:27:GLU:HG3  | 25:Y0:68:GLU:HA    | 1.94                     | 0.50              |
| 39:YF:62:ARG:HD2  | 39:YF:63:LYS:O     | 2.10                     | 0.50              |
| 46:YQ:30:GLY:HA2  | 46:YQ:107:ALA:HB2  | 1.94                     | 0.50              |
| 1:QA:765:G:N1     | 1:QA:812:C:O2'     | 2.38                     | 0.50              |
| 1:QA:1101:A:N6    | 2:QB:176:GLU:OE2   | 2.44                     | 0.50              |
| 35:RA:1056:G:H21  | 35:RA:1103:A:H62   | 1.59                     | 0.50              |
| 5:XE:48:ALA:HB2   | 5:XE:57:LYS:HD3    | 1.93                     | 0.50              |
| 35:YA:2302:G:N2   | 40:YG:126:ASP:OD1  | 2.40                     | 0.50              |
| 3:QC:175:LEU:HD21 | 3:QC:201:TYR:HE2   | 1.76                     | 0.50              |
| 5:QE:33:VAL:HG13  | 5:QE:112:LEU:HD22  | 1.92                     | 0.50              |
| 6:QF:11:ASN:HB3   | 6:QF:14:LEU:HG     | 1.93                     | 0.50              |
| 37:RD:148:GLU:HB3 | 37:RD:151:LYS:HD2  | 1.93                     | 0.50              |
| 41:RH:7:LEU:O     | 41:RH:69:ARG:NE    | 2.43                     | 0.50              |
| 43:RN:22:THR:HB   | 43:RN:25:ARG:HB2   | 1.93                     | 0.50              |
| 52:RW:86:LEU:HD22 | 52:RW:96:ILE:HD11  | 1.93                     | 0.50              |
| 22:XV:33:U:N3     | 22:XV:36:U:OP2     | 2.31                     | 0.50              |
| 33:Y8:14:VAL:HG12 | 33:Y8:24:ALA:HB2   | 1.93                     | 0.50              |
| 35:YA:1426:G:O2'  | 35:YA:1572:A:N6    | 2.45                     | 0.50              |
| 48:YS:10:ARG:HG3  | 48:YS:13:ARG:HH21  | 1.76                     | 0.50              |
| 35:RA:1043:C:HO2' | 35:RA:1048:A:HO2'  | 1.59                     | 0.50              |
| 35:RA:2291:U:O2'  | 35:RA:2374:C:O2    | 2.28                     | 0.50              |
| 46:RQ:30:GLY:HA2  | 46:RQ:107:ALA:HB2  | 1.92                     | 0.50              |
| 26:Y1:4:VAL:HG12  | 26:Y1:11:ARG:HG2   | 1.94                     | 0.50              |
| 35:RA:1779:U:OP2  | 35:RA:1784:A:N6    | 2.34                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RA:2199:A:N1    | 35:RA:2226:C:N4    | 2.57                     | 0.50              |
| 30:Y5:41:PRO:O     | 30:Y5:44:THR:OG1   | 2.30                     | 0.50              |
| 39:YF:46:ARG:HB3   | 39:YF:48:THR:HG23  | 1.94                     | 0.50              |
| 1:QA:626:U:H5''    | 16:QP:38:TYR:CD2   | 2.45                     | 0.50              |
| 10:QJ:53:PRO:O     | 14:QN:41:ARG:NH2   | 2.44                     | 0.50              |
| 26:R1:50:ARG:HG2   | 26:R1:59:THR:HG22  | 1.93                     | 0.50              |
| 35:RA:2816:C:O2    | 35:RA:2883:A:O2'   | 2.29                     | 0.50              |
| 1:XA:978:A:OP2     | 1:XA:1363(A):C:N4  | 2.43                     | 0.50              |
| 1:XA:1289:A:N1     | 1:XA:1371:G:O2'    | 2.42                     | 0.50              |
| 39:YF:168:ARG:HG2  | 39:YF:175:THR:HG21 | 1.93                     | 0.50              |
| 2:QB:88:ALA:O      | 2:QB:226:ARG:NH2   | 2.45                     | 0.50              |
| 11:QK:32:ILE:HG13  | 11:QK:72:ALA:HB2   | 1.94                     | 0.50              |
| 33:R8:12:LYS:NZ    | 35:RA:249:C:O2     | 2.40                     | 0.50              |
| 2:XB:84:GLU:HB3    | 2:XB:219:VAL:HG21  | 1.92                     | 0.50              |
| 2:XB:121:LEU:HD23  | 2:XB:127:ILE:HD12  | 1.94                     | 0.50              |
| 35:YA:1223:G:O6    | 51:YV:69:LYS:NZ    | 2.44                     | 0.50              |
| 39:YF:155:LEU:HD23 | 39:YF:192:LEU:HD13 | 1.93                     | 0.50              |
| 1:QA:1149:C:OP2    | 9:QI:9:ARG:NH2     | 2.45                     | 0.50              |
| 35:RA:221:A:N1     | 35:RA:265:A:O2'    | 2.44                     | 0.50              |
| 43:RN:15:LEU:HB2   | 43:RN:135:PRO:HB2  | 1.93                     | 0.50              |
| 1:XA:618:C:H5'     | 1:XA:619:U:H5''    | 1.94                     | 0.50              |
| 1:XA:1330:U:H4'    | 13:XM:23:TYR:CE1   | 2.46                     | 0.50              |
| 26:Y1:3:LYS:HB2    | 26:Y1:61:ARG:HH11  | 1.77                     | 0.50              |
| 29:Y4:1:MET:SD     | 40:YG:98:ARG:NH1   | 2.85                     | 0.50              |
| 35:RA:693:C:O2'    | 35:RA:1353:A:N3    | 2.41                     | 0.50              |
| 1:XA:1005:A:O3'    | 1:XA:1037:C:O2'    | 2.30                     | 0.50              |
| 35:YA:1801:G:OP2   | 37:YD:154:LYS:NZ   | 2.44                     | 0.50              |
| 1:QA:975:A:H4'     | 1:QA:976:G:H5''    | 1.93                     | 0.49              |
| 18:QR:23:LYS:HD2   | 18:QR:58:LEU:HD23  | 1.94                     | 0.49              |
| 35:RA:299:A:N3     | 35:RA:319:C:O2'    | 2.45                     | 0.49              |
| 6:XF:11:ASN:HB3    | 6:XF:14:LEU:HG     | 1.94                     | 0.49              |
| 35:YA:601:C:O2'    | 35:YA:605:C:OP1    | 2.28                     | 0.49              |
| 35:YA:1296:G:OP1   | 35:YA:2709:G:O2'   | 2.26                     | 0.49              |
| 1:QA:278:G:OP2     | 17:QQ:92:ARG:NH2   | 2.40                     | 0.49              |
| 1:QA:993:G:O2'     | 1:QA:994:A:N7      | 2.44                     | 0.49              |
| 35:RA:2882:A:H5'   | 47:RR:96:ARG:HG3   | 1.93                     | 0.49              |
| 1:XA:757:U:O2'     | 1:XA:879:C:O2      | 2.30                     | 0.49              |
| 8:XH:41:ARG:NH2    | 8:XH:123:GLU:OE2   | 2.45                     | 0.49              |
| 35:YA:116:C:O2'    | 35:YA:126:A:N3     | 2.37                     | 0.49              |
| 54:YY:20:TYR:HB3   | 54:YY:23:ARG:HG3   | 1.94                     | 0.49              |
| 1:QA:769:G:H4'     | 1:QA:1513:A:H4'    | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:953:G:N7     | 13:QM:104:ARG:NH2 | 2.53                     | 0.49              |
| 35:RA:1853:A:N3   | 35:RA:2233:U:O2'  | 2.41                     | 0.49              |
| 44:RO:19:ILE:HG22 | 44:RO:43:VAL:HA   | 1.93                     | 0.49              |
| 35:YA:1098:A:H3'  | 35:YA:1099:G:H8   | 1.77                     | 0.49              |
| 35:YA:2875:C:OP1  | 49:YT:3:ARG:NH1   | 2.45                     | 0.49              |
| 38:YE:7:VAL:HG23  | 38:YE:51:PHE:HE2  | 1.77                     | 0.49              |
| 52:YW:86:LEU:HD22 | 52:YW:96:ILE:HD11 | 1.95                     | 0.49              |
| 54:YY:14:LEU:HB2  | 54:YY:75:ILE:HD11 | 1.92                     | 0.49              |
| 1:QA:410:G:H21    | 1:QA:432:A:H62    | 1.59                     | 0.49              |
| 13:QM:24:GLY:O    | 13:QM:29:ARG:NH1  | 2.46                     | 0.49              |
| 35:RA:392:C:H5''  | 35:RA:409:C:H5''  | 1.93                     | 0.49              |
| 35:YA:2680:C:H5'  | 38:YE:189:PRO:HA  | 1.95                     | 0.49              |
| 39:YF:11:VAL:HG22 | 39:YF:125:LEU:HB2 | 1.93                     | 0.49              |
| 35:RA:336:C:HO2'  | 54:RY:35:TYR:HH   | 1.60                     | 0.49              |
| 35:RA:831:G:O2'   | 45:RP:38:GLN:OE1  | 2.27                     | 0.49              |
| 1:XA:28:G:O2'     | 1:XA:296:U:OP1    | 2.28                     | 0.49              |
| 1:XA:1129:C:OP1   | 9:XI:16:ARG:NH1   | 2.46                     | 0.49              |
| 10:XJ:11:PHE:HE1  | 10:XJ:67:THR:HG22 | 1.77                     | 0.49              |
| 10:XJ:67:THR:O    | 10:XJ:67:THR:OG1  | 2.30                     | 0.49              |
| 26:Y1:25:LYS:NZ   | 35:YA:2396:G:OP1  | 2.45                     | 0.49              |
| 35:YA:1047:G:H21  | 35:YA:1111:A:H62  | 1.59                     | 0.49              |
| 1:QA:1255:G:OP2   | 10:QJ:45:ARG:NH2  | 2.45                     | 0.49              |
| 18:XR:32:ARG:HA   | 18:XR:69:THR:HG21 | 1.94                     | 0.49              |
| 35:YA:1277:G:O2'  | 47:YR:24:GLN:OE1  | 2.23                     | 0.49              |
| 39:YF:6:VAL:N     | 39:YF:22:ALA:O    | 2.45                     | 0.49              |
| 53:YX:59:VAL:HB   | 53:YX:76:ARG:HG3  | 1.95                     | 0.49              |
| 1:QA:28:G:O2'     | 1:QA:296:U:OP1    | 2.29                     | 0.49              |
| 1:QA:407:G:H5''   | 4:QD:115:ARG:HG2  | 1.94                     | 0.49              |
| 4:QD:88:VAL:HA    | 5:QE:97:GLY:HA3   | 1.94                     | 0.49              |
| 35:RA:1490:A:O2'  | 37:RD:99:ASP:OD1  | 2.30                     | 0.49              |
| 1:XA:501:C:O2     | 1:XA:549:C:O2'    | 2.29                     | 0.49              |
| 1:XA:1098:C:OP2   | 2:XB:144:ARG:NH1  | 2.46                     | 0.49              |
| 35:YA:994:C:OP1   | 50:YU:53:ARG:NH2  | 2.45                     | 0.49              |
| 35:RA:299:A:N1    | 35:RA:322:A:O2'   | 2.42                     | 0.49              |
| 2:XB:69:LEU:HB3   | 2:XB:162:ILE:HG22 | 1.95                     | 0.49              |
| 2:XB:122:PHE:CE2  | 2:XB:139:LYS:HD3  | 2.43                     | 0.49              |
| 1:QA:1219:U:OP1   | 14:QN:19:ARG:NH2  | 2.46                     | 0.49              |
| 8:QH:91:ARG:NE    | 17:QQ:32:TYR:O    | 2.45                     | 0.49              |
| 9:QI:118:LYS:HB2  | 9:QI:121:ARG:HB3  | 1.93                     | 0.49              |
| 29:R4:31:ILE:HG21 | 40:RG:142:PRO:HB2 | 1.95                     | 0.49              |
| 33:Y8:26:LYS:HD3  | 33:Y8:44:LYS:HG2  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YA:955:C:OP1    | 46:YQ:87:LYS:NZ    | 2.40                     | 0.49              |
| 57:QA:1821:PAR:N64 | 57:QA:1821:PAR:O44 | 2.44                     | 0.49              |
| 25:R0:32:ARG:H     | 25:R0:35:ASN:ND2   | 2.09                     | 0.49              |
| 35:RA:1022:G:N2    | 35:RA:1023:U:O4    | 2.41                     | 0.49              |
| 39:RF:165:ARG:HG3  | 39:RF:168:ARG:HH12 | 1.78                     | 0.49              |
| 51:RV:72:VAL:HG13  | 51:RV:85:LYS:HB3   | 1.94                     | 0.49              |
| 1:XA:792:A:O2'     | 1:XA:794:A:N7      | 2.40                     | 0.49              |
| 2:XB:16:HIS:HB2    | 2:XB:204:ASN:HB3   | 1.94                     | 0.49              |
| 13:XM:23:TYR:HE2   | 13:XM:71:ARG:HG2   | 1.78                     | 0.49              |
| 13:XM:102:ARG:NH2  | 13:XM:105:THR:OG1  | 2.43                     | 0.49              |
| 41:YH:159:GLU:HG2  | 41:YH:169:VAL:HG11 | 1.94                     | 0.49              |
| 1:QA:380:G:N2      | 1:QA:383:A:OP2     | 2.39                     | 0.48              |
| 1:QA:401:C:O2'     | 1:QA:621:A:N3      | 2.42                     | 0.48              |
| 35:RA:643:A:N1     | 35:RA:2369:A:O2'   | 2.43                     | 0.48              |
| 39:RF:167:ALA:HB1  | 39:RF:173:VAL:HG11 | 1.95                     | 0.48              |
| 45:RP:89:ALA:O     | 45:RP:121:LYS:NZ   | 2.36                     | 0.48              |
| 6:XF:50:TYR:CE1    | 18:XR:77:GLY:HA2   | 2.43                     | 0.48              |
| 8:XH:34:GLU:OE1    | 8:XH:37:ARG:NH2    | 2.46                     | 0.48              |
| 35:YA:996:A:OP2    | 50:YU:93:LYS:NZ    | 2.39                     | 0.48              |
| 44:YO:16:ALA:HA    | 44:YO:46:ALA:HA    | 1.94                     | 0.48              |
| 1:QA:186:C:O2'     | 20:QT:85:MET:SD    | 2.69                     | 0.48              |
| 1:QA:811:C:O2'     | 1:QA:901:A:N1      | 2.46                     | 0.48              |
| 33:R8:27:THR:HG22  | 45:RP:63:PRO:HD3   | 1.94                     | 0.48              |
| 34:R9:25:VAL:HB    | 34:R9:34:GLN:HB2   | 1.94                     | 0.48              |
| 1:QA:663:A:H61     | 1:QA:742:G:H1      | 1.59                     | 0.48              |
| 1:QA:978:A:H61     | 1:QA:1316:G:H1'    | 1.78                     | 0.48              |
| 13:QM:8:GLU:OE2    | 13:QM:11:ARG:NH1   | 2.46                     | 0.48              |
| 35:RA:271:A:N3     | 35:RA:365:C:O2'    | 2.43                     | 0.48              |
| 45:RP:19:VAL:HG12  | 45:RP:27:HIS:HB3   | 1.95                     | 0.48              |
| 2:XB:126:GLU:O     | 2:XB:130:ARG:NH1   | 2.46                     | 0.48              |
| 3:XC:9:GLY:HA3     | 14:YN:49:HIS:HA    | 1.95                     | 0.48              |
| 14:YN:24:CYS:HB3   | 14:YN:29:ARG:H     | 1.78                     | 0.48              |
| 39:YF:167:ALA:HA   | 39:YF:170:LEU:HD23 | 1.95                     | 0.48              |
| 2:QB:27:LYS:O      | 2:QB:30:ARG:NH1    | 2.46                     | 0.48              |
| 6:QF:37:VAL:HA     | 6:QF:65:VAL:HG12   | 1.95                     | 0.48              |
| 3:XC:152:ILE:HG12  | 3:XC:199:LYS:HB2   | 1.94                     | 0.48              |
| 35:YA:1022:G:N2    | 35:YA:1023:U:O4    | 2.40                     | 0.48              |
| 35:YA:1657:C:OP1   | 38:YE:136:ARG:N    | 2.46                     | 0.48              |
| 37:RD:168:ARG:HG2  | 37:RD:173:VAL:HG12 | 1.95                     | 0.48              |
| 52:RW:18:ARG:NH1   | 52:RW:76:VAL:O     | 2.46                     | 0.48              |
| 1:QA:978:A:OP2     | 1:QA:1363(A):C:N4  | 2.42                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:R4:18:CYS:SG    | 29:R4:20:ASN:ND2   | 2.87                     | 0.48              |
| 35:RA:1082:U:O4    | 35:RA:1086:A:N6    | 2.47                     | 0.48              |
| 42:RI:4:ILE:HG12   | 42:RI:18:VAL:HG22  | 1.95                     | 0.48              |
| 51:RV:21:ARG:HD3   | 51:RV:91:TYR:CE2   | 2.48                     | 0.48              |
| 28:Y3:8:LEU:HD13   | 28:Y3:23:LEU:HD11  | 1.95                     | 0.48              |
| 41:YH:106:THR:O    | 41:YH:106:THR:OG1  | 2.31                     | 0.48              |
| 7:QG:57:GLU:HG3    | 7:QG:60:LYS:H      | 1.79                     | 0.48              |
| 39:RF:164:ARG:HG3  | 39:RF:175:THR:HB   | 1.96                     | 0.48              |
| 41:RH:3:ARG:HE     | 41:RH:4:ILE:H      | 1.62                     | 0.48              |
| 1:XA:1309:G:N7     | 13:XM:99:ARG:NH2   | 2.61                     | 0.48              |
| 10:XJ:9:ARG:HG2    | 10:XJ:69:ASN:HD22  | 1.79                     | 0.48              |
| 35:YA:139(A):G:H21 | 53:YX:41:ASN:HD21  | 1.61                     | 0.48              |
| 35:YA:919:G:N2     | 35:YA:2269:A:OP2   | 2.46                     | 0.48              |
| 1:QA:1414:U:H3     | 1:QA:1486:G:H1     | 1.61                     | 0.48              |
| 35:RA:220:G:O2'    | 35:RA:233:A:N3     | 2.40                     | 0.48              |
| 44:RO:16:ALA:HA    | 44:RO:46:ALA:HA    | 1.95                     | 0.48              |
| 51:RV:41:GLY:HA2   | 51:RV:45:THR:HA    | 1.95                     | 0.48              |
| 35:YA:223:A:O2'    | 35:YA:420:C:O2     | 2.29                     | 0.48              |
| 35:YA:1682:G:OP1   | 35:YA:1699:G:N1    | 2.46                     | 0.48              |
| 44:YO:1:MET:HG3    | 44:YO:67:LYS:HG2   | 1.95                     | 0.48              |
| 54:YY:39:VAL:HB    | 54:YY:42:VAL:HB    | 1.96                     | 0.48              |
| 33:R8:26:LYS:HD3   | 33:R8:44:LYS:HG2   | 1.95                     | 0.48              |
| 35:RA:307:G:N1     | 35:RA:310:A:OP2    | 2.47                     | 0.48              |
| 37:RD:71:ASP:HB2   | 37:RD:103:ARG:HH12 | 1.79                     | 0.48              |
| 1:XA:280:C:OP1     | 17:XQ:91:ARG:NH1   | 2.43                     | 0.48              |
| 1:XA:461:A:O2'     | 1:XA:471:G:N7      | 2.44                     | 0.48              |
| 1:XA:1085:U:H5''   | 1:XA:1086:U:H5     | 1.79                     | 0.48              |
| 6:XF:80:ARG:NH1    | 6:XF:88:VAL:O      | 2.47                     | 0.48              |
| 35:YA:861:A:N3     | 36:YB:79:C:O2'     | 2.45                     | 0.48              |
| 35:YA:1568:G:H5''  | 37:YD:61:LEU:HG    | 1.95                     | 0.48              |
| 39:YF:167:ALA:HB1  | 39:YF:173:VAL:HG11 | 1.96                     | 0.48              |
| 35:RA:117:G:OP2    | 35:RA:119:A:O2'    | 2.26                     | 0.48              |
| 35:RA:579:G:O2'    | 35:RA:2019:A:OP1   | 2.30                     | 0.48              |
| 35:RA:2751:G:H4'   | 41:RH:4:ILE:HD11   | 1.96                     | 0.48              |
| 38:RE:134:ILE:HA   | 38:RE:137:HIS:HD2  | 1.77                     | 0.48              |
| 1:XA:380:G:N2      | 1:XA:383:A:OP2     | 2.35                     | 0.48              |
| 17:XQ:28:PRO:HA    | 17:XQ:35:VAL:HA    | 1.96                     | 0.48              |
| 41:YH:154:PRO:HB3  | 41:YH:163:TYR:CZ   | 2.48                     | 0.48              |
| 49:YT:34:VAL:O     | 49:YT:41:ARG:N     | 2.43                     | 0.48              |
| 55:YZ:69:THR:HG22  | 55:YZ:90:VAL:HA    | 1.95                     | 0.48              |
| 16:QP:20:VAL:HG23  | 16:QP:35:LYS:HA    | 1.95                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:R5:41:PRO:O    | 30:R5:44:THR:OG1   | 2.32                     | 0.47              |
| 33:R8:19:SER:OG   | 35:RA:651:G:OP1    | 2.31                     | 0.47              |
| 35:RA:1155:A:P    | 50:RU:55:ARG:HG2   | 2.54                     | 0.47              |
| 42:RI:90:GLY:O    | 42:RI:121:LYS:NZ   | 2.37                     | 0.47              |
| 1:XA:718:G:O6     | 18:XR:74:ARG:NH1   | 2.47                     | 0.47              |
| 3:XC:8:ILE:HG23   | 3:XC:16:ARG:HE     | 1.78                     | 0.47              |
| 27:Y2:22:GLU:OE2  | 27:Y2:68:ARG:NH2   | 2.47                     | 0.47              |
| 35:YA:2572:A:OP1  | 35:YA:2574:G:O2'   | 2.30                     | 0.47              |
| 1:QA:1261:A:H62   | 1:QA:1274:G:H21    | 1.62                     | 0.47              |
| 9:QI:46:ALA:HB2   | 9:QI:74:ILE:HG23   | 1.95                     | 0.47              |
| 27:R2:22:GLU:OE2  | 27:R2:68:ARG:NH2   | 2.46                     | 0.47              |
| 35:RA:918:A:N3    | 36:RB:80:U:O2'     | 2.46                     | 0.47              |
| 35:RA:1657:C:OP1  | 38:RE:136:ARG:N    | 2.47                     | 0.47              |
| 35:RA:2574:G:N3   | 38:RE:143:ASN:ND2  | 2.61                     | 0.47              |
| 45:RP:47:ASP:OD2  | 45:RP:49:ARG:NH2   | 2.43                     | 0.47              |
| 35:YA:535:C:O3'   | 50:YU:53:ARG:NH1   | 2.47                     | 0.47              |
| 37:YD:5:LYS:HG2   | 37:YD:17:THR:HG22  | 1.96                     | 0.47              |
| 44:YO:80:ASP:OD2  | 49:YT:64:ARG:NH2   | 2.47                     | 0.47              |
| 49:YT:73:GLU:OE2  | 49:YT:103:ARG:NH2  | 2.46                     | 0.47              |
| 1:QA:376:G:H1     | 1:QA:387:U:H3      | 1.62                     | 0.47              |
| 1:QA:1172:C:H2'   | 1:QA:1173:G:H8     | 1.79                     | 0.47              |
| 1:QA:1422:G:O3'   | 44:RO:49:ARG:NH1   | 2.46                     | 0.47              |
| 35:RA:1833:U:O2'  | 35:RA:1969:A:N1    | 2.46                     | 0.47              |
| 35:RA:1859:A:N6   | 35:RA:1883:G:O2'   | 2.46                     | 0.47              |
| 19:XS:43:GLU:N    | 19:XS:43:GLU:CD    | 2.71                     | 0.47              |
| 25:Y0:33:ALA:N    | 25:Y0:64:ASP:OD1   | 2.45                     | 0.47              |
| 35:YA:1250:G:OP2  | 45:YP:21:ARG:NH1   | 2.47                     | 0.47              |
| 35:YA:1490:A:O2'  | 37:YD:99:ASP:OD1   | 2.29                     | 0.47              |
| 35:YA:1798:U:OP2  | 37:YD:274:ARG:NH2  | 2.42                     | 0.47              |
| 1:QA:642:A:N3     | 8:QH:113:SER:OG    | 2.44                     | 0.47              |
| 32:R7:37:LYS:NZ   | 35:RA:468:G:OP2    | 2.47                     | 0.47              |
| 35:RA:1155:A:OP1  | 50:RU:55:ARG:HG2   | 2.14                     | 0.47              |
| 35:RA:1394:U:O2   | 53:RX:16:LYS:NZ    | 2.45                     | 0.47              |
| 37:RD:183:ARG:HG3 | 37:RD:270:ILE:HG12 | 1.96                     | 0.47              |
| 44:RO:1:MET:HG3   | 44:RO:67:LYS:HG2   | 1.95                     | 0.47              |
| 5:XE:94:ALA:HB1   | 5:XE:98:THR:HG21   | 1.97                     | 0.47              |
| 19:XS:41:VAL:HG22 | 19:XS:44:MET:HE3   | 1.96                     | 0.47              |
| 25:Y0:32:ARG:H    | 25:Y0:35:ASN:ND2   | 2.12                     | 0.47              |
| 38:YE:144:ARG:HB3 | 38:YE:145:LYS:H    | 1.51                     | 0.47              |
| 29:R4:37:SER:HB2  | 40:RG:108:ASN:HA   | 1.95                     | 0.47              |
| 35:RA:223:A:O2'   | 35:RA:420:C:O2     | 2.33                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RA:660:G:H5''   | 39:RF:99:TYR:CD2   | 2.47                     | 0.47              |
| 48:RS:27:SER:HA    | 48:RS:88:ASP:HB3   | 1.96                     | 0.47              |
| 4:XD:68:TYR:OH     | 4:XD:98:GLU:OE2    | 2.21                     | 0.47              |
| 10:XJ:50:ILE:HB    | 14:XN:41:ARG:HE    | 1.79                     | 0.47              |
| 19:XS:63:THR:HG22  | 19:XS:66:MET:HE3   | 1.97                     | 0.47              |
| 35:YA:2853:C:H2'   | 35:YA:2854:G:H8    | 1.79                     | 0.47              |
| 38:YE:104:VAL:HG22 | 38:YE:198:VAL:HG22 | 1.97                     | 0.47              |
| 40:YG:106:LEU:HA   | 40:YG:110:ALA:HB3  | 1.96                     | 0.47              |
| 1:QA:1442(B):G:C8  | 49:RT:118:ARG:HG2  | 2.50                     | 0.47              |
| 22:QV:16:C:H4'     | 22:QV:17(A):U:H5'' | 1.95                     | 0.47              |
| 35:RA:2144:U:O2    | 35:RA:2148:G:N1    | 2.43                     | 0.47              |
| 46:RQ:39:PRO:HB3   | 46:RQ:99:PRO:HD3   | 1.96                     | 0.47              |
| 53:RX:59:VAL:HB    | 53:RX:76:ARG:HG3   | 1.96                     | 0.47              |
| 9:XI:19:LEU:HB3    | 9:XI:59:PHE:HD2    | 1.79                     | 0.47              |
| 1:QA:123:C:OP1     | 1:QA:311:C:O2'     | 2.27                     | 0.47              |
| 1:QA:562:C:H1'     | 12:QL:15:ARG:HB3   | 1.96                     | 0.47              |
| 1:QA:593:G:H1      | 1:QA:646:U:H3      | 1.63                     | 0.47              |
| 6:QF:50:TYR:OH     | 18:QR:74:ARG:O     | 2.32                     | 0.47              |
| 7:QG:28:ASN:OD1    | 7:QG:36:LYS:NZ     | 2.48                     | 0.47              |
| 7:QG:51:GLN:NE2    | 7:QG:56:GLN:O      | 2.47                     | 0.47              |
| 8:QH:85:ARG:NE     | 8:QH:87:SER:O      | 2.30                     | 0.47              |
| 20:QT:50:GLU:HG3   | 20:QT:100:ILE:HD11 | 1.95                     | 0.47              |
| 25:R0:27:GLU:HG3   | 25:R0:68:GLU:HA    | 1.96                     | 0.47              |
| 34:R9:16:VAL:HG22  | 34:R9:25:VAL:HG22  | 1.96                     | 0.47              |
| 1:XA:235:C:H2'     | 1:XA:236:G:H8      | 1.79                     | 0.47              |
| 1:XA:261:U:OP2     | 20:XT:79:ARG:NH2   | 2.48                     | 0.47              |
| 2:XB:71:VAL:HA     | 2:XB:93:VAL:HG22   | 1.97                     | 0.47              |
| 3:XC:58:GLU:HB3    | 10:XJ:92:THR:HG21  | 1.95                     | 0.47              |
| 26:Y1:18:ILE:HG12  | 26:Y1:37:ILE:HG12  | 1.97                     | 0.47              |
| 35:YA:463:G:N2     | 35:YA:466:A:OP2    | 2.39                     | 0.47              |
| 44:YO:19:ILE:HG22  | 44:YO:43:VAL:HA    | 1.97                     | 0.47              |
| 49:YT:24:PRO:HA    | 49:YT:49:VAL:HG13  | 1.97                     | 0.47              |
| 1:QA:1005:A:O2'    | 1:QA:1036:G:N2     | 2.47                     | 0.47              |
| 1:QA:1358:U:H5''   | 14:QN:34:TYR:HA    | 1.95                     | 0.47              |
| 35:RA:1074:G:C2    | 35:RA:1075:C:H1'   | 2.50                     | 0.47              |
| 46:RQ:26:TYR:O     | 46:RQ:67:ARG:NH1   | 2.43                     | 0.47              |
| 16:XP:38:TYR:CE1   | 16:XP:50:LYS:CB    | 2.97                     | 0.47              |
| 27:Y2:55:ARG:HH12  | 35:YA:74:A:H5'     | 1.80                     | 0.47              |
| 22:QV:56:C:O2      | 40:RG:78:SER:OG    | 2.32                     | 0.47              |
| 25:R0:43:THR:HG22  | 35:RA:2336:A:H61   | 1.79                     | 0.47              |
| 33:R8:26:LYS:HD3   | 33:R8:44:LYS:HA    | 1.97                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:R9:1:MET:SD    | 34:R9:35:ARG:HB2   | 2.55                     | 0.47              |
| 1:XA:949:A:N7     | 13:XM:106:ASN:ND2  | 2.63                     | 0.47              |
| 13:XM:94:ARG:HB3  | 13:XM:96:LEU:HD13  | 1.96                     | 0.47              |
| 16:XP:8:ARG:NH1   | 16:XP:9:PHE:O      | 2.48                     | 0.47              |
| 35:YA:530:G:N1    | 35:YA:2023:G:OP1   | 2.37                     | 0.47              |
| 38:YE:134:ILE:HA  | 38:YE:137:HIS:HD2  | 1.80                     | 0.47              |
| 1:QA:73:G:H1      | 1:QA:96:U:H3       | 1.63                     | 0.47              |
| 35:RA:321:G:O2'   | 35:RA:340:A:N3     | 2.46                     | 0.47              |
| 35:RA:854:G:H2'   | 35:RA:855:G:H8     | 1.80                     | 0.47              |
| 1:XA:1220:G:N2    | 19:XS:54:GLY:O     | 2.46                     | 0.47              |
| 18:XR:23:LYS:HD2  | 18:XR:58:LEU:HD23  | 1.97                     | 0.47              |
| 35:YA:745:G:O6    | 35:YA:746:A:N6     | 2.48                     | 0.47              |
| 51:YV:21:ARG:NE   | 51:YV:91:TYR:CE2   | 2.79                     | 0.47              |
| 52:YW:35:ILE:O    | 52:YW:39:THR:OG1   | 2.29                     | 0.47              |
| 1:QA:689:C:OP1    | 11:QK:27:ASN:ND2   | 2.44                     | 0.46              |
| 4:QD:166:LYS:HD2  | 4:QD:178:VAL:HG11  | 1.97                     | 0.46              |
| 19:QS:40:ILE:HG22 | 19:QS:67:VAL:HG13  | 1.97                     | 0.46              |
| 24:QY:75:C:O2     | 35:RA:2507:C:O2'   | 2.29                     | 0.46              |
| 35:RA:2483:C:N3   | 46:RQ:124:LYS:NZ   | 2.55                     | 0.46              |
| 35:RA:2718:G:O2'  | 35:RA:2847:U:OP1   | 2.33                     | 0.46              |
| 1:XA:975:A:H4'    | 1:XA:976:G:H5''    | 1.96                     | 0.46              |
| 2:XB:212:GLN:O    | 2:XB:216:SER:OG    | 2.27                     | 0.46              |
| 35:YA:2405:G:O2'  | 35:YA:2411:A:N6    | 2.45                     | 0.46              |
| 35:YA:2680:C:O2'  | 38:YE:11:MET:SD    | 2.72                     | 0.46              |
| 37:YD:71:ASP:HB2  | 37:YD:103:ARG:HH12 | 1.80                     | 0.46              |
| 45:YP:88:LEU:HD11 | 45:YP:114:ILE:HD12 | 1.98                     | 0.46              |
| 1:QA:932:C:H5''   | 7:QG:4:ARG:HE      | 1.80                     | 0.46              |
| 3:QC:184:TYR:HD1  | 3:QC:201:TYR:CD1   | 2.34                     | 0.46              |
| 20:QT:43:LEU:HD13 | 20:QT:51:GLU:HB3   | 1.97                     | 0.46              |
| 30:R5:12:SER:HB3  | 35:RA:2020:A:H5'   | 1.98                     | 0.46              |
| 1:XA:634:C:H2'    | 1:XA:635:G:H8      | 1.80                     | 0.46              |
| 1:XA:1330:U:H5'   | 13:XM:23:TYR:HD1   | 1.80                     | 0.46              |
| 6:XF:46:ARG:HH21  | 18:XR:78:LEU:HD22  | 1.80                     | 0.46              |
| 10:XJ:6:ILE:HB    | 10:XJ:72:VAL:HG13  | 1.97                     | 0.46              |
| 12:XL:57:LYS:HE3  | 12:XL:65:GLU:HG2   | 1.96                     | 0.46              |
| 16:QP:32:TYR:CE2  | 16:QP:35:LYS:HB2   | 2.51                     | 0.46              |
| 35:RA:1769:G:O2'  | 35:RA:1958:C:OP1   | 2.28                     | 0.46              |
| 45:RP:20:GLY:HA2  | 45:RP:28:GLY:HA2   | 1.98                     | 0.46              |
| 49:RT:27:THR:HG22 | 49:RT:48:ILE:HG12  | 1.96                     | 0.46              |
| 1:XA:345:C:OP2    | 49:YT:39:ARG:NH2   | 2.47                     | 0.46              |
| 12:XL:5:PRO:HD2   | 12:XL:15:ARG:HH22  | 1.80                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YA:586:A:N1     | 35:YA:809:G:O2'    | 2.45                     | 0.46              |
| 35:YA:793:A:OP2    | 35:YA:2071:A:O2'   | 2.33                     | 0.46              |
| 35:YA:1453:U:O2'   | 35:YA:1455:G:N7    | 2.46                     | 0.46              |
| 35:YA:2816:C:O2    | 35:YA:2883:A:O2'   | 2.29                     | 0.46              |
| 39:YF:157:VAL:HG22 | 39:YF:176:LEU:HB2  | 1.98                     | 0.46              |
| 3:QC:71:ALA:HA     | 3:QC:106:VAL:HG22  | 1.96                     | 0.46              |
| 35:RA:1266:G:O2'   | 35:RA:2012:G:O6    | 2.28                     | 0.46              |
| 35:RA:1288:U:O2'   | 35:RA:1647:G:N2    | 2.47                     | 0.46              |
| 1:XA:619:U:N3      | 4:XD:134:ASP:OD1   | 2.38                     | 0.46              |
| 1:XA:1414:U:H2'    | 1:XA:1415:G:H8     | 1.80                     | 0.46              |
| 35:YA:2503:2MA:O2' | 35:YA:2505:G:OP2   | 2.25                     | 0.46              |
| 38:YE:84:PHE:CZ    | 38:YE:86:PRO:HB3   | 2.51                     | 0.46              |
| 1:QA:35:G:N3       | 12:QL:118:SER:OG   | 2.48                     | 0.46              |
| 35:RA:2105:C:H2'   | 35:RA:2106:G:C8    | 2.51                     | 0.46              |
| 35:RA:2689:U:H4'   | 35:RA:2690:C:H5'   | 1.97                     | 0.46              |
| 51:RV:49:THR:O     | 51:RV:51:VAL:N     | 2.49                     | 0.46              |
| 1:XA:867:G:O2'     | 1:XA:873:A:N1      | 2.43                     | 0.46              |
| 1:XA:1251:A:N3     | 1:XA:1369:C:O2'    | 2.41                     | 0.46              |
| 4:XD:63:LYS:HD2    | 4:XD:198:VAL:HG12  | 1.97                     | 0.46              |
| 5:XE:76:ILE:HG13   | 5:XE:93:PRO:HG3    | 1.96                     | 0.46              |
| 8:XH:110:ALA:HB3   | 8:XH:121:ASP:HB3   | 1.97                     | 0.46              |
| 16:XP:43:LYS:HG2   | 16:XP:48:TRP:CD2   | 2.51                     | 0.46              |
| 35:YA:694:U:OP1    | 37:YD:59:LYS:NZ    | 2.44                     | 0.46              |
| 35:YA:2304:G:H22   | 35:YA:2312:U:H3    | 1.61                     | 0.46              |
| 35:YA:2685:G:H5'   | 44:YO:68:GLU:OE2   | 2.15                     | 0.46              |
| 55:YZ:108:PRO:HG2  | 55:YZ:117:LEU:HD21 | 1.96                     | 0.46              |
| 1:QA:1329:A:N7     | 21:QU:7:ARG:NH2    | 2.63                     | 0.46              |
| 33:R8:64:TYR:OH    | 35:RA:592:G:O2'    | 2.28                     | 0.46              |
| 35:RA:521:G:H2'    | 35:RA:522:G:H8     | 1.81                     | 0.46              |
| 35:RA:2478:A:O2'   | 35:RA:2536:G:N2    | 2.49                     | 0.46              |
| 1:XA:486:U:H2'     | 1:XA:487:A:C8      | 2.50                     | 0.46              |
| 1:XA:689:C:OP1     | 11:XK:27:ASN:ND2   | 2.48                     | 0.46              |
| 1:XA:769:G:OP2     | 1:XA:803:G:O2'     | 2.32                     | 0.46              |
| 8:XH:33:GLU:HG2    | 8:XH:59:LEU:HD21   | 1.96                     | 0.46              |
| 11:XK:18:ARG:NH2   | 11:XK:35:PRO:O     | 2.48                     | 0.46              |
| 14:XN:29:ARG:HG2   | 14:XN:31:ARG:H     | 1.80                     | 0.46              |
| 35:YA:958:U:O2     | 36:YB:90:A:O2'     | 2.27                     | 0.46              |
| 35:YA:1815:A:OP2   | 37:YD:54:ARG:NH2   | 2.42                     | 0.46              |
| 38:YE:111:ARG:HG3  | 47:YR:1:MET:HE1    | 1.97                     | 0.46              |
| 43:YN:12:ARG:NH1   | 43:YN:50:ASP:OD2   | 2.48                     | 0.46              |
| 52:YW:14:PRO:HG2   | 52:YW:78:GLU:HG2   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 2:QB:68:ILE:HD12  | 2:QB:161:ALA:HB3     | 1.96                     | 0.46              |
| 9:QI:10:ARG:NH1   | 9:QI:105:ASP:OD2     | 2.48                     | 0.46              |
| 10:QJ:12:ASP:HB3  | 10:QJ:15:THR:HG22    | 1.98                     | 0.46              |
| 30:R5:7:PRO:O     | 35:RA:2016:U:O2'     | 2.31                     | 0.46              |
| 33:R8:7:HIS:CD2   | 45:RP:50:ARG:HD3     | 2.51                     | 0.46              |
| 35:RA:530:G:N1    | 35:RA:2023:G:OP1     | 2.36                     | 0.46              |
| 35:RA:743:G:O2'   | 35:RA:1659:U:OP1     | 2.32                     | 0.46              |
| 35:RA:1084:A:H8   | 35:RA:1085:A:H4'     | 1.80                     | 0.46              |
| 35:RA:1666:G:O2'  | 44:RO:6:THR:OG1      | 2.27                     | 0.46              |
| 35:RA:2711:A:H5'' | 35:RA:2712(A):U:H5'' | 1.98                     | 0.46              |
| 35:RA:2788:C:OP1  | 38:RE:61:ARG:NH2     | 2.49                     | 0.46              |
| 54:RY:9:LYS:NZ    | 54:RY:28:LYS:O       | 2.43                     | 0.46              |
| 1:XA:1498:UR3:OP2 | 23:XX:16:A:O2'       | 2.32                     | 0.46              |
| 13:XM:82:MET:HE3  | 13:XM:93:ARG:HG2     | 1.98                     | 0.46              |
| 35:YA:1394:U:O2   | 53:YX:16:LYS:NZ      | 2.45                     | 0.46              |
| 44:YO:8:LEU:HB2   | 44:YO:19:ILE:HG13    | 1.97                     | 0.46              |
| 46:YQ:43:THR:HG22 | 46:YQ:94:VAL:HG12    | 1.98                     | 0.46              |
| 1:QA:824:C:H2'    | 1:QA:825:G:H8        | 1.81                     | 0.46              |
| 35:RA:2059:A:HO2' | 39:RF:69:HIS:HD1     | 1.63                     | 0.46              |
| 39:RF:6:VAL:N     | 39:RF:22:ALA:O       | 2.48                     | 0.46              |
| 41:RH:3:ARG:HE    | 41:RH:5:GLY:H        | 1.64                     | 0.46              |
| 41:RH:7:LEU:HD22  | 41:RH:69:ARG:HH21    | 1.80                     | 0.46              |
| 1:XA:1518:MA6:O5' | 1:XA:1518:MA6:H8     | 2.15                     | 0.46              |
| 28:Y3:51:ALA:HA   | 28:Y3:54:VAL:HG12    | 1.98                     | 0.46              |
| 35:YA:630:G:N2    | 35:YA:633:A:OP2      | 2.41                     | 0.46              |
| 37:YD:108:PRO:HA  | 37:YD:196:VAL:HA     | 1.97                     | 0.46              |
| 1:QA:1222:G:H5''  | 19:QS:78:ARG:HD2     | 1.97                     | 0.46              |
| 7:QG:79:ARG:HA    | 7:QG:84:ASN:HA       | 1.98                     | 0.46              |
| 9:QI:9:ARG:HB2    | 9:QI:104:ARG:HE      | 1.81                     | 0.46              |
| 35:RA:660:G:OP1   | 39:RF:99:TYR:HD2     | 1.99                     | 0.46              |
| 35:RA:675:A:N3    | 35:RA:2443:C:O2'     | 2.48                     | 0.46              |
| 35:RA:1007:C:H5'' | 43:RN:35:ARG:NH1     | 2.31                     | 0.46              |
| 35:RA:2295:C:OP1  | 48:RS:10:ARG:NH1     | 2.49                     | 0.46              |
| 35:RA:2521:C:O2'  | 35:RA:2564:A:N3      | 2.45                     | 0.46              |
| 43:RN:94:HIS:HB3  | 43:RN:97:ARG:HD3     | 1.98                     | 0.46              |
| 1:XA:1000:U:H2'   | 1:XA:1001(A):A:H8    | 1.78                     | 0.46              |
| 19:XS:68:GLY:H    | 29:Y4:58:ARG:HH12    | 1.63                     | 0.46              |
| 35:YA:1423:G:H2'  | 35:YA:1424:G:H8      | 1.81                     | 0.46              |
| 26:R1:3:LYS:HB3   | 26:R1:61:ARG:HH22    | 1.81                     | 0.46              |
| 35:RA:776:G:N7    | 35:RA:793:A:O2'      | 2.49                     | 0.46              |
| 35:RA:1223:G:N2   | 35:RA:1226:A:OP2     | 2.37                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:RF:110:LEU:HD11 | 39:RF:181:LEU:HG  | 1.97                     | 0.46              |
| 1:XA:742:G:OP2     | 15:XO:35:ARG:NH2  | 2.49                     | 0.46              |
| 7:XG:15:ASP:OD1    | 7:XG:19:GLY:N     | 2.48                     | 0.46              |
| 35:YA:1936:A:OP2   | 35:YA:1962:5MC:N4 | 2.46                     | 0.46              |
| 1:QA:976:G:OP2     | 1:QA:1358:U:O2'   | 2.34                     | 0.45              |
| 1:QA:1122:U:O4     | 1:QA:1123:A:N6    | 2.49                     | 0.45              |
| 35:RA:1231:G:H2'   | 35:RA:1232:G:C8   | 2.51                     | 0.45              |
| 35:RA:2788:C:O2'   | 35:RA:2809:A:N3   | 2.42                     | 0.45              |
| 1:XA:148:G:H2'     | 1:XA:149:A:C8     | 2.51                     | 0.45              |
| 1:XA:278:G:OP2     | 17:XQ:92:ARG:NH2  | 2.44                     | 0.45              |
| 16:XP:53:VAL:HG12  | 16:XP:79:VAL:HG22 | 1.97                     | 0.45              |
| 35:YA:1394:U:H4'   | 35:YA:1603:A:H4'  | 1.98                     | 0.45              |
| 35:YA:1824:G:H5''  | 37:YD:52:ARG:HH21 | 1.80                     | 0.45              |
| 37:YD:145:VAL:HB   | 37:YD:155:LEU:HB2 | 1.98                     | 0.45              |
| 2:QB:178:ARG:HG2   | 8:QH:72:PRO:HA    | 1.98                     | 0.45              |
| 26:R1:72:GLU:OE2   | 26:R1:76:ARG:HD2  | 2.16                     | 0.45              |
| 35:RA:1012:U:O4    | 43:RN:28:THR:OG1  | 2.29                     | 0.45              |
| 1:XA:427:U:O2'     | 1:XA:541:G:OP1    | 2.30                     | 0.45              |
| 1:XA:475:G:H2'     | 1:XA:476:G:H8     | 1.82                     | 0.45              |
| 4:XD:133:VAL:HG11  | 4:XD:138:TYR:HD2  | 1.80                     | 0.45              |
| 35:YA:2314:C:H2'   | 35:YA:2315:G:C8   | 2.52                     | 0.45              |
| 40:YG:97:ASP:HA    | 40:YG:100:TRP:HD1 | 1.80                     | 0.45              |
| 43:YN:71:ILE:HA    | 43:YN:86:PRO:HA   | 1.98                     | 0.45              |
| 35:RA:276:A:H5''   | 35:RA:277:C:H5'   | 1.98                     | 0.45              |
| 35:RA:1568:G:H5''  | 37:RD:61:LEU:HG   | 1.98                     | 0.45              |
| 35:RA:2735:G:H2'   | 35:RA:2736:G:H8   | 1.81                     | 0.45              |
| 1:XA:1129:C:H2'    | 1:XA:1139:G:N7    | 2.31                     | 0.45              |
| 1:XA:1458:G:OP1    | 20:XT:35:THR:OG1  | 2.31                     | 0.45              |
| 4:XD:148:VAL:HG11  | 4:XD:158:ILE:HG21 | 1.99                     | 0.45              |
| 35:YA:956:G:OP2    | 46:YQ:14:ARG:NH2  | 2.49                     | 0.45              |
| 35:YA:1541:G:OP2   | 35:YA:1542:A:O2'  | 2.31                     | 0.45              |
| 35:YA:1567:A:H3'   | 37:YD:86:PRO:HG3  | 1.99                     | 0.45              |
| 35:YA:1816:G:O6    | 37:YD:35:LYS:NZ   | 2.42                     | 0.45              |
| 36:YB:74:U:H1'     | 55:YZ:34:ASN:HD21 | 1.82                     | 0.45              |
| 1:QA:279:A:OP2     | 17:QQ:95:TYR:OH   | 2.34                     | 0.45              |
| 2:QB:164:VAL:HG21  | 2:QB:174:VAL:HG12 | 1.99                     | 0.45              |
| 5:QE:145:LYS:NZ    | 5:QE:149:GLU:OE2  | 2.49                     | 0.45              |
| 7:QG:22:LEU:HD21   | 7:QG:66:VAL:HG11  | 1.98                     | 0.45              |
| 12:QL:70:ILE:HG12  | 12:QL:77:LEU:HD12 | 1.98                     | 0.45              |
| 27:R2:29:LYS:HG2   | 27:R2:57:ILE:HD13 | 1.98                     | 0.45              |
| 32:R7:34:ARG:HG3   | 32:R7:39:ARG:HG3  | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RA:805:G:N2     | 35:RA:829:A:OP1    | 2.50                     | 0.45              |
| 35:RA:1798:U:OP2   | 37:RD:273:ARG:NH2  | 2.49                     | 0.45              |
| 35:YA:220:G:O2'    | 35:YA:233:A:N3     | 2.41                     | 0.45              |
| 35:YA:621:A:OP2    | 45:YP:108:LYS:NZ   | 2.50                     | 0.45              |
| 35:YA:1020:A:N1    | 35:YA:1141:U:O2'   | 2.45                     | 0.45              |
| 5:QE:48:ALA:HB2    | 5:QE:57:LYS:HD3    | 1.98                     | 0.45              |
| 15:QO:5:LYS:O      | 15:QO:9:GLN:HG2    | 2.17                     | 0.45              |
| 22:QV:24:U:O2'     | 35:RA:1923:U:OP1   | 2.34                     | 0.45              |
| 35:RA:641:C:O2'    | 35:RA:2350:C:OP1   | 2.26                     | 0.45              |
| 35:RA:995:C:O2     | 43:RN:3:THR:OG1    | 2.32                     | 0.45              |
| 35:RA:2431:U:N3    | 35:RA:2434:A:OP2   | 2.36                     | 0.45              |
| 37:RD:72:LYS:HE3   | 37:RD:101:GLU:HB3  | 1.97                     | 0.45              |
| 39:RF:150:GLY:HA2  | 39:RF:172:TRP:CD2  | 2.52                     | 0.45              |
| 39:RF:160:ASN:HB3  | 39:RF:163:VAL:HG12 | 1.98                     | 0.45              |
| 17:XQ:9:VAL:HG22   | 17:XQ:56:VAL:HG22  | 1.99                     | 0.45              |
| 3:QC:24:ALA:HB3    | 3:QC:29:TYR:HB2    | 1.98                     | 0.45              |
| 13:QM:60:VAL:HG12  | 13:QM:64:TRP:HZ3   | 1.80                     | 0.45              |
| 41:RH:159:GLU:HG2  | 41:RH:169:VAL:HG11 | 1.98                     | 0.45              |
| 48:RS:35:ILE:HB    | 48:RS:97:ARG:HH21  | 1.81                     | 0.45              |
| 50:RU:66:ASN:HD21  | 50:RU:70:ARG:HH21  | 1.65                     | 0.45              |
| 55:RZ:8:TYR:C      | 55:RZ:38:TYR:HD1   | 2.24                     | 0.45              |
| 1:XA:520:A:O2'     | 12:XL:73:GLU:OE1   | 2.34                     | 0.45              |
| 1:XA:736:C:O2'     | 6:XF:90:VAL:O      | 2.32                     | 0.45              |
| 1:XA:744:C:O2'     | 1:XA:851:G:N2      | 2.48                     | 0.45              |
| 6:XF:35:ALA:HA     | 6:XF:67:MET:HB3    | 1.99                     | 0.45              |
| 22:XV:58:A:O2'     | 22:XV:60:U:OP2     | 2.26                     | 0.45              |
| 35:YA:698:C:O2'    | 35:YA:734:A:N6     | 2.50                     | 0.45              |
| 35:YA:1035:U:OP1   | 41:YH:59:ARG:NH2   | 2.49                     | 0.45              |
| 35:YA:1288:U:O2'   | 35:YA:1647:G:N2    | 2.48                     | 0.45              |
| 35:YA:2133:G:O2'   | 35:YA:2158:A:N1    | 2.49                     | 0.45              |
| 1:QA:1255:G:O2'    | 1:QA:1258:G:N3     | 2.45                     | 0.45              |
| 1:QA:1393:U:HO2'   | 1:QA:1501:C:HO2'   | 1.62                     | 0.45              |
| 1:QA:1485:U:H2'    | 1:QA:1486:G:C8     | 2.52                     | 0.45              |
| 3:QC:184:TYR:CD1   | 3:QC:201:TYR:CE1   | 3.05                     | 0.45              |
| 35:RA:1754:C:N3    | 35:RA:2716:U:O2'   | 2.38                     | 0.45              |
| 39:RF:178:PRO:HB2  | 39:RF:201:VAL:HG11 | 1.98                     | 0.45              |
| 1:XA:181:G:O2'     | 1:XA:183:G:N7      | 2.49                     | 0.45              |
| 1:XA:1199:U:O2'    | 1:XA:1202:G:OP1    | 2.33                     | 0.45              |
| 35:YA:1098:A:H3'   | 35:YA:1099:G:C8    | 2.52                     | 0.45              |
| 35:YA:1853:A:N3    | 35:YA:2233:U:O2'   | 2.39                     | 0.45              |
| 55:YZ:126:VAL:HG11 | 55:YZ:161:VAL:HG13 | 1.99                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:1069:C:O2'    | 1:QA:1192:C:O2    | 2.27                     | 0.45              |
| 8:QH:33:GLU:OE2    | 8:QH:50:ARG:NE    | 2.47                     | 0.45              |
| 14:QN:24:CYS:HB3   | 14:QN:29:ARG:H    | 1.81                     | 0.45              |
| 35:RA:1312:U:O4    | 53:RX:60:ARG:HD3  | 2.17                     | 0.45              |
| 37:RD:132:PRO:HG3  | 37:RD:190:TYR:CE1 | 2.52                     | 0.45              |
| 54:RY:28:LYS:N     | 54:RY:38:ILE:O    | 2.44                     | 0.45              |
| 1:XA:1192:C:O2     | 5:XE:25:ARG:NH2   | 2.50                     | 0.45              |
| 31:Y6:37:ARG:HA    | 31:Y6:48:VAL:HA   | 1.99                     | 0.45              |
| 35:YA:1415:U:O2'   | 35:YA:1417:C:OP1  | 2.30                     | 0.45              |
| 35:YA:2581:G:OP2   | 35:YA:2581:G:N2   | 2.41                     | 0.45              |
| 1:QA:1456:G:O3'    | 20:QT:39:LYS:NZ   | 2.50                     | 0.45              |
| 7:QG:27:ILE:HD12   | 7:QG:40:ALA:HA    | 1.98                     | 0.45              |
| 32:R7:24:THR:HG23  | 32:R7:27:GLY:H    | 1.82                     | 0.45              |
| 35:RA:265:A:N1     | 35:RA:427:U:O2'   | 2.46                     | 0.45              |
| 46:RQ:30:GLY:N     | 46:RQ:105:GLU:OE2 | 2.48                     | 0.45              |
| 22:XV:49:G:H1      | 22:XV:65:C:H42    | 1.63                     | 0.45              |
| 26:Y1:86:SER:OG    | 26:Y1:89:GLU:OE1  | 2.29                     | 0.45              |
| 35:YA:30:G:O2'     | 35:YA:1214:A:N3   | 2.42                     | 0.45              |
| 35:YA:272(L):U:P   | 42:YI:50:ARG:HH22 | 2.40                     | 0.45              |
| 35:YA:2352:A:N6    | 35:YA:2365:G:O2'  | 2.50                     | 0.45              |
| 51:YV:21:ARG:CD    | 51:YV:91:TYR:CE2  | 3.00                     | 0.45              |
| 51:YV:21:ARG:CZ    | 51:YV:91:TYR:HE2  | 2.29                     | 0.45              |
| 4:QD:105:VAL:HG13  | 4:QD:110:PHE:HB2  | 1.99                     | 0.45              |
| 13:QM:19:LEU:HD11  | 13:QM:56:LEU:HD21 | 1.99                     | 0.45              |
| 20:QT:89:ARG:O     | 20:QT:93:GLU:HG2  | 2.17                     | 0.45              |
| 35:RA:557:U:O2'    | 43:RN:45:ASN:O    | 2.35                     | 0.45              |
| 35:RA:1417:C:O2'   | 35:RA:1587:A:N3   | 2.45                     | 0.45              |
| 39:RF:101:LEU:HD23 | 39:RF:106:ARG:HG2 | 2.00                     | 0.45              |
| 1:XA:1073:U:O2     | 2:XB:104:ASN:ND2  | 2.50                     | 0.45              |
| 5:XE:6:PHE:HD1     | 5:XE:36:ASP:HB3   | 1.82                     | 0.45              |
| 5:XE:33:VAL:HG13   | 5:XE:112:LEU:HD22 | 1.98                     | 0.45              |
| 6:XF:30:LEU:HB3    | 6:XF:35:ALA:HB3   | 1.99                     | 0.45              |
| 9:XI:9:ARG:HG2     | 9:XI:14:VAL:HG12  | 1.99                     | 0.45              |
| 13:XM:86:CYS:SG    | 13:XM:89:GLY:N    | 2.87                     | 0.45              |
| 35:YA:964:C:O2'    | 35:YA:2273:A:N3   | 2.46                     | 0.45              |
| 35:YA:2012:G:OP1   | 52:YW:11:ARG:NH2  | 2.49                     | 0.45              |
| 37:YD:132:PRO:HG3  | 37:YD:190:TYR:CE1 | 2.52                     | 0.45              |
| 38:YE:84:PHE:CE2   | 38:YE:86:PRO:CB   | 3.00                     | 0.45              |
| 35:RA:984:A:H5''   | 35:RA:985:C:H5    | 1.81                     | 0.44              |
| 43:RN:25:ARG:O     | 43:RN:29:LYS:NZ   | 2.45                     | 0.44              |
| 1:XA:1309:G:P      | 13:XM:88:ARG:HH21 | 2.40                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YA:1105:U:H2'   | 35:YA:1106:G:H8    | 1.80                     | 0.44              |
| 38:YE:176:ILE:HB   | 38:YE:181:LEU:HB2  | 1.99                     | 0.44              |
| 51:YV:21:ARG:HD3   | 51:YV:91:TYR:CE2   | 2.52                     | 0.44              |
| 1:QA:447:G:O6      | 1:QA:485:G:O2'     | 2.34                     | 0.44              |
| 1:QA:806:C:H2'     | 1:QA:807:A:H8      | 1.82                     | 0.44              |
| 10:QJ:61:GLU:OE1   | 14:QN:45:ARG:NE    | 2.47                     | 0.44              |
| 35:RA:588:U:H1'    | 39:RF:90:PHE:HB3   | 1.99                     | 0.44              |
| 35:RA:1651:G:N7    | 47:RR:11:ASN:ND2   | 2.64                     | 0.44              |
| 35:RA:1939:5MU:OP1 | 35:RA:2604:U:O2'   | 2.34                     | 0.44              |
| 38:RE:24:THR:OG1   | 38:RE:186:GLY:O    | 2.30                     | 0.44              |
| 1:XA:543:C:OP2     | 4:XD:10:ARG:NH2    | 2.48                     | 0.44              |
| 18:XR:51:LEU:HD13  | 18:XR:55:ARG:HG2   | 2.00                     | 0.44              |
| 35:YA:2119:A:H61   | 35:YA:2168:G:H21   | 1.64                     | 0.44              |
| 37:YD:77:ALA:HA    | 37:YD:97:TYR:HA    | 2.00                     | 0.44              |
| 37:YD:183:ARG:HG3  | 37:YD:270:ILE:HG12 | 1.99                     | 0.44              |
| 1:QA:426:G:OP1     | 4:QD:38:TYR:OH     | 2.36                     | 0.44              |
| 9:QI:36:TYR:HE1    | 9:QI:70:LYS:HE2    | 1.83                     | 0.44              |
| 35:RA:728:G:H4'    | 37:RD:13:ARG:HE    | 1.82                     | 0.44              |
| 35:RA:1327:C:HO2'  | 47:RR:105:ARG:HH12 | 1.59                     | 0.44              |
| 35:RA:1514:U:H2'   | 35:RA:1515:G:H8    | 1.82                     | 0.44              |
| 35:RA:2441:C:OP2   | 35:RA:2586:C:O2'   | 2.28                     | 0.44              |
| 37:RD:75:ILE:HG21  | 37:RD:99:ASP:HB2   | 2.00                     | 0.44              |
| 1:XA:790:A:OP1     | 22:XV:38:A:O2'     | 2.24                     | 0.44              |
| 5:XE:105:VAL:HG21  | 5:XE:128:PRO:HB3   | 1.99                     | 0.44              |
| 7:XG:79:ARG:HA     | 7:XG:84:ASN:HA     | 1.99                     | 0.44              |
| 11:XK:45:GLY:HA2   | 11:XK:48:ILE:HD12  | 2.00                     | 0.44              |
| 36:YB:87:G:N2      | 36:YB:90:A:OP2     | 2.40                     | 0.44              |
| 43:YN:21:LYS:NZ    | 43:YN:140:VAL:OXT  | 2.39                     | 0.44              |
| 1:QA:718:G:H5'     | 11:QK:117:ASN:OD1  | 2.18                     | 0.44              |
| 2:QB:9:GLU:HG2     | 2:QB:11:LEU:H      | 1.82                     | 0.44              |
| 5:QE:78:HIS:HA     | 8:QH:105:ARG:HG3   | 1.99                     | 0.44              |
| 20:QT:22:ARG:O     | 20:QT:26:ASN:ND2   | 2.51                     | 0.44              |
| 35:RA:586:A:N1     | 35:RA:809:G:O2'    | 2.46                     | 0.44              |
| 35:RA:1188:U:H2'   | 35:RA:1189:A:H8    | 1.81                     | 0.44              |
| 35:RA:1792:G:O2'   | 35:RA:1830:C:OP1   | 2.33                     | 0.44              |
| 35:RA:2200:C:O2    | 35:RA:2226:C:N4    | 2.49                     | 0.44              |
| 1:XA:624:C:H2'     | 1:XA:625:G:H8      | 1.82                     | 0.44              |
| 1:XA:978:A:O2'     | 1:XA:1322:C:N3     | 2.47                     | 0.44              |
| 5:XE:110:LEU:HD13  | 5:XE:118:ILE:HG21  | 1.97                     | 0.44              |
| 32:Y7:13:ALA:HB2   | 32:Y7:46:VAL:HG11  | 1.99                     | 0.44              |
| 35:YA:1792:G:O2'   | 35:YA:1830:C:OP1   | 2.35                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:YG:38:VAL:HG22  | 40:YG:93:THR:HG23  | 1.99                     | 0.44              |
| 1:QA:184:G:H2'     | 1:QA:185:A:H8      | 1.81                     | 0.44              |
| 1:QA:790:A:OP1     | 22:QV:38:A:O2'     | 2.30                     | 0.44              |
| 9:QI:16:ARG:HB2    | 9:QI:64:THR:HG22   | 1.99                     | 0.44              |
| 10:QJ:16:LEU:HD22  | 10:QJ:94:VAL:HG12  | 2.00                     | 0.44              |
| 35:RA:463:G:N2     | 35:RA:466:A:OP2    | 2.39                     | 0.44              |
| 38:RE:1:MET:HE1    | 38:RE:202:LYS:HG2  | 1.99                     | 0.44              |
| 1:XA:328:C:H4'     | 1:XA:329:A:H5'     | 1.99                     | 0.44              |
| 9:XI:5:TYR:N       | 9:XI:87:GLN:OE1    | 2.50                     | 0.44              |
| 41:YH:154:PRO:HB3  | 41:YH:163:TYR:CE1  | 2.53                     | 0.44              |
| 47:YR:63:ARG:HG2   | 47:YR:80:PHE:CE2   | 2.53                     | 0.44              |
| 1:QA:396:G:O2'     | 1:QA:398:C:OP1     | 2.26                     | 0.44              |
| 43:RN:36:GLY:HA2   | 43:RN:38:HIS:CE1   | 2.53                     | 0.44              |
| 1:XA:1368:G:OP1    | 9:XI:111:ARG:NH2   | 2.50                     | 0.44              |
| 6:XF:95:GLU:O      | 18:XR:32:ARG:NH1   | 2.50                     | 0.44              |
| 13:XM:17:VAL:O     | 13:XM:20:THR:OG1   | 2.27                     | 0.44              |
| 35:YA:2522:U:O2'   | 35:YA:2647:U:OP1   | 2.31                     | 0.44              |
| 37:YD:108:PRO:HB3  | 37:YD:143:HIS:CE1  | 2.53                     | 0.44              |
| 54:YY:83:THR:OG1   | 54:YY:84:ARG:N     | 2.51                     | 0.44              |
| 1:QA:128:G:O2'     | 17:QQ:3:LYS:NZ     | 2.38                     | 0.44              |
| 35:RA:184:C:O2'    | 35:RA:217:G:N3     | 2.50                     | 0.44              |
| 35:RA:807:U:OP2    | 45:RP:41:ARG:NH2   | 2.51                     | 0.44              |
| 35:RA:1936:A:OP2   | 35:RA:1962:5MC:N4  | 2.48                     | 0.44              |
| 35:RA:2404:C:O3'   | 45:RP:77:ARG:NH2   | 2.51                     | 0.44              |
| 41:RH:126:PRO:HG2  | 41:RH:130:ARG:HH21 | 1.82                     | 0.44              |
| 45:RP:3:LEU:HD23   | 45:RP:6:LEU:HD12   | 2.00                     | 0.44              |
| 1:XA:111:G:H5''    | 16:XP:27:LYS:HG2   | 1.99                     | 0.44              |
| 1:XA:297:G:N2      | 1:XA:300:A:OP2     | 2.48                     | 0.44              |
| 2:XB:71:VAL:HG13   | 2:XB:164:VAL:HA    | 1.99                     | 0.44              |
| 2:XB:207:ALA:O     | 2:XB:210:SER:OG    | 2.32                     | 0.44              |
| 6:XF:33:TYR:HE2    | 6:XF:78:GLU:HG3    | 1.82                     | 0.44              |
| 9:XI:50:LEU:HD23   | 9:XI:85:LEU:HD11   | 1.98                     | 0.44              |
| 35:YA:2377:A:O2'   | 48:YS:112:PHE:O    | 2.30                     | 0.44              |
| 35:YA:2500:U:O2'   | 35:YA:2504:U:OP1   | 2.32                     | 0.44              |
| 1:QA:1073:U:O2     | 2:QB:104:ASN:ND2   | 2.51                     | 0.44              |
| 35:RA:139(A):G:H21 | 53:RX:41:ASN:HD21  | 1.66                     | 0.44              |
| 35:RA:729:G:C5     | 37:RD:208:LYS:HB2  | 2.52                     | 0.44              |
| 35:RA:873:G:O3'    | 46:RQ:63:LYS:NZ    | 2.50                     | 0.44              |
| 9:XI:16:ARG:HH21   | 9:XI:18:PHE:HZ     | 1.66                     | 0.44              |
| 35:YA:956:G:H2'    | 35:YA:957:A:H2'    | 1.99                     | 0.44              |
| 47:YR:100:LEU:HD12 | 47:YR:111:LEU:HB3  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1377:A:OP2    | 7:QG:94:ARG:NE     | 2.51                     | 0.44              |
| 26:R1:11:ARG:NH2   | 35:RA:1365:A:O2'   | 2.51                     | 0.44              |
| 35:RA:475:U:H4'    | 35:RA:510:C:H5'    | 2.00                     | 0.44              |
| 51:RV:14:VAL:HB    | 51:RV:96:ILE:HG13  | 2.00                     | 0.44              |
| 1:XA:1074:G:H1     | 1:XA:1083:U:H3     | 1.66                     | 0.44              |
| 1:XA:1240:U:OP1    | 7:XG:119:ARG:NH2   | 2.46                     | 0.44              |
| 1:XA:1316:G:N1     | 1:XA:1319:A:OP2    | 2.51                     | 0.44              |
| 16:XP:19:ILE:HB    | 16:XP:37:GLY:HA3   | 1.99                     | 0.44              |
| 19:XS:68:GLY:H     | 29:Y4:58:ARG:NH1   | 2.16                     | 0.44              |
| 35:YA:639:U:H3     | 35:YA:649:G:H1     | 1.66                     | 0.44              |
| 35:YA:992:C:OP1    | 50:YU:47:TYR:OH    | 2.32                     | 0.44              |
| 1:QA:189(C):C:H42  | 1:QA:189(J):G:H1   | 1.66                     | 0.43              |
| 11:QK:20:TYR:CE1   | 11:QK:83:ILE:HD13  | 2.53                     | 0.43              |
| 35:RA:814:C:O2'    | 35:RA:1224:C:N3    | 2.51                     | 0.43              |
| 49:RT:9:LEU:O      | 49:RT:12:SER:OG    | 2.27                     | 0.43              |
| 55:RZ:102:LEU:HD11 | 55:RZ:124:ILE:HG12 | 2.00                     | 0.43              |
| 1:XA:96:U:H2'      | 1:XA:97:G:H8       | 1.82                     | 0.43              |
| 1:XA:123:C:OP1     | 1:XA:311:C:O2'     | 2.31                     | 0.43              |
| 6:XF:61:LEU:HD12   | 6:XF:63:TYR:HE1    | 1.83                     | 0.43              |
| 29:Y4:11:PRO:HG3   | 29:Y4:25:TYR:CD2   | 2.53                     | 0.43              |
| 33:Y8:12:LYS:NZ    | 35:YA:249:C:O2     | 2.35                     | 0.43              |
| 45:YP:19:VAL:HG12  | 45:YP:27:HIS:HB3   | 2.00                     | 0.43              |
| 11:QK:34:ASP:OD1   | 11:QK:38:ASN:N     | 2.51                     | 0.43              |
| 18:QR:34:TYR:HD1   | 18:QR:34:TYR:H     | 1.64                     | 0.43              |
| 32:R7:9:ARG:NH2    | 35:RA:1311:G:N7    | 2.65                     | 0.43              |
| 41:RH:68:THR:O     | 41:RH:72:ILE:HG12  | 2.18                     | 0.43              |
| 41:RH:126:PRO:HG2  | 41:RH:130:ARG:HE   | 1.83                     | 0.43              |
| 42:RI:114:LEU:HD11 | 42:RI:128:LEU:HB3  | 2.00                     | 0.43              |
| 4:XD:20:TYR:HD1    | 4:XD:26:CYS:HB3    | 1.83                     | 0.43              |
| 4:XD:59:ARG:HA     | 4:XD:59:ARG:HE     | 1.83                     | 0.43              |
| 7:XG:16:LEU:HD11   | 9:XI:45:ALA:HB2    | 2.00                     | 0.43              |
| 17:XQ:52:LYS:HE3   | 17:XQ:52:LYS:HB3   | 1.83                     | 0.43              |
| 35:YA:1664:A:H61   | 35:YA:1996:C:H42   | 1.66                     | 0.43              |
| 35:YA:2773:C:H5''  | 38:YE:164:ARG:HG2  | 2.00                     | 0.43              |
| 55:YZ:52:SER:OG    | 55:YZ:53:ILE:N     | 2.51                     | 0.43              |
| 1:QA:142:G:H2'     | 1:QA:143:A:H8      | 1.82                     | 0.43              |
| 4:QD:10:ARG:HB2    | 4:QD:40:PRO:HG3    | 2.00                     | 0.43              |
| 4:QD:140:VAL:HG11  | 4:QD:146:ILE:HD11  | 2.00                     | 0.43              |
| 49:RT:50:ILE:HB    | 49:RT:99:LEU:HB2   | 1.99                     | 0.43              |
| 15:XO:5:LYS:O      | 15:XO:9:GLN:HG2    | 2.19                     | 0.43              |
| 29:Y4:43:TYR:CZ    | 40:YG:179:PRO:HG3  | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YA:2115:G:O2'   | 35:YA:2166:G:N2    | 2.51                     | 0.43              |
| 35:YA:2635:C:O2'   | 38:YE:80:GLU:OE1   | 2.32                     | 0.43              |
| 39:YF:155:LEU:HD11 | 39:YF:176:LEU:HD12 | 1.99                     | 0.43              |
| 40:YG:109:VAL:HG11 | 40:YG:142:PRO:HB3  | 2.00                     | 0.43              |
| 1:QA:1516:G:N2     | 1:QA:1519:MA6:OP2  | 2.49                     | 0.43              |
| 2:QB:179:LYS:HD3   | 8:QH:72:PRO:HG3    | 1.99                     | 0.43              |
| 35:RA:955:C:OP1    | 46:RQ:87:LYS:NZ    | 2.43                     | 0.43              |
| 35:RA:956:G:OP2    | 46:RQ:14:ARG:NH2   | 2.52                     | 0.43              |
| 49:RT:24:PRO:HA    | 49:RT:49:VAL:HG13  | 2.00                     | 0.43              |
| 1:XA:107:G:N7      | 20:XT:15:ARG:NH2   | 2.67                     | 0.43              |
| 1:XA:824:C:H2'     | 1:XA:825:G:C8      | 2.53                     | 0.43              |
| 1:XA:986:A:H1'     | 19:XS:55:LYS:HA    | 1.99                     | 0.43              |
| 13:XM:23:TYR:CE2   | 13:XM:71:ARG:HG2   | 2.52                     | 0.43              |
| 34:Y9:2:LYS:NZ     | 35:YA:2478:A:OP2   | 2.48                     | 0.43              |
| 49:YT:35:LYS:HA    | 49:YT:40:THR:HA    | 1.99                     | 0.43              |
| 49:YT:93:ARG:HB3   | 49:YT:117:ASP:HB2  | 2.00                     | 0.43              |
| 1:QA:1129:C:H2'    | 1:QA:1139:G:N7     | 2.33                     | 0.43              |
| 5:QE:6:PHE:HD1     | 5:QE:36:ASP:HB3    | 1.83                     | 0.43              |
| 8:QH:112:LEU:HB3   | 8:QH:133:LEU:HA    | 2.00                     | 0.43              |
| 27:R2:36:ARG:NH2   | 53:RX:5:TYR:O      | 2.40                     | 0.43              |
| 30:R5:12:SER:OG    | 35:RA:2021:C:OP1   | 2.32                     | 0.43              |
| 35:RA:647:G:N3     | 35:RA:2350:C:O2'   | 2.51                     | 0.43              |
| 35:RA:1151:G:O2'   | 50:RU:77:SER:O     | 2.37                     | 0.43              |
| 35:RA:2572:A:H2'   | 38:RE:144:ARG:HD3  | 2.01                     | 0.43              |
| 52:RW:35:ILE:O     | 52:RW:39:THR:OG1   | 2.31                     | 0.43              |
| 1:XA:601:C:H2'     | 1:XA:602:A:H8      | 1.83                     | 0.43              |
| 1:XA:626:U:H4'     | 16:XP:38:TYR:CD2   | 2.53                     | 0.43              |
| 4:XD:98:GLU:HG3    | 4:XD:194:LEU:HD11  | 2.01                     | 0.43              |
| 5:XE:78:HIS:ND1    | 8:XH:104:ARG:HD2   | 2.33                     | 0.43              |
| 33:Y8:23:VAL:HG22  | 33:Y8:49:VAL:HG22  | 2.01                     | 0.43              |
| 33:Y8:30:ARG:NH2   | 45:YP:64:LYS:O     | 2.52                     | 0.43              |
| 35:YA:1009:A:N3    | 35:YA:1153:C:O2'   | 2.42                     | 0.43              |
| 35:YA:2164:C:H3'   | 35:YA:2165:G:H8    | 1.83                     | 0.43              |
| 1:QA:444:C:H2'     | 1:QA:445:G:H8      | 1.84                     | 0.43              |
| 1:QA:1005:A:O3'    | 1:QA:1037:C:O2'    | 2.37                     | 0.43              |
| 44:RO:8:LEU:HB2    | 44:RO:19:ILE:HG13  | 2.00                     | 0.43              |
| 48:RS:3:ARG:HH21   | 48:RS:9:ARG:HH12   | 1.67                     | 0.43              |
| 1:XA:1133:G:H2'    | 1:XA:1134:G:H8     | 1.82                     | 0.43              |
| 1:XA:1133:G:H2'    | 1:XA:1134:G:C8     | 2.54                     | 0.43              |
| 35:YA:743:G:O2'    | 35:YA:1659:U:OP1   | 2.31                     | 0.43              |
| 41:YH:87:LEU:HD23  | 41:YH:164:TYR:HA   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:YS:24:LEU:O     | 48:YS:86:ALA:N     | 2.48                     | 0.43              |
| 1:QA:1031:G:H2'    | 1:QA:1032:G:C8     | 2.53                     | 0.43              |
| 12:QL:71:PRO:HB2   | 12:QL:120:TYR:HE1  | 1.84                     | 0.43              |
| 35:RA:1466:G:O2'   | 35:RA:1546:C:O2'   | 2.28                     | 0.43              |
| 35:RA:1566:A:OP1   | 37:RD:211:ARG:NH1  | 2.51                     | 0.43              |
| 35:RA:1816:G:O6    | 37:RD:35:LYS:NZ    | 2.50                     | 0.43              |
| 35:RA:2013:A:H2    | 52:RW:88:ARG:HH22  | 1.66                     | 0.43              |
| 48:RS:26:LEU:HD23  | 48:RS:87:PHE:HD1   | 1.84                     | 0.43              |
| 49:RT:50:ILE:HA    | 49:RT:99:LEU:HD12  | 2.00                     | 0.43              |
| 1:XA:943:U:H1'     | 9:XI:124:GLN:HE22  | 1.84                     | 0.43              |
| 35:YA:297:C:OP1    | 54:YY:87:LYS:NZ    | 2.43                     | 0.43              |
| 35:YA:380:U:H2'    | 35:YA:381:G:H8     | 1.83                     | 0.43              |
| 35:YA:1779:U:OP2   | 35:YA:1784:A:N6    | 2.34                     | 0.43              |
| 35:YA:2438:U:O2'   | 35:YA:2440:C:OP1   | 2.36                     | 0.43              |
| 41:YH:28:GLY:HA3   | 41:YH:79:VAL:HB    | 2.01                     | 0.43              |
| 1:QA:730:G:C5      | 1:QA:731:G:H1'     | 2.54                     | 0.43              |
| 12:QL:70:ILE:HG13  | 12:QL:100:ILE:HD12 | 1.99                     | 0.43              |
| 35:RA:906:G:O2'    | 46:RQ:67:ARG:NH2   | 2.46                     | 0.43              |
| 22:XV:76:A:H2'     | 35:YA:2602:A:N6    | 2.33                     | 0.43              |
| 24:XY:37:A:O2'     | 35:YA:1913:A:N1    | 2.50                     | 0.43              |
| 35:YA:453:C:O2     | 35:YA:457:A:O2'    | 2.35                     | 0.43              |
| 35:YA:1156:A:OP1   | 50:YU:55:ARG:HD2   | 2.19                     | 0.43              |
| 35:YA:1327:C:HO2'  | 47:YR:105:ARG:HH12 | 1.60                     | 0.43              |
| 1:QA:522:C:H41     | 12:QL:53:ARG:HH22  | 1.67                     | 0.43              |
| 1:QA:640:A:N3      | 8:QH:115:SER:OG    | 2.40                     | 0.43              |
| 1:QA:806:C:H2'     | 1:QA:807:A:C8      | 2.54                     | 0.43              |
| 1:QA:985:C:H2'     | 1:QA:986:A:C8      | 2.54                     | 0.43              |
| 29:R4:14:ILE:HB    | 29:R4:22:ILE:HB    | 2.00                     | 0.43              |
| 29:R4:34:GLU:OE1   | 29:R4:35:VAL:CG2   | 2.66                     | 0.43              |
| 35:RA:2728:U:H2'   | 35:RA:2729:G:C8    | 2.54                     | 0.43              |
| 40:RG:77:ILE:HG23  | 40:RG:80:PHE:HB2   | 2.01                     | 0.43              |
| 1:XA:626:U:H5''    | 16:XP:38:TYR:CD2   | 2.52                     | 0.43              |
| 1:XA:1030(D):G:H2' | 1:XA:1030(E):A:C8  | 2.54                     | 0.43              |
| 44:YO:122:LEU:HD13 | 49:YT:72:VAL:HG11  | 2.00                     | 0.43              |
| 2:QB:54:THR:O      | 2:QB:58:ILE:HG12   | 2.19                     | 0.43              |
| 4:QD:168:ARG:HH22  | 37:YD:134:ARG:NH2  | 2.17                     | 0.43              |
| 35:RA:2880:C:O3'   | 47:RR:90:ARG:NH1   | 2.52                     | 0.43              |
| 37:RD:275:LYS:HD3  | 37:RD:275:LYS:HA   | 1.80                     | 0.43              |
| 44:RO:2:ILE:HB     | 44:RO:33:ALA:HB3   | 2.01                     | 0.43              |
| 50:RU:83:LEU:HD13  | 50:RU:88:ILE:HB    | 2.01                     | 0.43              |
| 1:XA:410:G:H3'     | 4:XD:25:ARG:HH22   | 1.84                     | 0.43              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:XA:919:A:O2'    | 1:XA:1080:A:N1      | 2.41                     | 0.43              |
| 2:XB:80:ILE:HG21  | 2:XB:211:ILE:HD12   | 2.01                     | 0.43              |
| 7:XG:150:ALA:HB1  | 11:XK:57:THR:HG21   | 2.01                     | 0.43              |
| 8:XH:36:LEU:HD12  | 8:XH:59:LEU:HD23    | 2.01                     | 0.43              |
| 31:Y6:6:ARG:HA    | 31:Y6:6:ARG:HD2     | 1.88                     | 0.43              |
| 35:YA:244:A:H4'   | 45:YP:74:GLU:HB2    | 2.01                     | 0.43              |
| 35:YA:869:G:H1'   | 46:YQ:8:LYS:HD2     | 2.01                     | 0.43              |
| 35:YA:2839:G:H5'  | 47:YR:46:GLY:HA2    | 2.01                     | 0.43              |
| 40:YG:5:VAL:HG23  | 40:YG:8:LYS:H       | 1.84                     | 0.43              |
| 1:QA:522:C:OP2    | 12:QL:69:TYR:OH     | 2.28                     | 0.42              |
| 3:QC:159:GLY:HA2  | 3:QC:193:TYR:HD2    | 1.75                     | 0.42              |
| 8:QH:25:ASP:HB3   | 8:QH:58:TYR:HD2     | 1.83                     | 0.42              |
| 26:R1:30:VAL:O    | 35:RA:2395:C:O2'    | 2.35                     | 0.42              |
| 27:R2:36:ARG:NH2  | 53:RX:8:ILE:O       | 2.51                     | 0.42              |
| 35:RA:1231:G:H2'  | 35:RA:1232:G:H8     | 1.84                     | 0.42              |
| 1:XA:148:G:H2'    | 1:XA:149:A:H8       | 1.83                     | 0.42              |
| 1:XA:237:C:O3'    | 17:XQ:25:ARG:NH2    | 2.51                     | 0.42              |
| 1:XA:403:C:H4'    | 4:XD:122:ARG:HH11   | 1.84                     | 0.42              |
| 1:XA:1131:G:OP1   | 9:XI:20:ARG:NH2     | 2.52                     | 0.42              |
| 35:YA:2502:G:H5'' | 35:YA:2503:2MA:H5'' | 2.00                     | 0.42              |
| 35:YA:2679:A:H5'  | 38:YE:165:VAL:HG21  | 2.01                     | 0.42              |
| 39:YF:155:LEU:HB2 | 39:YF:189:THR:HG21  | 2.01                     | 0.42              |
| 44:YO:68:GLU:HB3  | 44:YO:78:ARG:HB2    | 2.00                     | 0.42              |
| 45:YP:20:GLY:HA2  | 45:YP:28:GLY:HA2    | 2.01                     | 0.42              |
| 49:YT:94:ALA:HB1  | 49:YT:99:LEU:HD21   | 2.01                     | 0.42              |
| 3:QC:37:GLN:NE2   | 14:QN:52:GLN:OE1    | 2.36                     | 0.42              |
| 35:RA:576:U:H2'   | 35:RA:577:G:C8      | 2.54                     | 0.42              |
| 35:RA:685:A:OP1   | 35:RA:686:G:N2      | 2.52                     | 0.42              |
| 35:RA:1567:A:H3'  | 37:RD:86:PRO:HG3    | 2.01                     | 0.42              |
| 38:RE:134:ILE:HA  | 38:RE:137:HIS:CD2   | 2.54                     | 0.42              |
| 50:RU:102:GLU:HG3 | 51:RV:2:PHE:CZ      | 2.54                     | 0.42              |
| 55:RZ:58:VAL:HA   | 55:RZ:68:PRO:HA     | 2.01                     | 0.42              |
| 1:XA:184:G:H2'    | 1:XA:185:A:H8       | 1.84                     | 0.42              |
| 1:XA:624:C:H2'    | 1:XA:625:G:C8       | 2.54                     | 0.42              |
| 15:XO:3:ILE:HG22  | 15:XO:38:ARG:HH21   | 1.84                     | 0.42              |
| 35:YA:83:G:O2'    | 35:YA:102:G:N2      | 2.51                     | 0.42              |
| 35:YA:226:G:H21   | 35:YA:228:A:H62     | 1.67                     | 0.42              |
| 35:YA:335:C:O2    | 54:YY:70:SER:OG     | 2.38                     | 0.42              |
| 35:YA:1277:G:H2'  | 35:YA:1278:A:C8     | 2.54                     | 0.42              |
| 55:YZ:30:ASN:OD1  | 55:YZ:33:LEU:N      | 2.41                     | 0.42              |
| 35:RA:602:G:N2    | 35:RA:655:A:OP2     | 2.46                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:RD:245:PRO:HA   | 37:RD:246:PRO:HD3 | 1.94                     | 0.42              |
| 37:RD:247:ALA:HA   | 37:RD:253:GLN:HA  | 2.00                     | 0.42              |
| 1:XA:946:A:O2'     | 1:XA:1333:A:N3    | 2.45                     | 0.42              |
| 1:XA:1286:A:N6     | 1:XA:1354:C:O3'   | 2.52                     | 0.42              |
| 12:XL:117:ARG:HB2  | 12:XL:122:THR:HB  | 2.02                     | 0.42              |
| 13:XM:4:ILE:HG13   | 13:XM:5:ALA:H     | 1.84                     | 0.42              |
| 41:YH:46:GLU:OE2   | 41:YH:51:ARG:NH2  | 2.50                     | 0.42              |
| 41:YH:149:ARG:NH2  | 41:YH:167:GLU:OE2 | 2.47                     | 0.42              |
| 51:YV:52:VAL:HG21  | 51:YV:55:ALA:HB3  | 2.01                     | 0.42              |
| 55:YZ:13:GLU:HG3   | 55:YZ:18:LEU:HD21 | 2.01                     | 0.42              |
| 1:QA:328:C:H4'     | 1:QA:329:A:H5'    | 2.00                     | 0.42              |
| 1:QA:977:A:O2'     | 1:QA:979:C:OP2    | 2.34                     | 0.42              |
| 4:QD:61:LYS:HE2    | 4:QD:206:PHE:CE2  | 2.54                     | 0.42              |
| 27:R2:38:GLN:HA    | 27:R2:41:ILE:HG12 | 2.01                     | 0.42              |
| 30:R5:51:TYR:HE1   | 30:R5:56:LYS:HD3  | 1.84                     | 0.42              |
| 35:RA:1682:G:OP2   | 35:RA:1699:G:N2   | 2.52                     | 0.42              |
| 35:RA:2564:A:OP1   | 35:RA:2648:C:O2'  | 2.37                     | 0.42              |
| 39:RF:161:GLU:O    | 39:RF:165:ARG:HB2 | 2.20                     | 0.42              |
| 44:RO:68:GLU:HB3   | 44:RO:78:ARG:HB2  | 2.02                     | 0.42              |
| 46:RQ:52:VAL:HA    | 46:RQ:55:VAL:HG22 | 2.01                     | 0.42              |
| 50:RU:66:ASN:OD1   | 50:RU:70:ARG:NE   | 2.51                     | 0.42              |
| 11:XK:20:TYR:CE1   | 11:XK:83:ILE:HD12 | 2.54                     | 0.42              |
| 16:XP:3:LYS:HG2    | 16:XP:65:GLN:HB2  | 2.01                     | 0.42              |
| 27:Y2:37:PHE:CD1   | 53:YX:11:PRO:HD3  | 2.55                     | 0.42              |
| 35:YA:272(R):G:H2' | 35:YA:272(S):G:H8 | 1.84                     | 0.42              |
| 35:YA:414:C:H2'    | 35:YA:415:A:C8    | 2.54                     | 0.42              |
| 35:YA:616:G:O2'    | 39:YF:205:ARG:NH1 | 2.53                     | 0.42              |
| 35:YA:626:U:O4     | 45:YP:81:GLN:NE2  | 2.53                     | 0.42              |
| 35:YA:2328:A:H2'   | 35:YA:2329:G:C8   | 2.54                     | 0.42              |
| 40:YG:78:SER:OG    | 40:YG:79:ASN:N    | 2.52                     | 0.42              |
| 41:YH:54:ARG:HD2   | 41:YH:65:HIS:ND1  | 2.35                     | 0.42              |
| 41:YH:86:GLU:OE2   | 41:YH:132:ARG:NH2 | 2.52                     | 0.42              |
| 1:QA:346:G:OP1     | 49:RT:41:ARG:NH1  | 2.52                     | 0.42              |
| 1:QA:522:C:H41     | 12:QL:53:ARG:NH2  | 2.17                     | 0.42              |
| 1:QA:552:U:H4'     | 12:QL:87:GLY:HA3  | 2.02                     | 0.42              |
| 1:QA:626:U:C5'     | 16:QP:38:TYR:HD2  | 2.30                     | 0.42              |
| 1:QA:652:U:O4      | 1:QA:752:G:O2'    | 2.32                     | 0.42              |
| 3:QC:153:VAL:HG22  | 3:QC:198:VAL:HG22 | 2.00                     | 0.42              |
| 4:QD:18:LYS:HE3    | 4:QD:20:TYR:CE2   | 2.54                     | 0.42              |
| 35:RA:698:C:O2'    | 35:RA:734:A:N6    | 2.52                     | 0.42              |
| 35:RA:1423:G:H2'   | 35:RA:1424:G:H8   | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RA:2543:G:H2'   | 35:RA:2544:G:C8    | 2.54                     | 0.42              |
| 45:RP:65:ARG:O     | 45:RP:68:GLN:NE2   | 2.53                     | 0.42              |
| 53:RX:53:LYS:HB3   | 53:RX:82:GLN:HB3   | 2.01                     | 0.42              |
| 1:XA:96:U:H2'      | 1:XA:97:G:C8       | 2.55                     | 0.42              |
| 6:XF:30:LEU:HD23   | 6:XF:75:LEU:HD11   | 2.02                     | 0.42              |
| 35:YA:1028:A:N3    | 35:YA:2486:G:O2'   | 2.49                     | 0.42              |
| 35:YA:1665:A:H1'   | 44:YO:1:MET:HB2    | 2.01                     | 0.42              |
| 35:YA:1666:G:HO2'  | 44:YO:6:THR:HG1    | 1.59                     | 0.42              |
| 46:YQ:104:PHE:HE2  | 46:YQ:125:LEU:HD11 | 1.85                     | 0.42              |
| 1:QA:1106:G:H5''   | 3:QC:172:ARG:HG2   | 2.01                     | 0.42              |
| 1:QA:1412:C:H2'    | 1:QA:1413:A:C8     | 2.55                     | 0.42              |
| 2:QB:84:GLU:HB3    | 2:QB:219:VAL:HG21  | 2.02                     | 0.42              |
| 3:QC:19:GLU:HG2    | 3:QC:55:VAL:O      | 2.18                     | 0.42              |
| 9:QI:4:TYR:HB2     | 9:QI:19:LEU:HB2    | 2.00                     | 0.42              |
| 25:R0:77:ARG:NH2   | 35:RA:857:C:OP2    | 2.52                     | 0.42              |
| 35:RA:442:G:N3     | 39:RF:48:THR:OG1   | 2.42                     | 0.42              |
| 35:RA:2633:G:H5''  | 35:RA:2812:G:H5'   | 2.02                     | 0.42              |
| 39:RF:165:ARG:HG3  | 39:RF:168:ARG:NH1  | 2.35                     | 0.42              |
| 39:RF:184:TYR:CE2  | 39:RF:188:ARG:HD2  | 2.55                     | 0.42              |
| 1:XA:142:G:H2'     | 1:XA:143:A:H8      | 1.84                     | 0.42              |
| 1:XA:673:G:H4'     | 6:XF:87:ARG:HH12   | 1.84                     | 0.42              |
| 14:YN:4:LYS:HA     | 14:YN:7:ILE:HG12   | 2.02                     | 0.42              |
| 30:Y5:7:PRO:O      | 35:YA:2016:U:O2'   | 2.37                     | 0.42              |
| 35:YA:78:A:H2'     | 35:YA:79:G:H8      | 1.83                     | 0.42              |
| 35:YA:200:U:O2     | 35:YA:386:G:N2     | 2.52                     | 0.42              |
| 13:QM:66:LEU:HD13  | 13:QM:66:LEU:HA    | 1.88                     | 0.42              |
| 33:R8:2:PRO:O      | 35:RA:666:G:N2     | 2.52                     | 0.42              |
| 35:RA:1638:C:OP1   | 35:RA:2710:C:O2'   | 2.36                     | 0.42              |
| 40:RG:37:VAL:HG13  | 40:RG:94:LEU:HB2   | 2.02                     | 0.42              |
| 40:RG:173:LEU:HD13 | 40:RG:176:LEU:HD12 | 2.01                     | 0.42              |
| 1:XA:769:G:H4'     | 1:XA:1513:A:H4'    | 2.02                     | 0.42              |
| 17:XQ:62:SER:OG    | 17:XQ:72:ARG:NE    | 2.43                     | 0.42              |
| 28:Y3:52:HIS:CD2   | 28:Y3:53:LEU:HG    | 2.55                     | 0.42              |
| 35:YA:1223:G:N2    | 35:YA:1226:A:OP2   | 2.43                     | 0.42              |
| 35:YA:1500:G:H21   | 37:YD:100:GLY:HA3  | 1.85                     | 0.42              |
| 35:YA:2441:C:OP2   | 35:YA:2586:C:O2'   | 2.35                     | 0.42              |
| 35:YA:2602:A:H4'   | 35:YA:2603:G:C5'   | 2.50                     | 0.42              |
| 39:YF:178:PRO:HB2  | 39:YF:201:VAL:HG21 | 2.01                     | 0.42              |
| 1:QA:523:A:H61     | 12:QL:92:OTD:CG    | 2.31                     | 0.42              |
| 1:QA:981:U:O4      | 1:QA:1223:C:N4     | 2.53                     | 0.42              |
| 2:QB:163:PHE:HA    | 2:QB:185:ILE:HG13  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:QE:6:PHE:CD1     | 5:QE:36:ASP:HB3    | 2.54                     | 0.42              |
| 35:RA:572:A:OP2    | 51:RV:78:LYS:NZ    | 2.41                     | 0.42              |
| 41:RH:3:ARG:NE     | 41:RH:5:GLY:H      | 2.18                     | 0.42              |
| 7:XG:113:GLU:OE2   | 7:XG:122:HIS:ND1   | 2.38                     | 0.42              |
| 8:XH:104:ARG:HA    | 8:XH:104:ARG:HD3   | 1.85                     | 0.42              |
| 10:XJ:40:LEU:HB2   | 10:XJ:69:ASN:HB2   | 2.02                     | 0.42              |
| 28:Y3:52:HIS:CG    | 36:YB:83:G:H4'     | 2.54                     | 0.42              |
| 35:YA:1069:A:C6    | 35:YA:1095:A:H4'   | 2.55                     | 0.42              |
| 35:YA:2679:A:OP2   | 38:YE:160:TYR:OH   | 2.27                     | 0.42              |
| 1:QA:165:C:H2'     | 1:QA:166:G:H8      | 1.85                     | 0.42              |
| 35:RA:411:G:OP2    | 35:RA:2406:U:O2'   | 2.37                     | 0.42              |
| 35:RA:1296:G:OP1   | 35:RA:2709:G:O2'   | 2.26                     | 0.42              |
| 1:XA:192:U:H5'     | 20:XT:101:GLY:HA3  | 2.01                     | 0.42              |
| 4:XD:50:ARG:HA     | 4:XD:51:PRO:HD3    | 1.92                     | 0.42              |
| 9:XI:42:ARG:NH2    | 9:XI:71:SER:OG     | 2.53                     | 0.42              |
| 9:XI:73:GLN:O      | 9:XI:77:ILE:HG12   | 2.20                     | 0.42              |
| 35:YA:2633:G:H5''  | 35:YA:2812:G:H5'   | 2.00                     | 0.42              |
| 39:YF:31:HIS:NE2   | 39:YF:35:GLU:OE2   | 2.53                     | 0.42              |
| 16:QP:18:ARG:NH1   | 16:QP:32:TYR:OH    | 2.53                     | 0.42              |
| 19:QS:22:LEU:HA    | 19:QS:22:LEU:HD13  | 1.82                     | 0.42              |
| 35:RA:1478:G:O2'   | 35:RA:1558:A:N7    | 2.50                     | 0.42              |
| 38:RE:5:LEU:HD11   | 38:RE:79:ARG:HB2   | 2.02                     | 0.42              |
| 41:RH:99:VAL:N     | 41:RH:102:ALA:O    | 2.51                     | 0.42              |
| 42:RI:115:ALA:HB2  | 42:RI:131:LYS:HE2  | 2.02                     | 0.42              |
| 46:RQ:34:LEU:HB2   | 46:RQ:118:LEU:HD22 | 2.01                     | 0.42              |
| 50:RU:44:ASN:HD21  | 51:RV:75:PHE:HB3   | 1.84                     | 0.42              |
| 1:XA:356:A:N3      | 1:XA:368:U:O2'     | 2.37                     | 0.42              |
| 1:XA:476:G:H2'     | 1:XA:477:A:H8      | 1.84                     | 0.42              |
| 1:XA:779:C:H5''    | 11:XK:122:LYS:HG2  | 2.02                     | 0.42              |
| 1:XA:1356:G:H2'    | 1:XA:1357:A:C8     | 2.55                     | 0.42              |
| 1:XA:1408:A:N1     | 57:XA:1794:PAR:O61 | 2.51                     | 0.42              |
| 9:XI:9:ARG:H       | 9:XI:79:LEU:HD23   | 1.85                     | 0.42              |
| 17:XQ:6:LEU:HD23   | 17:XQ:23:VAL:HG11  | 2.02                     | 0.42              |
| 35:YA:602:G:O2'    | 35:YA:604:G:O2'    | 2.33                     | 0.42              |
| 35:YA:1188:U:H2'   | 35:YA:1189:A:H8    | 1.84                     | 0.42              |
| 35:YA:1309:G:O2'   | 35:YA:1611:C:O2'   | 2.33                     | 0.42              |
| 35:YA:1567:A:C6    | 37:YD:84:TYR:CD2   | 3.08                     | 0.42              |
| 35:YA:1790:C:H2'   | 35:YA:1791:A:C5    | 2.55                     | 0.42              |
| 37:YD:253:GLN:HB2  | 37:YD:257:LEU:HD12 | 2.01                     | 0.42              |
| 38:YE:34:VAL:HG12  | 38:YE:72:VAL:HG21  | 2.01                     | 0.42              |
| 40:YG:101:ILE:HG22 | 40:YG:105:LYS:HE2  | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:142:G:H2'     | 1:QA:143:A:C8      | 2.54                     | 0.41              |
| 1:QA:673:G:H5''    | 6:QF:87:ARG:NH1    | 2.35                     | 0.41              |
| 1:QA:1366:C:O2'    | 10:QJ:60:ARG:NH2   | 2.47                     | 0.41              |
| 31:R6:10:LEU:HD13  | 31:R6:19:ARG:HG2   | 2.02                     | 0.41              |
| 35:RA:1466:G:HO2'  | 35:RA:1546:C:HO2'  | 1.59                     | 0.41              |
| 35:RA:2503:2MA:O2' | 35:RA:2505:G:OP2   | 2.25                     | 0.41              |
| 41:RH:24:VAL:HG21  | 41:RH:72:ILE:HD12  | 2.02                     | 0.41              |
| 48:RS:10:ARG:HG3   | 48:RS:13:ARG:HH21  | 1.84                     | 0.41              |
| 1:XA:407:G:H2'     | 1:XA:408:A:C8      | 2.54                     | 0.41              |
| 1:XA:407:G:OP1     | 4:XD:115:ARG:NH1   | 2.53                     | 0.41              |
| 1:XA:684:A:O2'     | 11:XK:39:PRO:O     | 2.35                     | 0.41              |
| 1:XA:1060:C:H5''   | 10:XJ:51:ARG:HG2   | 2.02                     | 0.41              |
| 1:XA:1491:G:N7     | 57:XA:1794:PAR:O53 | 2.47                     | 0.41              |
| 25:Y0:31:VAL:HB    | 25:Y0:35:ASN:HD22  | 1.85                     | 0.41              |
| 35:YA:557:U:O2'    | 43:YN:45:ASN:O     | 2.34                     | 0.41              |
| 35:YA:1057:A:H62   | 35:YA:1086:A:H3'   | 1.84                     | 0.41              |
| 2:QB:181:PHE:CE1   | 8:QH:71:GLY:HA2    | 2.55                     | 0.41              |
| 35:RA:1688:U:O2    | 35:RA:1700:A:H5'   | 2.20                     | 0.41              |
| 35:RA:2857:G:N2    | 35:RA:2860:A:OP2   | 2.34                     | 0.41              |
| 1:XA:1031:G:H2'    | 1:XA:1032:G:C8     | 2.55                     | 0.41              |
| 1:XA:1179:A:O3'    | 9:XI:103:THR:OG1   | 2.37                     | 0.41              |
| 24:XY:75:C:O2      | 35:YA:2507:C:O2'   | 2.28                     | 0.41              |
| 28:Y3:6:VAL:HG12   | 28:Y3:28:LEU:HD11  | 2.01                     | 0.41              |
| 35:YA:2405:G:H5'   | 45:YP:75:ILE:HD13  | 2.03                     | 0.41              |
| 40:YG:3:LEU:HD11   | 40:YG:101:ILE:HD11 | 2.01                     | 0.41              |
| 41:YH:8:PRO:O      | 41:YH:69:ARG:NH2   | 2.46                     | 0.41              |
| 1:QA:749:C:H2'     | 1:QA:750:G:H8      | 1.85                     | 0.41              |
| 14:QN:29:ARG:HG2   | 14:QN:31:ARG:H     | 1.84                     | 0.41              |
| 35:RA:1657:C:H4'   | 38:RE:133:LYS:HB3  | 2.03                     | 0.41              |
| 35:RA:1889:A:H2'   | 35:RA:1890:A:C8    | 2.55                     | 0.41              |
| 1:XA:966:M2G:HM13  | 1:XA:967:5MC:H1'   | 2.02                     | 0.41              |
| 1:XA:1149:C:P      | 9:XI:9:ARG:HH21    | 2.43                     | 0.41              |
| 3:XC:150:LYS:HG3   | 3:XC:169:ALA:HB2   | 2.02                     | 0.41              |
| 4:XD:194:LEU:HB3   | 4:XD:196:LEU:HD12  | 2.01                     | 0.41              |
| 10:XJ:61:GLU:OE1   | 14:XN:45:ARG:NE    | 2.48                     | 0.41              |
| 10:XJ:61:GLU:OE2   | 14:XN:49:HIS:NE2   | 2.40                     | 0.41              |
| 28:Y3:8:LEU:HA     | 28:Y3:54:VAL:HG23  | 2.01                     | 0.41              |
| 35:YA:87:C:H5''    | 35:YA:88:G:H5'     | 2.03                     | 0.41              |
| 39:YF:39:TRP:NE1   | 39:YF:99:TYR:O     | 2.52                     | 0.41              |
| 47:YR:87:TYR:OH    | 47:YR:117:VAL:O    | 2.37                     | 0.41              |
| 2:QB:155:LEU:HD21  | 2:QB:159:PRO:HG3   | 2.03                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:QE:76:ILE:HG13   | 5:QE:93:PRO:HG3   | 2.02                     | 0.41              |
| 11:QK:65:ALA:HB1   | 11:QK:98:LEU:HD12 | 2.03                     | 0.41              |
| 35:RA:272(Q):G:H2' | 35:RA:272(R):G:C8 | 2.55                     | 0.41              |
| 35:RA:581:C:H2'    | 35:RA:582:G:C8    | 2.55                     | 0.41              |
| 35:RA:1082:U:H6    | 35:RA:1082:U:H2'  | 1.71                     | 0.41              |
| 35:RA:1516:C:H2'   | 35:RA:1517:G:H8   | 1.85                     | 0.41              |
| 35:RA:2302:G:O2'   | 40:RG:126:ASP:O   | 2.33                     | 0.41              |
| 37:RD:72:LYS:NZ    | 37:RD:99:ASP:OD2  | 2.53                     | 0.41              |
| 37:RD:260:ARG:NH2  | 37:RD:266:SER:OG  | 2.53                     | 0.41              |
| 46:RQ:110:THR:HG23 | 46:RQ:113:GLN:H   | 1.85                     | 0.41              |
| 1:XA:652:U:O4      | 1:XA:752:G:O2'    | 2.30                     | 0.41              |
| 1:XA:1005:A:O2'    | 1:XA:1036:G:N2    | 2.53                     | 0.41              |
| 25:Y0:43:THR:HG22  | 35:YA:2336:A:H61  | 1.86                     | 0.41              |
| 30:Y5:4:HIS:O      | 35:YA:2056:G:N2   | 2.53                     | 0.41              |
| 35:YA:184:C:H1'    | 35:YA:217:G:H1'   | 2.01                     | 0.41              |
| 35:YA:579:G:O2'    | 35:YA:2019:A:OP1  | 2.38                     | 0.41              |
| 35:YA:2136:C:N4    | 35:YA:2155:G:O6   | 2.52                     | 0.41              |
| 45:YP:65:ARG:O     | 45:YP:68:GLN:NE2  | 2.52                     | 0.41              |
| 1:QA:521:G:N7      | 12:QL:53:ARG:NH1  | 2.67                     | 0.41              |
| 1:QA:1230:C:H5'    | 22:QV:30:G:H5''   | 2.03                     | 0.41              |
| 1:QA:1403:C:N4     | 23:QX:18:G:OP1    | 2.52                     | 0.41              |
| 4:QD:79:PHE:HE1    | 4:QD:204:ILE:HD13 | 1.85                     | 0.41              |
| 8:QH:34:GLU:HB3    | 8:QH:118:VAL:HG21 | 2.01                     | 0.41              |
| 19:QS:63:THR:OG1   | 19:QS:65:ASN:OD1  | 2.35                     | 0.41              |
| 35:RA:1593:G:H2'   | 35:RA:1594:G:C8   | 2.56                     | 0.41              |
| 35:RA:1638:C:O3'   | 35:RA:2709:G:N2   | 2.53                     | 0.41              |
| 1:XA:476:G:H2'     | 1:XA:477:A:C8     | 2.55                     | 0.41              |
| 1:XA:673:G:H2'     | 1:XA:674:G:C8     | 2.55                     | 0.41              |
| 33:Y8:10:ALA:HA    | 45:YP:59:LEU:HD11 | 2.01                     | 0.41              |
| 35:YA:483:A:O2'    | 54:YY:49:VAL:O    | 2.25                     | 0.41              |
| 35:YA:801:G:O6     | 39:YF:53:THR:OG1  | 2.38                     | 0.41              |
| 35:YA:1538:G:H2'   | 35:YA:1539:G:H8   | 1.86                     | 0.41              |
| 35:YA:1567:A:C6    | 37:YD:84:TYR:CE2  | 3.06                     | 0.41              |
| 36:YB:37:C:O2      | 48:YS:95:HIS:NE2  | 2.48                     | 0.41              |
| 1:QA:1179:A:O3'    | 9:QI:103:THR:OG1  | 2.34                     | 0.41              |
| 1:QA:1343:G:H4'    | 9:QI:122:ALA:HB3  | 2.02                     | 0.41              |
| 2:QB:101:MET:HA    | 2:QB:108:ILE:HG21 | 2.02                     | 0.41              |
| 4:QD:103:ASN:CG    | 4:QD:114:ARG:HE   | 2.28                     | 0.41              |
| 30:R5:7:PRO:HA     | 35:RA:2615:U:C2   | 2.56                     | 0.41              |
| 35:RA:323:G:C8     | 39:RF:171:PRO:HG3 | 2.55                     | 0.41              |
| 35:RA:1057:A:N6    | 35:RA:1087:G:OP2  | 2.53                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:RD:13:ARG:NH1   | 37:RD:16:MET:SD    | 2.94                     | 0.41              |
| 39:RF:182:ASN:OD1  | 39:RF:182:ASN:N    | 2.44                     | 0.41              |
| 53:RX:55:ASN:HB2   | 53:RX:80:ILE:HB    | 2.03                     | 0.41              |
| 1:XA:1524:C:H5''   | 11:XK:120:ARG:HH12 | 1.85                     | 0.41              |
| 9:XI:50:LEU:HB3    | 9:XI:56:LEU:HA     | 2.02                     | 0.41              |
| 35:YA:1243:G:O2'   | 45:YP:7:ARG:NH2    | 2.52                     | 0.41              |
| 42:YI:114:LEU:HD23 | 42:YI:130:TYR:HA   | 2.02                     | 0.41              |
| 1:QA:237:C:O3'     | 17:QQ:25:ARG:NH2   | 2.54                     | 0.41              |
| 2:QB:82:ARG:HG3    | 2:QB:92:TYR:CZ     | 2.55                     | 0.41              |
| 3:QC:130:VAL:HG21  | 3:QC:157:ILE:HG23  | 2.02                     | 0.41              |
| 3:QC:184:TYR:CD1   | 3:QC:201:TYR:CD1   | 3.08                     | 0.41              |
| 9:QI:78:LYS:HB2    | 9:QI:78:LYS:HE2    | 1.84                     | 0.41              |
| 26:R1:18:ILE:HG12  | 26:R1:37:ILE:HG12  | 2.03                     | 0.41              |
| 35:RA:451:C:OP1    | 39:RF:52:LYS:NZ    | 2.46                     | 0.41              |
| 35:RA:2305:A:H5''  | 40:RG:134:GLY:HA3  | 2.02                     | 0.41              |
| 35:RA:2513:G:N2    | 38:RE:143:ASN:HD21 | 2.19                     | 0.41              |
| 38:RE:34:VAL:HG12  | 38:RE:72:VAL:HG21  | 2.03                     | 0.41              |
| 47:RR:12:ARG:HB3   | 47:RR:16:HIS:HB3   | 2.02                     | 0.41              |
| 47:RR:87:TYR:OH    | 47:RR:117:VAL:O    | 2.27                     | 0.41              |
| 52:RW:69:LEU:HB3   | 52:RW:107:LEU:HD23 | 2.03                     | 0.41              |
| 1:XA:84:U:O2'      | 1:XA:89:C:N4       | 2.54                     | 0.41              |
| 1:XA:677:U:O2      | 1:XA:777:A:O2'     | 2.35                     | 0.41              |
| 1:XA:719:C:O2'     | 18:XR:50:ILE:O     | 2.33                     | 0.41              |
| 5:XE:102:ALA:H     | 5:XE:107:ARG:HH21  | 1.67                     | 0.41              |
| 7:XG:150:ALA:O     | 11:XK:57:THR:OG1   | 2.29                     | 0.41              |
| 13:XM:91:ARG:HH22  | 13:XM:103:THR:HG21 | 1.84                     | 0.41              |
| 35:YA:108:U:H2'    | 35:YA:109:G:H8     | 1.86                     | 0.41              |
| 35:YA:1889:A:H2'   | 35:YA:1890:A:C8    | 2.56                     | 0.41              |
| 44:YO:120:GLU:OE1  | 49:YT:67:SER:OG    | 2.37                     | 0.41              |
| 1:QA:6:G:H4'       | 1:QA:298:A:H4'     | 2.03                     | 0.41              |
| 1:QA:444:C:H2'     | 1:QA:445:G:C8      | 2.55                     | 0.41              |
| 1:QA:943:U:H1'     | 9:QI:124:GLN:HE22  | 1.85                     | 0.41              |
| 2:QB:84:GLU:HG3    | 2:QB:215:LEU:HB3   | 2.02                     | 0.41              |
| 33:R8:31:HIS:ND1   | 33:R8:32:LEU:HG    | 2.36                     | 0.41              |
| 35:RA:252:G:OP1    | 45:RP:50:ARG:NH1   | 2.53                     | 0.41              |
| 35:RA:635:C:O2'    | 35:RA:639:U:OP1    | 2.36                     | 0.41              |
| 44:RO:34:THR:OG1   | 44:RO:35:VAL:N     | 2.54                     | 0.41              |
| 1:XA:108:G:N1      | 20:XT:15:ARG:HG2   | 2.36                     | 0.41              |
| 1:XA:673:G:H4'     | 6:XF:87:ARG:NH1    | 2.36                     | 0.41              |
| 33:Y8:27:THR:HG22  | 45:YP:63:PRO:HD3   | 2.03                     | 0.41              |
| 35:YA:1657:C:H4'   | 38:YE:133:LYS:HB3  | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:YZ:5:LEU:HD11   | 55:YZ:44:PHE:HA    | 2.02                     | 0.41              |
| 1:QA:9:G:H2'       | 1:QA:10:A:H8       | 1.86                     | 0.41              |
| 1:QA:744:C:O2'     | 1:QA:851:G:N2      | 2.51                     | 0.41              |
| 2:QB:158:LEU:HA    | 2:QB:159:PRO:HD3   | 1.98                     | 0.41              |
| 6:QF:24:GLU:O      | 6:QF:28:ARG:N      | 2.52                     | 0.41              |
| 9:QI:25:LYS:N      | 9:QI:60:ASP:OD1    | 2.50                     | 0.41              |
| 10:QJ:50:ILE:HB    | 14:QN:41:ARG:HE    | 1.85                     | 0.41              |
| 11:QK:43:SER:HB3   | 11:QK:68:ALA:HB2   | 2.03                     | 0.41              |
| 17:QQ:6:LEU:HD23   | 17:QQ:23:VAL:HG11  | 2.03                     | 0.41              |
| 27:R2:37:PHE:CD1   | 53:RX:11:PRO:HD3   | 2.55                     | 0.41              |
| 35:RA:679:C:H2'    | 35:RA:680:G:C8     | 2.56                     | 0.41              |
| 35:RA:2500:U:O2'   | 35:RA:2504:U:OP1   | 2.30                     | 0.41              |
| 38:RE:1:MET:HG3    | 38:RE:200:GLU:HB3  | 2.03                     | 0.41              |
| 48:RS:25:ARG:NE    | 48:RS:88:ASP:OD2   | 2.50                     | 0.41              |
| 1:XA:881:G:P       | 12:XL:12:ARG:HH22  | 2.44                     | 0.41              |
| 1:XA:1510:U:H2'    | 1:XA:1511:G:C8     | 2.55                     | 0.41              |
| 7:XG:65:ALA:HB1    | 7:XG:127:ALA:HB3   | 2.03                     | 0.41              |
| 18:XR:34:TYR:H     | 18:XR:34:TYR:HD1   | 1.69                     | 0.41              |
| 19:XS:52:TYR:HB2   | 19:XS:57:HIS:CE1   | 2.56                     | 0.41              |
| 22:XV:15:G:N2      | 22:XV:21:A:N3      | 2.69                     | 0.41              |
| 25:Y0:14:ARG:O     | 35:YA:2278:A:N6    | 2.54                     | 0.41              |
| 34:Y9:37:GLY:HA2   | 35:YA:1125:G:H5'   | 2.03                     | 0.41              |
| 35:YA:143(A):G:H4' | 53:YX:35:THR:HG21  | 2.02                     | 0.41              |
| 35:YA:251:A:C5     | 35:YA:252:G:H1'    | 2.56                     | 0.41              |
| 35:YA:277:C:H4'    | 35:YA:278:A:H8     | 1.86                     | 0.41              |
| 35:YA:321:G:O2'    | 35:YA:340:A:N3     | 2.53                     | 0.41              |
| 35:YA:776:G:N7     | 35:YA:793:A:O2'    | 2.54                     | 0.41              |
| 35:YA:825:C:O2     | 45:YP:55:ARG:NH1   | 2.54                     | 0.41              |
| 35:YA:1082:U:H6    | 35:YA:1082:U:H2'   | 1.73                     | 0.41              |
| 35:YA:1538:G:H2'   | 35:YA:1539:G:C8    | 2.56                     | 0.41              |
| 35:YA:2071:A:H2'   | 35:YA:2072:G:H8    | 1.85                     | 0.41              |
| 35:YA:2513:G:N2    | 38:YE:143:ASN:HD21 | 2.19                     | 0.41              |
| 1:QA:41:G:H2'      | 1:QA:42:G:H8       | 1.85                     | 0.41              |
| 1:QA:1287:A:H2     | 1:QA:1353:G:H1'    | 1.86                     | 0.41              |
| 7:QG:67:GLU:HA     | 7:QG:70:LYS:HD3    | 2.01                     | 0.41              |
| 37:RD:260:ARG:HH22 | 37:RD:270:ILE:HD12 | 1.85                     | 0.41              |
| 55:RZ:14:LYS:HA    | 55:RZ:15:PRO:HD3   | 1.97                     | 0.41              |
| 34:Y9:1:MET:SD     | 34:Y9:35:ARG:HB2   | 2.61                     | 0.41              |
| 35:YA:276:A:H5''   | 35:YA:277:C:H5'    | 2.03                     | 0.41              |
| 35:YA:729:G:O5'    | 37:YD:208:LYS:NZ   | 2.54                     | 0.41              |
| 35:YA:854:G:H2'    | 35:YA:855:G:H8     | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YA:1568:G:OP1   | 37:YD:63:ARG:NH1   | 2.42                     | 0.41              |
| 35:YA:2144:U:HO2'  | 35:YA:2147:G:H1    | 1.66                     | 0.41              |
| 49:YT:16:ARG:HH21  | 49:YT:81:PRO:HA    | 1.86                     | 0.41              |
| 1:QA:624:C:H2'     | 1:QA:625:G:C8      | 2.56                     | 0.40              |
| 1:QA:924:C:H2'     | 1:QA:925:G:C8      | 2.56                     | 0.40              |
| 1:QA:1226:C:P      | 13:QM:91:ARG:HH12  | 2.44                     | 0.40              |
| 7:QG:26:PHE:O      | 7:QG:30:ILE:HG12   | 2.21                     | 0.40              |
| 8:QH:104:ARG:HD3   | 8:QH:104:ARG:HA    | 1.91                     | 0.40              |
| 35:RA:483:A:O2'    | 54:RY:49:VAL:O     | 2.35                     | 0.40              |
| 35:RA:855:G:H1     | 35:RA:922:U:H3     | 1.68                     | 0.40              |
| 35:RA:2161:C:H2'   | 35:RA:2162:G:H8    | 1.86                     | 0.40              |
| 35:RA:2405:G:H5'   | 45:RP:75:ILE:HD13  | 2.02                     | 0.40              |
| 38:RE:2:LYS:HG2    | 38:RE:200:GLU:HB2  | 2.03                     | 0.40              |
| 49:RT:30:VAL:HG22  | 49:RT:86:ILE:HG12  | 2.02                     | 0.40              |
| 1:XA:157:G:H1      | 1:XA:164:U:H3      | 1.68                     | 0.40              |
| 1:XA:1000:U:H2'    | 1:XA:1001(A):A:C8  | 2.56                     | 0.40              |
| 2:XB:54:THR:HG22   | 2:XB:199:TYR:HB3   | 2.02                     | 0.40              |
| 8:XH:105:ARG:HD3   | 8:XH:105:ARG:HA    | 1.94                     | 0.40              |
| 9:XI:48:GLU:OE2    | 9:XI:51:ARG:NE     | 2.44                     | 0.40              |
| 35:YA:2805:G:H2'   | 35:YA:2807:G:C8    | 2.56                     | 0.40              |
| 38:YE:21:VAL:HA    | 38:YE:22:PRO:HD3   | 1.94                     | 0.40              |
| 44:YO:8:LEU:HD13   | 44:YO:82:ASN:HB3   | 2.03                     | 0.40              |
| 1:QA:1294:G:H2'    | 1:QA:1295:G:H8     | 1.86                     | 0.40              |
| 1:QA:1484:C:O2'    | 35:RA:1960:A:O2'   | 2.24                     | 0.40              |
| 2:QB:177:ALA:HB1   | 2:QB:182:ILE:HB    | 2.03                     | 0.40              |
| 3:QC:3:ASN:OD1     | 3:QC:3:ASN:N       | 2.54                     | 0.40              |
| 7:QG:16:LEU:HD21   | 9:QI:45:ALA:HB2    | 2.02                     | 0.40              |
| 25:R0:23:VAL:HG22  | 25:R0:38:VAL:HG22  | 2.03                     | 0.40              |
| 30:R5:19:ARG:HH11  | 30:R5:19:ARG:HD3   | 1.78                     | 0.40              |
| 35:RA:459:U:H2'    | 35:RA:460:A:H8     | 1.86                     | 0.40              |
| 35:RA:535:C:O3'    | 50:RU:53:ARG:NH1   | 2.54                     | 0.40              |
| 37:RD:133:LEU:HB3  | 37:RD:173:VAL:HG21 | 2.03                     | 0.40              |
| 37:RD:231:HIS:CD2  | 37:RD:249:PRO:HG3  | 2.55                     | 0.40              |
| 42:RI:72:LEU:HA    | 42:RI:75:LEU:HD22  | 2.03                     | 0.40              |
| 44:RO:104:ARG:HH22 | 49:RT:43:GLN:CD    | 2.29                     | 0.40              |
| 46:RQ:119:ARG:O    | 46:RQ:123:HIS:ND1  | 2.50                     | 0.40              |
| 48:RS:15:ARG:O     | 48:RS:19:LYS:HG2   | 2.21                     | 0.40              |
| 55:RZ:151:HIS:CE1  | 55:RZ:153:SER:HB2  | 2.57                     | 0.40              |
| 13:XM:99:ARG:HB2   | 13:XM:101:GLN:NE2  | 2.36                     | 0.40              |
| 16:XP:20:VAL:HG21  | 16:XP:32:TYR:CE2   | 2.50                     | 0.40              |
| 24:XY:62:C:H2'     | 24:XY:63:G:C8      | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:Y2:55:ARG:HB3  | 27:Y2:59:ARG:HH12  | 1.87                     | 0.40              |
| 35:YA:85:G:O2'    | 35:YA:103:A:N1     | 2.42                     | 0.40              |
| 35:YA:323:G:C8    | 39:YF:171:PRO:HG3  | 2.56                     | 0.40              |
| 38:YE:3:GLY:HA2   | 38:YE:199:ARG:HA   | 2.03                     | 0.40              |
| 49:YT:24:PRO:HD3  | 49:YT:52:ILE:HD12  | 2.03                     | 0.40              |
| 1:QA:537:G:H5''   | 12:QL:113:ARG:HH12 | 1.86                     | 0.40              |
| 1:QA:718:G:C8     | 11:QK:116:HIS:HB3  | 2.56                     | 0.40              |
| 5:QE:50:GLU:HB2   | 5:QE:53:LEU:HD13   | 2.02                     | 0.40              |
| 13:QM:40:ASN:HB3  | 13:QM:43:THR:HG23  | 2.02                     | 0.40              |
| 25:R0:39:ARG:HH21 | 35:RA:2355:C:H1'   | 1.85                     | 0.40              |
| 35:RA:1500:G:H21  | 37:RD:100:GLY:HA3  | 1.86                     | 0.40              |
| 35:RA:2572:A:O2'  | 38:RE:144:ARG:NH1  | 2.54                     | 0.40              |
| 37:RD:16:MET:SD   | 37:RD:211:ARG:NH2  | 2.88                     | 0.40              |
| 51:RV:62:LEU:HD11 | 51:RV:95:LEU:HB2   | 2.03                     | 0.40              |
| 1:XA:1229:A:O2'   | 22:XV:30:G:OP1     | 2.38                     | 0.40              |
| 1:XA:1239:A:O2'   | 7:XG:114:ARG:O     | 2.36                     | 0.40              |
| 3:XC:108:ASN:HD21 | 3:XC:144:SER:HB3   | 1.87                     | 0.40              |
| 28:Y3:8:LEU:HB2   | 28:Y3:28:LEU:HD13  | 2.02                     | 0.40              |
| 35:YA:192:C:O2'   | 35:YA:802:A:N3     | 2.47                     | 0.40              |
| 35:YA:1007:C:H5'' | 43:YN:35:ARG:NH1   | 2.36                     | 0.40              |
| 35:YA:1084:A:H8   | 35:YA:1085:A:H4'   | 1.86                     | 0.40              |
| 35:YA:1316:U:H2'  | 35:YA:1317:A:H8    | 1.86                     | 0.40              |
| 35:YA:1754:C:OP1  | 49:YT:96:ARG:NH1   | 2.55                     | 0.40              |
| 37:YD:69:ARG:HH11 | 37:YD:105:ILE:HG21 | 1.87                     | 0.40              |
| 1:QA:392:G:OP1    | 16:QP:8:ARG:NH2    | 2.51                     | 0.40              |
| 1:QA:1184:G:H2'   | 1:QA:1185:G:H8     | 1.86                     | 0.40              |
| 4:QD:53:ASP:HB3   | 4:QD:57:ARG:NH1    | 2.36                     | 0.40              |
| 11:QK:99:GLN:HG2  | 11:QK:105:VAL:HG21 | 2.04                     | 0.40              |
| 33:R8:5:LYS:HG2   | 35:RA:242:G:C8     | 2.56                     | 0.40              |
| 35:RA:521:G:H2'   | 35:RA:522:G:C8     | 2.57                     | 0.40              |
| 54:RY:27:VAL:HG12 | 54:RY:39:VAL:HG22  | 2.04                     | 0.40              |
| 5:XE:6:PHE:CD1    | 5:XE:36:ASP:HB3    | 2.57                     | 0.40              |
| 25:Y0:46:LYS:HB2  | 25:Y0:78:TYR:CD1   | 2.56                     | 0.40              |
| 35:YA:1593:G:H2'  | 35:YA:1594:G:C8    | 2.57                     | 0.40              |
| 1:QA:56:U:H2'     | 1:QA:57:G:C8       | 2.56                     | 0.40              |
| 29:R4:28:LYS:HD2  | 29:R4:31:ILE:HD11  | 2.03                     | 0.40              |
| 35:RA:390:A:C6    | 45:RP:71:VAL:HG21  | 2.56                     | 0.40              |
| 35:RA:614(D):A:C4 | 39:RF:180:GLY:HA3  | 2.57                     | 0.40              |
| 40:RG:32:PRO:HB3  | 40:RG:163:ALA:HB2  | 2.03                     | 0.40              |
| 1:XA:107:G:OP1    | 1:XA:325:A:N6      | 2.55                     | 0.40              |
| 1:XA:1053:G:N7    | 1:XA:1200:C:H5''   | 2.37                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:1095:U:P      | 1:XA:1108:G:H1    | 2.44                     | 0.40              |
| 9:XI:24:GLY:N      | 9:XI:60:ASP:OD1   | 2.37                     | 0.40              |
| 10:XJ:61:GLU:OE2   | 14:YN:58:LYS:NZ   | 2.51                     | 0.40              |
| 35:YA:787:U:H5''   | 35:YA:788:A:H5'   | 2.03                     | 0.40              |
| 35:YA:1012:U:C4    | 43:YN:25:ARG:HD3  | 2.56                     | 0.40              |
| 35:YA:1400:G:H2'   | 35:YA:1401:G:C8   | 2.57                     | 0.40              |
| 37:YD:206:LEU:HA   | 37:YD:211:ARG:HD2 | 2.03                     | 0.40              |
| 37:YD:245:PRO:HA   | 37:YD:246:PRO:HD3 | 1.94                     | 0.40              |
| 38:YE:134:ILE:HA   | 38:YE:137:HIS:CD2 | 2.57                     | 0.40              |
| 39:YF:13:SER:OG    | 39:YF:16:GLY:O    | 2.29                     | 0.40              |
| 45:YP:106:LEU:HD11 | 45:YP:112:LEU:HB2 | 2.04                     | 0.40              |
| 46:YQ:39:PRO:HB3   | 46:YQ:99:PRO:HD3  | 2.03                     | 0.40              |
| 55:YZ:108:PRO:HB3  | 55:YZ:144:LEU:HB2 | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | QB    | 229/256 (90%) | 202 (88%) | 19 (8%)  | 8 (4%)   | 3           | 16  |
| 2   | XB    | 229/256 (90%) | 204 (89%) | 22 (10%) | 3 (1%)   | 9           | 35  |
| 3   | QC    | 204/239 (85%) | 197 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 3   | XC    | 204/239 (85%) | 195 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 4   | QD    | 206/209 (99%) | 195 (95%) | 10 (5%)  | 1 (0%)   | 24          | 57  |
| 4   | XD    | 206/209 (99%) | 199 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 5   | QE    | 146/162 (90%) | 140 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 5   | XE    | 146/162 (90%) | 141 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 6   | QF    | 98/101 (97%)  | 98 (100%) | 0        | 0        | 100         | 100 |
| 6   | XF    | 98/101 (97%)  | 97 (99%)  | 1 (1%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7   | QG    | 153/156 (98%) | 149 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 7   | XG    | 153/156 (98%) | 147 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 8   | QH    | 135/138 (98%) | 132 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 8   | XH    | 135/138 (98%) | 133 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 9   | QI    | 125/128 (98%) | 110 (88%) | 15 (12%) | 0        | 100         | 100 |
| 9   | XI    | 124/128 (97%) | 111 (90%) | 13 (10%) | 0        | 100         | 100 |
| 10  | QJ    | 95/105 (90%)  | 81 (85%)  | 11 (12%) | 3 (3%)   | 3           | 18  |
| 10  | XJ    | 94/105 (90%)  | 84 (89%)  | 8 (8%)   | 2 (2%)   | 5           | 25  |
| 11  | QK    | 112/129 (87%) | 107 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 11  | XK    | 112/129 (87%) | 108 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 12  | QL    | 119/132 (90%) | 105 (88%) | 12 (10%) | 2 (2%)   | 7           | 30  |
| 12  | XL    | 119/132 (90%) | 109 (92%) | 6 (5%)   | 4 (3%)   | 3           | 16  |
| 13  | QM    | 114/126 (90%) | 107 (94%) | 4 (4%)   | 3 (3%)   | 4           | 21  |
| 13  | XM    | 112/126 (89%) | 106 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 14  | QN    | 58/61 (95%)   | 57 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 14  | XN    | 58/61 (95%)   | 57 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 15  | QO    | 86/89 (97%)   | 82 (95%)  | 3 (4%)   | 1 (1%)   | 10          | 37  |
| 15  | XO    | 86/89 (97%)   | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 16  | QP    | 80/88 (91%)   | 79 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 16  | XP    | 80/88 (91%)   | 76 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 17  | QQ    | 97/105 (92%)  | 90 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 17  | XQ    | 97/105 (92%)  | 92 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 18  | QR    | 66/88 (75%)   | 66 (100%) | 0        | 0        | 100         | 100 |
| 18  | XR    | 66/88 (75%)   | 66 (100%) | 0        | 0        | 100         | 100 |
| 19  | QS    | 81/93 (87%)   | 78 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 19  | XS    | 81/93 (87%)   | 77 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 20  | QT    | 94/106 (89%)  | 91 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 20  | XT    | 96/106 (91%)  | 92 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 21  | QU    | 21/27 (78%)   | 20 (95%)  | 1 (5%)   | 0        | 100         | 100 |
| 21  | XU    | 21/27 (78%)   | 20 (95%)  | 1 (5%)   | 0        | 100         | 100 |
| 25  | R0    | 75/85 (88%)   | 74 (99%)  | 1 (1%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 25  | Y0    | 75/85 (88%)   | 74 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 26  | R1    | 95/98 (97%)   | 93 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 26  | Y1    | 95/98 (97%)   | 94 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 27  | R2    | 68/72 (94%)   | 68 (100%) | 0       | 0        | 100         | 100 |
| 27  | Y2    | 68/72 (94%)   | 68 (100%) | 0       | 0        | 100         | 100 |
| 28  | R3    | 57/60 (95%)   | 56 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 28  | Y3    | 57/60 (95%)   | 56 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 29  | R4    | 67/71 (94%)   | 59 (88%)  | 7 (10%) | 1 (2%)   | 8           | 32  |
| 29  | Y4    | 67/71 (94%)   | 54 (81%)  | 8 (12%) | 5 (8%)   | 1           | 4   |
| 30  | R5    | 57/60 (95%)   | 56 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 30  | Y5    | 57/60 (95%)   | 56 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 31  | R6    | 51/54 (94%)   | 49 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 31  | Y6    | 51/54 (94%)   | 49 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 32  | R7    | 46/49 (94%)   | 46 (100%) | 0       | 0        | 100         | 100 |
| 32  | Y7    | 46/49 (94%)   | 46 (100%) | 0       | 0        | 100         | 100 |
| 33  | R8    | 62/65 (95%)   | 61 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 33  | Y8    | 62/65 (95%)   | 60 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 34  | R9    | 35/37 (95%)   | 35 (100%) | 0       | 0        | 100         | 100 |
| 34  | Y9    | 35/37 (95%)   | 35 (100%) | 0       | 0        | 100         | 100 |
| 37  | RD    | 273/276 (99%) | 263 (96%) | 10 (4%) | 0        | 100         | 100 |
| 37  | YD    | 273/276 (99%) | 264 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 38  | RE    | 202/206 (98%) | 195 (96%) | 6 (3%)  | 1 (0%)   | 24          | 57  |
| 38  | YE    | 202/206 (98%) | 192 (95%) | 9 (4%)  | 1 (0%)   | 24          | 57  |
| 39  | RF    | 200/210 (95%) | 196 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 39  | YF    | 200/210 (95%) | 198 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 40  | RG    | 179/182 (98%) | 163 (91%) | 13 (7%) | 3 (2%)   | 7           | 30  |
| 40  | YG    | 179/182 (98%) | 161 (90%) | 16 (9%) | 2 (1%)   | 11          | 39  |
| 41  | RH    | 172/180 (96%) | 166 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 41  | YH    | 171/180 (95%) | 165 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 42  | RI    | 145/148 (98%) | 134 (92%) | 11 (8%) | 0        | 100         | 100 |
| 42  | YI    | 144/148 (97%) | 140 (97%) | 4 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 43  | RN    | 138/140 (99%)     | 133 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 43  | YN    | 138/140 (99%)     | 133 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 44  | RO    | 120/122 (98%)     | 115 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 44  | YO    | 120/122 (98%)     | 114 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 45  | RP    | 147/150 (98%)     | 139 (95%)   | 8 (5%)   | 0        | 100         | 100 |
| 45  | YP    | 147/150 (98%)     | 139 (95%)   | 8 (5%)   | 0        | 100         | 100 |
| 46  | RQ    | 139/141 (99%)     | 134 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 46  | YQ    | 139/141 (99%)     | 136 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 47  | RR    | 116/118 (98%)     | 112 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 47  | YR    | 116/118 (98%)     | 114 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 48  | RS    | 108/112 (96%)     | 103 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 48  | YS    | 108/112 (96%)     | 106 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 49  | RT    | 129/146 (88%)     | 121 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 49  | YT    | 129/146 (88%)     | 126 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 50  | RU    | 114/118 (97%)     | 111 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 50  | YU    | 114/118 (97%)     | 112 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 51  | RV    | 99/101 (98%)      | 93 (94%)    | 5 (5%)   | 1 (1%)   | 12          | 41  |
| 51  | YV    | 99/101 (98%)      | 91 (92%)    | 7 (7%)   | 1 (1%)   | 12          | 41  |
| 52  | RW    | 110/113 (97%)     | 107 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 52  | YW    | 110/113 (97%)     | 109 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 53  | RX    | 93/96 (97%)       | 90 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 53  | YX    | 93/96 (97%)       | 90 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 54  | RY    | 105/110 (96%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 54  | YY    | 105/110 (96%)     | 98 (93%)    | 7 (7%)   | 0        | 100         | 100 |
| 55  | RZ    | 176/206 (85%)     | 164 (93%)   | 11 (6%)  | 1 (1%)   | 21          | 52  |
| 55  | YZ    | 175/206 (85%)     | 165 (94%)   | 8 (5%)   | 2 (1%)   | 11          | 39  |
| All | All   | 11389/12128 (94%) | 10866 (95%) | 478 (4%) | 45 (0%)  | 30          | 61  |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 17  | PHE  |
| 2   | QB    | 127 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | QD    | 5   | ILE  |
| 10  | QJ    | 32  | ALA  |
| 10  | QJ    | 79  | ARG  |
| 12  | QL    | 48  | PRO  |
| 13  | QM    | 106 | ASN  |
| 40  | RG    | 48  | GLU  |
| 40  | RG    | 49  | ASP  |
| 51  | RV    | 50  | PRO  |
| 10  | XJ    | 79  | ARG  |
| 12  | XL    | 47  | LYS  |
| 29  | Y4    | 47  | GLN  |
| 29  | Y4    | 49  | PHE  |
| 29  | Y4    | 59  | PHE  |
| 40  | YG    | 96  | ARG  |
| 55  | YZ    | 52  | SER  |
| 2   | QB    | 9   | GLU  |
| 2   | QB    | 21  | ARG  |
| 2   | QB    | 126 | GLU  |
| 10  | QJ    | 55  | LYS  |
| 12  | QL    | 49  | ASN  |
| 29  | R4    | 56  | VAL  |
| 40  | RG    | 50  | ALA  |
| 10  | XJ    | 55  | LYS  |
| 12  | XL    | 48  | PRO  |
| 29  | Y4    | 58  | ARG  |
| 2   | QB    | 22  | LYS  |
| 13  | QM    | 107 | ALA  |
| 15  | QO    | 88  | ARG  |
| 2   | XB    | 9   | GLU  |
| 2   | XB    | 126 | GLU  |
| 55  | YZ    | 51  | ALA  |
| 2   | QB    | 8   | LYS  |
| 13  | QM    | 105 | THR  |
| 55  | RZ    | 52  | SER  |
| 12  | XL    | 46  | LYS  |
| 29  | Y4    | 48  | ARG  |
| 40  | YG    | 97  | ASP  |
| 51  | YV    | 50  | PRO  |
| 38  | RE    | 52  | LEU  |
| 38  | YE    | 52  | LEU  |
| 12  | XL    | 88  | GLY  |
| 2   | XB    | 125 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 125 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2   | QB    | 191/220 (87%) | 191 (100%) | 0        | 100         | 100 |
| 2   | XB    | 187/220 (85%) | 187 (100%) | 0        | 100         | 100 |
| 3   | QC    | 144/188 (77%) | 144 (100%) | 0        | 100         | 100 |
| 3   | XC    | 140/188 (74%) | 140 (100%) | 0        | 100         | 100 |
| 4   | QD    | 171/181 (94%) | 171 (100%) | 0        | 100         | 100 |
| 4   | XD    | 172/181 (95%) | 172 (100%) | 0        | 100         | 100 |
| 5   | QE    | 114/123 (93%) | 114 (100%) | 0        | 100         | 100 |
| 5   | XE    | 114/123 (93%) | 114 (100%) | 0        | 100         | 100 |
| 6   | QF    | 85/90 (94%)   | 85 (100%)  | 0        | 100         | 100 |
| 6   | XF    | 85/90 (94%)   | 85 (100%)  | 0        | 100         | 100 |
| 7   | QG    | 120/127 (94%) | 120 (100%) | 0        | 100         | 100 |
| 7   | XG    | 119/127 (94%) | 119 (100%) | 0        | 100         | 100 |
| 8   | QH    | 116/119 (98%) | 116 (100%) | 0        | 100         | 100 |
| 8   | XH    | 114/119 (96%) | 114 (100%) | 0        | 100         | 100 |
| 9   | QI    | 91/99 (92%)   | 91 (100%)  | 0        | 100         | 100 |
| 9   | XI    | 88/99 (89%)   | 88 (100%)  | 0        | 100         | 100 |
| 10  | QJ    | 68/92 (74%)   | 68 (100%)  | 0        | 100         | 100 |
| 10  | XJ    | 68/92 (74%)   | 68 (100%)  | 0        | 100         | 100 |
| 11  | QK    | 83/99 (84%)   | 83 (100%)  | 0        | 100         | 100 |
| 11  | XK    | 83/99 (84%)   | 83 (100%)  | 0        | 100         | 100 |
| 12  | QL    | 96/108 (89%)  | 96 (100%)  | 0        | 100         | 100 |
| 12  | XL    | 96/108 (89%)  | 96 (100%)  | 0        | 100         | 100 |
| 13  | QM    | 90/101 (89%)  | 90 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 13  | XM    | 87/101 (86%) | 87 (100%) | 0        | 100         | 100 |
| 14  | QN    | 49/50 (98%)  | 49 (100%) | 0        | 100         | 100 |
| 14  | XN    | 49/50 (98%)  | 49 (100%) | 0        | 100         | 100 |
| 15  | QO    | 78/80 (98%)  | 78 (100%) | 0        | 100         | 100 |
| 15  | XO    | 78/80 (98%)  | 78 (100%) | 0        | 100         | 100 |
| 16  | QP    | 69/74 (93%)  | 69 (100%) | 0        | 100         | 100 |
| 16  | XP    | 68/74 (92%)  | 68 (100%) | 0        | 100         | 100 |
| 17  | QQ    | 94/97 (97%)  | 94 (100%) | 0        | 100         | 100 |
| 17  | XQ    | 94/97 (97%)  | 94 (100%) | 0        | 100         | 100 |
| 18  | QR    | 59/77 (77%)  | 59 (100%) | 0        | 100         | 100 |
| 18  | XR    | 59/77 (77%)  | 59 (100%) | 0        | 100         | 100 |
| 19  | QS    | 68/80 (85%)  | 68 (100%) | 0        | 100         | 100 |
| 19  | XS    | 67/80 (84%)  | 67 (100%) | 0        | 100         | 100 |
| 20  | QT    | 71/82 (87%)  | 70 (99%)  | 1 (1%)   | 59          | 76  |
| 20  | XT    | 70/82 (85%)  | 70 (100%) | 0        | 100         | 100 |
| 21  | QU    | 18/22 (82%)  | 18 (100%) | 0        | 100         | 100 |
| 21  | XU    | 18/22 (82%)  | 18 (100%) | 0        | 100         | 100 |
| 25  | R0    | 61/67 (91%)  | 61 (100%) | 0        | 100         | 100 |
| 25  | Y0    | 61/67 (91%)  | 61 (100%) | 0        | 100         | 100 |
| 26  | R1    | 79/83 (95%)  | 79 (100%) | 0        | 100         | 100 |
| 26  | Y1    | 81/83 (98%)  | 81 (100%) | 0        | 100         | 100 |
| 27  | R2    | 65/67 (97%)  | 65 (100%) | 0        | 100         | 100 |
| 27  | Y2    | 66/67 (98%)  | 66 (100%) | 0        | 100         | 100 |
| 28  | R3    | 51/52 (98%)  | 51 (100%) | 0        | 100         | 100 |
| 28  | Y3    | 50/52 (96%)  | 50 (100%) | 0        | 100         | 100 |
| 29  | R4    | 58/63 (92%)  | 58 (100%) | 0        | 100         | 100 |
| 29  | Y4    | 54/63 (86%)  | 54 (100%) | 0        | 100         | 100 |
| 30  | R5    | 51/52 (98%)  | 51 (100%) | 0        | 100         | 100 |
| 30  | Y5    | 50/52 (96%)  | 50 (100%) | 0        | 100         | 100 |
| 31  | R6    | 51/52 (98%)  | 51 (100%) | 0        | 100         | 100 |
| 31  | Y6    | 50/52 (96%)  | 50 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 32  | R7    | 41/42 (98%)    | 41 (100%)  | 0        | 100         | 100 |
| 32  | Y7    | 41/42 (98%)    | 41 (100%)  | 0        | 100         | 100 |
| 33  | R8    | 54/55 (98%)    | 54 (100%)  | 0        | 100         | 100 |
| 33  | Y8    | 54/55 (98%)    | 54 (100%)  | 0        | 100         | 100 |
| 34  | R9    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 34  | Y9    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 37  | RD    | 214/218 (98%)  | 214 (100%) | 0        | 100         | 100 |
| 37  | YD    | 215/218 (99%)  | 215 (100%) | 0        | 100         | 100 |
| 38  | RE    | 164/166 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 38  | YE    | 164/166 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 39  | RF    | 160/166 (96%)  | 160 (100%) | 0        | 100         | 100 |
| 39  | YF    | 159/166 (96%)  | 159 (100%) | 0        | 100         | 100 |
| 40  | RG    | 144/156 (92%)  | 144 (100%) | 0        | 100         | 100 |
| 40  | YG    | 142/156 (91%)  | 142 (100%) | 0        | 100         | 100 |
| 41  | RH    | 144/148 (97%)  | 144 (100%) | 0        | 100         | 100 |
| 41  | YH    | 143/148 (97%)  | 143 (100%) | 0        | 100         | 100 |
| 42  | RI    | 111/124 (90%)  | 111 (100%) | 0        | 100         | 100 |
| 42  | YI    | 108/124 (87%)  | 108 (100%) | 0        | 100         | 100 |
| 43  | RN    | 119/119 (100%) | 119 (100%) | 0        | 100         | 100 |
| 43  | YN    | 118/119 (99%)  | 118 (100%) | 0        | 100         | 100 |
| 44  | RO    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 44  | YO    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 45  | RP    | 115/116 (99%)  | 115 (100%) | 0        | 100         | 100 |
| 45  | YP    | 115/116 (99%)  | 115 (100%) | 0        | 100         | 100 |
| 46  | RQ    | 111/111 (100%) | 111 (100%) | 0        | 100         | 100 |
| 46  | YQ    | 111/111 (100%) | 111 (100%) | 0        | 100         | 100 |
| 47  | RR    | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 47  | YR    | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 48  | RS    | 87/88 (99%)    | 87 (100%)  | 0        | 100         | 100 |
| 48  | YS    | 85/88 (97%)    | 85 (100%)  | 0        | 100         | 100 |
| 49  | RT    | 115/127 (91%)  | 115 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 49  | YT    | 113/127 (89%)    | 113 (100%)  | 0        | 100         | 100 |
| 50  | RU    | 93/94 (99%)      | 93 (100%)   | 0        | 100         | 100 |
| 50  | YU    | 93/94 (99%)      | 93 (100%)   | 0        | 100         | 100 |
| 51  | RV    | 81/82 (99%)      | 81 (100%)   | 0        | 100         | 100 |
| 51  | YV    | 80/82 (98%)      | 80 (100%)   | 0        | 100         | 100 |
| 52  | RW    | 90/92 (98%)      | 90 (100%)   | 0        | 100         | 100 |
| 52  | YW    | 90/92 (98%)      | 90 (100%)   | 0        | 100         | 100 |
| 53  | RX    | 77/78 (99%)      | 77 (100%)   | 0        | 100         | 100 |
| 53  | YX    | 77/78 (99%)      | 77 (100%)   | 0        | 100         | 100 |
| 54  | RY    | 86/91 (94%)      | 86 (100%)   | 0        | 100         | 100 |
| 54  | YY    | 86/91 (94%)      | 86 (100%)   | 0        | 100         | 100 |
| 55  | RZ    | 152/179 (85%)    | 152 (100%)  | 0        | 100         | 100 |
| 55  | YZ    | 148/179 (83%)    | 148 (100%)  | 0        | 100         | 100 |
| All | All   | 9329/10064 (93%) | 9328 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | QT    | 60  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | QC    | 108 | ASN  |
| 4   | QD    | 45  | GLN  |
| 4   | QD    | 129 | ASN  |
| 4   | QD    | 201 | GLN  |
| 5   | QE    | 127 | ASN  |
| 6   | QF    | 73  | ASN  |
| 7   | QG    | 148 | ASN  |
| 9   | QI    | 73  | GLN  |
| 9   | QI    | 124 | GLN  |
| 10  | QJ    | 69  | ASN  |
| 12  | QL    | 80  | HIS  |
| 13  | QM    | 101 | GLN  |
| 14  | QN    | 49  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | QO    | 37  | ASN  |
| 16  | QP    | 13  | HIS  |
| 19  | QS    | 23  | ASN  |
| 19  | QS    | 57  | HIS  |
| 20  | QT    | 16  | HIS  |
| 31  | R6    | 26  | ASN  |
| 33  | R8    | 35  | GLN  |
| 34  | R9    | 34  | GLN  |
| 37  | RD    | 166 | GLN  |
| 38  | RE    | 48  | GLN  |
| 38  | RE    | 137 | HIS  |
| 39  | RF    | 8   | GLN  |
| 39  | RF    | 40  | GLN  |
| 40  | RG    | 26  | GLN  |
| 40  | RG    | 108 | ASN  |
| 41  | RH    | 74  | ASN  |
| 42  | RI    | 133 | HIS  |
| 42  | RI    | 139 | GLN  |
| 43  | RN    | 94  | HIS  |
| 44  | RO    | 89  | ASN  |
| 45  | RP    | 70  | GLN  |
| 46  | RQ    | 57  | HIS  |
| 47  | RR    | 13  | HIS  |
| 47  | RR    | 71  | GLN  |
| 49  | RT    | 90  | GLN  |
| 52  | RW    | 61  | ASN  |
| 53  | RX    | 41  | ASN  |
| 55  | RZ    | 73  | GLN  |
| 55  | RZ    | 75  | ASN  |
| 2   | XB    | 113 | HIS  |
| 3   | XC    | 108 | ASN  |
| 3   | XC    | 139 | GLN  |
| 5   | XE    | 20  | GLN  |
| 5   | XE    | 127 | ASN  |
| 6   | XF    | 73  | ASN  |
| 6   | XF    | 100 | ASN  |
| 7   | XG    | 64  | GLN  |
| 9   | XI    | 73  | GLN  |
| 9   | XI    | 124 | GLN  |
| 10  | XJ    | 69  | ASN  |
| 12  | XL    | 80  | HIS  |
| 13  | XM    | 106 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | XO    | 9   | GLN  |
| 15  | XO    | 37  | ASN  |
| 15  | XO    | 62  | GLN  |
| 19  | XS    | 65  | ASN  |
| 20  | XT    | 16  | HIS  |
| 34  | Y9    | 34  | GLN  |
| 37  | YD    | 87  | ASN  |
| 39  | YF    | 29  | ASN  |
| 39  | YF    | 40  | GLN  |
| 43  | YN    | 94  | HIS  |
| 45  | YP    | 70  | GLN  |
| 47  | YR    | 13  | HIS  |
| 47  | YR    | 71  | GLN  |
| 49  | YT    | 58  | ASN  |
| 52  | YW    | 61  | ASN  |
| 53  | YX    | 41  | ASN  |
| 55  | YZ    | 55  | HIS  |
| 55  | YZ    | 121 | HIS  |
| 55  | YZ    | 151 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | QA    | 1497/1522 (98%) | 239 (15%)         | 15 (1%)         |
| 1   | XA    | 1501/1522 (98%) | 230 (15%)         | 15 (0%)         |
| 22  | QV    | 76/77 (98%)     | 15 (19%)          | 0               |
| 22  | XV    | 76/77 (98%)     | 13 (17%)          | 0               |
| 23  | QX    | 17/19 (89%)     | 6 (35%)           | 1 (5%)          |
| 23  | XX    | 17/19 (89%)     | 8 (47%)           | 1 (5%)          |
| 24  | QY    | 75/76 (98%)     | 31 (41%)          | 0               |
| 24  | XY    | 75/76 (98%)     | 33 (44%)          | 0               |
| 35  | RA    | 2858/2915 (98%) | 453 (15%)         | 16 (0%)         |
| 35  | YA    | 2858/2915 (98%) | 454 (15%)         | 15 (0%)         |
| 36  | RB    | 119/122 (97%)   | 10 (8%)           | 0               |
| 36  | YB    | 119/122 (97%)   | 11 (9%)           | 0               |
| All | All   | 9288/9462 (98%) | 1503 (16%)        | 63 (0%)         |

All (1503) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 5   | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 6      | G    |
| 1   | QA    | 9      | G    |
| 1   | QA    | 22     | G    |
| 1   | QA    | 32     | A    |
| 1   | QA    | 39     | G    |
| 1   | QA    | 47     | C    |
| 1   | QA    | 48     | C    |
| 1   | QA    | 50     | A    |
| 1   | QA    | 51     | A    |
| 1   | QA    | 52     | G    |
| 1   | QA    | 61     | G    |
| 1   | QA    | 66     | G    |
| 1   | QA    | 78     | G    |
| 1   | QA    | 101    | A    |
| 1   | QA    | 105    | G    |
| 1   | QA    | 116    | A    |
| 1   | QA    | 121    | C    |
| 1   | QA    | 129(B) | G    |
| 1   | QA    | 131    | C    |
| 1   | QA    | 151    | A    |
| 1   | QA    | 163    | C    |
| 1   | QA    | 174    | C    |
| 1   | QA    | 182    | U    |
| 1   | QA    | 189(F) | U    |
| 1   | QA    | 189(G) | U    |
| 1   | QA    | 189(H) | G    |
| 1   | QA    | 195    | A    |
| 1   | QA    | 197    | A    |
| 1   | QA    | 202    | U    |
| 1   | QA    | 203    | U    |
| 1   | QA    | 204    | U    |
| 1   | QA    | 216    | G    |
| 1   | QA    | 220    | G    |
| 1   | QA    | 247    | G    |
| 1   | QA    | 251    | G    |
| 1   | QA    | 266    | G    |
| 1   | QA    | 267    | C    |
| 1   | QA    | 289    | G    |
| 1   | QA    | 301    | G    |
| 1   | QA    | 321    | A    |
| 1   | QA    | 328    | C    |
| 1   | QA    | 332    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 346 | G    |
| 1   | QA    | 350 | G    |
| 1   | QA    | 351 | G    |
| 1   | QA    | 352 | C    |
| 1   | QA    | 353 | A    |
| 1   | QA    | 354 | G    |
| 1   | QA    | 356 | A    |
| 1   | QA    | 367 | U    |
| 1   | QA    | 372 | C    |
| 1   | QA    | 373 | A    |
| 1   | QA    | 384 | G    |
| 1   | QA    | 388 | G    |
| 1   | QA    | 397 | A    |
| 1   | QA    | 398 | C    |
| 1   | QA    | 406 | G    |
| 1   | QA    | 412 | A    |
| 1   | QA    | 413 | G    |
| 1   | QA    | 424 | G    |
| 1   | QA    | 429 | U    |
| 1   | QA    | 439 | A    |
| 1   | QA    | 452 | A    |
| 1   | QA    | 461 | A    |
| 1   | QA    | 470 | C    |
| 1   | QA    | 482 | A    |
| 1   | QA    | 484 | G    |
| 1   | QA    | 485 | G    |
| 1   | QA    | 496 | A    |
| 1   | QA    | 498 | U    |
| 1   | QA    | 508 | C    |
| 1   | QA    | 509 | A    |
| 1   | QA    | 510 | A    |
| 1   | QA    | 511 | C    |
| 1   | QA    | 518 | C    |
| 1   | QA    | 521 | G    |
| 1   | QA    | 532 | A    |
| 1   | QA    | 533 | A    |
| 1   | QA    | 547 | A    |
| 1   | QA    | 559 | A    |
| 1   | QA    | 560 | U    |
| 1   | QA    | 561 | U    |
| 1   | QA    | 564 | C    |
| 1   | QA    | 567 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 572 | A    |
| 1   | QA    | 573 | A    |
| 1   | QA    | 576 | G    |
| 1   | QA    | 577 | G    |
| 1   | QA    | 596 | C    |
| 1   | QA    | 630 | G    |
| 1   | QA    | 631 | G    |
| 1   | QA    | 653 | A    |
| 1   | QA    | 665 | A    |
| 1   | QA    | 666 | G    |
| 1   | QA    | 687 | A    |
| 1   | QA    | 688 | G    |
| 1   | QA    | 695 | A    |
| 1   | QA    | 721 | G    |
| 1   | QA    | 723 | U    |
| 1   | QA    | 731 | G    |
| 1   | QA    | 734 | G    |
| 1   | QA    | 749 | C    |
| 1   | QA    | 755 | G    |
| 1   | QA    | 760 | G    |
| 1   | QA    | 774 | G    |
| 1   | QA    | 777 | A    |
| 1   | QA    | 793 | U    |
| 1   | QA    | 794 | A    |
| 1   | QA    | 815 | A    |
| 1   | QA    | 816 | A    |
| 1   | QA    | 817 | C    |
| 1   | QA    | 821 | G    |
| 1   | QA    | 828 | A    |
| 1   | QA    | 829 | G    |
| 1   | QA    | 836 | G    |
| 1   | QA    | 840 | C    |
| 1   | QA    | 841 | U    |
| 1   | QA    | 848 | C    |
| 1   | QA    | 851 | G    |
| 1   | QA    | 902 | G    |
| 1   | QA    | 914 | A    |
| 1   | QA    | 916 | G    |
| 1   | QA    | 926 | G    |
| 1   | QA    | 927 | G    |
| 1   | QA    | 934 | C    |
| 1   | QA    | 942 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 960     | U    |
| 1   | QA    | 961     | U    |
| 1   | QA    | 968     | A    |
| 1   | QA    | 969     | A    |
| 1   | QA    | 971     | G    |
| 1   | QA    | 974     | A    |
| 1   | QA    | 975     | A    |
| 1   | QA    | 976     | G    |
| 1   | QA    | 977     | A    |
| 1   | QA    | 981     | U    |
| 1   | QA    | 982     | U    |
| 1   | QA    | 992     | U    |
| 1   | QA    | 993     | G    |
| 1   | QA    | 1002    | G    |
| 1   | QA    | 1004    | A    |
| 1   | QA    | 1005    | A    |
| 1   | QA    | 1006    | C    |
| 1   | QA    | 1009    | G    |
| 1   | QA    | 1020    | U    |
| 1   | QA    | 1022    | G    |
| 1   | QA    | 1023    | G    |
| 1   | QA    | 1025    | U    |
| 1   | QA    | 1026    | G    |
| 1   | QA    | 1027    | C    |
| 1   | QA    | 1028    | C    |
| 1   | QA    | 1029    | C    |
| 1   | QA    | 1030(B) | G    |
| 1   | QA    | 1030(C) | C    |
| 1   | QA    | 1031    | G    |
| 1   | QA    | 1036    | G    |
| 1   | QA    | 1044    | A    |
| 1   | QA    | 1053    | G    |
| 1   | QA    | 1054    | C    |
| 1   | QA    | 1065    | U    |
| 1   | QA    | 1066    | C    |
| 1   | QA    | 1068    | G    |
| 1   | QA    | 1070    | U    |
| 1   | QA    | 1081    | G    |
| 1   | QA    | 1094    | G    |
| 1   | QA    | 1095    | U    |
| 1   | QA    | 1101    | A    |
| 1   | QA    | 1108    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | QA    | 1117 | G    |
| 1   | QA    | 1125 | U    |
| 1   | QA    | 1129 | C    |
| 1   | QA    | 1130 | A    |
| 1   | QA    | 1136 | U    |
| 1   | QA    | 1137 | C    |
| 1   | QA    | 1139 | G    |
| 1   | QA    | 1146 | A    |
| 1   | QA    | 1147 | C    |
| 1   | QA    | 1152 | A    |
| 1   | QA    | 1157 | A    |
| 1   | QA    | 1159 | U    |
| 1   | QA    | 1183 | A    |
| 1   | QA    | 1187 | G    |
| 1   | QA    | 1196 | U    |
| 1   | QA    | 1197 | G    |
| 1   | QA    | 1201 | A    |
| 1   | QA    | 1211 | U    |
| 1   | QA    | 1214 | C    |
| 1   | QA    | 1224 | G    |
| 1   | QA    | 1227 | A    |
| 1   | QA    | 1228 | C    |
| 1   | QA    | 1236 | A    |
| 1   | QA    | 1238 | A    |
| 1   | QA    | 1250 | A    |
| 1   | QA    | 1256 | A    |
| 1   | QA    | 1257 | U    |
| 1   | QA    | 1258 | G    |
| 1   | QA    | 1260 | C    |
| 1   | QA    | 1270 | C    |
| 1   | QA    | 1278 | U    |
| 1   | QA    | 1279 | A    |
| 1   | QA    | 1280 | A    |
| 1   | QA    | 1282 | C    |
| 1   | QA    | 1287 | A    |
| 1   | QA    | 1300 | G    |
| 1   | QA    | 1302 | U    |
| 1   | QA    | 1303 | C    |
| 1   | QA    | 1305 | G    |
| 1   | QA    | 1320 | C    |
| 1   | QA    | 1340 | A    |
| 1   | QA    | 1346 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 1347    | G    |
| 1   | QA    | 1353    | G    |
| 1   | QA    | 1363(A) | C    |
| 1   | QA    | 1370    | G    |
| 1   | QA    | 1397    | C    |
| 1   | QA    | 1399    | C    |
| 1   | QA    | 1404    | 5MC  |
| 1   | QA    | 1419    | G    |
| 1   | QA    | 1442(A) | G    |
| 1   | QA    | 1442(B) | G    |
| 1   | QA    | 1447    | A    |
| 1   | QA    | 1452    | C    |
| 1   | QA    | 1456    | G    |
| 1   | QA    | 1469    | G    |
| 1   | QA    | 1487    | G    |
| 1   | QA    | 1490    | C    |
| 1   | QA    | 1492    | A    |
| 1   | QA    | 1497    | G    |
| 1   | QA    | 1499    | A    |
| 1   | QA    | 1503    | A    |
| 1   | QA    | 1504    | G    |
| 1   | QA    | 1506    | U    |
| 1   | QA    | 1517    | G    |
| 1   | QA    | 1519    | MA6  |
| 1   | QA    | 1520    | G    |
| 1   | QA    | 1529    | G    |
| 1   | QA    | 1530    | G    |
| 1   | QA    | 1531    | A    |
| 22  | QV    | 3       | C    |
| 22  | QV    | 8       | U    |
| 22  | QV    | 14      | A    |
| 22  | QV    | 16      | C    |
| 22  | QV    | 17      | C    |
| 22  | QV    | 17(A)   | U    |
| 22  | QV    | 18      | G    |
| 22  | QV    | 19      | G    |
| 22  | QV    | 20      | U    |
| 22  | QV    | 21      | A    |
| 22  | QV    | 47      | U    |
| 22  | QV    | 48      | C    |
| 22  | QV    | 49      | G    |
| 22  | QV    | 65      | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | QV    | 76  | A    |
| 23  | QX    | 7   | G    |
| 23  | QX    | 10  | G    |
| 23  | QX    | 11  | U    |
| 23  | QX    | 13  | A    |
| 23  | QX    | 15  | A    |
| 23  | QX    | 19  | G    |
| 24  | QY    | 2   | G    |
| 24  | QY    | 8   | U    |
| 24  | QY    | 9   | A    |
| 24  | QY    | 16  | C    |
| 24  | QY    | 17  | U    |
| 24  | QY    | 18  | G    |
| 24  | QY    | 19  | G    |
| 24  | QY    | 21  | A    |
| 24  | QY    | 29  | U    |
| 24  | QY    | 30  | G    |
| 24  | QY    | 43  | G    |
| 24  | QY    | 46  | G    |
| 24  | QY    | 47  | U    |
| 24  | QY    | 48  | C    |
| 24  | QY    | 49  | A    |
| 24  | QY    | 50  | G    |
| 24  | QY    | 51  | C    |
| 24  | QY    | 52  | G    |
| 24  | QY    | 55  | U    |
| 24  | QY    | 56  | C    |
| 24  | QY    | 57  | G    |
| 24  | QY    | 58  | A    |
| 24  | QY    | 61  | C    |
| 24  | QY    | 67  | A    |
| 24  | QY    | 68  | G    |
| 24  | QY    | 69  | C    |
| 24  | QY    | 71  | C    |
| 24  | QY    | 72  | C    |
| 24  | QY    | 73  | A    |
| 24  | QY    | 74  | C    |
| 24  | QY    | 75  | C    |
| 35  | RA    | 10  | G    |
| 35  | RA    | 15  | G    |
| 35  | RA    | 34  | C    |
| 35  | RA    | 45  | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | RA    | 51     | G    |
| 35  | RA    | 71     | A    |
| 35  | RA    | 74     | A    |
| 35  | RA    | 75     | G    |
| 35  | RA    | 84     | A    |
| 35  | RA    | 102    | G    |
| 35  | RA    | 118    | A    |
| 35  | RA    | 119    | A    |
| 35  | RA    | 120    | U    |
| 35  | RA    | 131    | G    |
| 35  | RA    | 157    | U    |
| 35  | RA    | 182    | A    |
| 35  | RA    | 188    | G    |
| 35  | RA    | 196    | A    |
| 35  | RA    | 199    | A    |
| 35  | RA    | 205    | G    |
| 35  | RA    | 214    | G    |
| 35  | RA    | 216    | A    |
| 35  | RA    | 221    | A    |
| 35  | RA    | 222    | A    |
| 35  | RA    | 229    | A    |
| 35  | RA    | 230    | U    |
| 35  | RA    | 248    | G    |
| 35  | RA    | 265    | A    |
| 35  | RA    | 272(K) | U    |
| 35  | RA    | 272(N) | U    |
| 35  | RA    | 273(B) | U    |
| 35  | RA    | 273(C) | G    |
| 35  | RA    | 278    | A    |
| 35  | RA    | 311    | A    |
| 35  | RA    | 317    | G    |
| 35  | RA    | 324    | A    |
| 35  | RA    | 329    | G    |
| 35  | RA    | 330    | A    |
| 35  | RA    | 331    | A    |
| 35  | RA    | 338    | G    |
| 35  | RA    | 342    | G    |
| 35  | RA    | 345    | A    |
| 35  | RA    | 352    | G    |
| 35  | RA    | 362    | U    |
| 35  | RA    | 363(A) | G    |
| 35  | RA    | 372    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | RA    | 386    | G    |
| 35  | RA    | 396    | G    |
| 35  | RA    | 405    | U    |
| 35  | RA    | 411    | G    |
| 35  | RA    | 412    | A    |
| 35  | RA    | 428    | A    |
| 35  | RA    | 444    | C    |
| 35  | RA    | 455    | C    |
| 35  | RA    | 457    | A    |
| 35  | RA    | 467    | G    |
| 35  | RA    | 470    | A    |
| 35  | RA    | 481    | G    |
| 35  | RA    | 491    | G    |
| 35  | RA    | 505    | A    |
| 35  | RA    | 508    | G    |
| 35  | RA    | 509    | C    |
| 35  | RA    | 530    | G    |
| 35  | RA    | 531    | C    |
| 35  | RA    | 532    | A    |
| 35  | RA    | 533    | G    |
| 35  | RA    | 563    | G    |
| 35  | RA    | 573    | G    |
| 35  | RA    | 575    | A    |
| 35  | RA    | 583    | G    |
| 35  | RA    | 586    | A    |
| 35  | RA    | 603    | A    |
| 35  | RA    | 604    | G    |
| 35  | RA    | 607    | U    |
| 35  | RA    | 614(B) | U    |
| 35  | RA    | 614(C) | G    |
| 35  | RA    | 615    | G    |
| 35  | RA    | 620    | G    |
| 35  | RA    | 627    | A    |
| 35  | RA    | 634    | C    |
| 35  | RA    | 637    | A    |
| 35  | RA    | 645    | C    |
| 35  | RA    | 646    | A    |
| 35  | RA    | 652(C) | A    |
| 35  | RA    | 652(D) | G    |
| 35  | RA    | 652(V) | G    |
| 35  | RA    | 669    | G    |
| 35  | RA    | 686    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | RA    | 717 | G    |
| 35  | RA    | 726 | G    |
| 35  | RA    | 730 | C    |
| 35  | RA    | 734 | A    |
| 35  | RA    | 753 | C    |
| 35  | RA    | 764 | A    |
| 35  | RA    | 765 | G    |
| 35  | RA    | 775 | G    |
| 35  | RA    | 776 | G    |
| 35  | RA    | 782 | A    |
| 35  | RA    | 784 | A    |
| 35  | RA    | 785 | G    |
| 35  | RA    | 788 | A    |
| 35  | RA    | 789 | A    |
| 35  | RA    | 792 | G    |
| 35  | RA    | 805 | G    |
| 35  | RA    | 812 | C    |
| 35  | RA    | 827 | U    |
| 35  | RA    | 828 | U    |
| 35  | RA    | 831 | G    |
| 35  | RA    | 857 | C    |
| 35  | RA    | 859 | G    |
| 35  | RA    | 881 | G    |
| 35  | RA    | 886 | C    |
| 35  | RA    | 887 | A    |
| 35  | RA    | 888 | C    |
| 35  | RA    | 889 | C    |
| 35  | RA    | 890 | A    |
| 35  | RA    | 893 | C    |
| 35  | RA    | 896 | A    |
| 35  | RA    | 897 | C    |
| 35  | RA    | 898 | C    |
| 35  | RA    | 899 | A    |
| 35  | RA    | 907 | U    |
| 35  | RA    | 910 | A    |
| 35  | RA    | 915 | C    |
| 35  | RA    | 917 | A    |
| 35  | RA    | 932 | G    |
| 35  | RA    | 941 | A    |
| 35  | RA    | 945 | A    |
| 35  | RA    | 946 | G    |
| 35  | RA    | 953 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | RA           | 957        | A           |
| 35         | RA           | 959        | A           |
| 35         | RA           | 961        | C           |
| 35         | RA           | 974        | G           |
| 35         | RA           | 975(A)     | C           |
| 35         | RA           | 983        | A           |
| 35         | RA           | 996        | A           |
| 35         | RA           | 1005       | C           |
| 35         | RA           | 1012       | U           |
| 35         | RA           | 1013       | C           |
| 35         | RA           | 1022       | G           |
| 35         | RA           | 1025       | G           |
| 35         | RA           | 1026       | U           |
| 35         | RA           | 1033       | U           |
| 35         | RA           | 1045       | A           |
| 35         | RA           | 1046       | A           |
| 35         | RA           | 1047       | G           |
| 35         | RA           | 1051       | G           |
| 35         | RA           | 1052       | C           |
| 35         | RA           | 1054       | A           |
| 35         | RA           | 1058       | G           |
| 35         | RA           | 1060       | U           |
| 35         | RA           | 1063       | G           |
| 35         | RA           | 1064       | C           |
| 35         | RA           | 1065       | U           |
| 35         | RA           | 1066       | U           |
| 35         | RA           | 1067       | A           |
| 35         | RA           | 1068       | G           |
| 35         | RA           | 1070       | A           |
| 35         | RA           | 1071       | G           |
| 35         | RA           | 1073       | A           |
| 35         | RA           | 1074       | G           |
| 35         | RA           | 1076       | C           |
| 35         | RA           | 1077       | A           |
| 35         | RA           | 1079       | C           |
| 35         | RA           | 1082       | U           |
| 35         | RA           | 1083       | U           |
| 35         | RA           | 1084       | A           |
| 35         | RA           | 1085       | A           |
| 35         | RA           | 1086       | A           |
| 35         | RA           | 1088       | A           |
| 35         | RA           | 1090       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | RA           | 1092       | C           |
| 35         | RA           | 1094       | U           |
| 35         | RA           | 1096       | A           |
| 35         | RA           | 1097       | U           |
| 35         | RA           | 1098       | A           |
| 35         | RA           | 1108       | U           |
| 35         | RA           | 1109       | C           |
| 35         | RA           | 1110       | G           |
| 35         | RA           | 1112       | G           |
| 35         | RA           | 1128       | A           |
| 35         | RA           | 1130       | U           |
| 35         | RA           | 1135       | C           |
| 35         | RA           | 1136       | G           |
| 35         | RA           | 1155       | A           |
| 35         | RA           | 1171       | G           |
| 35         | RA           | 1188       | U           |
| 35         | RA           | 1206       | G           |
| 35         | RA           | 1211       | U           |
| 35         | RA           | 1220       | A           |
| 35         | RA           | 1236       | G           |
| 35         | RA           | 1247       | A           |
| 35         | RA           | 1250       | G           |
| 35         | RA           | 1253       | A           |
| 35         | RA           | 1256       | G           |
| 35         | RA           | 1265       | A           |
| 35         | RA           | 1271       | G           |
| 35         | RA           | 1272       | A           |
| 35         | RA           | 1273       | U           |
| 35         | RA           | 1300       | U           |
| 35         | RA           | 1301       | A           |
| 35         | RA           | 1314       | C           |
| 35         | RA           | 1341       | U           |
| 35         | RA           | 1352       | U           |
| 35         | RA           | 1359       | A           |
| 35         | RA           | 1360       | A           |
| 35         | RA           | 1365       | A           |
| 35         | RA           | 1368       | G           |
| 35         | RA           | 1379       | A           |
| 35         | RA           | 1384       | A           |
| 35         | RA           | 1385       | G           |
| 35         | RA           | 1395       | A           |
| 35         | RA           | 1416       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | RA    | 1417    | C    |
| 35  | RA    | 1419    | A    |
| 35  | RA    | 1420    | U    |
| 35  | RA    | 1421    | G    |
| 35  | RA    | 1427    | A    |
| 35  | RA    | 1428    | C    |
| 35  | RA    | 1429    | G    |
| 35  | RA    | 1445(A) | A    |
| 35  | RA    | 1450(A) | G    |
| 35  | RA    | 1455    | G    |
| 35  | RA    | 1459    | G    |
| 35  | RA    | 1460    | A    |
| 35  | RA    | 1461    | G    |
| 35  | RA    | 1467    | C    |
| 35  | RA    | 1471    | A    |
| 35  | RA    | 1482    | G    |
| 35  | RA    | 1490    | A    |
| 35  | RA    | 1493    | C    |
| 35  | RA    | 1494    | A    |
| 35  | RA    | 1497    | U    |
| 35  | RA    | 1508    | A    |
| 35  | RA    | 1509(A) | C    |
| 35  | RA    | 1509(B) | A    |
| 35  | RA    | 1542    | A    |
| 35  | RA    | 1543    | C    |
| 35  | RA    | 1554    | A    |
| 35  | RA    | 1558    | A    |
| 35  | RA    | 1566    | A    |
| 35  | RA    | 1569    | A    |
| 35  | RA    | 1578    | U    |
| 35  | RA    | 1580    | A    |
| 35  | RA    | 1584    | C    |
| 35  | RA    | 1586    | A    |
| 35  | RA    | 1608    | A    |
| 35  | RA    | 1609    | A    |
| 35  | RA    | 1640    | C    |
| 35  | RA    | 1648    | C    |
| 35  | RA    | 1674    | G    |
| 35  | RA    | 1696    | G    |
| 35  | RA    | 1700    | A    |
| 35  | RA    | 1701    | A    |
| 35  | RA    | 1721    | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | RA           | 1722       | A           |
| 35         | RA           | 1750       | G           |
| 35         | RA           | 1756       | G           |
| 35         | RA           | 1762       | A           |
| 35         | RA           | 1763       | G           |
| 35         | RA           | 1764       | G           |
| 35         | RA           | 1773       | A           |
| 35         | RA           | 1774       | C           |
| 35         | RA           | 1780       | A           |
| 35         | RA           | 1786       | A           |
| 35         | RA           | 1791       | A           |
| 35         | RA           | 1800       | C           |
| 35         | RA           | 1801       | G           |
| 35         | RA           | 1816       | G           |
| 35         | RA           | 1828       | G           |
| 35         | RA           | 1829       | A           |
| 35         | RA           | 1835       | G           |
| 35         | RA           | 1847       | A           |
| 35         | RA           | 1848       | A           |
| 35         | RA           | 1877       | A           |
| 35         | RA           | 1878       | G           |
| 35         | RA           | 1900       | A           |
| 35         | RA           | 1906       | G           |
| 35         | RA           | 1913       | A           |
| 35         | RA           | 1914       | C           |
| 35         | RA           | 1927       | A           |
| 35         | RA           | 1929       | G           |
| 35         | RA           | 1930       | G           |
| 35         | RA           | 1936       | A           |
| 35         | RA           | 1938       | A           |
| 35         | RA           | 1955       | U           |
| 35         | RA           | 1963       | U           |
| 35         | RA           | 1967       | C           |
| 35         | RA           | 1970       | A           |
| 35         | RA           | 1971       | A           |
| 35         | RA           | 1972       | A           |
| 35         | RA           | 1984       | G           |
| 35         | RA           | 1992       | G           |
| 35         | RA           | 1993       | U           |
| 35         | RA           | 1997       | G           |
| 35         | RA           | 2004       | G           |
| 35         | RA           | 2020       | A           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | RA    | 2023 | G    |
| 35  | RA    | 2031 | A    |
| 35  | RA    | 2032 | G    |
| 35  | RA    | 2033 | A    |
| 35  | RA    | 2043 | C    |
| 35  | RA    | 2055 | C    |
| 35  | RA    | 2056 | G    |
| 35  | RA    | 2060 | A    |
| 35  | RA    | 2061 | G    |
| 35  | RA    | 2062 | A    |
| 35  | RA    | 2069 | G    |
| 35  | RA    | 2093 | G    |
| 35  | RA    | 2096 | U    |
| 35  | RA    | 2099 | U    |
| 35  | RA    | 2103 | C    |
| 35  | RA    | 2104 | G    |
| 35  | RA    | 2105 | C    |
| 35  | RA    | 2107 | C    |
| 35  | RA    | 2108 | C    |
| 35  | RA    | 2112 | G    |
| 35  | RA    | 2116 | G    |
| 35  | RA    | 2117 | A    |
| 35  | RA    | 2119 | A    |
| 35  | RA    | 2120 | G    |
| 35  | RA    | 2123 | G    |
| 35  | RA    | 2126 | A    |
| 35  | RA    | 2127 | G    |
| 35  | RA    | 2129 | C    |
| 35  | RA    | 2131 | G    |
| 35  | RA    | 2132 | U    |
| 35  | RA    | 2133 | G    |
| 35  | RA    | 2134 | A    |
| 35  | RA    | 2136 | C    |
| 35  | RA    | 2137 | C    |
| 35  | RA    | 2145 | C    |
| 35  | RA    | 2146 | C    |
| 35  | RA    | 2147 | G    |
| 35  | RA    | 2148 | G    |
| 35  | RA    | 2151 | G    |
| 35  | RA    | 2161 | C    |
| 35  | RA    | 2165 | G    |
| 35  | RA    | 2172 | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | RA           | 2173       | A           |
| 35         | RA           | 2176       | A           |
| 35         | RA           | 2186       | G           |
| 35         | RA           | 2189       | U           |
| 35         | RA           | 2192       | G           |
| 35         | RA           | 2198       | A           |
| 35         | RA           | 2206       | G           |
| 35         | RA           | 2207       | G           |
| 35         | RA           | 2208       | A           |
| 35         | RA           | 2218       | U           |
| 35         | RA           | 2219       | G           |
| 35         | RA           | 2225       | A           |
| 35         | RA           | 2238       | G           |
| 35         | RA           | 2239       | G           |
| 35         | RA           | 2249       | U           |
| 35         | RA           | 2269       | A           |
| 35         | RA           | 2275       | C           |
| 35         | RA           | 2278       | A           |
| 35         | RA           | 2279       | G           |
| 35         | RA           | 2283       | C           |
| 35         | RA           | 2287       | A           |
| 35         | RA           | 2288       | A           |
| 35         | RA           | 2292       | C           |
| 35         | RA           | 2305       | A           |
| 35         | RA           | 2308       | G           |
| 35         | RA           | 2319       | G           |
| 35         | RA           | 2320       | A           |
| 35         | RA           | 2321       | G           |
| 35         | RA           | 2322       | A           |
| 35         | RA           | 2325       | G           |
| 35         | RA           | 2334       | G           |
| 35         | RA           | 2335       | A           |
| 35         | RA           | 2336       | A           |
| 35         | RA           | 2343       | C           |
| 35         | RA           | 2345       | G           |
| 35         | RA           | 2347       | C           |
| 35         | RA           | 2350       | C           |
| 35         | RA           | 2354       | G           |
| 35         | RA           | 2372       | G           |
| 35         | RA           | 2383       | G           |
| 35         | RA           | 2385       | C           |
| 35         | RA           | 2391       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | RA           | 2396       | G           |
| 35         | RA           | 2406       | U           |
| 35         | RA           | 2407       | G           |
| 35         | RA           | 2410       | G           |
| 35         | RA           | 2422       | A           |
| 35         | RA           | 2424       | C           |
| 35         | RA           | 2425       | A           |
| 35         | RA           | 2426       | A           |
| 35         | RA           | 2429       | G           |
| 35         | RA           | 2430       | A           |
| 35         | RA           | 2435       | A           |
| 35         | RA           | 2439       | A           |
| 35         | RA           | 2441       | C           |
| 35         | RA           | 2445       | G           |
| 35         | RA           | 2448       | A           |
| 35         | RA           | 2476       | A           |
| 35         | RA           | 2478       | A           |
| 35         | RA           | 2491       | U           |
| 35         | RA           | 2494       | G           |
| 35         | RA           | 2502       | G           |
| 35         | RA           | 2505       | G           |
| 35         | RA           | 2518       | A           |
| 35         | RA           | 2520       | C           |
| 35         | RA           | 2529       | G           |
| 35         | RA           | 2554       | U           |
| 35         | RA           | 2564       | A           |
| 35         | RA           | 2566       | A           |
| 35         | RA           | 2567       | G           |
| 35         | RA           | 2572       | A           |
| 35         | RA           | 2582       | G           |
| 35         | RA           | 2602       | A           |
| 35         | RA           | 2603       | G           |
| 35         | RA           | 2611       | U           |
| 35         | RA           | 2612       | C           |
| 35         | RA           | 2615       | U           |
| 35         | RA           | 2621       | A           |
| 35         | RA           | 2629       | A           |
| 35         | RA           | 2630       | G           |
| 35         | RA           | 2646       | C           |
| 35         | RA           | 2654       | A           |
| 35         | RA           | 2663       | G           |
| 35         | RA           | 2686       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | RA    | 2689    | U    |
| 35  | RA    | 2690    | C    |
| 35  | RA    | 2702    | U    |
| 35  | RA    | 2703    | C    |
| 35  | RA    | 2712(B) | A    |
| 35  | RA    | 2713    | A    |
| 35  | RA    | 2714    | G    |
| 35  | RA    | 2718    | G    |
| 35  | RA    | 2726    | U    |
| 35  | RA    | 2732    | G    |
| 35  | RA    | 2733    | A    |
| 35  | RA    | 2748    | A    |
| 35  | RA    | 2758    | A    |
| 35  | RA    | 2765    | A    |
| 35  | RA    | 2778    | A    |
| 35  | RA    | 2818    | G    |
| 35  | RA    | 2820    | A    |
| 35  | RA    | 2821    | A    |
| 35  | RA    | 2823    | A    |
| 35  | RA    | 2833    | G    |
| 35  | RA    | 2835    | A    |
| 35  | RA    | 2839    | G    |
| 35  | RA    | 2866    | U    |
| 35  | RA    | 2872    | G    |
| 35  | RA    | 2880    | C    |
| 35  | RA    | 2892    | A    |
| 35  | RA    | 2894    | G    |
| 35  | RA    | 2896    | C    |
| 35  | RA    | 2897    | U    |
| 36  | RB    | 8       | U    |
| 36  | RB    | 9       | G    |
| 36  | RB    | 12      | C    |
| 36  | RB    | 13      | A    |
| 36  | RB    | 30      | C    |
| 36  | RB    | 33      | G    |
| 36  | RB    | 51      | G    |
| 36  | RB    | 56      | G    |
| 36  | RB    | 73      | A    |
| 36  | RB    | 110     | G    |
| 1   | XA    | 5       | U    |
| 1   | XA    | 7       | G    |
| 1   | XA    | 9       | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | XA    | 31     | G    |
| 1   | XA    | 32     | A    |
| 1   | XA    | 39     | G    |
| 1   | XA    | 47     | C    |
| 1   | XA    | 48     | C    |
| 1   | XA    | 51     | A    |
| 1   | XA    | 59     | A    |
| 1   | XA    | 61     | G    |
| 1   | XA    | 66     | G    |
| 1   | XA    | 88     | A    |
| 1   | XA    | 89     | C    |
| 1   | XA    | 101    | A    |
| 1   | XA    | 105    | G    |
| 1   | XA    | 116    | A    |
| 1   | XA    | 121    | C    |
| 1   | XA    | 129(B) | G    |
| 1   | XA    | 131    | C    |
| 1   | XA    | 144    | G    |
| 1   | XA    | 151    | A    |
| 1   | XA    | 163    | C    |
| 1   | XA    | 174    | C    |
| 1   | XA    | 182    | U    |
| 1   | XA    | 189(G) | U    |
| 1   | XA    | 189(I) | G    |
| 1   | XA    | 195    | A    |
| 1   | XA    | 197    | A    |
| 1   | XA    | 202    | U    |
| 1   | XA    | 203    | U    |
| 1   | XA    | 204    | U    |
| 1   | XA    | 216    | G    |
| 1   | XA    | 220    | G    |
| 1   | XA    | 247    | G    |
| 1   | XA    | 250    | A    |
| 1   | XA    | 251    | G    |
| 1   | XA    | 266    | G    |
| 1   | XA    | 267    | C    |
| 1   | XA    | 289    | G    |
| 1   | XA    | 301    | G    |
| 1   | XA    | 321    | A    |
| 1   | XA    | 328    | C    |
| 1   | XA    | 332    | G    |
| 1   | XA    | 346    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 350 | G    |
| 1   | XA    | 351 | G    |
| 1   | XA    | 352 | C    |
| 1   | XA    | 353 | A    |
| 1   | XA    | 354 | G    |
| 1   | XA    | 356 | A    |
| 1   | XA    | 367 | U    |
| 1   | XA    | 372 | C    |
| 1   | XA    | 373 | A    |
| 1   | XA    | 384 | G    |
| 1   | XA    | 388 | G    |
| 1   | XA    | 397 | A    |
| 1   | XA    | 398 | C    |
| 1   | XA    | 406 | G    |
| 1   | XA    | 412 | A    |
| 1   | XA    | 413 | G    |
| 1   | XA    | 424 | G    |
| 1   | XA    | 429 | U    |
| 1   | XA    | 439 | A    |
| 1   | XA    | 452 | A    |
| 1   | XA    | 461 | A    |
| 1   | XA    | 470 | C    |
| 1   | XA    | 482 | A    |
| 1   | XA    | 484 | G    |
| 1   | XA    | 485 | G    |
| 1   | XA    | 496 | A    |
| 1   | XA    | 498 | U    |
| 1   | XA    | 509 | A    |
| 1   | XA    | 510 | A    |
| 1   | XA    | 511 | C    |
| 1   | XA    | 518 | C    |
| 1   | XA    | 521 | G    |
| 1   | XA    | 532 | A    |
| 1   | XA    | 533 | A    |
| 1   | XA    | 547 | A    |
| 1   | XA    | 559 | A    |
| 1   | XA    | 561 | U    |
| 1   | XA    | 564 | C    |
| 1   | XA    | 572 | A    |
| 1   | XA    | 573 | A    |
| 1   | XA    | 576 | G    |
| 1   | XA    | 577 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 596 | C    |
| 1   | XA    | 630 | G    |
| 1   | XA    | 631 | G    |
| 1   | XA    | 653 | A    |
| 1   | XA    | 665 | A    |
| 1   | XA    | 666 | G    |
| 1   | XA    | 687 | A    |
| 1   | XA    | 688 | G    |
| 1   | XA    | 695 | A    |
| 1   | XA    | 703 | G    |
| 1   | XA    | 721 | G    |
| 1   | XA    | 723 | U    |
| 1   | XA    | 731 | G    |
| 1   | XA    | 749 | C    |
| 1   | XA    | 755 | G    |
| 1   | XA    | 759 | A    |
| 1   | XA    | 777 | A    |
| 1   | XA    | 793 | U    |
| 1   | XA    | 794 | A    |
| 1   | XA    | 815 | A    |
| 1   | XA    | 816 | A    |
| 1   | XA    | 817 | C    |
| 1   | XA    | 821 | G    |
| 1   | XA    | 828 | A    |
| 1   | XA    | 829 | G    |
| 1   | XA    | 836 | G    |
| 1   | XA    | 840 | C    |
| 1   | XA    | 841 | U    |
| 1   | XA    | 848 | C    |
| 1   | XA    | 851 | G    |
| 1   | XA    | 891 | U    |
| 1   | XA    | 902 | G    |
| 1   | XA    | 914 | A    |
| 1   | XA    | 916 | G    |
| 1   | XA    | 926 | G    |
| 1   | XA    | 927 | G    |
| 1   | XA    | 934 | C    |
| 1   | XA    | 960 | U    |
| 1   | XA    | 961 | U    |
| 1   | XA    | 968 | A    |
| 1   | XA    | 969 | A    |
| 1   | XA    | 971 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 974     | A    |
| 1   | XA    | 975     | A    |
| 1   | XA    | 976     | G    |
| 1   | XA    | 977     | A    |
| 1   | XA    | 992     | U    |
| 1   | XA    | 993     | G    |
| 1   | XA    | 1002    | G    |
| 1   | XA    | 1003    | G    |
| 1   | XA    | 1004    | A    |
| 1   | XA    | 1005    | A    |
| 1   | XA    | 1006    | C    |
| 1   | XA    | 1020    | U    |
| 1   | XA    | 1023    | G    |
| 1   | XA    | 1025    | U    |
| 1   | XA    | 1026    | G    |
| 1   | XA    | 1027    | C    |
| 1   | XA    | 1028    | C    |
| 1   | XA    | 1030(B) | G    |
| 1   | XA    | 1030(C) | C    |
| 1   | XA    | 1031    | G    |
| 1   | XA    | 1043    | C    |
| 1   | XA    | 1044    | A    |
| 1   | XA    | 1053    | G    |
| 1   | XA    | 1054    | C    |
| 1   | XA    | 1065    | U    |
| 1   | XA    | 1066    | C    |
| 1   | XA    | 1068    | G    |
| 1   | XA    | 1081    | G    |
| 1   | XA    | 1094    | G    |
| 1   | XA    | 1095    | U    |
| 1   | XA    | 1100    | C    |
| 1   | XA    | 1101    | A    |
| 1   | XA    | 1117    | G    |
| 1   | XA    | 1125    | U    |
| 1   | XA    | 1129    | C    |
| 1   | XA    | 1130    | A    |
| 1   | XA    | 1136    | U    |
| 1   | XA    | 1137    | C    |
| 1   | XA    | 1138    | G    |
| 1   | XA    | 1139    | G    |
| 1   | XA    | 1146    | A    |
| 1   | XA    | 1147    | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 1152    | A    |
| 1   | XA    | 1157    | A    |
| 1   | XA    | 1158    | C    |
| 1   | XA    | 1159    | U    |
| 1   | XA    | 1183    | A    |
| 1   | XA    | 1196    | U    |
| 1   | XA    | 1197    | G    |
| 1   | XA    | 1201    | A    |
| 1   | XA    | 1211    | U    |
| 1   | XA    | 1214    | C    |
| 1   | XA    | 1224    | G    |
| 1   | XA    | 1227    | A    |
| 1   | XA    | 1236    | A    |
| 1   | XA    | 1238    | A    |
| 1   | XA    | 1250    | A    |
| 1   | XA    | 1256    | A    |
| 1   | XA    | 1257    | U    |
| 1   | XA    | 1258    | G    |
| 1   | XA    | 1260    | C    |
| 1   | XA    | 1270    | C    |
| 1   | XA    | 1278    | U    |
| 1   | XA    | 1279    | A    |
| 1   | XA    | 1280    | A    |
| 1   | XA    | 1282    | C    |
| 1   | XA    | 1285    | A    |
| 1   | XA    | 1286    | A    |
| 1   | XA    | 1287    | A    |
| 1   | XA    | 1300    | G    |
| 1   | XA    | 1302    | U    |
| 1   | XA    | 1303    | C    |
| 1   | XA    | 1305    | G    |
| 1   | XA    | 1317    | C    |
| 1   | XA    | 1320    | C    |
| 1   | XA    | 1340    | A    |
| 1   | XA    | 1347    | G    |
| 1   | XA    | 1353    | G    |
| 1   | XA    | 1363(A) | C    |
| 1   | XA    | 1363(B) | A    |
| 1   | XA    | 1370    | G    |
| 1   | XA    | 1397    | C    |
| 1   | XA    | 1399    | C    |
| 1   | XA    | 1419    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 1442(A) | G    |
| 1   | XA    | 1442(B) | G    |
| 1   | XA    | 1447    | A    |
| 1   | XA    | 1456    | G    |
| 1   | XA    | 1469    | G    |
| 1   | XA    | 1487    | G    |
| 1   | XA    | 1492    | A    |
| 1   | XA    | 1497    | G    |
| 1   | XA    | 1499    | A    |
| 1   | XA    | 1503    | A    |
| 1   | XA    | 1504    | G    |
| 1   | XA    | 1506    | U    |
| 1   | XA    | 1517    | G    |
| 1   | XA    | 1520    | G    |
| 1   | XA    | 1529    | G    |
| 1   | XA    | 1530    | G    |
| 1   | XA    | 1531    | A    |
| 22  | XV    | 3       | C    |
| 22  | XV    | 8       | U    |
| 22  | XV    | 16      | C    |
| 22  | XV    | 17(A)   | U    |
| 22  | XV    | 18      | G    |
| 22  | XV    | 19      | G    |
| 22  | XV    | 20      | U    |
| 22  | XV    | 21      | A    |
| 22  | XV    | 47      | U    |
| 22  | XV    | 48      | C    |
| 22  | XV    | 49      | G    |
| 22  | XV    | 65      | C    |
| 22  | XV    | 76      | A    |
| 23  | XX    | 7       | G    |
| 23  | XX    | 10      | G    |
| 23  | XX    | 11      | U    |
| 23  | XX    | 13      | A    |
| 23  | XX    | 14      | A    |
| 23  | XX    | 15      | A    |
| 23  | XX    | 19      | G    |
| 23  | XX    | 23      | A    |
| 24  | XY    | 2       | G    |
| 24  | XY    | 8       | U    |
| 24  | XY    | 9       | A    |
| 24  | XY    | 12      | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | XY    | 16  | C    |
| 24  | XY    | 17  | U    |
| 24  | XY    | 18  | G    |
| 24  | XY    | 19  | G    |
| 24  | XY    | 21  | A    |
| 24  | XY    | 23  | A    |
| 24  | XY    | 29  | U    |
| 24  | XY    | 31  | C    |
| 24  | XY    | 43  | G    |
| 24  | XY    | 46  | G    |
| 24  | XY    | 47  | U    |
| 24  | XY    | 48  | C    |
| 24  | XY    | 49  | A    |
| 24  | XY    | 50  | G    |
| 24  | XY    | 51  | C    |
| 24  | XY    | 52  | G    |
| 24  | XY    | 54  | U    |
| 24  | XY    | 55  | U    |
| 24  | XY    | 56  | C    |
| 24  | XY    | 57  | G    |
| 24  | XY    | 58  | A    |
| 24  | XY    | 61  | C    |
| 24  | XY    | 67  | A    |
| 24  | XY    | 68  | G    |
| 24  | XY    | 69  | C    |
| 24  | XY    | 71  | C    |
| 24  | XY    | 73  | A    |
| 24  | XY    | 74  | C    |
| 24  | XY    | 75  | C    |
| 35  | YA    | 10  | G    |
| 35  | YA    | 34  | C    |
| 35  | YA    | 45  | C    |
| 35  | YA    | 51  | G    |
| 35  | YA    | 55  | G    |
| 35  | YA    | 71  | A    |
| 35  | YA    | 74  | A    |
| 35  | YA    | 75  | G    |
| 35  | YA    | 84  | A    |
| 35  | YA    | 92  | A    |
| 35  | YA    | 95  | G    |
| 35  | YA    | 102 | G    |
| 35  | YA    | 118 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | YA    | 119    | A    |
| 35  | YA    | 120    | U    |
| 35  | YA    | 131    | G    |
| 35  | YA    | 157    | U    |
| 35  | YA    | 182    | A    |
| 35  | YA    | 188    | G    |
| 35  | YA    | 196    | A    |
| 35  | YA    | 199    | A    |
| 35  | YA    | 205    | G    |
| 35  | YA    | 215    | G    |
| 35  | YA    | 216    | A    |
| 35  | YA    | 221    | A    |
| 35  | YA    | 222    | A    |
| 35  | YA    | 228    | A    |
| 35  | YA    | 229    | A    |
| 35  | YA    | 230    | U    |
| 35  | YA    | 233    | A    |
| 35  | YA    | 248    | G    |
| 35  | YA    | 265    | A    |
| 35  | YA    | 272(J) | C    |
| 35  | YA    | 272(K) | U    |
| 35  | YA    | 272(N) | U    |
| 35  | YA    | 273(B) | U    |
| 35  | YA    | 273(C) | G    |
| 35  | YA    | 277    | C    |
| 35  | YA    | 278    | A    |
| 35  | YA    | 311    | A    |
| 35  | YA    | 317    | G    |
| 35  | YA    | 324    | A    |
| 35  | YA    | 329    | G    |
| 35  | YA    | 330    | A    |
| 35  | YA    | 338    | G    |
| 35  | YA    | 342    | G    |
| 35  | YA    | 345    | A    |
| 35  | YA    | 352    | G    |
| 35  | YA    | 362    | U    |
| 35  | YA    | 363(A) | G    |
| 35  | YA    | 372    | G    |
| 35  | YA    | 386    | G    |
| 35  | YA    | 396    | G    |
| 35  | YA    | 405    | U    |
| 35  | YA    | 411    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | YA    | 412    | A    |
| 35  | YA    | 428    | A    |
| 35  | YA    | 444    | C    |
| 35  | YA    | 455    | C    |
| 35  | YA    | 457    | A    |
| 35  | YA    | 467    | G    |
| 35  | YA    | 470    | A    |
| 35  | YA    | 481    | G    |
| 35  | YA    | 505    | A    |
| 35  | YA    | 508    | G    |
| 35  | YA    | 509    | C    |
| 35  | YA    | 530    | G    |
| 35  | YA    | 531    | C    |
| 35  | YA    | 532    | A    |
| 35  | YA    | 533    | G    |
| 35  | YA    | 563    | G    |
| 35  | YA    | 573    | G    |
| 35  | YA    | 575    | A    |
| 35  | YA    | 603    | A    |
| 35  | YA    | 604    | G    |
| 35  | YA    | 607    | U    |
| 35  | YA    | 614(C) | G    |
| 35  | YA    | 615    | G    |
| 35  | YA    | 620    | G    |
| 35  | YA    | 627    | A    |
| 35  | YA    | 634    | C    |
| 35  | YA    | 637    | A    |
| 35  | YA    | 645    | C    |
| 35  | YA    | 646    | A    |
| 35  | YA    | 652(C) | A    |
| 35  | YA    | 652(D) | G    |
| 35  | YA    | 652(V) | G    |
| 35  | YA    | 669    | G    |
| 35  | YA    | 686    | G    |
| 35  | YA    | 717    | G    |
| 35  | YA    | 726    | G    |
| 35  | YA    | 730    | C    |
| 35  | YA    | 734    | A    |
| 35  | YA    | 738    | G    |
| 35  | YA    | 753    | C    |
| 35  | YA    | 764    | A    |
| 35  | YA    | 765    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | YA    | 775    | G    |
| 35  | YA    | 776    | G    |
| 35  | YA    | 782    | A    |
| 35  | YA    | 784    | A    |
| 35  | YA    | 785    | G    |
| 35  | YA    | 788    | A    |
| 35  | YA    | 789    | A    |
| 35  | YA    | 792    | G    |
| 35  | YA    | 805    | G    |
| 35  | YA    | 812    | C    |
| 35  | YA    | 827    | U    |
| 35  | YA    | 828    | U    |
| 35  | YA    | 831    | G    |
| 35  | YA    | 857    | C    |
| 35  | YA    | 859    | G    |
| 35  | YA    | 869    | G    |
| 35  | YA    | 881    | G    |
| 35  | YA    | 886    | C    |
| 35  | YA    | 887    | A    |
| 35  | YA    | 888    | C    |
| 35  | YA    | 889    | C    |
| 35  | YA    | 890    | A    |
| 35  | YA    | 893    | C    |
| 35  | YA    | 896    | A    |
| 35  | YA    | 897    | C    |
| 35  | YA    | 898    | C    |
| 35  | YA    | 907    | U    |
| 35  | YA    | 910    | A    |
| 35  | YA    | 915    | C    |
| 35  | YA    | 917    | A    |
| 35  | YA    | 932    | G    |
| 35  | YA    | 941    | A    |
| 35  | YA    | 945    | A    |
| 35  | YA    | 946    | G    |
| 35  | YA    | 953    | A    |
| 35  | YA    | 957    | A    |
| 35  | YA    | 959    | A    |
| 35  | YA    | 961    | C    |
| 35  | YA    | 973    | A    |
| 35  | YA    | 974    | G    |
| 35  | YA    | 975(A) | C    |
| 35  | YA    | 983    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | YA           | 996        | A           |
| 35         | YA           | 1005       | C           |
| 35         | YA           | 1008       | C           |
| 35         | YA           | 1012       | U           |
| 35         | YA           | 1013       | C           |
| 35         | YA           | 1025       | G           |
| 35         | YA           | 1026       | U           |
| 35         | YA           | 1033       | U           |
| 35         | YA           | 1045       | A           |
| 35         | YA           | 1046       | A           |
| 35         | YA           | 1047       | G           |
| 35         | YA           | 1052       | C           |
| 35         | YA           | 1054       | A           |
| 35         | YA           | 1058       | G           |
| 35         | YA           | 1060       | U           |
| 35         | YA           | 1063       | G           |
| 35         | YA           | 1064       | C           |
| 35         | YA           | 1065       | U           |
| 35         | YA           | 1066       | U           |
| 35         | YA           | 1067       | A           |
| 35         | YA           | 1068       | G           |
| 35         | YA           | 1070       | A           |
| 35         | YA           | 1071       | G           |
| 35         | YA           | 1073       | A           |
| 35         | YA           | 1074       | G           |
| 35         | YA           | 1076       | C           |
| 35         | YA           | 1077       | A           |
| 35         | YA           | 1079       | C           |
| 35         | YA           | 1082       | U           |
| 35         | YA           | 1083       | U           |
| 35         | YA           | 1084       | A           |
| 35         | YA           | 1085       | A           |
| 35         | YA           | 1086       | A           |
| 35         | YA           | 1088       | A           |
| 35         | YA           | 1092       | C           |
| 35         | YA           | 1096       | A           |
| 35         | YA           | 1097       | U           |
| 35         | YA           | 1098       | A           |
| 35         | YA           | 1108       | U           |
| 35         | YA           | 1109       | C           |
| 35         | YA           | 1110       | G           |
| 35         | YA           | 1112       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | YA    | 1128    | A    |
| 35  | YA    | 1129    | A    |
| 35  | YA    | 1130    | U    |
| 35  | YA    | 1135    | C    |
| 35  | YA    | 1136    | G    |
| 35  | YA    | 1143    | A    |
| 35  | YA    | 1171    | G    |
| 35  | YA    | 1206    | G    |
| 35  | YA    | 1211    | U    |
| 35  | YA    | 1220    | A    |
| 35  | YA    | 1236    | G    |
| 35  | YA    | 1250    | G    |
| 35  | YA    | 1253    | A    |
| 35  | YA    | 1256    | G    |
| 35  | YA    | 1265    | A    |
| 35  | YA    | 1271    | G    |
| 35  | YA    | 1272    | A    |
| 35  | YA    | 1273    | U    |
| 35  | YA    | 1300    | U    |
| 35  | YA    | 1301    | A    |
| 35  | YA    | 1313    | U    |
| 35  | YA    | 1314    | C    |
| 35  | YA    | 1352    | U    |
| 35  | YA    | 1359    | A    |
| 35  | YA    | 1360    | A    |
| 35  | YA    | 1365    | A    |
| 35  | YA    | 1368    | G    |
| 35  | YA    | 1378    | A    |
| 35  | YA    | 1379    | A    |
| 35  | YA    | 1380    | G    |
| 35  | YA    | 1384    | A    |
| 35  | YA    | 1385    | G    |
| 35  | YA    | 1395    | A    |
| 35  | YA    | 1416    | G    |
| 35  | YA    | 1417    | C    |
| 35  | YA    | 1419    | A    |
| 35  | YA    | 1420    | U    |
| 35  | YA    | 1421    | G    |
| 35  | YA    | 1427    | A    |
| 35  | YA    | 1428    | C    |
| 35  | YA    | 1445(A) | A    |
| 35  | YA    | 1450(A) | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 35  | YA    | 1455    | G    |
| 35  | YA    | 1459    | G    |
| 35  | YA    | 1460    | A    |
| 35  | YA    | 1467    | C    |
| 35  | YA    | 1471    | A    |
| 35  | YA    | 1482    | G    |
| 35  | YA    | 1493    | C    |
| 35  | YA    | 1494    | A    |
| 35  | YA    | 1497    | U    |
| 35  | YA    | 1508    | A    |
| 35  | YA    | 1509(A) | C    |
| 35  | YA    | 1509(B) | A    |
| 35  | YA    | 1525    | G    |
| 35  | YA    | 1542    | A    |
| 35  | YA    | 1543    | C    |
| 35  | YA    | 1547    | C    |
| 35  | YA    | 1558    | A    |
| 35  | YA    | 1566    | A    |
| 35  | YA    | 1569    | A    |
| 35  | YA    | 1578    | U    |
| 35  | YA    | 1580    | A    |
| 35  | YA    | 1584    | C    |
| 35  | YA    | 1586    | A    |
| 35  | YA    | 1607    | C    |
| 35  | YA    | 1608    | A    |
| 35  | YA    | 1609    | A    |
| 35  | YA    | 1640    | C    |
| 35  | YA    | 1648    | C    |
| 35  | YA    | 1674    | G    |
| 35  | YA    | 1693    | U    |
| 35  | YA    | 1696    | G    |
| 35  | YA    | 1698    | A    |
| 35  | YA    | 1700    | A    |
| 35  | YA    | 1701    | A    |
| 35  | YA    | 1721    | G    |
| 35  | YA    | 1722    | A    |
| 35  | YA    | 1750    | G    |
| 35  | YA    | 1756    | G    |
| 35  | YA    | 1757    | U    |
| 35  | YA    | 1762    | A    |
| 35  | YA    | 1763    | G    |
| 35  | YA    | 1764    | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | YA           | 1769       | G           |
| 35         | YA           | 1773       | A           |
| 35         | YA           | 1774       | C           |
| 35         | YA           | 1780       | A           |
| 35         | YA           | 1786       | A           |
| 35         | YA           | 1791       | A           |
| 35         | YA           | 1800       | C           |
| 35         | YA           | 1801       | G           |
| 35         | YA           | 1811       | G           |
| 35         | YA           | 1816       | G           |
| 35         | YA           | 1828       | G           |
| 35         | YA           | 1829       | A           |
| 35         | YA           | 1835       | G           |
| 35         | YA           | 1847       | A           |
| 35         | YA           | 1848       | A           |
| 35         | YA           | 1877       | A           |
| 35         | YA           | 1878       | G           |
| 35         | YA           | 1889       | A           |
| 35         | YA           | 1900       | A           |
| 35         | YA           | 1914       | C           |
| 35         | YA           | 1929       | G           |
| 35         | YA           | 1930       | G           |
| 35         | YA           | 1936       | A           |
| 35         | YA           | 1937       | A           |
| 35         | YA           | 1938       | A           |
| 35         | YA           | 1955       | U           |
| 35         | YA           | 1963       | U           |
| 35         | YA           | 1967       | C           |
| 35         | YA           | 1970       | A           |
| 35         | YA           | 1971       | A           |
| 35         | YA           | 1972       | A           |
| 35         | YA           | 1984       | G           |
| 35         | YA           | 1992       | G           |
| 35         | YA           | 1993       | U           |
| 35         | YA           | 1997       | G           |
| 35         | YA           | 2020       | A           |
| 35         | YA           | 2023       | G           |
| 35         | YA           | 2031       | A           |
| 35         | YA           | 2032       | G           |
| 35         | YA           | 2033       | A           |
| 35         | YA           | 2043       | C           |
| 35         | YA           | 2055       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | YA           | 2056       | G           |
| 35         | YA           | 2060       | A           |
| 35         | YA           | 2061       | G           |
| 35         | YA           | 2062       | A           |
| 35         | YA           | 2069       | G           |
| 35         | YA           | 2093       | G           |
| 35         | YA           | 2096       | U           |
| 35         | YA           | 2099       | U           |
| 35         | YA           | 2103       | C           |
| 35         | YA           | 2104       | G           |
| 35         | YA           | 2105       | C           |
| 35         | YA           | 2107       | C           |
| 35         | YA           | 2108       | C           |
| 35         | YA           | 2116       | G           |
| 35         | YA           | 2117       | A           |
| 35         | YA           | 2119       | A           |
| 35         | YA           | 2120       | G           |
| 35         | YA           | 2121       | G           |
| 35         | YA           | 2123       | G           |
| 35         | YA           | 2127       | G           |
| 35         | YA           | 2129       | C           |
| 35         | YA           | 2131       | G           |
| 35         | YA           | 2132       | U           |
| 35         | YA           | 2133       | G           |
| 35         | YA           | 2134       | A           |
| 35         | YA           | 2136       | C           |
| 35         | YA           | 2145       | C           |
| 35         | YA           | 2146       | C           |
| 35         | YA           | 2147       | G           |
| 35         | YA           | 2148       | G           |
| 35         | YA           | 2151       | G           |
| 35         | YA           | 2158       | A           |
| 35         | YA           | 2161       | C           |
| 35         | YA           | 2165       | G           |
| 35         | YA           | 2172       | U           |
| 35         | YA           | 2173       | A           |
| 35         | YA           | 2186       | G           |
| 35         | YA           | 2189       | U           |
| 35         | YA           | 2192       | G           |
| 35         | YA           | 2198       | A           |
| 35         | YA           | 2206       | G           |
| 35         | YA           | 2207       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | YA    | 2208 | A    |
| 35  | YA    | 2218 | U    |
| 35  | YA    | 2219 | G    |
| 35  | YA    | 2225 | A    |
| 35  | YA    | 2238 | G    |
| 35  | YA    | 2239 | G    |
| 35  | YA    | 2249 | U    |
| 35  | YA    | 2269 | A    |
| 35  | YA    | 2275 | C    |
| 35  | YA    | 2278 | A    |
| 35  | YA    | 2279 | G    |
| 35  | YA    | 2283 | C    |
| 35  | YA    | 2287 | A    |
| 35  | YA    | 2288 | A    |
| 35  | YA    | 2305 | A    |
| 35  | YA    | 2308 | G    |
| 35  | YA    | 2309 | A    |
| 35  | YA    | 2312 | U    |
| 35  | YA    | 2319 | G    |
| 35  | YA    | 2320 | A    |
| 35  | YA    | 2321 | G    |
| 35  | YA    | 2322 | A    |
| 35  | YA    | 2325 | G    |
| 35  | YA    | 2334 | G    |
| 35  | YA    | 2335 | A    |
| 35  | YA    | 2336 | A    |
| 35  | YA    | 2343 | C    |
| 35  | YA    | 2347 | C    |
| 35  | YA    | 2350 | C    |
| 35  | YA    | 2354 | G    |
| 35  | YA    | 2372 | G    |
| 35  | YA    | 2383 | G    |
| 35  | YA    | 2385 | C    |
| 35  | YA    | 2391 | G    |
| 35  | YA    | 2396 | G    |
| 35  | YA    | 2406 | U    |
| 35  | YA    | 2410 | G    |
| 35  | YA    | 2422 | A    |
| 35  | YA    | 2424 | C    |
| 35  | YA    | 2425 | A    |
| 35  | YA    | 2427 | C    |
| 35  | YA    | 2428 | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | YA           | 2429       | G           |
| 35         | YA           | 2430       | A           |
| 35         | YA           | 2435       | A           |
| 35         | YA           | 2439       | A           |
| 35         | YA           | 2441       | C           |
| 35         | YA           | 2445       | G           |
| 35         | YA           | 2448       | A           |
| 35         | YA           | 2476       | A           |
| 35         | YA           | 2491       | U           |
| 35         | YA           | 2494       | G           |
| 35         | YA           | 2502       | G           |
| 35         | YA           | 2505       | G           |
| 35         | YA           | 2518       | A           |
| 35         | YA           | 2520       | C           |
| 35         | YA           | 2529       | G           |
| 35         | YA           | 2554       | U           |
| 35         | YA           | 2564       | A           |
| 35         | YA           | 2566       | A           |
| 35         | YA           | 2567       | G           |
| 35         | YA           | 2582       | G           |
| 35         | YA           | 2586       | C           |
| 35         | YA           | 2602       | A           |
| 35         | YA           | 2604       | U           |
| 35         | YA           | 2609       | U           |
| 35         | YA           | 2611       | U           |
| 35         | YA           | 2612       | C           |
| 35         | YA           | 2615       | U           |
| 35         | YA           | 2629       | A           |
| 35         | YA           | 2630       | G           |
| 35         | YA           | 2633       | G           |
| 35         | YA           | 2646       | C           |
| 35         | YA           | 2654       | A           |
| 35         | YA           | 2663       | G           |
| 35         | YA           | 2673       | G           |
| 35         | YA           | 2686       | G           |
| 35         | YA           | 2689       | U           |
| 35         | YA           | 2690       | C           |
| 35         | YA           | 2691       | C           |
| 35         | YA           | 2702       | U           |
| 35         | YA           | 2703       | C           |
| 35         | YA           | 2712(B)    | A           |
| 35         | YA           | 2713       | A           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | YA    | 2714 | G    |
| 35  | YA    | 2726 | U    |
| 35  | YA    | 2732 | G    |
| 35  | YA    | 2733 | A    |
| 35  | YA    | 2748 | A    |
| 35  | YA    | 2758 | A    |
| 35  | YA    | 2764 | A    |
| 35  | YA    | 2765 | A    |
| 35  | YA    | 2766 | G    |
| 35  | YA    | 2778 | A    |
| 35  | YA    | 2818 | G    |
| 35  | YA    | 2820 | A    |
| 35  | YA    | 2821 | A    |
| 35  | YA    | 2833 | G    |
| 35  | YA    | 2835 | A    |
| 35  | YA    | 2866 | U    |
| 35  | YA    | 2872 | G    |
| 35  | YA    | 2892 | A    |
| 35  | YA    | 2894 | G    |
| 35  | YA    | 2896 | C    |
| 35  | YA    | 2897 | U    |
| 36  | YB    | 8    | U    |
| 36  | YB    | 9    | G    |
| 36  | YB    | 12   | C    |
| 36  | YB    | 13   | A    |
| 36  | YB    | 24   | G    |
| 36  | YB    | 30   | C    |
| 36  | YB    | 33   | G    |
| 36  | YB    | 51   | G    |
| 36  | YB    | 56   | G    |
| 36  | YB    | 73   | A    |
| 36  | YB    | 110  | G    |

All (63) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 60  | A    |
| 1   | QA    | 65  | U    |
| 1   | QA    | 115 | G    |
| 1   | QA    | 266 | G    |
| 1   | QA    | 509 | A    |
| 1   | QA    | 560 | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | QA           | 687        | A           |
| 1          | QA           | 748        | C           |
| 1          | QA           | 840        | C           |
| 1          | QA           | 913        | A           |
| 1          | QA           | 991        | U           |
| 1          | QA           | 992        | U           |
| 1          | QA           | 1065       | U           |
| 1          | QA           | 1067       | A           |
| 1          | QA           | 1442(A)    | G           |
| 23         | QX           | 18         | G           |
| 35         | RA           | 272(M)     | G           |
| 35         | RA           | 277        | C           |
| 35         | RA           | 752        | A           |
| 35         | RA           | 827        | U           |
| 35         | RA           | 856        | C           |
| 35         | RA           | 1057       | A           |
| 35         | RA           | 1065       | U           |
| 35         | RA           | 1073       | A           |
| 35         | RA           | 1210       | A           |
| 35         | RA           | 1992       | G           |
| 35         | RA           | 2126       | A           |
| 35         | RA           | 2171       | A           |
| 35         | RA           | 2172       | U           |
| 35         | RA           | 2406       | U           |
| 35         | RA           | 2601       | C           |
| 35         | RA           | 2689       | U           |
| 1          | XA           | 60         | A           |
| 1          | XA           | 65         | U           |
| 1          | XA           | 115        | G           |
| 1          | XA           | 266        | G           |
| 1          | XA           | 509        | A           |
| 1          | XA           | 560        | U           |
| 1          | XA           | 687        | A           |
| 1          | XA           | 748        | C           |
| 1          | XA           | 840        | C           |
| 1          | XA           | 913        | A           |
| 1          | XA           | 991        | U           |
| 1          | XA           | 992        | U           |
| 1          | XA           | 1065       | U           |
| 1          | XA           | 1067       | A           |
| 1          | XA           | 1442(A)    | G           |
| 23         | XX           | 18         | G           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 35  | YA    | 272(M) | G    |
| 35  | YA    | 277    | C    |
| 35  | YA    | 752    | A    |
| 35  | YA    | 827    | U    |
| 35  | YA    | 856    | C    |
| 35  | YA    | 1057   | A    |
| 35  | YA    | 1065   | U    |
| 35  | YA    | 1073   | A    |
| 35  | YA    | 1210   | A    |
| 35  | YA    | 1992   | G    |
| 35  | YA    | 2126   | A    |
| 35  | YA    | 2171   | A    |
| 35  | YA    | 2172   | U    |
| 35  | YA    | 2406   | U    |
| 35  | YA    | 2689   | U    |

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

48 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$ |
| 12  | 0TD  | XL    | 92   | 12    | 8,9,10       | 3.41 | 3 (37%)     | 6,11,13     | 1.49 | 1 (16%)     |
| 1   | MA6  | QA    | 1519 | 1     | 23,26,27     | 1.51 | 5 (21%)     | 33,38,41    | 2.41 | 13 (39%)    |
| 1   | 2MG  | QA    | 1207 | 1     | 23,26,27     | 1.27 | 4 (17%)     | 33,38,41    | 2.26 | 10 (30%)    |
| 1   | 2MG  | XA    | 1207 | 1     | 23,26,27     | 1.27 | 3 (13%)     | 33,38,41    | 2.29 | 10 (30%)    |
| 1   | 5MC  | QA    | 967  | 1     | 19,22,23     | 1.56 | 3 (15%)     | 26,32,35    | 1.18 | 3 (11%)     |
| 35  | 2MA  | RA    | 2503 | 35,56 | 22,25,26     | 1.44 | 5 (22%)     | 32,37,40    | 2.44 | 8 (25%)     |
| 35  | OMC  | RA    | 1920 | 35    | 19,22,23     | 0.83 | 1 (5%)      | 25,31,34    | 1.17 | 3 (12%)     |
| 35  | 5MU  | RA    | 1939 | 35    | 19,22,23     | 1.42 | 4 (21%)     | 27,32,35    | 2.30 | 6 (22%)     |
| 35  | OMC  | YA    | 1920 | 35    | 19,22,23     | 0.86 | 2 (10%)     | 25,31,34    | 1.19 | 3 (12%)     |
| 1   | MA6  | QA    | 1518 | 1     | 23,26,27     | 1.60 | 6 (26%)     | 33,38,41    | 2.35 | 10 (30%)    |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MA6  | XA    | 1518 | 1        | 23,26,27     | 1.60 | 6 (26%)  | 33,38,41    | 2.41 | 12 (36%) |
| 1   | 5MC  | XA    | 1404 | 1        | 19,22,23     | 1.28 | 2 (10%)  | 26,32,35    | 1.18 | 3 (11%)  |
| 35  | 2MA  | YA    | 2503 | 35,56    | 22,25,26     | 1.43 | 5 (22%)  | 32,37,40    | 2.31 | 8 (25%)  |
| 35  | 5MU  | YA    | 1939 | 35       | 19,22,23     | 1.39 | 4 (21%)  | 27,32,35    | 2.26 | 6 (22%)  |
| 35  | 5MU  | YA    | 1915 | 35       | 19,22,23     | 1.48 | 5 (26%)  | 27,32,35    | 2.66 | 9 (33%)  |
| 12  | 0TD  | QL    | 92   | 12       | 8,9,10       | 3.79 | 1 (12%)  | 6,11,13     | 2.26 | 3 (50%)  |
| 35  | PSU  | RA    | 1911 | 35       | 18,21,22     | 1.42 | 4 (22%)  | 21,30,33    | 2.09 | 4 (19%)  |
| 1   | PSU  | XA    | 516  | 1        | 18,21,22     | 1.44 | 4 (22%)  | 21,30,33    | 2.06 | 5 (23%)  |
| 1   | M2G  | XA    | 966  | 1        | 24,27,28     | 1.29 | 5 (20%)  | 33,40,43    | 1.82 | 5 (15%)  |
| 1   | 5MC  | XA    | 967  | 1        | 19,22,23     | 1.24 | 2 (10%)  | 26,32,35    | 1.18 | 3 (11%)  |
| 1   | MA6  | XA    | 1519 | 1        | 23,26,27     | 1.51 | 6 (26%)  | 33,38,41    | 2.40 | 13 (39%) |
| 1   | 5MC  | XA    | 1400 | 1        | 19,22,23     | 1.44 | 3 (15%)  | 26,32,35    | 1.21 | 2 (7%)   |
| 1   | G7M  | XA    | 527  | 56,1     | 23,26,27     | 2.27 | 5 (21%)  | 34,39,42    | 3.28 | 10 (29%) |
| 1   | 4OC  | XA    | 1402 | 1        | 20,23,24     | 0.81 | 1 (5%)   | 25,32,35    | 1.03 | 1 (4%)   |
| 1   | 5MC  | QA    | 1407 | 1        | 19,22,23     | 1.33 | 3 (15%)  | 26,32,35    | 1.45 | 2 (7%)   |
| 1   | UR3  | XA    | 1498 | 1        | 19,22,23     | 0.98 | 2 (10%)  | 26,32,35    | 1.71 | 3 (11%)  |
| 35  | PSU  | RA    | 2605 | 35       | 18,21,22     | 1.47 | 4 (22%)  | 21,30,33    | 2.03 | 4 (19%)  |
| 35  | PSU  | YA    | 2605 | 35       | 18,21,22     | 1.51 | 4 (22%)  | 21,30,33    | 2.11 | 4 (19%)  |
| 35  | 5MU  | RA    | 1915 | 35       | 19,22,23     | 1.54 | 5 (26%)  | 27,32,35    | 2.68 | 9 (33%)  |
| 35  | 5MC  | RA    | 1942 | 35       | 19,22,23     | 1.50 | 3 (15%)  | 26,32,35    | 1.22 | 3 (11%)  |
| 35  | OMG  | RA    | 2251 | 22,35,56 | 23,26,27     | 1.25 | 3 (13%)  | 32,38,41    | 1.98 | 6 (18%)  |
| 35  | OMG  | YA    | 2251 | 22,35,56 | 23,26,27     | 1.27 | 3 (13%)  | 32,38,41    | 2.08 | 6 (18%)  |
| 1   | G7M  | QA    | 527  | 56,1     | 23,26,27     | 2.32 | 5 (21%)  | 34,39,42    | 3.15 | 11 (32%) |
| 35  | PSU  | YA    | 1917 | 35,56    | 18,21,22     | 1.45 | 4 (22%)  | 21,30,33    | 2.01 | 3 (14%)  |
| 1   | 5MC  | QA    | 1400 | 1        | 19,22,23     | 1.41 | 3 (15%)  | 26,32,35    | 1.17 | 2 (7%)   |
| 35  | 5MC  | RA    | 1962 | 35,56    | 19,22,23     | 1.30 | 3 (15%)  | 26,32,35    | 1.23 | 2 (7%)   |
| 35  | 5MC  | YA    | 1942 | 35       | 19,22,23     | 1.41 | 2 (10%)  | 26,32,35    | 1.31 | 4 (15%)  |
| 1   | 4OC  | QA    | 1402 | 1        | 20,23,24     | 0.79 | 0        | 25,32,35    | 1.13 | 2 (8%)   |
| 1   | UR3  | QA    | 1498 | 1        | 19,22,23     | 0.93 | 1 (5%)   | 26,32,35    | 1.70 | 2 (7%)   |
| 1   | 5MC  | QA    | 1404 | 1        | 19,22,23     | 1.35 | 3 (15%)  | 26,32,35    | 1.12 | 3 (11%)  |
| 35  | 5MC  | YA    | 1962 | 35,56    | 19,22,23     | 1.34 | 3 (15%)  | 26,32,35    | 1.17 | 2 (7%)   |
| 1   | 5MC  | XA    | 1407 | 1        | 19,22,23     | 1.15 | 2 (10%)  | 26,32,35    | 1.30 | 2 (7%)   |
| 35  | PSU  | RA    | 1917 | 35,56    | 18,21,22     | 1.43 | 4 (22%)  | 21,30,33    | 1.96 | 4 (19%)  |
| 35  | OMU  | RA    | 2552 | 35,56    | 19,22,23     | 1.31 | 2 (10%)  | 25,31,34    | 1.87 | 5 (20%)  |
| 1   | M2G  | QA    | 966  | 1        | 24,27,28     | 1.30 | 5 (20%)  | 33,40,43    | 1.78 | 5 (15%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | OMU  | YA    | 2552 | 35,56 | 19,22,23     | 1.35 | 3 (15%)  | 25,31,34    | 1.89 | 5 (20%)  |
| 1   | PSU  | QA    | 516  | 1     | 18,21,22     | 1.40 | 5 (27%)  | 21,30,33    | 1.88 | 3 (14%)  |
| 35  | PSU  | YA    | 1911 | 35    | 18,21,22     | 1.44 | 4 (22%)  | 21,30,33    | 2.03 | 4 (19%)  |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 12  | 0TD  | XL    | 92   | 12    | -       | 3/7/12/14  | -       |
| 1   | MA6  | QA    | 1519 | 1     | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | 2MG  | QA    | 1207 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 2MG  | XA    | 1207 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 5MC  | QA    | 967  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 2MA  | RA    | 2503 | 35,56 | -       | 0/7/25/26  | 0/3/3/3 |
| 35  | OMC  | RA    | 1920 | 35    | -       | 0/9/27/28  | 0/2/2/2 |
| 35  | 5MU  | RA    | 1939 | 35    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | OMC  | YA    | 1920 | 35    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | MA6  | QA    | 1518 | 1     | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | MA6  | XA    | 1518 | 1     | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | 5MC  | XA    | 1404 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 2MA  | YA    | 2503 | 35,56 | -       | 0/7/25/26  | 0/3/3/3 |
| 35  | 5MU  | YA    | 1939 | 35    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 5MU  | YA    | 1915 | 35    | -       | 2/7/25/26  | 0/2/2/2 |
| 12  | 0TD  | QL    | 92   | 12    | -       | 1/7/12/14  | -       |
| 35  | PSU  | RA    | 1911 | 35    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | XA    | 516  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | M2G  | XA    | 966  | 1     | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | 5MC  | XA    | 967  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | XA    | 1519 | 1     | -       | 4/11/29/30 | 0/3/3/3 |
| 1   | 5MC  | XA    | 1400 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | G7M  | XA    | 527  | 56,1  | -       | 3/7/25/26  | 0/3/3/3 |
| 1   | 4OC  | XA    | 1402 | 1     | -       | 2/9/29/30  | 0/2/2/2 |
| 1   | 5MC  | QA    | 1407 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | UR3  | XA    | 1498 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | PSU  | RA    | 2605 | 35    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | PSU  | YA    | 2605 | 35    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 5MU  | RA    | 1915 | 35    | -       | 2/7/25/26  | 0/2/2/2 |
| 35  | 5MC  | RA    | 1942 | 35    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 35  | OMG  | RA    | 2251 | 22,35,56 | -       | 0/9/27/28  | 0/3/3/3 |
| 35  | OMG  | YA    | 2251 | 22,35,56 | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | G7M  | QA    | 527  | 56,1     | -       | 2/7/25/26  | 0/3/3/3 |
| 35  | PSU  | YA    | 1917 | 35,56    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | QA    | 1400 | 1        | -       | 2/7/25/26  | 0/2/2/2 |
| 35  | 5MC  | RA    | 1962 | 35,56    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | 5MC  | YA    | 1942 | 35       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | QA    | 1402 | 1        | -       | 2/9/29/30  | 0/2/2/2 |
| 1   | UR3  | QA    | 1498 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | QA    | 1404 | 1        | -       | 2/7/25/26  | 0/2/2/2 |
| 35  | 5MC  | YA    | 1962 | 35,56    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | XA    | 1407 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | PSU  | RA    | 1917 | 35,56    | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | OMU  | RA    | 2552 | 35,56    | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | M2G  | QA    | 966  | 1        | -       | 0/11/29/30 | 0/3/3/3 |
| 35  | OMU  | YA    | 2552 | 35,56    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | QA    | 516  | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 35  | PSU  | YA    | 1911 | 35       | -       | 0/7/25/26  | 0/2/2/2 |

All (165) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 12  | QL    | 92   | 0TD  | CB-CA | -10.41 | 1.51        | 1.54     |
| 12  | XL    | 92   | 0TD  | CB-CA | -8.91  | 1.51        | 1.54     |
| 1   | QA    | 527  | G7M  | C8-N7 | 7.07   | 1.45        | 1.33     |
| 1   | XA    | 527  | G7M  | C8-N7 | 6.77   | 1.44        | 1.33     |
| 1   | QA    | 967  | 5MC  | C5-C4 | 5.55   | 1.48        | 1.44     |
| 1   | QA    | 527  | G7M  | C5-N7 | -5.26  | 1.33        | 1.39     |
| 1   | XA    | 527  | G7M  | C5-N7 | -5.15  | 1.33        | 1.39     |
| 35  | RA    | 1942 | 5MC  | C5-C4 | 5.13   | 1.48        | 1.44     |
| 1   | XA    | 1400 | 5MC  | C5-C4 | 4.81   | 1.47        | 1.44     |
| 35  | YA    | 1942 | 5MC  | C5-C4 | 4.75   | 1.47        | 1.44     |
| 1   | QA    | 1518 | MA6  | C5-C4 | 4.70   | 1.47        | 1.39     |
| 1   | QA    | 1400 | 5MC  | C5-C4 | 4.67   | 1.47        | 1.44     |
| 1   | XA    | 1518 | MA6  | C5-C4 | 4.51   | 1.47        | 1.39     |
| 1   | QA    | 1519 | MA6  | C5-C4 | 4.49   | 1.47        | 1.39     |
| 1   | QA    | 1404 | 5MC  | C5-C4 | 4.43   | 1.47        | 1.44     |
| 35  | YA    | 1962 | 5MC  | C5-C4 | 4.36   | 1.47        | 1.44     |
| 1   | QA    | 1407 | 5MC  | C5-C4 | 4.32   | 1.47        | 1.44     |
| 1   | XA    | 1519 | MA6  | C5-C4 | 4.25   | 1.46        | 1.39     |
| 35  | YA    | 2503 | 2MA  | C5-C4 | 4.06   | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 35  | RA    | 1962 | 5MC  | C5-C4 | 4.04  | 1.47        | 1.44     |
| 1   | XA    | 1404 | 5MC  | C5-C4 | 3.98  | 1.47        | 1.44     |
| 1   | QA    | 527  | G7M  | C8-N9 | 3.93  | 1.46        | 1.35     |
| 1   | XA    | 527  | G7M  | C8-N9 | 3.91  | 1.46        | 1.35     |
| 35  | RA    | 2503 | 2MA  | C5-C4 | 3.85  | 1.46        | 1.39     |
| 1   | XA    | 967  | 5MC  | C5-C4 | 3.81  | 1.47        | 1.44     |
| 1   | XA    | 527  | G7M  | C5-C4 | 3.56  | 1.47        | 1.38     |
| 35  | YA    | 2552 | OMU  | C4-N3 | -3.56 | 1.32        | 1.38     |
| 35  | RA    | 1915 | 5MU  | C4-N3 | -3.49 | 1.32        | 1.38     |
| 35  | YA    | 1915 | 5MU  | C4-N3 | -3.42 | 1.32        | 1.38     |
| 1   | QA    | 527  | G7M  | C5-C4 | 3.34  | 1.46        | 1.38     |
| 1   | QA    | 1518 | MA6  | C5-C6 | 3.32  | 1.49        | 1.41     |
| 1   | XA    | 1407 | 5MC  | C5-C4 | 3.31  | 1.46        | 1.44     |
| 1   | XA    | 1518 | MA6  | C5-C6 | 3.24  | 1.49        | 1.41     |
| 35  | RA    | 2552 | OMU  | C4-N3 | -3.24 | 1.33        | 1.38     |
| 35  | RA    | 1939 | 5MU  | C4-N3 | -3.22 | 1.32        | 1.38     |
| 35  | YA    | 2605 | PSU  | C4-N3 | -3.16 | 1.32        | 1.38     |
| 35  | RA    | 2605 | PSU  | C4-N3 | -3.07 | 1.33        | 1.38     |
| 35  | RA    | 1915 | 5MU  | C2-N1 | 3.07  | 1.43        | 1.38     |
| 35  | YA    | 1939 | 5MU  | C4-N3 | -3.03 | 1.33        | 1.38     |
| 1   | QA    | 966  | M2G  | C5-C4 | 3.02  | 1.47        | 1.38     |
| 35  | YA    | 1939 | 5MU  | C6-N1 | -3.01 | 1.32        | 1.38     |
| 35  | YA    | 1917 | PSU  | C4-N3 | -3.01 | 1.33        | 1.38     |
| 35  | RA    | 1962 | 5MC  | C6-N1 | -3.00 | 1.32        | 1.38     |
| 35  | YA    | 2251 | OMG  | C5-C4 | 3.00  | 1.47        | 1.38     |
| 1   | XA    | 516  | PSU  | C6-C5 | 2.99  | 1.38        | 1.35     |
| 1   | XA    | 516  | PSU  | C4-N3 | -2.96 | 1.33        | 1.38     |
| 1   | XA    | 967  | 5MC  | C6-N1 | -2.94 | 1.33        | 1.38     |
| 35  | RA    | 2251 | OMG  | C6-N1 | -2.93 | 1.33        | 1.38     |
| 35  | YA    | 2251 | OMG  | C6-N1 | -2.93 | 1.33        | 1.38     |
| 35  | RA    | 1911 | PSU  | C4-N3 | -2.91 | 1.33        | 1.38     |
| 35  | YA    | 1915 | 5MU  | C2-N1 | 2.91  | 1.43        | 1.38     |
| 1   | QA    | 1207 | 2MG  | C5-C4 | 2.91  | 1.46        | 1.38     |
| 1   | XA    | 966  | M2G  | C6-N1 | -2.89 | 1.33        | 1.38     |
| 35  | RA    | 2251 | OMG  | C5-C4 | 2.89  | 1.46        | 1.38     |
| 35  | YA    | 1962 | 5MC  | C6-N1 | -2.88 | 1.33        | 1.38     |
| 35  | YA    | 1942 | 5MC  | C6-N1 | -2.88 | 1.33        | 1.38     |
| 1   | XA    | 1404 | 5MC  | C6-N1 | -2.88 | 1.33        | 1.38     |
| 35  | YA    | 1911 | PSU  | C4-N3 | -2.88 | 1.33        | 1.38     |
| 1   | QA    | 1519 | MA6  | C5-C6 | 2.87  | 1.48        | 1.41     |
| 35  | YA    | 1939 | 5MU  | C2-N3 | -2.86 | 1.33        | 1.38     |
| 35  | RA    | 1939 | 5MU  | C6-N1 | -2.86 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 35  | RA    | 1917 | PSU  | C4-N3 | -2.85 | 1.33        | 1.38     |
| 35  | YA    | 2605 | PSU  | C6-C5 | 2.83  | 1.38        | 1.35     |
| 1   | XA    | 1207 | 2MG  | C6-N1 | -2.82 | 1.33        | 1.38     |
| 1   | XA    | 1519 | MA6  | C5-C6 | 2.77  | 1.48        | 1.41     |
| 1   | XA    | 1207 | 2MG  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 1   | QA    | 527  | G7M  | C6-N1 | -2.76 | 1.33        | 1.38     |
| 35  | RA    | 1939 | 5MU  | C2-N3 | -2.76 | 1.33        | 1.38     |
| 35  | RA    | 1942 | 5MC  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 1   | XA    | 966  | M2G  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 1   | QA    | 1207 | 2MG  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 35  | YA    | 1911 | PSU  | C6-C5 | 2.72  | 1.38        | 1.35     |
| 1   | QA    | 967  | 5MC  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 1   | QA    | 1400 | 5MC  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 1   | XA    | 527  | G7M  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 35  | RA    | 2503 | 2MA  | C5-N7 | -2.68 | 1.34        | 1.39     |
| 1   | XA    | 1400 | 5MC  | C6-N1 | -2.68 | 1.33        | 1.38     |
| 35  | YA    | 2251 | OMG  | C5-N7 | -2.68 | 1.33        | 1.39     |
| 1   | QA    | 516  | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 35  | RA    | 2605 | PSU  | C6-C5 | 2.66  | 1.38        | 1.35     |
| 1   | QA    | 966  | M2G  | C6-N1 | -2.66 | 1.33        | 1.38     |
| 35  | RA    | 1911 | PSU  | C6-C5 | 2.66  | 1.38        | 1.35     |
| 35  | YA    | 2503 | 2MA  | C5-N7 | -2.66 | 1.34        | 1.39     |
| 35  | RA    | 1917 | PSU  | C6-C5 | 2.64  | 1.38        | 1.35     |
| 1   | XA    | 1519 | MA6  | C4-N9 | -2.64 | 1.32        | 1.37     |
| 1   | QA    | 516  | PSU  | C6-C5 | 2.59  | 1.38        | 1.35     |
| 1   | QA    | 1404 | 5MC  | C6-N1 | -2.59 | 1.33        | 1.38     |
| 35  | RA    | 1915 | 5MU  | C6-C5 | 2.55  | 1.38        | 1.34     |
| 1   | QA    | 1519 | MA6  | C5-N7 | -2.55 | 1.34        | 1.39     |
| 1   | XA    | 1400 | 5MC  | C6-C5 | 2.54  | 1.38        | 1.34     |
| 1   | XA    | 1407 | 5MC  | C6-N1 | -2.53 | 1.33        | 1.38     |
| 35  | YA    | 1915 | 5MU  | C6-N1 | -2.52 | 1.33        | 1.38     |
| 1   | XA    | 1518 | MA6  | C4-N9 | -2.51 | 1.32        | 1.37     |
| 35  | RA    | 1915 | 5MU  | C2-N3 | -2.50 | 1.33        | 1.38     |
| 35  | YA    | 2605 | PSU  | C2-N1 | -2.49 | 1.33        | 1.36     |
| 1   | XA    | 1519 | MA6  | C5-N7 | -2.47 | 1.34        | 1.39     |
| 35  | YA    | 1915 | 5MU  | C2-N3 | -2.46 | 1.33        | 1.38     |
| 35  | YA    | 2552 | OMU  | C2-N3 | -2.46 | 1.33        | 1.38     |
| 35  | RA    | 2251 | OMG  | C5-N7 | -2.45 | 1.34        | 1.39     |
| 1   | XA    | 966  | M2G  | C5-N7 | -2.44 | 1.34        | 1.39     |
| 35  | YA    | 1920 | OMC  | C5-C4 | -2.43 | 1.37        | 1.42     |
| 35  | RA    | 2503 | 2MA  | C5-C6 | 2.43  | 1.47        | 1.41     |
| 1   | XA    | 1207 | 2MG  | C5-N7 | -2.39 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 35  | RA    | 2605 | PSU  | C2-N1  | -2.39 | 1.33        | 1.36     |
| 1   | QA    | 1407 | 5MC  | C6-N1  | -2.39 | 1.33        | 1.38     |
| 35  | YA    | 1917 | PSU  | C2-N3  | -2.38 | 1.33        | 1.37     |
| 35  | RA    | 1915 | 5MU  | C6-N1  | -2.38 | 1.34        | 1.38     |
| 1   | QA    | 1400 | 5MC  | C6-C5  | 2.37  | 1.38        | 1.34     |
| 1   | QA    | 966  | M2G  | C5-N7  | -2.37 | 1.34        | 1.39     |
| 35  | YA    | 1911 | PSU  | C2-N3  | -2.36 | 1.33        | 1.37     |
| 35  | YA    | 1911 | PSU  | C2-N1  | -2.36 | 1.33        | 1.36     |
| 35  | YA    | 2605 | PSU  | C2-N3  | -2.36 | 1.33        | 1.37     |
| 35  | YA    | 1917 | PSU  | C2-N1  | -2.36 | 1.33        | 1.36     |
| 35  | RA    | 2552 | OMU  | C2-N3  | -2.36 | 1.33        | 1.38     |
| 1   | XA    | 1518 | MA6  | C8-N9  | -2.36 | 1.33        | 1.37     |
| 35  | RA    | 1939 | 5MU  | C6-C5  | 2.35  | 1.38        | 1.34     |
| 35  | RA    | 1942 | 5MC  | C6-C5  | 2.35  | 1.38        | 1.34     |
| 35  | YA    | 1917 | PSU  | C6-C5  | 2.33  | 1.37        | 1.35     |
| 35  | RA    | 2605 | PSU  | C2-N3  | -2.32 | 1.33        | 1.37     |
| 1   | XA    | 516  | PSU  | C2-N3  | -2.30 | 1.33        | 1.37     |
| 35  | RA    | 1911 | PSU  | C2-N3  | -2.30 | 1.33        | 1.37     |
| 35  | RA    | 1917 | PSU  | C2-N1  | -2.29 | 1.33        | 1.36     |
| 35  | YA    | 2503 | 2MA  | C5-C6  | 2.28  | 1.47        | 1.41     |
| 35  | RA    | 1917 | PSU  | C2-N3  | -2.28 | 1.33        | 1.37     |
| 1   | QA    | 1207 | 2MG  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 35  | YA    | 2503 | 2MA  | C4-N9  | -2.27 | 1.33        | 1.37     |
| 12  | XL    | 92   | 0TD  | OD2-CG | -2.27 | 1.23        | 1.30     |
| 1   | QA    | 1518 | MA6  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 35  | RA    | 1920 | OMC  | C5-C4  | -2.26 | 1.37        | 1.42     |
| 1   | QA    | 1404 | 5MC  | C6-C5  | 2.26  | 1.38        | 1.34     |
| 1   | QA    | 966  | M2G  | C2-N2  | 2.26  | 1.39        | 1.35     |
| 1   | QA    | 1407 | 5MC  | C6-C5  | 2.23  | 1.38        | 1.34     |
| 1   | XA    | 1498 | UR3  | C5-C4  | -2.23 | 1.38        | 1.43     |
| 1   | QA    | 1518 | MA6  | C4-N9  | -2.22 | 1.33        | 1.37     |
| 12  | XL    | 92   | 0TD  | CB-SB  | 2.21  | 1.84        | 1.82     |
| 1   | QA    | 967  | 5MC  | C6-C5  | 2.20  | 1.38        | 1.34     |
| 1   | QA    | 516  | PSU  | C2-N1  | -2.19 | 1.33        | 1.36     |
| 1   | XA    | 966  | M2G  | C2-N2  | 2.19  | 1.39        | 1.35     |
| 35  | YA    | 1920 | OMC  | C6-N1  | -2.17 | 1.32        | 1.38     |
| 35  | RA    | 1911 | PSU  | C2-N1  | -2.15 | 1.33        | 1.36     |
| 1   | XA    | 1498 | UR3  | C6-N1  | -2.15 | 1.33        | 1.38     |
| 1   | XA    | 1518 | MA6  | C5-N7  | -2.14 | 1.35        | 1.39     |
| 1   | QA    | 1519 | MA6  | C4-N9  | -2.14 | 1.33        | 1.37     |
| 1   | XA    | 516  | PSU  | C2-N1  | -2.13 | 1.33        | 1.36     |
| 1   | QA    | 1519 | MA6  | C8-N9  | -2.11 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | YA    | 1939 | 5MU  | C6-C5   | 2.10  | 1.38        | 1.34     |
| 1   | XA    | 1519 | MA6  | C8-N9   | -2.10 | 1.34        | 1.37     |
| 1   | QA    | 1498 | UR3  | C5-C4   | -2.10 | 1.38        | 1.43     |
| 35  | YA    | 1915 | 5MU  | C6-C5   | 2.09  | 1.38        | 1.34     |
| 1   | QA    | 1518 | MA6  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 35  | RA    | 2503 | 2MA  | C8-N9   | -2.09 | 1.34        | 1.37     |
| 1   | XA    | 1518 | MA6  | C6-N6   | 2.07  | 1.42        | 1.36     |
| 35  | RA    | 1962 | 5MC  | C6-C5   | 2.06  | 1.38        | 1.34     |
| 1   | XA    | 966  | M2G  | C4-N9   | -2.05 | 1.32        | 1.38     |
| 1   | QA    | 516  | PSU  | C2-N3   | -2.05 | 1.34        | 1.37     |
| 35  | RA    | 2503 | 2MA  | C4-N9   | -2.05 | 1.33        | 1.37     |
| 1   | QA    | 516  | PSU  | O4'-C1' | -2.05 | 1.41        | 1.43     |
| 1   | QA    | 966  | M2G  | C4-N9   | -2.03 | 1.32        | 1.38     |
| 1   | XA    | 1402 | 4OC  | C6-N1   | -2.03 | 1.33        | 1.38     |
| 1   | XA    | 1519 | MA6  | C8-N7   | 2.03  | 1.35        | 1.31     |
| 1   | QA    | 1207 | 2MG  | C4-N9   | -2.02 | 1.32        | 1.38     |
| 35  | YA    | 1962 | 5MC  | C6-C5   | 2.02  | 1.37        | 1.34     |
| 35  | YA    | 2503 | 2MA  | C8-N7   | 2.01  | 1.35        | 1.31     |
| 35  | YA    | 2552 | OMU  | C6-N1   | -2.00 | 1.33        | 1.38     |
| 1   | QA    | 1518 | MA6  | C6-N6   | 2.00  | 1.42        | 1.36     |

All (247) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | XA    | 527  | G7M  | CN7-N7-C8 | -10.02 | 109.61      | 124.79   |
| 35  | RA    | 2503 | 2MA  | C5-C4-N3  | -9.19  | 117.50      | 127.18   |
| 1   | QA    | 527  | G7M  | CN7-N7-C8 | -8.85  | 111.39      | 124.79   |
| 35  | YA    | 2503 | 2MA  | C5-C4-N3  | -8.42  | 118.31      | 127.18   |
| 1   | XA    | 1207 | 2MG  | C2-N3-C4  | 7.36   | 121.20      | 112.00   |
| 35  | RA    | 2503 | 2MA  | N3-C4-N9  | 7.06   | 135.95      | 126.99   |
| 1   | XA    | 527  | G7M  | C8-N7-C5  | 6.97   | 116.49      | 107.78   |
| 35  | YA    | 2251 | OMG  | C5-C4-N3  | -6.96  | 117.31      | 128.39   |
| 1   | QA    | 1207 | 2MG  | C2-N3-C4  | 6.93   | 120.67      | 112.00   |
| 1   | QA    | 527  | G7M  | N9-C8-N7  | -6.79  | 95.99       | 112.48   |
| 1   | QA    | 527  | G7M  | C8-N7-C5  | 6.76   | 116.24      | 107.78   |
| 1   | XA    | 527  | G7M  | N9-C8-N7  | -6.73  | 96.14       | 112.48   |
| 1   | QA    | 1498 | UR3  | C4-N3-C2  | -6.62  | 119.26      | 124.58   |
| 1   | XA    | 1498 | UR3  | C4-N3-C2  | -6.58  | 119.28      | 124.58   |
| 35  | RA    | 1911 | PSU  | N1-C2-N3  | 6.50   | 122.02      | 115.17   |
| 1   | XA    | 1207 | 2MG  | C5-C4-N3  | -6.44  | 118.13      | 128.39   |
| 35  | YA    | 2503 | 2MA  | N3-C4-N9  | 6.43   | 135.15      | 126.99   |
| 35  | RA    | 2251 | OMG  | C5-C4-N3  | -6.39  | 118.22      | 128.39   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 35  | RA    | 1915 | 5MU  | C1'-N1-C2 | 6.35  | 129.00      | 117.59   |
| 1   | QA    | 527  | G7M  | N9-C4-N3  | 6.35  | 138.65      | 125.95   |
| 35  | YA    | 2605 | PSU  | N1-C2-N3  | 6.33  | 121.84      | 115.17   |
| 1   | XA    | 516  | PSU  | N1-C2-N3  | 6.30  | 121.81      | 115.17   |
| 35  | YA    | 1915 | 5MU  | C1'-N1-C2 | 6.27  | 128.84      | 117.59   |
| 35  | YA    | 1917 | PSU  | N1-C2-N3  | 6.20  | 121.71      | 115.17   |
| 35  | YA    | 1911 | PSU  | N1-C2-N3  | 6.13  | 121.64      | 115.17   |
| 1   | QA    | 1207 | 2MG  | C5-C4-N3  | -6.11 | 118.66      | 128.39   |
| 1   | XA    | 527  | G7M  | N9-C4-N3  | 6.11  | 138.16      | 125.95   |
| 35  | RA    | 1917 | PSU  | N1-C2-N3  | 6.04  | 121.54      | 115.17   |
| 1   | QA    | 966  | M2G  | C5-C4-N3  | -5.95 | 118.92      | 128.39   |
| 1   | XA    | 966  | M2G  | C5-C4-N3  | -5.88 | 119.03      | 128.39   |
| 35  | RA    | 2605 | PSU  | N1-C2-N3  | 5.87  | 121.36      | 115.17   |
| 35  | RA    | 1915 | 5MU  | N3-C2-N1  | 5.87  | 122.53      | 114.89   |
| 35  | YA    | 2552 | OMU  | N3-C2-N1  | 5.80  | 122.44      | 114.89   |
| 1   | QA    | 516  | PSU  | N1-C2-N3  | 5.79  | 121.28      | 115.17   |
| 1   | QA    | 1519 | MA6  | C5-C4-N3  | -5.78 | 118.75      | 126.72   |
| 35  | RA    | 1939 | 5MU  | C4-N3-C2  | -5.73 | 119.82      | 127.34   |
| 1   | XA    | 527  | G7M  | CN7-N7-C5 | 5.69  | 133.90      | 126.80   |
| 1   | QA    | 527  | G7M  | C5-C4-N3  | -5.61 | 117.55      | 128.15   |
| 35  | RA    | 1939 | 5MU  | N3-C2-N1  | 5.56  | 122.13      | 114.89   |
| 35  | YA    | 1939 | 5MU  | C4-N3-C2  | -5.53 | 120.09      | 127.34   |
| 1   | XA    | 527  | G7M  | C5-C4-N3  | -5.46 | 117.84      | 128.15   |
| 1   | QA    | 1518 | MA6  | C5-C4-N3  | -5.36 | 119.34      | 126.72   |
| 1   | QA    | 1518 | MA6  | C4-C5-N7  | -5.35 | 104.47      | 110.58   |
| 1   | XA    | 1519 | MA6  | C5-C4-N3  | -5.32 | 119.39      | 126.72   |
| 1   | XA    | 1518 | MA6  | C4-C5-N7  | -5.32 | 104.50      | 110.58   |
| 35  | RA    | 2552 | OMU  | N3-C2-N1  | 5.31  | 121.81      | 114.89   |
| 35  | YA    | 1915 | 5MU  | N3-C2-N1  | 5.31  | 121.80      | 114.89   |
| 35  | YA    | 1915 | 5MU  | C1'-N1-C6 | -5.29 | 112.44      | 121.15   |
| 35  | YA    | 1939 | 5MU  | N3-C2-N1  | 5.15  | 121.59      | 114.89   |
| 35  | YA    | 2251 | OMG  | N9-C4-N3  | 5.13  | 136.20      | 125.95   |
| 1   | XA    | 1518 | MA6  | C5-C4-N3  | -5.12 | 119.66      | 126.72   |
| 35  | YA    | 2251 | OMG  | C2-N3-C4  | 5.10  | 121.09      | 112.30   |
| 35  | RA    | 2251 | OMG  | C2-N3-C4  | 5.00  | 120.91      | 112.30   |
| 35  | RA    | 1915 | 5MU  | C1'-N1-C6 | -4.83 | 113.20      | 121.15   |
| 35  | YA    | 1915 | 5MU  | C4-N3-C2  | -4.82 | 121.02      | 127.34   |
| 35  | RA    | 2251 | OMG  | N9-C4-N3  | 4.80  | 135.56      | 125.95   |
| 35  | RA    | 1939 | 5MU  | C5-C4-N3  | 4.77  | 119.47      | 115.32   |
| 1   | QA    | 527  | G7M  | C2-N3-C4  | 4.74  | 120.46      | 112.30   |
| 35  | RA    | 1915 | 5MU  | C4-N3-C2  | -4.69 | 121.19      | 127.34   |
| 1   | XA    | 1518 | MA6  | C2-N1-C6  | 4.69  | 123.29      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 35  | YA    | 1939 | 5MU  | C5-C4-N3  | 4.61  | 119.33      | 115.32   |
| 1   | QA    | 1518 | MA6  | C2-N1-C6  | 4.60  | 123.06      | 111.83   |
| 35  | RA    | 1915 | 5MU  | O2-C2-N3  | -4.59 | 113.03      | 121.49   |
| 35  | YA    | 2552 | OMU  | C4-N3-C2  | -4.59 | 120.92      | 126.61   |
| 1   | XA    | 1207 | 2MG  | N9-C4-N3  | 4.55  | 135.05      | 125.95   |
| 1   | QA    | 1519 | MA6  | C2-N1-C6  | 4.53  | 122.89      | 111.83   |
| 1   | XA    | 1519 | MA6  | C2-N1-C6  | 4.50  | 122.83      | 111.83   |
| 1   | QA    | 966  | M2G  | N9-C4-N3  | 4.50  | 134.94      | 125.95   |
| 1   | QA    | 527  | G7M  | CN7-N7-C5 | 4.47  | 132.37      | 126.80   |
| 1   | XA    | 527  | G7M  | C2-N3-C4  | 4.47  | 119.99      | 112.30   |
| 1   | XA    | 1518 | MA6  | C9-N6-C6  | -4.44 | 109.22      | 120.52   |
| 35  | YA    | 1939 | 5MU  | O4-C4-C5  | -4.44 | 119.84      | 124.92   |
| 1   | XA    | 966  | M2G  | N9-C4-N3  | 4.43  | 134.81      | 125.95   |
| 1   | QA    | 1519 | MA6  | C4-C5-N7  | -4.40 | 105.55      | 110.58   |
| 35  | RA    | 2552 | OMU  | C4-N3-C2  | -4.38 | 121.17      | 126.61   |
| 1   | QA    | 1518 | MA6  | C9-N6-C6  | -4.33 | 109.51      | 120.52   |
| 35  | YA    | 1915 | 5MU  | C5-C4-N3  | 4.32  | 119.08      | 115.32   |
| 35  | RA    | 1911 | PSU  | C4-N3-C2  | -4.28 | 120.47      | 126.37   |
| 1   | XA    | 966  | M2G  | C2-N3-C4  | 4.28  | 120.43      | 112.51   |
| 35  | RA    | 1939 | 5MU  | C5-C6-N1  | -4.26 | 118.69      | 123.31   |
| 35  | YA    | 1939 | 5MU  | C5-C6-N1  | -4.24 | 118.71      | 123.31   |
| 1   | QA    | 1207 | 2MG  | N9-C4-N3  | 4.20  | 134.35      | 125.95   |
| 35  | YA    | 2605 | PSU  | C4-N3-C2  | -4.16 | 120.64      | 126.37   |
| 1   | QA    | 527  | G7M  | C8-N9-C4  | 4.15  | 117.37      | 107.09   |
| 1   | QA    | 1519 | MA6  | N3-C4-N9  | 4.14  | 134.21      | 127.17   |
| 1   | XA    | 1519 | MA6  | C4-C5-N7  | -4.13 | 105.86      | 110.58   |
| 1   | XA    | 527  | G7M  | C8-N9-C4  | 4.11  | 117.26      | 107.09   |
| 35  | RA    | 1939 | 5MU  | O4-C4-C5  | -4.11 | 120.22      | 124.92   |
| 1   | QA    | 1407 | 5MC  | O2-C2-N3  | -4.10 | 115.86      | 122.33   |
| 35  | RA    | 2605 | PSU  | C4-N3-C2  | -4.10 | 120.72      | 126.37   |
| 1   | XA    | 1519 | MA6  | C10-N6-C6 | -4.09 | 110.11      | 120.52   |
| 35  | YA    | 1911 | PSU  | C4-N3-C2  | -4.07 | 120.77      | 126.37   |
| 1   | QA    | 1519 | MA6  | C10-N6-C6 | -4.06 | 110.19      | 120.52   |
| 1   | QA    | 966  | M2G  | C2-N3-C4  | 4.06  | 120.01      | 112.51   |
| 35  | YA    | 1917 | PSU  | C4-N3-C2  | -4.05 | 120.79      | 126.37   |
| 1   | XA    | 1519 | MA6  | C9-N6-C6  | -4.03 | 110.26      | 120.52   |
| 1   | XA    | 516  | PSU  | C4-N3-C2  | -4.01 | 120.85      | 126.37   |
| 35  | RA    | 1962 | 5MC  | C5-C6-N1  | -3.98 | 118.98      | 123.31   |
| 35  | YA    | 1962 | 5MC  | C5-C6-N1  | -3.91 | 119.06      | 123.31   |
| 1   | XA    | 1400 | 5MC  | C5-C6-N1  | -3.88 | 119.10      | 123.31   |
| 35  | YA    | 2605 | PSU  | O2-C2-N1  | -3.87 | 118.80      | 122.79   |
| 35  | RA    | 1917 | PSU  | C4-N3-C2  | -3.87 | 121.05      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 35  | RA    | 1911 | PSU  | O2-C2-N1  | -3.84 | 118.83      | 122.79   |
| 35  | YA    | 1915 | 5MU  | O4-C4-C5  | -3.83 | 120.53      | 124.92   |
| 35  | RA    | 1915 | 5MU  | C5-C4-N3  | 3.82  | 118.65      | 115.32   |
| 35  | YA    | 1915 | 5MU  | O2-C2-N3  | -3.81 | 114.45      | 121.49   |
| 35  | YA    | 1917 | PSU  | O2-C2-N1  | -3.80 | 118.87      | 122.79   |
| 1   | XA    | 516  | PSU  | O2-C2-N1  | -3.78 | 118.89      | 122.79   |
| 1   | QA    | 1400 | 5MC  | C5-C6-N1  | -3.76 | 119.23      | 123.31   |
| 1   | XA    | 1518 | MA6  | C2-N3-C4  | 3.75  | 120.98      | 111.83   |
| 35  | YA    | 1911 | PSU  | O2-C2-N1  | -3.75 | 118.92      | 122.79   |
| 1   | QA    | 516  | PSU  | O2-C2-N1  | -3.72 | 118.95      | 122.79   |
| 35  | RA    | 2605 | PSU  | O2-C2-N1  | -3.71 | 118.96      | 122.79   |
| 1   | QA    | 1519 | MA6  | C2-N3-C4  | 3.69  | 120.83      | 111.83   |
| 1   | XA    | 1519 | MA6  | C2-N3-C4  | 3.68  | 120.82      | 111.83   |
| 1   | XA    | 1519 | MA6  | N3-C4-N9  | 3.68  | 133.43      | 127.17   |
| 35  | RA    | 2503 | 2MA  | C4-C5-N7  | -3.66 | 106.40      | 110.58   |
| 1   | XA    | 1518 | MA6  | C10-N6-C9 | -3.63 | 104.53      | 116.18   |
| 1   | XA    | 527  | G7M  | C1'-N9-C8 | -3.60 | 114.59      | 126.74   |
| 1   | QA    | 1518 | MA6  | C2-N3-C4  | 3.59  | 120.60      | 111.83   |
| 1   | XA    | 1519 | MA6  | C10-N6-C9 | -3.59 | 104.66      | 116.18   |
| 1   | XA    | 1518 | MA6  | N1-C2-N3  | -3.56 | 123.19      | 128.58   |
| 35  | RA    | 1942 | 5MC  | C5-C6-N1  | -3.56 | 119.44      | 123.31   |
| 1   | XA    | 1519 | MA6  | N1-C2-N3  | -3.56 | 123.19      | 128.58   |
| 1   | QA    | 516  | PSU  | C4-N3-C2  | -3.56 | 121.47      | 126.37   |
| 1   | QA    | 527  | G7M  | C1'-N9-C8 | -3.54 | 114.79      | 126.74   |
| 35  | RA    | 1915 | 5MU  | C6-N1-C2  | -3.52 | 117.79      | 121.30   |
| 1   | QA    | 1407 | 5MC  | C5-C4-N3  | -3.48 | 118.19      | 121.75   |
| 35  | YA    | 1939 | 5MU  | O2-C2-N1  | -3.47 | 118.28      | 122.80   |
| 1   | QA    | 1519 | MA6  | C10-N6-C9 | -3.44 | 105.13      | 116.18   |
| 35  | RA    | 1939 | 5MU  | O2-C2-N1  | -3.44 | 118.33      | 122.80   |
| 1   | QA    | 1498 | UR3  | C5-C4-N3  | 3.41  | 119.53      | 115.04   |
| 35  | RA    | 1917 | PSU  | O2-C2-N1  | -3.41 | 119.27      | 122.79   |
| 1   | QA    | 1518 | MA6  | C10-N6-C9 | -3.38 | 105.33      | 116.18   |
| 35  | YA    | 2503 | 2MA  | C4-C5-N7  | -3.38 | 106.72      | 110.58   |
| 1   | QA    | 1519 | MA6  | N1-C2-N3  | -3.36 | 123.50      | 128.58   |
| 1   | QA    | 967  | 5MC  | C5-C6-N1  | -3.36 | 119.67      | 123.31   |
| 1   | QA    | 1207 | 2MG  | C6-C5-N7  | 3.35  | 136.38      | 130.29   |
| 1   | XA    | 1518 | MA6  | C6-C5-N7  | 3.34  | 138.77      | 133.43   |
| 35  | RA    | 1915 | 5MU  | O4-C4-C5  | -3.30 | 121.14      | 124.92   |
| 1   | QA    | 1518 | MA6  | C5-N7-C8  | 3.29  | 108.62      | 103.45   |
| 1   | XA    | 1498 | UR3  | C5-C4-N3  | 3.28  | 119.36      | 115.04   |
| 1   | XA    | 1404 | 5MC  | C5-C6-N1  | -3.28 | 119.75      | 123.31   |
| 1   | XA    | 1207 | 2MG  | C6-C5-N7  | 3.25  | 136.21      | 130.29   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | XA    | 1518 | MA6  | C5-N7-C8  | 3.25  | 108.56      | 103.45   |
| 1   | QA    | 1518 | MA6  | N3-C4-N9  | 3.24  | 132.67      | 127.17   |
| 12  | QL    | 92   | 0TD  | OD1-CG-CB | -3.23 | 115.68      | 122.44   |
| 35  | YA    | 2552 | OMU  | O2-C2-N1  | -3.23 | 118.60      | 122.80   |
| 1   | XA    | 1518 | MA6  | N3-C4-N9  | 3.22  | 132.64      | 127.17   |
| 1   | XA    | 1407 | 5MC  | O2-C2-N3  | -3.22 | 117.26      | 122.33   |
| 35  | RA    | 2552 | OMU  | O2-C2-N1  | -3.19 | 118.65      | 122.80   |
| 1   | QA    | 1518 | MA6  | C6-C5-N7  | 3.19  | 138.52      | 133.43   |
| 1   | QA    | 1518 | MA6  | N1-C2-N3  | -3.13 | 123.84      | 128.58   |
| 1   | XA    | 967  | 5MC  | C5-C6-N1  | -3.13 | 119.92      | 123.31   |
| 1   | QA    | 1404 | 5MC  | C5-C6-N1  | -3.12 | 119.93      | 123.31   |
| 1   | XA    | 966  | M2G  | C6-C5-N7  | 3.11  | 135.96      | 130.29   |
| 1   | QA    | 1519 | MA6  | C9-N6-C6  | -3.11 | 112.61      | 120.52   |
| 1   | XA    | 1407 | 5MC  | C5-C4-N3  | -3.10 | 118.58      | 121.75   |
| 12  | QL    | 92   | 0TD  | OD2-CG-CB | 3.09  | 119.83      | 113.15   |
| 35  | YA    | 1942 | 5MC  | C5-C6-N1  | -2.99 | 120.07      | 123.31   |
| 35  | YA    | 2503 | 2MA  | N6-C6-N1  | 2.98  | 121.05      | 117.03   |
| 12  | XL    | 92   | 0TD  | O-C-CA    | -2.98 | 117.11      | 124.77   |
| 1   | QA    | 1519 | MA6  | C5-N7-C8  | 2.94  | 108.08      | 103.45   |
| 1   | XA    | 1519 | MA6  | N1-C6-N6  | 2.94  | 120.44      | 116.86   |
| 35  | YA    | 1942 | 5MC  | C5-C4-N3  | -2.93 | 118.75      | 121.75   |
| 12  | QL    | 92   | 0TD  | O-C-CA    | -2.92 | 117.26      | 124.77   |
| 1   | QA    | 966  | M2G  | C6-C5-N7  | 2.88  | 135.53      | 130.29   |
| 35  | RA    | 2251 | OMG  | C6-C5-N7  | 2.87  | 135.52      | 130.29   |
| 1   | QA    | 1402 | 4OC  | O2-C2-N3  | -2.87 | 117.81      | 122.33   |
| 1   | QA    | 1207 | 2MG  | C4-C5-N7  | -2.87 | 106.13      | 110.67   |
| 1   | QA    | 1207 | 2MG  | N2-C2-N3  | -2.85 | 116.88      | 120.51   |
| 1   | XA    | 1404 | 5MC  | C5-C4-N3  | -2.84 | 118.85      | 121.75   |
| 1   | XA    | 1207 | 2MG  | C4-C5-N7  | -2.81 | 106.21      | 110.67   |
| 35  | RA    | 2552 | OMU  | C5-C4-N3  | 2.79  | 118.71      | 114.80   |
| 1   | QA    | 1207 | 2MG  | N1-C2-N2  | 2.78  | 119.40      | 116.56   |
| 35  | RA    | 2552 | OMU  | O4-C4-C5  | -2.74 | 120.44      | 125.16   |
| 35  | RA    | 2503 | 2MA  | C5-N7-C8  | 2.72  | 107.72      | 103.45   |
| 35  | YA    | 1920 | OMC  | O2-C2-N3  | -2.71 | 118.06      | 122.33   |
| 1   | XA    | 1400 | 5MC  | C5-C4-N3  | -2.70 | 118.99      | 121.75   |
| 35  | RA    | 1920 | OMC  | O2-C2-N3  | -2.67 | 118.13      | 122.33   |
| 1   | QA    | 967  | 5MC  | C5-C4-N3  | -2.63 | 119.06      | 121.75   |
| 35  | YA    | 1942 | 5MC  | O2-C2-N3  | -2.62 | 118.20      | 122.33   |
| 35  | YA    | 1915 | 5MU  | C6-N1-C2  | -2.60 | 118.71      | 121.30   |
| 35  | YA    | 2552 | OMU  | C5-C4-N3  | 2.56  | 118.39      | 114.80   |
| 35  | YA    | 2251 | OMG  | C6-C5-N7  | 2.54  | 134.92      | 130.29   |
| 1   | XA    | 1519 | MA6  | C5-N7-C8  | 2.54  | 107.45      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 35  | YA    | 2552 | OMU  | O4-C4-C5  | -2.53 | 120.79      | 125.16   |
| 35  | RA    | 2503 | 2MA  | C4-N9-C8  | 2.53  | 108.39      | 105.74   |
| 35  | YA    | 2251 | OMG  | C4-C5-N7  | -2.51 | 106.69      | 110.67   |
| 1   | XA    | 1402 | 4OC  | O2-C2-N3  | -2.50 | 118.38      | 122.33   |
| 1   | QA    | 966  | M2G  | C4-C5-N7  | -2.47 | 106.75      | 110.67   |
| 1   | QA    | 1207 | 2MG  | C2-N1-C6  | -2.47 | 121.56      | 124.55   |
| 1   | QA    | 1404 | 5MC  | C5-C4-N3  | -2.46 | 119.23      | 121.75   |
| 1   | QA    | 1519 | MA6  | N1-C6-N6  | 2.46  | 119.86      | 116.86   |
| 1   | XA    | 967  | 5MC  | C5-C4-N3  | -2.46 | 119.24      | 121.75   |
| 1   | XA    | 966  | M2G  | C4-C5-N7  | -2.45 | 106.79      | 110.67   |
| 1   | QA    | 527  | G7M  | O6-C6-C5  | -2.44 | 122.56      | 128.01   |
| 35  | RA    | 1942 | 5MC  | C5-C4-N3  | -2.44 | 119.25      | 121.75   |
| 1   | XA    | 1519 | MA6  | C6-C5-N7  | 2.43  | 137.31      | 133.43   |
| 35  | RA    | 2605 | PSU  | C6-C5-C4  | -2.43 | 116.53      | 118.17   |
| 35  | YA    | 2503 | 2MA  | C4-N9-C8  | 2.42  | 108.27      | 105.74   |
| 35  | YA    | 1920 | OMC  | C1'-N1-C2 | 2.41  | 123.77      | 118.44   |
| 35  | YA    | 1942 | 5MC  | CM5-C5-C6 | -2.40 | 119.60      | 122.85   |
| 35  | RA    | 1920 | OMC  | C1'-N1-C2 | 2.40  | 123.75      | 118.44   |
| 35  | YA    | 2503 | 2MA  | C2-N1-C6  | 2.40  | 121.79      | 118.10   |
| 1   | QA    | 1207 | 2MG  | CM2-N2-C2 | -2.39 | 118.51      | 123.65   |
| 35  | YA    | 2503 | 2MA  | C5-N7-C8  | 2.39  | 107.20      | 103.45   |
| 1   | XA    | 1518 | MA6  | C4-N9-C8  | 2.38  | 108.24      | 105.74   |
| 1   | XA    | 1519 | MA6  | C4-N9-C8  | 2.36  | 108.21      | 105.74   |
| 35  | RA    | 2251 | OMG  | C4-C5-N7  | -2.34 | 106.95      | 110.67   |
| 1   | XA    | 527  | G7M  | O6-C6-C5  | -2.34 | 122.80      | 128.01   |
| 1   | XA    | 1207 | 2MG  | C2-N1-C6  | -2.33 | 121.73      | 124.55   |
| 35  | YA    | 1920 | OMC  | N4-C4-N3  | 2.33  | 122.08      | 117.91   |
| 1   | QA    | 1404 | 5MC  | O2-C2-N3  | -2.33 | 118.65      | 122.33   |
| 1   | QA    | 527  | G7M  | C5-C6-N1  | 2.33  | 116.65      | 111.84   |
| 1   | XA    | 1207 | 2MG  | N1-C2-N2  | 2.33  | 118.94      | 116.56   |
| 35  | YA    | 1911 | PSU  | C6-C5-C4  | -2.28 | 116.63      | 118.17   |
| 35  | RA    | 1920 | OMC  | N4-C4-N3  | 2.28  | 121.99      | 117.91   |
| 1   | QA    | 1400 | 5MC  | C5-C4-N3  | -2.28 | 119.42      | 121.75   |
| 35  | RA    | 1942 | 5MC  | O2-C2-N3  | -2.27 | 118.75      | 122.33   |
| 35  | YA    | 1915 | 5MU  | C5-C6-N1  | -2.25 | 120.86      | 123.31   |
| 1   | XA    | 1207 | 2MG  | CM2-N2-C2 | -2.23 | 118.86      | 123.65   |
| 1   | QA    | 1519 | MA6  | C4-N9-C8  | 2.21  | 108.06      | 105.74   |
| 35  | RA    | 2251 | OMG  | O6-C6-C5  | -2.21 | 120.71      | 126.53   |
| 35  | RA    | 1917 | PSU  | C6-C5-C4  | -2.20 | 116.69      | 118.17   |
| 35  | YA    | 1962 | 5MC  | C5-C4-N3  | -2.20 | 119.50      | 121.75   |
| 1   | XA    | 1498 | UR3  | C1'-N1-C2 | 2.19  | 120.63      | 117.04   |
| 1   | QA    | 1519 | MA6  | C6-C5-N7  | 2.19  | 136.93      | 133.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | XA    | 967  | 5MC  | C1'-N1-C6   | -2.18 | 117.55      | 121.15   |
| 35  | YA    | 2605 | PSU  | C6-C5-C4    | -2.18 | 116.70      | 118.17   |
| 1   | QA    | 1207 | 2MG  | O6-C6-C5    | -2.18 | 120.78      | 126.53   |
| 35  | YA    | 2251 | OMG  | O6-C6-C5    | -2.13 | 120.91      | 126.53   |
| 35  | RA    | 2503 | 2MA  | N6-C6-N1    | 2.11  | 119.88      | 117.03   |
| 35  | RA    | 2503 | 2MA  | N9-C8-N7    | -2.11 | 110.94      | 113.94   |
| 1   | QA    | 1402 | 4OC  | C6-C5-C4    | 2.10  | 119.53      | 117.00   |
| 1   | XA    | 1207 | 2MG  | N2-C2-N3    | -2.10 | 117.84      | 120.51   |
| 1   | XA    | 516  | PSU  | O4'-C1'-C2' | 2.09  | 108.04      | 105.15   |
| 1   | XA    | 1518 | MA6  | N9-C8-N7    | -2.09 | 110.98      | 113.94   |
| 35  | RA    | 1962 | 5MC  | C5-C4-N3    | -2.08 | 119.62      | 121.75   |
| 35  | RA    | 2503 | 2MA  | C2-N1-C6    | 2.06  | 121.27      | 118.10   |
| 1   | QA    | 967  | 5MC  | CM5-C5-C6   | -2.05 | 120.08      | 122.85   |
| 35  | YA    | 2503 | 2MA  | C6-C5-N7    | 2.03  | 136.00      | 132.09   |
| 35  | RA    | 1915 | 5MU  | C5-C6-N1    | -2.02 | 121.12      | 123.31   |
| 1   | XA    | 1404 | 5MC  | CM5-C5-C6   | -2.02 | 120.12      | 122.85   |
| 1   | XA    | 1207 | 2MG  | O6-C6-C5    | -2.02 | 121.21      | 126.53   |
| 35  | RA    | 1911 | PSU  | C5-C6-N1    | -2.01 | 119.35      | 122.14   |
| 1   | XA    | 516  | PSU  | C6-C5-C4    | -2.01 | 116.82      | 118.17   |

There are no chirality outliers.

All (38) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | QA    | 1518 | MA6  | C5-C6-N6-C9     |
| 1   | XA    | 1518 | MA6  | C5-C6-N6-C9     |
| 1   | QA    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 1   | XA    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 35  | RA    | 1915 | 5MU  | O4'-C1'-N1-C2   |
| 35  | RA    | 1915 | 5MU  | O4'-C1'-N1-C6   |
| 35  | YA    | 1915 | 5MU  | O4'-C1'-N1-C2   |
| 35  | YA    | 1915 | 5MU  | O4'-C1'-N1-C6   |
| 1   | QA    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 1   | XA    | 1400 | 5MC  | O4'-C4'-C5'-O5' |
| 1   | XA    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 1   | QA    | 1518 | MA6  | N1-C6-N6-C9     |
| 1   | XA    | 1518 | MA6  | N1-C6-N6-C9     |
| 1   | QA    | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 1   | XA    | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 1   | XA    | 527  | G7M  | C3'-C4'-C5'-O5' |
| 1   | XA    | 1519 | MA6  | C5-C6-N6-C9     |
| 1   | QA    | 1400 | 5MC  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | XA    | 527  | G7M  | O4'-C4'-C5'-O5' |
| 1   | XA    | 1400 | 5MC  | C3'-C4'-C5'-O5' |
| 1   | QA    | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 1   | QA    | 1519 | MA6  | C5-C6-N6-C9     |
| 1   | QA    | 1404 | 5MC  | C3'-C4'-C5'-O5' |
| 12  | QL    | 92   | 0TD  | CG-CB-SB-CSB    |
| 12  | XL    | 92   | 0TD  | CG-CB-SB-CSB    |
| 12  | XL    | 92   | 0TD  | SB-CB-CG-OD1    |
| 35  | RA    | 2552 | OMU  | O4'-C4'-C5'-O5' |
| 1   | QA    | 1518 | MA6  | C5-C6-N6-C10    |
| 1   | XA    | 1518 | MA6  | C5-C6-N6-C10    |
| 1   | QA    | 1400 | 5MC  | C3'-C4'-C5'-O5' |
| 1   | QA    | 1404 | 5MC  | O4'-C4'-C5'-O5' |
| 1   | XA    | 1519 | MA6  | N1-C6-N6-C9     |
| 1   | XA    | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 1   | QA    | 527  | G7M  | C4'-C5'-O5'-P   |
| 1   | XA    | 527  | G7M  | C4'-C5'-O5'-P   |
| 12  | XL    | 92   | 0TD  | SB-CB-CG-OD2    |
| 1   | QA    | 527  | G7M  | C3'-C4'-C5'-O5' |
| 35  | YA    | 1962 | 5MC  | O4'-C4'-C5'-O5' |

There are no ring outliers.

12 monomers are involved in 13 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | QA    | 1519 | MA6  | 1       | 0            |
| 35  | RA    | 2503 | 2MA  | 2       | 0            |
| 35  | RA    | 1939 | 5MU  | 1       | 0            |
| 1   | QA    | 1518 | MA6  | 1       | 0            |
| 1   | XA    | 1518 | MA6  | 1       | 0            |
| 35  | YA    | 2503 | 2MA  | 2       | 0            |
| 12  | QL    | 92   | 0TD  | 1       | 0            |
| 1   | XA    | 966  | M2G  | 1       | 0            |
| 1   | XA    | 967  | 5MC  | 1       | 0            |
| 1   | XA    | 1498 | UR3  | 1       | 0            |
| 35  | RA    | 1962 | 5MC  | 1       | 0            |
| 35  | YA    | 1962 | 5MC  | 1       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 2027 ligands modelled in this entry, 2023 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | SF4  | QD    | 302  | -    | 0,12,12      | -    | -        | -           |      |          |
| 57  | PAR  | XA    | 1794 | -    | 44,45,45     | 0.65 | 0        | 63,67,67    | 1.22 | 7 (11%)  |
| 57  | PAR  | QA    | 1821 | -    | 44,45,45     | 0.68 | 0        | 63,67,67    | 1.47 | 10 (15%) |
| 58  | SF4  | XD    | 301  | -    | 0,12,12      | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 58  | SF4  | QD    | 302  | -    | -       | -          | 0/6/5/5 |
| 57  | PAR  | XA    | 1794 | -    | -       | 3/18/94/94 | 0/4/4/4 |
| 57  | PAR  | QA    | 1821 | -    | -       | 4/18/94/94 | 0/4/4/4 |
| 58  | SF4  | XD    | 301  | -    | -       | -          | 0/6/5/5 |

There are no bond length outliers.

All (17) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | QA    | 1821 | PAR  | C44-C34-C24 | 5.00  | 119.30      | 110.99   |
| 57  | XA    | 1794 | PAR  | C13-O52-C52 | -3.49 | 109.70      | 117.98   |
| 57  | QA    | 1821 | PAR  | C13-O52-C52 | -3.48 | 109.73      | 117.98   |
| 57  | XA    | 1794 | PAR  | C14-O33-C33 | -3.03 | 110.79      | 117.98   |
| 57  | XA    | 1794 | PAR  | C11-O51-C51 | 2.74  | 119.07      | 113.72   |
| 57  | QA    | 1821 | PAR  | O62-C62-C12 | -2.58 | 105.07      | 109.90   |
| 57  | QA    | 1821 | PAR  | C14-C24-N24 | -2.54 | 105.63      | 110.20   |
| 57  | QA    | 1821 | PAR  | O11-C42-C32 | -2.44 | 103.35      | 109.18   |
| 57  | QA    | 1821 | PAR  | C62-C12-N12 | -2.41 | 106.19      | 110.94   |
| 57  | QA    | 1821 | PAR  | O34-C34-C44 | -2.38 | 104.77      | 110.38   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | QA    | 1821 | PAR  | C14-O33-C33 | -2.36 | 112.38      | 117.98   |
| 57  | QA    | 1821 | PAR  | O52-C13-O43 | -2.31 | 109.00      | 111.37   |
| 57  | XA    | 1794 | PAR  | O11-C42-C32 | -2.21 | 103.90      | 109.18   |
| 57  | XA    | 1794 | PAR  | O33-C33-C23 | -2.18 | 104.30      | 111.32   |
| 57  | QA    | 1821 | PAR  | O54-C14-C24 | -2.18 | 105.26      | 110.08   |
| 57  | XA    | 1794 | PAR  | O33-C14-O54 | -2.12 | 105.11      | 110.69   |
| 57  | XA    | 1794 | PAR  | O11-C11-C21 | -2.12 | 104.61      | 108.08   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

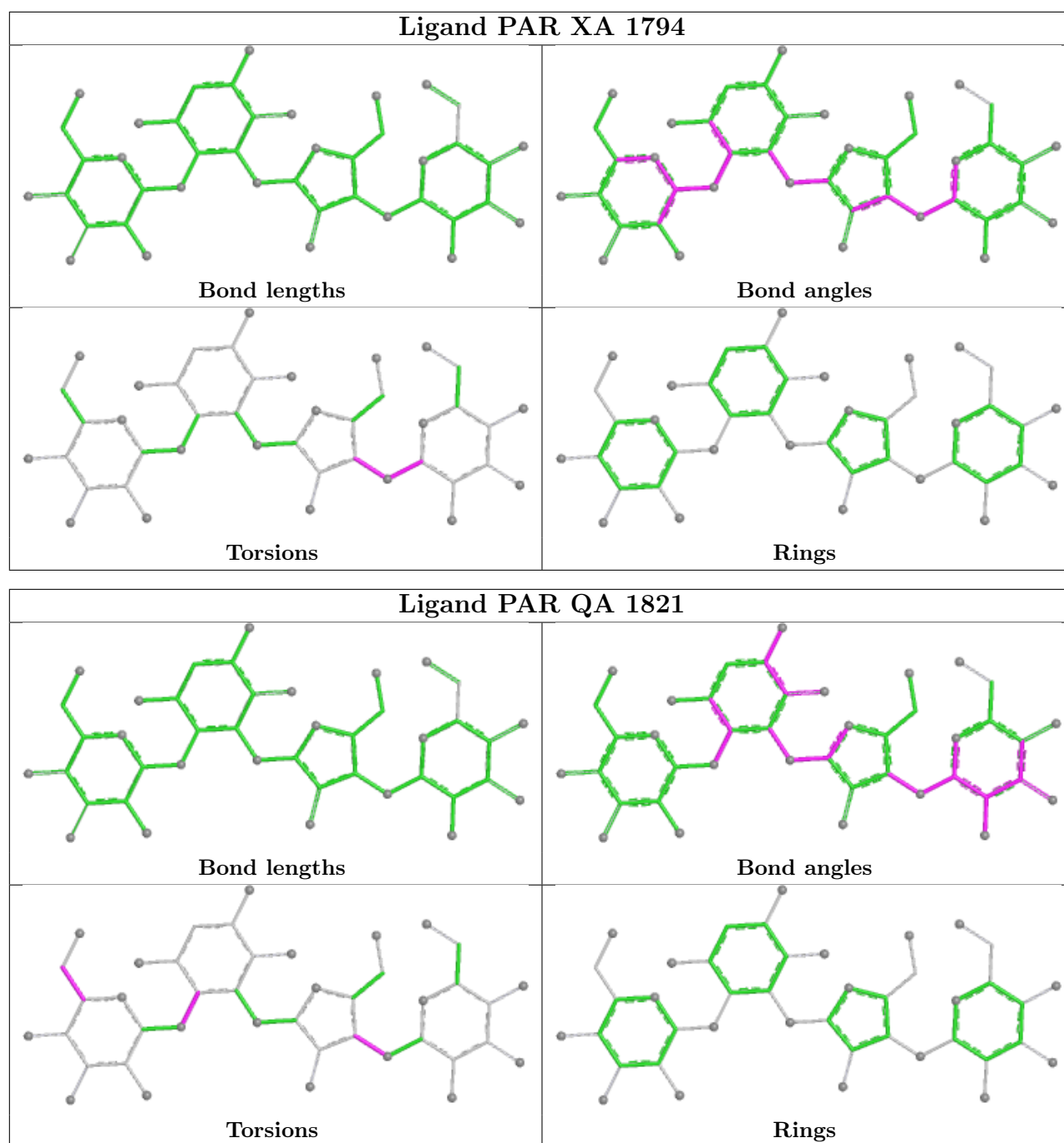
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 57  | QA    | 1821 | PAR  | O51-C51-C61-O61 |
| 57  | QA    | 1821 | PAR  | C41-C51-C61-O61 |
| 57  | XA    | 1794 | PAR  | O54-C14-O33-C33 |
| 57  | QA    | 1821 | PAR  | C23-C33-O33-C14 |
| 57  | QA    | 1821 | PAR  | C52-C42-O11-C11 |
| 57  | XA    | 1794 | PAR  | C23-C33-O33-C14 |
| 57  | XA    | 1794 | PAR  | C43-C33-O33-C14 |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57  | XA    | 1794 | PAR  | 2       | 0            |
| 57  | QA    | 1821 | PAR  | 1       | 0            |
| 58  | XD    | 301  | SF4  | 1       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | QA    | 1488/1522 (97%) | 0.05   | 19 (1%) 75 56 | 59, 101, 188, 338     | 0     |
| 1   | XA    | 1492/1522 (98%) | -0.12  | 11 (0%) 84 68 | 47, 90, 177, 328      | 0     |
| 2   | QB    | 231/256 (90%)   | 0.54   | 12 (5%) 33 17 | 76, 130, 166, 190     | 0     |
| 2   | XB    | 231/256 (90%)   | 0.45   | 8 (3%) 47 27  | 65, 117, 160, 194     | 0     |
| 3   | QC    | 206/239 (86%)   | 0.42   | 11 (5%) 32 17 | 100, 135, 171, 196    | 0     |
| 3   | XC    | 206/239 (86%)   | 0.33   | 11 (5%) 32 17 | 51, 105, 146, 163     | 0     |
| 4   | QD    | 208/209 (99%)   | 0.59   | 14 (6%) 24 13 | 58, 102, 144, 164     | 0     |
| 4   | XD    | 208/209 (99%)   | 0.70   | 19 (9%) 15 8  | 63, 99, 137, 171      | 0     |
| 5   | QE    | 148/162 (91%)   | 0.38   | 4 (2%) 56 35  | 70, 104, 141, 172     | 0     |
| 5   | XE    | 148/162 (91%)   | 0.30   | 2 (1%) 73 53  | 56, 91, 122, 138      | 0     |
| 6   | QF    | 100/101 (99%)   | 0.12   | 0 100 100     | 63, 92, 129, 145      | 0     |
| 6   | XF    | 100/101 (99%)   | 0.08   | 1 (1%) 79 61  | 64, 96, 127, 158      | 0     |
| 7   | QG    | 155/156 (99%)   | 0.46   | 7 (4%) 38 20  | 88, 124, 155, 209     | 0     |
| 7   | XG    | 155/156 (99%)   | 0.48   | 6 (3%) 43 24  | 75, 107, 147, 184     | 0     |
| 8   | QH    | 137/138 (99%)   | 0.53   | 6 (4%) 39 21  | 67, 104, 135, 156     | 0     |
| 8   | XH    | 137/138 (99%)   | 0.41   | 6 (4%) 39 21  | 59, 92, 127, 154      | 0     |
| 9   | QI    | 127/128 (99%)   | 1.16   | 26 (20%) 2 1  | 94, 141, 174, 200     | 0     |
| 9   | XI    | 126/128 (98%)   | 0.78   | 12 (9%) 14 7  | 70, 113, 147, 186     | 0     |
| 10  | QJ    | 97/105 (92%)    | 1.00   | 11 (11%) 10 5 | 94, 140, 188, 200     | 0     |
| 10  | XJ    | 96/105 (91%)    | 1.06   | 13 (13%) 7 4  | 87, 123, 160, 175     | 0     |
| 11  | QK    | 114/129 (88%)   | 0.32   | 5 (4%) 39 21  | 70, 100, 132, 154     | 0     |
| 11  | XK    | 114/129 (88%)   | 0.50   | 8 (7%) 22 12  | 58, 96, 141, 167      | 0     |
| 12  | QL    | 121/132 (91%)   | 0.81   | 13 (10%) 11 6 | 55, 92, 120, 149      | 0     |
| 12  | XL    | 121/132 (91%)   | 0.75   | 16 (13%) 7 4  | 52, 75, 112, 137      | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2  |         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------|---------|-----------------------|-------|
| 13  | QM    | 116/126 (92%) | 0.72   | 9 (7%)   | 19 10   | 88, 127, 162, 177     | 0     |
| 13  | XM    | 114/126 (90%) | 0.65   | 6 (5%)   | 32 17   | 75, 111, 156, 195     | 0     |
| 14  | QN    | 60/61 (98%)   | 1.45   | 14 (23%) | 2 1     | 81, 135, 179, 194     | 0     |
| 14  | XN    | 60/61 (98%)   | 1.01   | 10 (16%) | 4 2     | 76, 101, 135, 139     | 0     |
| 15  | QO    | 88/89 (98%)   | 0.49   | 1 (1%)   | 78 59   | 64, 94, 137, 167      | 0     |
| 15  | XO    | 88/89 (98%)   | 0.65   | 9 (10%)  | 12 6    | 58, 88, 136, 145      | 0     |
| 16  | QP    | 82/88 (93%)   | 0.89   | 6 (7%)   | 21 11   | 53, 94, 123, 156      | 0     |
| 16  | XP    | 82/88 (93%)   | 0.86   | 7 (8%)   | 16 9    | 65, 94, 138, 174      | 0     |
| 17  | QQ    | 99/105 (94%)  | 0.84   | 8 (8%)   | 18 10   | 71, 99, 140, 152      | 0     |
| 17  | XQ    | 99/105 (94%)  | 0.86   | 10 (10%) | 12 6    | 63, 93, 128, 153      | 0     |
| 18  | QR    | 68/88 (77%)   | 0.25   | 0        | 100 100 | 75, 97, 130, 163      | 0     |
| 18  | XR    | 68/88 (77%)   | 0.48   | 3 (4%)   | 39 21   | 62, 93, 139, 161      | 0     |
| 19  | QS    | 83/93 (89%)   | 0.86   | 10 (12%) | 9 5     | 101, 136, 184, 192    | 0     |
| 19  | XS    | 83/93 (89%)   | 0.74   | 10 (12%) | 9 5     | 75, 118, 155, 172     | 0     |
| 20  | QT    | 96/106 (90%)  | 1.02   | 10 (10%) | 11 6    | 65, 95, 144, 161      | 0     |
| 20  | XT    | 98/106 (92%)  | 0.82   | 9 (9%)   | 14 8    | 75, 97, 152, 165      | 0     |
| 21  | QU    | 23/27 (85%)   | 2.40   | 13 (56%) | 0 0     | 91, 122, 147, 158     | 0     |
| 21  | XU    | 23/27 (85%)   | 1.33   | 4 (17%)  | 4 2     | 90, 108, 124, 144     | 0     |
| 22  | QV    | 77/77 (100%)  | 0.10   | 1 (1%)   | 75 56   | 86, 122, 172, 240     | 0     |
| 22  | XV    | 77/77 (100%)  | 0.05   | 3 (3%)   | 43 24   | 58, 105, 164, 210     | 0     |
| 23  | QX    | 18/19 (94%)   | 1.03   | 4 (22%)  | 2 1     | 71, 163, 230, 231     | 0     |
| 23  | XX    | 18/19 (94%)   | 1.00   | 6 (33%)  | 1 0     | 64, 153, 241, 253     | 0     |
| 24  | QY    | 76/76 (100%)  | 0.80   | 9 (11%)  | 9 5     | 105, 192, 252, 287    | 0     |
| 24  | XY    | 76/76 (100%)  | 0.89   | 10 (13%) | 7 4     | 85, 162, 243, 269     | 0     |
| 25  | R0    | 77/85 (90%)   | 0.58   | 4 (5%)   | 33 17   | 54, 81, 100, 143      | 0     |
| 25  | Y0    | 77/85 (90%)   | 0.17   | 0        | 100 100 | 21, 55, 85, 93        | 0     |
| 26  | R1    | 97/98 (98%)   | 0.57   | 2 (2%)   | 63 42   | 52, 76, 116, 133      | 0     |
| 26  | Y1    | 97/98 (98%)   | 0.56   | 7 (7%)   | 21 11   | 30, 63, 106, 133      | 0     |
| 27  | R2    | 70/72 (97%)   | 0.42   | 2 (2%)   | 53 32   | 61, 93, 137, 159      | 0     |
| 27  | Y2    | 70/72 (97%)   | 0.36   | 4 (5%)   | 29 16   | 38, 69, 100, 154      | 0     |
| 28  | R3    | 59/60 (98%)   | 0.37   | 3 (5%)   | 33 18   | 50, 81, 129, 176      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|---------|-----------------------|-------|
| 28  | Y3    | 59/60 (98%)     | 0.25   | 4 (6%)  | 23 12   | 28, 51, 104, 137      | 0     |
| 29  | R4    | 69/71 (97%)     | 0.57   | 1 (1%)  | 73 53   | 104, 149, 191, 208    | 0     |
| 29  | Y4    | 69/71 (97%)     | 0.60   | 9 (13%) | 7 4     | 85, 126, 184, 223     | 0     |
| 30  | R5    | 59/60 (98%)     | 0.14   | 0       | 100 100 | 39, 73, 97, 152       | 0     |
| 30  | Y5    | 59/60 (98%)     | 0.13   | 1 (1%)  | 69 48   | 32, 57, 102, 184      | 0     |
| 31  | R6    | 53/54 (98%)     | 0.27   | 1 (1%)  | 66 45   | 60, 82, 120, 148      | 0     |
| 31  | Y6    | 53/54 (98%)     | -0.05  | 0       | 100 100 | 45, 65, 89, 92        | 0     |
| 32  | R7    | 48/49 (97%)     | 0.43   | 4 (8%)  | 17 9    | 32, 58, 82, 117       | 0     |
| 32  | Y7    | 48/49 (97%)     | 0.30   | 3 (6%)  | 26 14   | 34, 49, 74, 131       | 0     |
| 33  | R8    | 64/65 (98%)     | 0.81   | 6 (9%)  | 14 8    | 46, 70, 96, 129       | 0     |
| 33  | Y8    | 64/65 (98%)     | 0.48   | 6 (9%)  | 14 8    | 37, 51, 86, 111       | 0     |
| 34  | R9    | 37/37 (100%)    | 1.11   | 5 (13%) | 7 4     | 68, 96, 127, 185      | 0     |
| 34  | Y9    | 37/37 (100%)    | 0.58   | 1 (2%)  | 56 35   | 46, 60, 78, 101       | 0     |
| 35  | RA    | 2856/2915 (97%) | -0.01  | 64 (2%) | 62 41   | 45, 74, 216, 308      | 0     |
| 35  | YA    | 2856/2915 (97%) | -0.32  | 55 (1%) | 66 45   | 31, 53, 205, 329      | 0     |
| 36  | RB    | 120/122 (98%)   | -0.08  | 1 (0%)  | 82 65   | 79, 108, 141, 171     | 0     |
| 36  | YB    | 120/122 (98%)   | -0.25  | 1 (0%)  | 82 65   | 54, 75, 101, 137      | 0     |
| 37  | RD    | 275/276 (99%)   | 0.49   | 14 (5%) | 33 18   | 40, 64, 104, 121      | 0     |
| 37  | YD    | 275/276 (99%)   | 0.23   | 6 (2%)  | 62 41   | 33, 55, 86, 155       | 0     |
| 38  | RE    | 204/206 (99%)   | 0.40   | 9 (4%)  | 39 21   | 46, 76, 113, 157      | 0     |
| 38  | YE    | 204/206 (99%)   | 0.24   | 6 (2%)  | 53 32   | 35, 58, 96, 128       | 0     |
| 39  | RF    | 202/210 (96%)   | 0.29   | 4 (1%)  | 65 44   | 39, 81, 129, 184      | 0     |
| 39  | YF    | 202/210 (96%)   | 0.12   | 3 (1%)  | 72 52   | 27, 58, 111, 141      | 0     |
| 40  | RG    | 181/182 (99%)   | 0.48   | 7 (3%)  | 43 24   | 84, 121, 157, 203     | 0     |
| 40  | YG    | 181/182 (99%)   | 0.38   | 4 (2%)  | 62 41   | 63, 91, 139, 182      | 0     |
| 41  | RH    | 174/180 (96%)   | 0.54   | 3 (1%)  | 69 48   | 80, 124, 159, 185     | 0     |
| 41  | YH    | 173/180 (96%)   | 0.18   | 4 (2%)  | 61 39   | 38, 72, 108, 145      | 0     |
| 42  | RI    | 147/148 (99%)   | 0.31   | 3 (2%)  | 65 44   | 57, 106, 145, 165     | 0     |
| 42  | YI    | 146/148 (98%)   | 0.16   | 3 (2%)  | 63 42   | 55, 96, 141, 167      | 0     |
| 43  | RN    | 140/140 (100%)  | 0.45   | 6 (4%)  | 40 22   | 48, 83, 128, 153      | 0     |
| 43  | YN    | 140/140 (100%)  | 0.23   | 3 (2%)  | 63 42   | 35, 59, 97, 134       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | RO    | 122/122 (100%)    | 0.31   | 3 (2%) 58 37   | 43, 76, 104, 123      | 0     |
| 44  | YO    | 122/122 (100%)    | 0.21   | 2 (1%) 70 49   | 27, 57, 93, 108       | 0     |
| 45  | RP    | 149/150 (99%)     | 0.59   | 8 (5%) 31 17   | 38, 90, 138, 163      | 0     |
| 45  | YP    | 149/150 (99%)     | 0.45   | 8 (5%) 31 17   | 33, 65, 104, 133      | 0     |
| 46  | RQ    | 141/141 (100%)    | 0.76   | 15 (10%) 11 6  | 57, 89, 128, 180      | 0     |
| 46  | YQ    | 141/141 (100%)    | 0.42   | 4 (2%) 55 34   | 31, 60, 94, 157       | 0     |
| 47  | RR    | 118/118 (100%)    | 0.54   | 5 (4%) 40 22   | 45, 69, 103, 116      | 0     |
| 47  | YR    | 118/118 (100%)    | 0.35   | 1 (0%) 82 65   | 37, 53, 89, 129       | 0     |
| 48  | RS    | 110/112 (98%)     | 0.56   | 5 (4%) 38 20   | 61, 98, 132, 151      | 0     |
| 48  | YS    | 110/112 (98%)     | 0.26   | 4 (3%) 46 26   | 40, 72, 106, 130      | 0     |
| 49  | RT    | 131/146 (89%)     | 0.29   | 3 (2%) 61 39   | 49, 78, 130, 166      | 0     |
| 49  | YT    | 131/146 (89%)     | 0.25   | 4 (3%) 51 30   | 42, 70, 116, 148      | 0     |
| 50  | RU    | 116/118 (98%)     | 0.59   | 3 (2%) 57 36   | 44, 81, 123, 134      | 0     |
| 50  | YU    | 116/118 (98%)     | 0.16   | 1 (0%) 81 63   | 29, 49, 79, 115       | 0     |
| 51  | RV    | 101/101 (100%)    | 0.29   | 4 (3%) 42 23   | 55, 91, 130, 172      | 0     |
| 51  | YV    | 101/101 (100%)    | 0.03   | 1 (0%) 79 61   | 37, 62, 101, 168      | 0     |
| 52  | RW    | 112/113 (99%)     | 0.39   | 2 (1%) 67 47   | 36, 64, 105, 138      | 0     |
| 52  | YW    | 112/113 (99%)     | 0.16   | 2 (1%) 67 47   | 32, 50, 89, 184       | 0     |
| 53  | RX    | 95/96 (98%)       | 0.54   | 5 (5%) 32 17   | 42, 75, 116, 140      | 0     |
| 53  | YX    | 95/96 (98%)       | 0.24   | 4 (4%) 40 22   | 28, 56, 104, 134      | 0     |
| 54  | RY    | 107/110 (97%)     | 0.81   | 7 (6%) 25 13   | 59, 98, 129, 162      | 0     |
| 54  | YY    | 107/110 (97%)     | 0.35   | 4 (3%) 45 25   | 41, 73, 109, 157      | 0     |
| 55  | RZ    | 178/206 (86%)     | 0.86   | 18 (10%) 12 6  | 82, 136, 202, 263     | 0     |
| 55  | YZ    | 177/206 (85%)     | 0.77   | 27 (15%) 5 3   | 53, 108, 209, 266     | 0     |
| All | All   | 20859/21590 (96%) | 0.23   | 812 (3%) 43 24 | 21, 84, 164, 338      | 0     |

All (812) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | RA    | 2602 | A    | 8.1  |
| 20  | QT    | 9    | ASN  | 7.8  |
| 35  | YA    | 1091 | G    | 7.2  |
| 20  | XT    | 6    | PRO  | 6.6  |
| 9   | QI    | 126  | SER  | 6.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | R1    | 2    | SER  | 5.9  |
| 21  | QU    | 15   | ARG  | 5.9  |
| 9   | QI    | 105  | ASP  | 5.8  |
| 55  | RZ    | 176  | PRO  | 5.8  |
| 10  | XJ    | 46   | ARG  | 5.6  |
| 3   | XC    | 158  | GLY  | 5.5  |
| 54  | YY    | 1    | MET  | 5.5  |
| 9   | QI    | 106  | ALA  | 5.5  |
| 22  | QV    | 1    | C    | 5.5  |
| 38  | YE    | 146  | THR  | 5.3  |
| 22  | XV    | 1    | C    | 5.3  |
| 34  | R9    | 28   | GLU  | 5.2  |
| 21  | QU    | 14   | TRP  | 5.2  |
| 12  | XL    | 21   | LYS  | 5.2  |
| 26  | Y1    | 2    | SER  | 5.2  |
| 51  | RV    | 73   | SER  | 5.1  |
| 35  | YA    | 1092 | C    | 5.0  |
| 21  | QU    | 6    | ARG  | 5.0  |
| 45  | RP    | 15   | ARG  | 5.0  |
| 11  | XK    | 117  | ASN  | 4.9  |
| 4   | QD    | 24   | GLU  | 4.9  |
| 9   | QI    | 102  | LEU  | 4.9  |
| 1   | XA    | 1397 | C    | 4.9  |
| 55  | YZ    | 120  | ILE  | 4.8  |
| 54  | RY    | 1    | MET  | 4.8  |
| 35  | YA    | 1075 | C    | 4.8  |
| 10  | QJ    | 47   | PHE  | 4.8  |
| 12  | QL    | 32   | PHE  | 4.8  |
| 48  | RS    | 32   | LEU  | 4.7  |
| 35  | YA    | 1090 | U    | 4.7  |
| 35  | RA    | 2155 | G    | 4.7  |
| 9   | XI    | 125  | TYR  | 4.7  |
| 10  | XJ    | 64   | GLU  | 4.6  |
| 35  | YA    | 1077 | A    | 4.6  |
| 3   | QC    | 160  | ALA  | 4.6  |
| 7   | QG    | 84   | ASN  | 4.6  |
| 11  | XK    | 126  | ARG  | 4.5  |
| 47  | YR    | 7    | GLY  | 4.5  |
| 21  | QU    | 2    | GLY  | 4.4  |
| 16  | QP    | 22   | THR  | 4.3  |
| 16  | QP    | 68   | ASP  | 4.3  |
| 35  | RA    | 2319 | G    | 4.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 20         | QT           | 70         | SER         | 4.3         |
| 55         | YZ           | 177        | PRO         | 4.3         |
| 55         | YZ           | 166        | SER         | 4.3         |
| 8          | QH           | 99         | GLU         | 4.3         |
| 55         | RZ           | 115        | GLY         | 4.2         |
| 10         | QJ           | 76         | ASN         | 4.2         |
| 35         | YA           | 1067       | A           | 4.2         |
| 35         | YA           | 1093       | G           | 4.2         |
| 32         | R7           | 48         | LYS         | 4.2         |
| 55         | RZ           | 141        | VAL         | 4.1         |
| 21         | QU           | 5          | ASP         | 4.1         |
| 35         | RA           | 1171       | G           | 4.1         |
| 12         | QL           | 17         | LYS         | 4.1         |
| 14         | XN           | 2          | ALA         | 4.1         |
| 46         | RQ           | 22         | LYS         | 4.1         |
| 12         | XL           | 89         | ARG         | 4.1         |
| 55         | RZ           | 175        | VAL         | 4.1         |
| 14         | QN           | 35         | ARG         | 4.0         |
| 17         | QQ           | 24         | GLU         | 4.0         |
| 7          | XG           | 42         | ILE         | 4.0         |
| 16         | XP           | 28         | ARG         | 4.0         |
| 35         | YA           | 1078       | U           | 4.0         |
| 17         | XQ           | 24         | GLU         | 4.0         |
| 21         | QU           | 4          | GLY         | 4.0         |
| 2          | QB           | 101        | MET         | 4.0         |
| 16         | XP           | 68         | ASP         | 4.0         |
| 35         | RA           | 2062       | A           | 4.0         |
| 55         | RZ           | 113        | ALA         | 3.9         |
| 1          | QA           | 79         | G           | 3.9         |
| 3          | QC           | 157        | ILE         | 3.9         |
| 10         | XJ           | 73         | ASP         | 3.8         |
| 55         | RZ           | 117        | LEU         | 3.8         |
| 12         | QL           | 18         | VAL         | 3.8         |
| 19         | QS           | 9          | VAL         | 3.8         |
| 37         | RD           | 237        | GLU         | 3.8         |
| 45         | YP           | 70         | GLN         | 3.8         |
| 9          | XI           | 126        | SER         | 3.8         |
| 1          | XA           | 630        | G           | 3.8         |
| 1          | QA           | 1531       | A           | 3.8         |
| 35         | YA           | 1066       | U           | 3.8         |
| 4          | XD           | 2          | GLY         | 3.7         |
| 45         | RP           | 32         | THR         | 3.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 48         | YS           | 3          | ARG         | 3.7         |
| 1          | QA           | 1030(C)    | C           | 3.7         |
| 11         | QK           | 117        | ASN         | 3.7         |
| 4          | XD           | 24         | GLU         | 3.6         |
| 40         | YG           | 35         | GLU         | 3.6         |
| 29         | Y4           | 63         | TYR         | 3.6         |
| 46         | RQ           | 10         | ARG         | 3.6         |
| 24         | XY           | 54         | U           | 3.6         |
| 32         | Y7           | 48         | LYS         | 3.6         |
| 55         | RZ           | 120        | ILE         | 3.6         |
| 14         | XN           | 14         | PRO         | 3.6         |
| 12         | QL           | 16         | GLU         | 3.6         |
| 3          | QC           | 158        | GLY         | 3.6         |
| 4          | XD           | 23         | GLY         | 3.5         |
| 43         | RN           | 68         | GLU         | 3.5         |
| 4          | QD           | 4          | TYR         | 3.5         |
| 19         | QS           | 84         | GLY         | 3.5         |
| 55         | YZ           | 172        | ALA         | 3.5         |
| 54         | RY           | 62         | GLU         | 3.5         |
| 14         | QN           | 3          | ARG         | 3.5         |
| 12         | XL           | 62         | SER         | 3.5         |
| 46         | YQ           | 113        | GLN         | 3.5         |
| 1          | QA           | 90         | U           | 3.5         |
| 37         | RD           | 217        | ARG         | 3.5         |
| 14         | QN           | 18         | VAL         | 3.5         |
| 55         | YZ           | 174        | VAL         | 3.4         |
| 41         | YH           | 4          | ILE         | 3.4         |
| 33         | Y8           | 65         | GLU         | 3.4         |
| 4          | QD           | 154        | ASN         | 3.4         |
| 20         | XT           | 18         | GLN         | 3.4         |
| 38         | RE           | 146        | THR         | 3.4         |
| 20         | XT           | 73         | HIS         | 3.4         |
| 26         | Y1           | 38         | SER         | 3.4         |
| 13         | QM           | 117        | VAL         | 3.4         |
| 55         | YZ           | 117        | LEU         | 3.4         |
| 44         | RO           | 1          | MET         | 3.4         |
| 9          | QI           | 64         | THR         | 3.4         |
| 14         | QN           | 7          | ILE         | 3.4         |
| 11         | XK           | 13         | GLN         | 3.4         |
| 15         | XO           | 37         | ASN         | 3.4         |
| 35         | RA           | 2804       | C           | 3.4         |
| 55         | RZ           | 116        | VAL         | 3.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | RA    | 1046 | A    | 3.3  |
| 33  | R8    | 65   | GLU  | 3.3  |
| 34  | R9    | 37   | GLY  | 3.3  |
| 35  | RA    | 1091 | G    | 3.3  |
| 35  | RA    | 2182 | G    | 3.3  |
| 20  | QT    | 17   | ARG  | 3.3  |
| 5   | XE    | 81   | GLU  | 3.3  |
| 4   | XD    | 166  | LYS  | 3.3  |
| 14  | XN    | 22   | THR  | 3.3  |
| 12  | XL    | 19   | ARG  | 3.3  |
| 24  | XY    | 17   | U    | 3.3  |
| 14  | QN    | 16   | PHE  | 3.3  |
| 51  | YV    | 49   | THR  | 3.3  |
| 54  | RY    | 12   | THR  | 3.3  |
| 11  | QK    | 14   | VAL  | 3.3  |
| 14  | XN    | 18   | VAL  | 3.3  |
| 46  | RQ    | 112  | GLU  | 3.3  |
| 14  | QN    | 21   | TYR  | 3.2  |
| 20  | XT    | 74   | LYS  | 3.2  |
| 37  | RD    | 276  | LYS  | 3.2  |
| 35  | RA    | 1090 | U    | 3.2  |
| 23  | QX    | 12   | A    | 3.2  |
| 24  | QY    | 76   | A    | 3.2  |
| 4   | XD    | 120  | LEU  | 3.2  |
| 14  | QN    | 15   | LYS  | 3.2  |
| 13  | QM    | 9    | ILE  | 3.2  |
| 55  | RZ    | 98   | MET  | 3.2  |
| 8   | XH    | 136  | GLU  | 3.2  |
| 9   | QI    | 110  | GLU  | 3.2  |
| 55  | RZ    | 178  | GLU  | 3.2  |
| 23  | QX    | 23   | A    | 3.2  |
| 46  | RQ    | 104  | PHE  | 3.2  |
| 31  | R6    | 54   | ILE  | 3.2  |
| 26  | Y1    | 23   | LYS  | 3.2  |
| 4   | XD    | 73   | ARG  | 3.2  |
| 42  | RI    | 20   | ASP  | 3.2  |
| 46  | RQ    | 59   | ARG  | 3.2  |
| 35  | YA    | 1068 | G    | 3.2  |
| 35  | RA    | 2803 | C    | 3.2  |
| 35  | YA    | 1072 | C    | 3.2  |
| 35  | YA    | 1536 | C    | 3.2  |
| 7   | QG    | 4    | ARG  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | XS    | 39   | THR  | 3.2  |
| 1   | XA    | 88   | A    | 3.1  |
| 1   | XA    | 1531 | A    | 3.1  |
| 38  | RE    | 121  | ASN  | 3.1  |
| 48  | YS    | 12   | PHE  | 3.1  |
| 35  | RA    | 1043 | C    | 3.1  |
| 55  | YZ    | 144  | LEU  | 3.1  |
| 10  | XJ    | 47   | PHE  | 3.1  |
| 14  | XN    | 16   | PHE  | 3.1  |
| 55  | YZ    | 176  | PRO  | 3.1  |
| 11  | XK    | 53   | SER  | 3.1  |
| 12  | XL    | 63   | GLY  | 3.1  |
| 33  | Y8    | 56   | GLU  | 3.1  |
| 4   | XD    | 3    | ARG  | 3.1  |
| 24  | XY    | 55   | U    | 3.1  |
| 55  | YZ    | 109  | ALA  | 3.1  |
| 4   | XD    | 134  | ASP  | 3.1  |
| 9   | QI    | 18   | PHE  | 3.1  |
| 35  | YA    | 34   | C    | 3.1  |
| 17  | XQ    | 37   | LYS  | 3.1  |
| 3   | QC    | 159  | GLY  | 3.1  |
| 32  | Y7    | 47   | ARG  | 3.1  |
| 14  | XN    | 15   | LYS  | 3.1  |
| 26  | Y1    | 27   | GLU  | 3.1  |
| 23  | XX    | 23   | A    | 3.1  |
| 41  | YH    | 175  | LYS  | 3.1  |
| 46  | RQ    | 1    | MET  | 3.1  |
| 50  | YU    | 117  | GLN  | 3.0  |
| 13  | QM    | 100  | GLY  | 3.0  |
| 28  | R3    | 55   | ARG  | 3.0  |
| 24  | QY    | 17   | U    | 3.0  |
| 27  | Y2    | 11   | GLU  | 3.0  |
| 46  | YQ    | 112  | GLU  | 3.0  |
| 16  | XP    | 29   | ASP  | 3.0  |
| 29  | Y4    | 67   | TYR  | 3.0  |
| 10  | QJ    | 62   | HIS  | 3.0  |
| 55  | YZ    | 81   | ARG  | 3.0  |
| 35  | RA    | 1092 | C    | 3.0  |
| 35  | YA    | 2803 | C    | 3.0  |
| 55  | RZ    | 114  | GLY  | 3.0  |
| 11  | XK    | 42   | TRP  | 3.0  |
| 53  | YX    | 1    | MET  | 3.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 8   | QH    | 91     | ARG  | 3.0  |
| 16  | QP    | 21     | VAL  | 3.0  |
| 9   | XI    | 12     | GLU  | 3.0  |
| 41  | RH    | 155    | SER  | 3.0  |
| 3   | XC    | 162    | GLN  | 3.0  |
| 35  | RA    | 363(A) | G    | 3.0  |
| 35  | RA    | 1042   | G    | 3.0  |
| 4   | QD    | 181    | MET  | 3.0  |
| 35  | YA    | 1046   | A    | 3.0  |
| 35  | YA    | 1095   | A    | 3.0  |
| 55  | YZ    | 173    | ALA  | 3.0  |
| 24  | QY    | 61     | C    | 3.0  |
| 14  | QN    | 38     | GLY  | 3.0  |
| 27  | Y2    | 70     | GLN  | 3.0  |
| 16  | QP    | 19     | ILE  | 3.0  |
| 33  | Y8    | 40     | GLU  | 2.9  |
| 35  | RA    | 2156   | G    | 2.9  |
| 35  | RA    | 2805   | G    | 2.9  |
| 46  | RQ    | 61     | GLY  | 2.9  |
| 35  | YA    | 1076   | C    | 2.9  |
| 12  | XL    | 85     | ILE  | 2.9  |
| 15  | XO    | 64     | ARG  | 2.9  |
| 4   | QD    | 98     | GLU  | 2.9  |
| 9   | QI    | 127    | LYS  | 2.9  |
| 17  | QQ    | 96     | GLU  | 2.9  |
| 40  | RG    | 46     | ALA  | 2.9  |
| 11  | QK    | 13     | GLN  | 2.9  |
| 20  | QT    | 14     | LYS  | 2.9  |
| 21  | QU    | 17     | THR  | 2.9  |
| 9   | XI    | 106    | ALA  | 2.9  |
| 9   | XI    | 36     | TYR  | 2.9  |
| 26  | Y1    | 36     | GLY  | 2.9  |
| 37  | RD    | 231    | HIS  | 2.9  |
| 37  | RD    | 268    | ARG  | 2.9  |
| 43  | RN    | 26     | LEU  | 2.9  |
| 46  | RQ    | 113    | GLN  | 2.9  |
| 9   | XI    | 105    | ASP  | 2.9  |
| 21  | QU    | 3      | LYS  | 2.9  |
| 38  | RE    | 17     | ASP  | 2.9  |
| 43  | RN    | 83     | LYS  | 2.9  |
| 24  | XY    | 15     | G    | 2.9  |
| 35  | RA    | 2140   | C    | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | QH    | 84   | ARG  | 2.9  |
| 52  | RW    | 92   | ARG  | 2.9  |
| 10  | QJ    | 59   | SER  | 2.9  |
| 16  | XP    | 19   | ILE  | 2.9  |
| 4   | XD    | 76   | ARG  | 2.9  |
| 10  | QJ    | 63   | PHE  | 2.9  |
| 12  | QL    | 29   | GLY  | 2.9  |
| 34  | R9    | 22   | ARG  | 2.9  |
| 12  | XL    | 23   | LYS  | 2.9  |
| 38  | RE    | 203  | LYS  | 2.9  |
| 26  | R1    | 8    | SER  | 2.8  |
| 35  | RA    | 1053 | C    | 2.8  |
| 12  | XL    | 30   | ALA  | 2.8  |
| 37  | YD    | 276  | LYS  | 2.8  |
| 9   | QI    | 36   | TYR  | 2.8  |
| 35  | RA    | 1087 | G    | 2.8  |
| 5   | QE    | 81   | GLU  | 2.8  |
| 20  | XT    | 8    | ARG  | 2.8  |
| 35  | RA    | 2139 | C    | 2.8  |
| 35  | RA    | 2142 | C    | 2.8  |
| 35  | YA    | 277  | C    | 2.8  |
| 39  | RF    | 161  | GLU  | 2.8  |
| 17  | XQ    | 100  | LYS  | 2.8  |
| 3   | XC    | 2    | GLY  | 2.8  |
| 54  | RY    | 5    | MET  | 2.8  |
| 9   | QI    | 62   | TYR  | 2.8  |
| 3   | QC    | 174  | PRO  | 2.8  |
| 14  | QN    | 29   | ARG  | 2.8  |
| 20  | XT    | 7    | LYS  | 2.8  |
| 44  | RO    | 81   | ASP  | 2.8  |
| 45  | RP    | 76   | LYS  | 2.8  |
| 1   | QA    | 1364 | U    | 2.8  |
| 9   | QI    | 115  | GLY  | 2.8  |
| 12  | QL    | 64   | TYR  | 2.8  |
| 35  | RA    | 2151 | G    | 2.8  |
| 35  | YA    | 1071 | G    | 2.8  |
| 35  | YA    | 2178 | C    | 2.8  |
| 35  | YA    | 2805 | G    | 2.8  |
| 13  | QM    | 92   | HIS  | 2.8  |
| 12  | XL    | 104  | VAL  | 2.8  |
| 29  | Y4    | 66   | SER  | 2.8  |
| 34  | R9    | 16   | VAL  | 2.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | RD           | 265        | PRO         | 2.8         |
| 45         | YP           | 42         | SER         | 2.8         |
| 21         | QU           | 8          | THR         | 2.8         |
| 1          | QA           | 1363(B)    | A           | 2.8         |
| 9          | QI           | 125        | TYR         | 2.8         |
| 35         | RA           | 1103       | A           | 2.8         |
| 36         | YB           | 1          | U           | 2.8         |
| 14         | QN           | 2          | ALA         | 2.8         |
| 14         | XN           | 12         | ARG         | 2.8         |
| 9          | QI           | 11         | LYS         | 2.8         |
| 10         | QJ           | 33         | GLN         | 2.8         |
| 35         | RA           | 34         | C           | 2.8         |
| 55         | YZ           | 113        | ALA         | 2.8         |
| 15         | XO           | 60         | VAL         | 2.8         |
| 55         | YZ           | 116        | VAL         | 2.8         |
| 14         | QN           | 13         | THR         | 2.8         |
| 37         | RD           | 188        | GLU         | 2.8         |
| 12         | XL           | 29         | GLY         | 2.7         |
| 15         | XO           | 89         | GLY         | 2.7         |
| 17         | QQ           | 91         | ARG         | 2.7         |
| 47         | RR           | 68         | ARG         | 2.7         |
| 4          | QD           | 166        | LYS         | 2.7         |
| 1          | QA           | 1447       | A           | 2.7         |
| 19         | QS           | 11         | VAL         | 2.7         |
| 24         | QY           | 54         | U           | 2.7         |
| 3          | QC           | 166        | GLU         | 2.7         |
| 14         | XN           | 7          | ILE         | 2.7         |
| 19         | XS           | 38         | SER         | 2.7         |
| 48         | RS           | 8          | GLU         | 2.7         |
| 13         | XM           | 6          | GLY         | 2.7         |
| 19         | XS           | 68         | GLY         | 2.7         |
| 4          | QD           | 134        | ASP         | 2.7         |
| 27         | R2           | 52         | ASP         | 2.7         |
| 35         | YA           | 2318       | G           | 2.7         |
| 9          | QI           | 119        | ALA         | 2.7         |
| 9          | QI           | 14         | VAL         | 2.7         |
| 19         | XS           | 9          | VAL         | 2.7         |
| 4          | QD           | 165        | MET         | 2.7         |
| 47         | RR           | 1          | MET         | 2.7         |
| 2          | QB           | 12         | GLU         | 2.7         |
| 38         | YE           | 71         | GLY         | 2.7         |
| 53         | RX           | 68         | ARG         | 2.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | YA    | 2174 | C    | 2.7  |
| 4   | XD    | 188  | LEU  | 2.7  |
| 33  | R8    | 56   | GLU  | 2.7  |
| 13  | QM    | 102  | ARG  | 2.7  |
| 21  | XU    | 6    | ARG  | 2.7  |
| 37  | YD    | 267  | SER  | 2.7  |
| 35  | YA    | 1097 | U    | 2.7  |
| 1   | QA    | 532  | A    | 2.7  |
| 35  | YA    | 2602 | A    | 2.7  |
| 20  | QT    | 64   | ASP  | 2.7  |
| 49  | RT    | 131  | ALA  | 2.7  |
| 2   | XB    | 7    | VAL  | 2.7  |
| 7   | XG    | 38   | LEU  | 2.7  |
| 17  | XQ    | 35   | VAL  | 2.7  |
| 19  | QS    | 5    | LEU  | 2.7  |
| 12  | QL    | 95   | GLY  | 2.7  |
| 12  | XL    | 47   | LYS  | 2.7  |
| 55  | YZ    | 170  | THR  | 2.7  |
| 1   | QA    | 1202 | G    | 2.7  |
| 35  | RA    | 2894 | G    | 2.7  |
| 35  | YA    | 2807 | G    | 2.7  |
| 35  | YA    | 1101 | U    | 2.7  |
| 37  | RD    | 84   | TYR  | 2.7  |
| 38  | RE    | 25   | VAL  | 2.7  |
| 35  | RA    | 2117 | A    | 2.6  |
| 55  | RZ    | 146  | ILE  | 2.6  |
| 55  | YZ    | 118  | GLN  | 2.6  |
| 33  | Y8    | 15   | LYS  | 2.6  |
| 38  | RE    | 145  | LYS  | 2.6  |
| 35  | RA    | 1076 | C    | 2.6  |
| 9   | XI    | 102  | LEU  | 2.6  |
| 10  | QJ    | 20   | ALA  | 2.6  |
| 2   | QB    | 70   | PHE  | 2.6  |
| 14  | QN    | 12   | ARG  | 2.6  |
| 21  | XU    | 15   | ARG  | 2.6  |
| 24  | QY    | 15   | G    | 2.6  |
| 35  | RA    | 2100 | G    | 2.6  |
| 35  | RA    | 2154 | G    | 2.6  |
| 39  | RF    | 78   | ILE  | 2.6  |
| 28  | R3    | 60   | GLU  | 2.6  |
| 12  | XL    | 120  | TYR  | 2.6  |
| 40  | RG    | 39   | ILE  | 2.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 43         | RN           | 84         | LYS         | 2.6         |
| 21         | XU           | 16         | GLY         | 2.6         |
| 53         | RX           | 61         | GLY         | 2.6         |
| 17         | XQ           | 5          | VAL         | 2.6         |
| 41         | YH           | 113        | VAL         | 2.6         |
| 9          | XI           | 71         | SER         | 2.6         |
| 28         | Y3           | 38         | GLU         | 2.6         |
| 28         | Y3           | 60         | GLU         | 2.6         |
| 55         | YZ           | 175        | VAL         | 2.6         |
| 7          | XG           | 5          | ARG         | 2.6         |
| 10         | XJ           | 100        | THR         | 2.6         |
| 23         | XX           | 11         | U           | 2.6         |
| 27         | Y2           | 69         | ARG         | 2.6         |
| 37         | YD           | 27         | THR         | 2.6         |
| 32         | R7           | 1          | MET         | 2.6         |
| 35         | RA           | 171        | G           | 2.6         |
| 35         | RA           | 2116       | G           | 2.6         |
| 35         | YA           | 1533       | G           | 2.6         |
| 35         | YA           | 2792       | G           | 2.6         |
| 55         | YZ           | 104        | PHE         | 2.6         |
| 40         | YG           | 2          | PRO         | 2.6         |
| 35         | YA           | 1098       | A           | 2.6         |
| 4          | QD           | 23         | GLY         | 2.6         |
| 10         | XJ           | 10         | GLY         | 2.6         |
| 10         | QJ           | 40         | LEU         | 2.6         |
| 42         | YI           | 116        | LEU         | 2.6         |
| 4          | XD           | 122        | ARG         | 2.6         |
| 53         | YX           | 60         | ARG         | 2.6         |
| 54         | RY           | 19         | LYS         | 2.6         |
| 3          | XC           | 192        | THR         | 2.6         |
| 17         | XQ           | 15         | MET         | 2.5         |
| 20         | QT           | 73         | HIS         | 2.5         |
| 3          | QC           | 13         | GLY         | 2.5         |
| 19         | XS           | 84         | GLY         | 2.5         |
| 32         | R7           | 47         | ARG         | 2.5         |
| 9          | QI           | 15         | ALA         | 2.5         |
| 19         | XS           | 73         | GLU         | 2.5         |
| 1          | XA           | 89         | C           | 2.5         |
| 24         | QY           | 16         | C           | 2.5         |
| 35         | RA           | 2755       | C           | 2.5         |
| 12         | QL           | 31         | PRO         | 2.5         |
| 33         | R8           | 45         | GLY         | 2.5         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 13         | XM           | 88         | ARG         | 2.5         |
| 15         | XO           | 65         | ARG         | 2.5         |
| 33         | Y8           | 46         | ARG         | 2.5         |
| 37         | RD           | 262        | ARG         | 2.5         |
| 43         | RN           | 74         | ARG         | 2.5         |
| 14         | QN           | 25         | VAL         | 2.5         |
| 55         | RZ           | 174        | VAL         | 2.5         |
| 9          | XI           | 110        | GLU         | 2.5         |
| 17         | XQ           | 27         | PHE         | 2.5         |
| 24         | XY           | 1          | G           | 2.5         |
| 3          | QC           | 12         | LEU         | 2.5         |
| 1          | QA           | 1397       | C           | 2.5         |
| 4          | XD           | 159        | ARG         | 2.5         |
| 25         | R0           | 74         | ARG         | 2.5         |
| 45         | RP           | 45         | LEU         | 2.5         |
| 9          | QI           | 100        | GLY         | 2.5         |
| 19         | QS           | 68         | GLY         | 2.5         |
| 35         | RA           | 1052       | C           | 2.5         |
| 35         | YA           | 1102       | C           | 2.5         |
| 51         | RV           | 48         | GLY         | 2.5         |
| 45         | YP           | 117        | GLU         | 2.5         |
| 46         | RQ           | 48         | GLU         | 2.5         |
| 9          | XI           | 64         | THR         | 2.5         |
| 2          | XB           | 175        | ARG         | 2.5         |
| 10         | XJ           | 62         | HIS         | 2.5         |
| 51         | RV           | 50         | PRO         | 2.5         |
| 26         | Y1           | 98         | LEU         | 2.5         |
| 55         | RZ           | 70         | LEU         | 2.5         |
| 37         | YD           | 238        | GLY         | 2.5         |
| 7          | XG           | 80         | VAL         | 2.5         |
| 2          | XB           | 200        | ILE         | 2.5         |
| 10         | XJ           | 76         | ASN         | 2.5         |
| 52         | RW           | 94         | ASP         | 2.5         |
| 55         | YZ           | 123        | ASP         | 2.5         |
| 10         | XJ           | 60         | ARG         | 2.5         |
| 45         | YP           | 16         | ARG         | 2.5         |
| 55         | YZ           | 108        | PRO         | 2.5         |
| 48         | YS           | 8          | GLU         | 2.4         |
| 9          | XI           | 9          | ARG         | 2.4         |
| 12         | XL           | 20         | LYS         | 2.4         |
| 35         | RA           | 273(K)     | C           | 2.4         |
| 35         | RA           | 2146       | C           | 2.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 55         | YZ           | 157        | LEU         | 2.4         |
| 1          | XA           | 1532       | U           | 2.4         |
| 3          | XC           | 206        | GLU         | 2.4         |
| 15         | XO           | 41         | GLU         | 2.4         |
| 43         | YN           | 68         | GLU         | 2.4         |
| 45         | RP           | 74         | GLU         | 2.4         |
| 8          | QH           | 107        | LEU         | 2.4         |
| 48         | RS           | 16         | ASN         | 2.4         |
| 35         | YA           | 887        | A           | 2.4         |
| 55         | RZ           | 107        | THR         | 2.4         |
| 7          | XG           | 85         | TYR         | 2.4         |
| 19         | QS           | 41         | VAL         | 2.4         |
| 24         | QY           | 74         | C           | 2.4         |
| 35         | RA           | 1051       | G           | 2.4         |
| 35         | RA           | 1115       | G           | 2.4         |
| 35         | YA           | 1087       | G           | 2.4         |
| 42         | RI           | 1          | MET         | 2.4         |
| 9          | QI           | 128        | ARG         | 2.4         |
| 14         | XN           | 3          | ARG         | 2.4         |
| 19         | XS           | 78         | ARG         | 2.4         |
| 28         | Y3           | 55         | ARG         | 2.4         |
| 42         | YI           | 10         | GLU         | 2.4         |
| 4          | XD           | 27         | TYR         | 2.4         |
| 9          | QI           | 10         | ARG         | 2.4         |
| 47         | RR           | 2          | ARG         | 2.4         |
| 2          | XB           | 17         | PHE         | 2.4         |
| 1          | QA           | 723        | U           | 2.4         |
| 4          | XD           | 135        | LEU         | 2.4         |
| 22         | XV           | 47         | U           | 2.4         |
| 35         | RA           | 2150       | U           | 2.4         |
| 46         | YQ           | 41         | TRP         | 2.4         |
| 4          | XD           | 4          | TYR         | 2.4         |
| 6          | XF           | 55         | ASP         | 2.4         |
| 28         | R3           | 39         | ASP         | 2.4         |
| 46         | RQ           | 28         | ALA         | 2.4         |
| 53         | RX           | 63         | LYS         | 2.4         |
| 19         | XS           | 56         | GLN         | 2.4         |
| 55         | YZ           | 136        | PHE         | 2.4         |
| 35         | RA           | 1460       | A           | 2.4         |
| 35         | YA           | 1070       | A           | 2.4         |
| 35         | YA           | 9          | U           | 2.4         |
| 35         | RA           | 1100       | C           | 2.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | YZ    | 143  | GLY  | 2.3  |
| 11  | QK    | 123  | LYS  | 2.3  |
| 4   | QD    | 122  | ARG  | 2.3  |
| 11  | QK    | 126  | ARG  | 2.3  |
| 15  | XO    | 3    | ILE  | 2.3  |
| 21  | QU    | 20   | LYS  | 2.3  |
| 21  | QU    | 18   | TYR  | 2.3  |
| 37  | RD    | 54   | ARG  | 2.3  |
| 14  | QN    | 36   | PHE  | 2.3  |
| 16  | XP    | 34   | GLU  | 2.3  |
| 40  | YG    | 5    | VAL  | 2.3  |
| 19  | QS    | 38   | SER  | 2.3  |
| 12  | QL    | 13   | LYS  | 2.3  |
| 23  | QX    | 14   | A    | 2.3  |
| 23  | XX    | 12   | A    | 2.3  |
| 23  | XX    | 14   | A    | 2.3  |
| 2   | XB    | 172  | ILE  | 2.3  |
| 3   | XC    | 5    | ILE  | 2.3  |
| 18  | XR    | 82   | THR  | 2.3  |
| 25  | R0    | 19   | LYS  | 2.3  |
| 33  | R8    | 11   | LYS  | 2.3  |
| 54  | YY    | 80   | GLY  | 2.3  |
| 49  | YT    | 131  | ALA  | 2.3  |
| 52  | YW    | 111  | HIS  | 2.3  |
| 13  | XM    | 16   | ASP  | 2.3  |
| 35  | RA    | 2183 | C    | 2.3  |
| 5   | QE    | 20   | GLN  | 2.3  |
| 7   | QG    | 74   | GLU  | 2.3  |
| 1   | QA    | 1310 | G    | 2.3  |
| 23  | XX    | 9    | G    | 2.3  |
| 35  | YA    | 1074 | G    | 2.3  |
| 40  | RG    | 74   | LYS  | 2.3  |
| 19  | XS    | 2    | PRO  | 2.3  |
| 37  | RD    | 211  | ARG  | 2.3  |
| 45  | RP    | 21   | ARG  | 2.3  |
| 48  | RS    | 3    | ARG  | 2.3  |
| 37  | RD    | 224  | ALA  | 2.3  |
| 7   | QG    | 148  | ASN  | 2.3  |
| 8   | QH    | 112  | LEU  | 2.3  |
| 20  | XT    | 10   | LEU  | 2.3  |
| 23  | XX    | 13   | A    | 2.3  |
| 29  | Y4    | 59   | PHE  | 2.3  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 10  | QJ    | 58     | ASP  | 2.3  |
| 34  | R9    | 12     | ASP  | 2.3  |
| 35  | RA    | 273(B) | U    | 2.3  |
| 35  | YA    | 1065   | U    | 2.3  |
| 53  | YX    | 38     | GLU  | 2.3  |
| 13  | XM    | 98     | VAL  | 2.3  |
| 32  | R7    | 46     | VAL  | 2.3  |
| 37  | RD    | 153    | ALA  | 2.3  |
| 2   | QB    | 187    | LEU  | 2.3  |
| 13  | XM    | 90     | LEU  | 2.3  |
| 17  | QQ    | 98     | LEU  | 2.3  |
| 18  | XR    | 78     | LEU  | 2.3  |
| 23  | QX    | 10     | G    | 2.3  |
| 35  | RA    | 11     | G    | 2.3  |
| 35  | RA    | 2807   | G    | 2.3  |
| 4   | XD    | 77     | ASN  | 2.3  |
| 8   | XH    | 4      | ASP  | 2.3  |
| 33  | Y8    | 26     | LYS  | 2.3  |
| 7   | QG    | 80     | VAL  | 2.3  |
| 29  | Y4    | 64     | GLY  | 2.3  |
| 4   | XD    | 33     | MET  | 2.3  |
| 53  | RX    | 91     | ALA  | 2.3  |
| 55  | RZ    | 172    | ALA  | 2.3  |
| 35  | YA    | 1178   | C    | 2.3  |
| 12  | QL    | 47     | LYS  | 2.3  |
| 3   | XC    | 179    | ARG  | 2.3  |
| 33  | R8    | 35     | GLN  | 2.3  |
| 2   | QB    | 93     | VAL  | 2.3  |
| 8   | QH    | 136    | GLU  | 2.2  |
| 37  | YD    | 237    | GLU  | 2.2  |
| 44  | YO    | 120    | GLU  | 2.2  |
| 54  | YY    | 64     | GLU  | 2.2  |
| 1   | QA    | 1117   | G    | 2.2  |
| 35  | RA    | 2141   | G    | 2.2  |
| 35  | YA    | 1089   | G    | 2.2  |
| 20  | QT    | 101    | GLY  | 2.2  |
| 21  | XU    | 11     | GLY  | 2.2  |
| 54  | RY    | 16     | ALA  | 2.2  |
| 1   | XA    | 60     | A    | 2.2  |
| 5   | QE    | 12     | LEU  | 2.2  |
| 24  | XY    | 76     | A    | 2.2  |
| 35  | RA    | 362    | U    | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 35         | RA           | 2585       | U           | 2.2         |
| 20         | XT           | 19         | SER         | 2.2         |
| 1          | XA           | 63         | C           | 2.2         |
| 3          | QC           | 164        | ARG         | 2.2         |
| 24         | QY           | 60         | C           | 2.2         |
| 24         | XY           | 16         | C           | 2.2         |
| 35         | RA           | 2789       | C           | 2.2         |
| 55         | RZ           | 80         | ARG         | 2.2         |
| 15         | XO           | 62         | GLN         | 2.2         |
| 45         | YP           | 71         | VAL         | 2.2         |
| 4          | XD           | 80         | GLU         | 2.2         |
| 18         | XR           | 62         | GLU         | 2.2         |
| 27         | R2           | 11         | GLU         | 2.2         |
| 45         | YP           | 74         | GLU         | 2.2         |
| 15         | XO           | 87         | ILE         | 2.2         |
| 12         | QL           | 48         | PRO         | 2.2         |
| 42         | RI           | 84         | GLY         | 2.2         |
| 46         | YQ           | 15         | GLY         | 2.2         |
| 3          | QC           | 4          | LYS         | 2.2         |
| 13         | QM           | 103        | THR         | 2.2         |
| 24         | XY           | 57         | G           | 2.2         |
| 35         | YA           | 1171       | G           | 2.2         |
| 40         | RG           | 165        | THR         | 2.2         |
| 4          | XD           | 209        | ARG         | 2.2         |
| 1          | XA           | 1447       | A           | 2.2         |
| 19         | QS           | 4          | SER         | 2.2         |
| 49         | RT           | 28         | VAL         | 2.2         |
| 7          | QG           | 37         | ASN         | 2.2         |
| 13         | QM           | 78         | ILE         | 2.2         |
| 1          | QA           | 1195       | C           | 2.2         |
| 2          | XB           | 18         | GLY         | 2.2         |
| 9          | QI           | 8          | GLY         | 2.2         |
| 20         | XT           | 103        | GLY         | 2.2         |
| 39         | RF           | 81         | PRO         | 2.2         |
| 49         | YT           | 93         | ARG         | 2.2         |
| 12         | XL           | 42         | THR         | 2.2         |
| 9          | QI           | 65         | VAL         | 2.2         |
| 53         | YX           | 59         | VAL         | 2.2         |
| 1          | QA           | 1065       | U           | 2.2         |
| 1          | QA           | 485        | G           | 2.2         |
| 1          | XA           | 324        | G           | 2.2         |
| 2          | QB           | 118        | LEU         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | QG    | 73   | MET  | 2.2  |
| 22  | XV    | 38   | A    | 2.2  |
| 24  | XY    | 3    | G    | 2.2  |
| 54  | YY    | 40   | GLU  | 2.2  |
| 55  | YZ    | 119  | GLU  | 2.2  |
| 55  | YZ    | 150  | LEU  | 2.2  |
| 8   | XH    | 28   | ALA  | 2.2  |
| 11  | XK    | 118  | GLY  | 2.2  |
| 17  | XQ    | 33   | GLY  | 2.2  |
| 48  | RS    | 37   | ALA  | 2.2  |
| 49  | RT    | 130  | ALA  | 2.2  |
| 39  | YF    | 62   | ARG  | 2.2  |
| 53  | RX    | 60   | ARG  | 2.2  |
| 2   | QB    | 164  | VAL  | 2.2  |
| 17  | XQ    | 23   | VAL  | 2.2  |
| 12  | XL    | 116  | SER  | 2.2  |
| 9   | QI    | 99   | LEU  | 2.2  |
| 3   | XC    | 3    | ASN  | 2.2  |
| 16  | XP    | 54   | GLU  | 2.2  |
| 41  | RH    | 167  | GLU  | 2.2  |
| 43  | RN    | 92   | ALA  | 2.2  |
| 4   | QD    | 2    | GLY  | 2.2  |
| 7   | XG    | 81   | GLY  | 2.2  |
| 13  | QM    | 97   | PRO  | 2.2  |
| 26  | Y1    | 21   | ARG  | 2.2  |
| 39  | YF    | 74   | ARG  | 2.2  |
| 9   | XI    | 37   | PHE  | 2.2  |
| 19  | QS    | 12   | ASP  | 2.2  |
| 35  | RA    | 1088 | A    | 2.2  |
| 35  | RA    | 2802 | G    | 2.2  |
| 35  | YA    | 2141 | G    | 2.2  |
| 9   | QI    | 7    | THR  | 2.1  |
| 24  | XY    | 61   | C    | 2.1  |
| 35  | YA    | 2804 | C    | 2.1  |
| 3   | XC    | 188  | LEU  | 2.1  |
| 10  | XJ    | 33   | GLN  | 2.1  |
| 13  | QM    | 67   | GLU  | 2.1  |
| 17  | QQ    | 75   | ARG  | 2.1  |
| 28  | Y3    | 2    | PRO  | 2.1  |
| 29  | Y4    | 17   | GLY  | 2.1  |
| 39  | RF    | 85   | GLY  | 2.1  |
| 11  | XK    | 36   | ASP  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | YD    | 71   | ASP  | 2.1  |
| 42  | YI    | 20   | ASP  | 2.1  |
| 50  | RU    | 56   | ASP  | 2.1  |
| 1   | QA    | 1286 | A    | 2.1  |
| 35  | RA    | 896  | A    | 2.1  |
| 35  | YA    | 2062 | A    | 2.1  |
| 35  | YA    | 2117 | A    | 2.1  |
| 15  | QO    | 31   | LEU  | 2.1  |
| 20  | QT    | 74   | LYS  | 2.1  |
| 35  | YA    | 545  | G    | 2.1  |
| 35  | YA    | 2190 | G    | 2.1  |
| 46  | RQ    | 103  | MET  | 2.1  |
| 14  | XN    | 35   | ARG  | 2.1  |
| 48  | YS    | 15   | ARG  | 2.1  |
| 52  | YW    | 93   | ALA  | 2.1  |
| 3   | XC    | 161  | GLU  | 2.1  |
| 5   | XE    | 23   | GLY  | 2.1  |
| 38  | YE    | 163  | GLU  | 2.1  |
| 38  | YE    | 193  | GLY  | 2.1  |
| 41  | YH    | 58   | GLU  | 2.1  |
| 35  | RA    | 1102 | C    | 2.1  |
| 36  | RB    | 12   | C    | 2.1  |
| 10  | XJ    | 58   | ASP  | 2.1  |
| 2   | QB    | 102  | LEU  | 2.1  |
| 10  | QJ    | 75   | ILE  | 2.1  |
| 38  | RE    | 152  | LYS  | 2.1  |
| 10  | XJ    | 43   | ARG  | 2.1  |
| 43  | YN    | 124  | ALA  | 2.1  |
| 44  | RO    | 41   | ALA  | 2.1  |
| 29  | Y4    | 54   | GLY  | 2.1  |
| 29  | Y4    | 57   | GLU  | 2.1  |
| 35  | RA    | 1098 | A    | 2.1  |
| 40  | RG    | 35   | GLU  | 2.1  |
| 40  | YG    | 164  | GLU  | 2.1  |
| 2   | QB    | 55   | PHE  | 2.1  |
| 9   | QI    | 108  | VAL  | 2.1  |
| 30  | Y5    | 60   | VAL  | 2.1  |
| 35  | YA    | 2319 | G    | 2.1  |
| 35  | YA    | 2793 | G    | 2.1  |
| 50  | RU    | 90   | VAL  | 2.1  |
| 35  | RA    | 1075 | C    | 2.1  |
| 35  | RA    | 1886 | C    | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 35         | YA           | 2179       | C           | 2.1         |
| 27         | Y2           | 15         | LYS         | 2.1         |
| 50         | RU           | 13         | LYS         | 2.1         |
| 16         | XP           | 73         | LEU         | 2.1         |
| 19         | XS           | 15         | LEU         | 2.1         |
| 29         | R4           | 22         | ILE         | 2.1         |
| 40         | RG           | 52         | ILE         | 2.1         |
| 21         | QU           | 22         | ARG         | 2.1         |
| 16         | QP           | 82         | GLN         | 2.1         |
| 17         | XQ           | 26         | GLN         | 2.1         |
| 24         | QY           | 55         | U           | 2.1         |
| 35         | RA           | 1101       | U           | 2.1         |
| 38         | RE           | 139        | GLY         | 2.1         |
| 9          | QI           | 123        | PRO         | 2.1         |
| 47         | RR           | 43         | GLU         | 2.1         |
| 49         | YT           | 45         | PHE         | 2.1         |
| 49         | YT           | 46         | GLU         | 2.1         |
| 35         | RA           | 1445(A)    | A           | 2.1         |
| 35         | RA           | 1847       | A           | 2.1         |
| 35         | YA           | 2169       | A           | 2.1         |
| 43         | YN           | 83         | LYS         | 2.1         |
| 3          | QC           | 5          | ILE         | 2.1         |
| 8          | XH           | 133        | LEU         | 2.1         |
| 9          | QI           | 96         | LEU         | 2.1         |
| 10         | QJ           | 8          | LEU         | 2.1         |
| 45         | RP           | 79         | ARG         | 2.1         |
| 55         | YZ           | 125        | LEU         | 2.1         |
| 55         | YZ           | 155        | LEU         | 2.1         |
| 19         | QS           | 44         | MET         | 2.1         |
| 17         | QQ           | 42         | TYR         | 2.1         |
| 54         | RY           | 35         | TYR         | 2.1         |
| 35         | RA           | 1536       | C           | 2.1         |
| 35         | YA           | 1100       | C           | 2.1         |
| 1          | QA           | 630        | G           | 2.1         |
| 1          | QA           | 1030(B)    | G           | 2.1         |
| 35         | RA           | 2318       | G           | 2.1         |
| 3          | XC           | 159        | GLY         | 2.1         |
| 2          | QB           | 163        | PHE         | 2.1         |
| 5          | QE           | 79         | GLU         | 2.1         |
| 1          | XA           | 1196       | U           | 2.0         |
| 12         | QL           | 91         | LYS         | 2.0         |
| 45         | RP           | 71         | VAL         | 2.0         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | RD           | 22         | SER         | 2.0         |
| 17         | QQ           | 36         | ILE         | 2.0         |
| 21         | QU           | 13         | ILE         | 2.0         |
| 40         | RG           | 29         | TRP         | 2.0         |
| 33         | R8           | 25         | MET         | 2.0         |
| 38         | YE           | 1          | MET         | 2.0         |
| 2          | XB           | 237        | ALA         | 2.0         |
| 16         | QP           | 32         | TYR         | 2.0         |
| 35         | RA           | 1073       | A           | 2.0         |
| 35         | YA           | 529        | A           | 2.0         |
| 35         | YA           | 2135       | A           | 2.0         |
| 38         | YE           | 151        | TYR         | 2.0         |
| 46         | RQ           | 75         | THR         | 2.0         |
| 32         | Y7           | 26         | GLY         | 2.0         |
| 45         | YP           | 68         | GLN         | 2.0         |
| 12         | QL           | 94         | PRO         | 2.0         |
| 17         | QQ           | 69         | LYS         | 2.0         |
| 20         | QT           | 29         | LYS         | 2.0         |
| 44         | YO           | 108        | GLU         | 2.0         |
| 35         | YA           | 645        | C           | 2.0         |
| 45         | YP           | 76         | LYS         | 2.0         |
| 46         | RQ           | 85         | LYS         | 2.0         |
| 2          | XB           | 165        | VAL         | 2.0         |
| 12         | XL           | 18         | VAL         | 2.0         |
| 41         | RH           | 169        | VAL         | 2.0         |
| 55         | RZ           | 139        | VAL         | 2.0         |
| 10         | XJ           | 45         | ARG         | 2.0         |
| 11         | XK           | 98         | LEU         | 2.0         |
| 35         | RA           | 275        | G           | 2.0         |
| 35         | YA           | 2334       | G           | 2.0         |
| 46         | RQ           | 114        | ALA         | 2.0         |
| 4          | QD           | 54         | TYR         | 2.0         |
| 8          | XH           | 20         | TYR         | 2.0         |
| 13         | XM           | 21         | TYR         | 2.0         |
| 25         | R0           | 71         | ASP         | 2.0         |
| 29         | Y4           | 18         | CYS         | 2.0         |
| 2          | QB           | 131        | PRO         | 2.0         |
| 4          | QD           | 7          | PRO         | 2.0         |
| 34         | Y9           | 30         | PRO         | 2.0         |
| 46         | RQ           | 12         | GLN         | 2.0         |
| 4          | QD           | 73         | ARG         | 2.0         |
| 8          | XH           | 93         | VAL         | 2.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | RE    | 188  | VAL  | 2.0  |
| 39  | YF    | 35   | GLU  | 2.0  |
| 20  | QT    | 22   | ARG  | 2.0  |
| 25  | R0    | 77   | ARG  | 2.0  |
| 51  | RV    | 72   | VAL  | 2.0  |
| 55  | YZ    | 161  | VAL  | 2.0  |
| 2   | QB    | 11   | LEU  | 2.0  |
| 47  | RR    | 18   | LEU  | 2.0  |
| 35  | RA    | 1072 | C    | 2.0  |

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

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 35  | 5MU  | RA    | 1915 | 21/22 | 0.86 | 0.10 | 86,101,109,111             | 0     |
| 1   | PSU  | QA    | 516  | 20/21 | 0.87 | 0.10 | 94,102,120,123             | 0     |
| 1   | PSU  | XA    | 516  | 20/21 | 0.87 | 0.10 | 78,89,96,97                | 0     |
| 1   | 2MG  | QA    | 1207 | 24/25 | 0.87 | 0.11 | 126,135,147,148            | 0     |
| 12  | 0TD  | XL    | 92   | 10/11 | 0.87 | 0.14 | 65,73,88,113               | 0     |
| 1   | 5MC  | QA    | 967  | 21/22 | 0.89 | 0.12 | 97,98,105,116              | 0     |
| 1   | 2MG  | XA    | 1207 | 24/25 | 0.90 | 0.11 | 91,102,107,114             | 0     |
| 1   | G7M  | XA    | 527  | 24/25 | 0.90 | 0.12 | 64,72,87,114               | 0     |
| 35  | PSU  | RA    | 1911 | 20/21 | 0.91 | 0.09 | 72,85,93,99                | 0     |
| 1   | M2G  | QA    | 966  | 25/26 | 0.91 | 0.13 | 96,100,111,116             | 0     |
| 35  | 5MU  | YA    | 1915 | 21/22 | 0.91 | 0.09 | 60,70,89,93                | 0     |
| 35  | OMC  | RA    | 1920 | 21/22 | 0.91 | 0.10 | 67,70,77,83                | 0     |
| 12  | 0TD  | QL    | 92   | 10/11 | 0.92 | 0.21 | 131,143,166,185            | 0     |
| 35  | PSU  | RA    | 1917 | 20/21 | 0.92 | 0.08 | 84,91,97,106               | 0     |
| 1   | 5MC  | XA    | 1404 | 21/22 | 0.92 | 0.12 | 51,52,66,72                | 0     |
| 35  | PSU  | YA    | 1917 | 20/21 | 0.93 | 0.08 | 59,70,97,100               | 0     |
| 1   | G7M  | QA    | 527  | 24/25 | 0.93 | 0.12 | 79,88,104,109              | 0     |
| 35  | 5MC  | RA    | 1962 | 21/22 | 0.93 | 0.10 | 57,64,94,105               | 0     |
| 35  | OMU  | RA    | 2552 | 21/22 | 0.93 | 0.11 | 48,49,71,96                | 0     |
| 35  | PSU  | YA    | 1911 | 20/21 | 0.94 | 0.08 | 58,71,82,84                | 0     |
| 1   | 5MC  | XA    | 967  | 21/22 | 0.94 | 0.11 | 86,94,104,108              | 0     |
| 35  | 5MU  | YA    | 1939 | 21/22 | 0.94 | 0.10 | 37,44,55,61                | 0     |
| 35  | 5MC  | RA    | 1942 | 21/22 | 0.94 | 0.08 | 61,74,92,94                | 0     |
| 1   | 5MC  | QA    | 1407 | 21/22 | 0.94 | 0.10 | 68,70,78,81                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | 4OC  | QA    | 1402 | 22/23 | 0.94 | 0.10 | 77,82,90,101                | 0     |
| 1   | UR3  | QA    | 1498 | 21/22 | 0.95 | 0.10 | 68,69,75,86                 | 0     |
| 1   | UR3  | XA    | 1498 | 21/22 | 0.95 | 0.10 | 55,57,75,88                 | 0     |
| 1   | MA6  | XA    | 1518 | 24/25 | 0.95 | 0.11 | 52,59,86,88                 | 0     |
| 35  | 5MU  | RA    | 1939 | 21/22 | 0.95 | 0.10 | 53,61,75,83                 | 0     |
| 1   | 5MC  | QA    | 1404 | 21/22 | 0.95 | 0.09 | 67,68,69,70                 | 0     |
| 1   | 5MC  | XA    | 1400 | 21/22 | 0.95 | 0.09 | 65,75,89,94                 | 0     |
| 1   | 5MC  | QA    | 1400 | 21/22 | 0.95 | 0.09 | 78,79,92,100                | 0     |
| 35  | 2MA  | RA    | 2503 | 23/24 | 0.95 | 0.12 | 45,46,50,65                 | 0     |
| 1   | 5MC  | XA    | 1407 | 21/22 | 0.95 | 0.09 | 50,51,62,70                 | 0     |
| 35  | OMU  | YA    | 2552 | 21/22 | 0.95 | 0.09 | 35,43,55,65                 | 0     |
| 35  | PSU  | RA    | 2605 | 20/21 | 0.95 | 0.10 | 47,48,65,66                 | 0     |
| 35  | PSU  | YA    | 2605 | 20/21 | 0.95 | 0.09 | 35,38,53,57                 | 0     |
| 1   | M2G  | XA    | 966  | 25/26 | 0.96 | 0.11 | 73,82,100,102               | 0     |
| 35  | 5MC  | YA    | 1962 | 21/22 | 0.96 | 0.08 | 37,38,52,72                 | 0     |
| 35  | OMG  | RA    | 2251 | 24/25 | 0.96 | 0.09 | 47,49,65,68                 | 0     |
| 35  | OMG  | YA    | 2251 | 24/25 | 0.96 | 0.09 | 34,35,41,43                 | 0     |
| 35  | OMC  | YA    | 1920 | 21/22 | 0.96 | 0.08 | 59,67,75,79                 | 0     |
| 1   | MA6  | XA    | 1519 | 24/25 | 0.96 | 0.10 | 55,60,73,80                 | 0     |
| 1   | 4OC  | XA    | 1402 | 22/23 | 0.96 | 0.10 | 62,72,90,95                 | 0     |
| 1   | MA6  | QA    | 1518 | 24/25 | 0.96 | 0.09 | 64,65,71,75                 | 0     |
| 35  | 5MC  | YA    | 1942 | 21/22 | 0.96 | 0.07 | 43,53,69,74                 | 0     |
| 1   | MA6  | QA    | 1519 | 24/25 | 0.97 | 0.11 | 65,66,70,80                 | 0     |
| 35  | 2MA  | YA    | 2503 | 23/24 | 0.97 | 0.08 | 36,39,50,79                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3424 | 1/1   | -0.12 | 0.53 | 121,121,121,121             | 0     |
| 56  | MG   | RA    | 3256 | 1/1   | -0.02 | 0.52 | 96,96,96,96                 | 0     |
| 56  | MG   | RA    | 3301 | 1/1   | 0.10  | 0.30 | 98,98,98,98                 | 0     |
| 56  | MG   | RA    | 3189 | 1/1   | 0.11  | 0.24 | 86,86,86,86                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3309 | 1/1   | 0.13 | 0.20 | 99,99,99,99                 | 0     |
| 56  | MG   | RA    | 3205 | 1/1   | 0.19 | 0.43 | 136,136,136,136             | 0     |
| 56  | MG   | QA    | 1737 | 1/1   | 0.24 | 0.36 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3666 | 1/1   | 0.25 | 0.28 | 116,116,116,116             | 0     |
| 56  | MG   | RA    | 3579 | 1/1   | 0.26 | 0.19 | 87,87,87,87                 | 0     |
| 56  | MG   | RA    | 3369 | 1/1   | 0.26 | 0.34 | 119,119,119,119             | 0     |
| 56  | MG   | RA    | 3536 | 1/1   | 0.33 | 0.22 | 114,114,114,114             | 0     |
| 56  | MG   | RA    | 3450 | 1/1   | 0.34 | 0.55 | 94,94,94,94                 | 0     |
| 56  | MG   | RB    | 205  | 1/1   | 0.34 | 0.17 | 75,75,75,75                 | 0     |
| 56  | MG   | QA    | 1607 | 1/1   | 0.35 | 0.37 | 73,73,73,73                 | 0     |
| 56  | MG   | QA    | 1658 | 1/1   | 0.36 | 0.24 | 91,91,91,91                 | 0     |
| 56  | MG   | QA    | 1796 | 1/1   | 0.36 | 0.34 | 111,111,111,111             | 0     |
| 56  | MG   | XR    | 101  | 1/1   | 0.36 | 0.27 | 89,89,89,89                 | 0     |
| 56  | MG   | YA    | 3607 | 1/1   | 0.36 | 0.31 | 105,105,105,105             | 0     |
| 56  | MG   | RA    | 3159 | 1/1   | 0.37 | 0.63 | 97,97,97,97                 | 0     |
| 56  | MG   | QE    | 201  | 1/1   | 0.37 | 0.39 | 114,114,114,114             | 0     |
| 56  | MG   | RA    | 3058 | 1/1   | 0.37 | 0.23 | 83,83,83,83                 | 0     |
| 56  | MG   | RA    | 3400 | 1/1   | 0.37 | 0.36 | 88,88,88,88                 | 0     |
| 56  | MG   | RA    | 3083 | 1/1   | 0.37 | 0.16 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3272 | 1/1   | 0.37 | 0.19 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3221 | 1/1   | 0.39 | 0.41 | 89,89,89,89                 | 0     |
| 56  | MG   | RA    | 3381 | 1/1   | 0.40 | 0.43 | 87,87,87,87                 | 0     |
| 56  | MG   | RA    | 3513 | 1/1   | 0.40 | 0.27 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3053 | 1/1   | 0.40 | 0.51 | 108,108,108,108             | 0     |
| 56  | MG   | RA    | 3213 | 1/1   | 0.40 | 0.30 | 105,105,105,105             | 0     |
| 56  | MG   | RA    | 3214 | 1/1   | 0.41 | 0.36 | 105,105,105,105             | 0     |
| 56  | MG   | RA    | 3155 | 1/1   | 0.41 | 0.18 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3153 | 1/1   | 0.42 | 0.61 | 127,127,127,127             | 0     |
| 56  | MG   | XA    | 1671 | 1/1   | 0.42 | 0.17 | 96,96,96,96                 | 0     |
| 56  | MG   | QO    | 101  | 1/1   | 0.42 | 0.63 | 113,113,113,113             | 0     |
| 56  | MG   | YA    | 3024 | 1/1   | 0.42 | 0.23 | 102,102,102,102             | 0     |
| 56  | MG   | RA    | 3322 | 1/1   | 0.42 | 0.42 | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3069 | 1/1   | 0.43 | 0.71 | 144,144,144,144             | 0     |
| 56  | MG   | QA    | 1705 | 1/1   | 0.43 | 0.21 | 103,103,103,103             | 0     |
| 56  | MG   | RA    | 3096 | 1/1   | 0.43 | 0.28 | 102,102,102,102             | 0     |
| 56  | MG   | RA    | 3350 | 1/1   | 0.44 | 0.56 | 127,127,127,127             | 0     |
| 56  | MG   | RA    | 3591 | 1/1   | 0.47 | 0.42 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3163 | 1/1   | 0.47 | 0.28 | 80,80,80,80                 | 0     |
| 56  | MG   | XA    | 1718 | 1/1   | 0.47 | 0.42 | 116,116,116,116             | 0     |
| 56  | MG   | RA    | 3460 | 1/1   | 0.48 | 0.47 | 89,89,89,89                 | 0     |
| 56  | MG   | XA    | 1723 | 1/1   | 0.48 | 0.26 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3152 | 1/1   | 0.48 | 0.78 | 92,92,92,92                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3011 | 1/1   | 0.48 | 0.41 | 106,106,106,106             | 0     |
| 56  | MG   | YA    | 3480 | 1/1   | 0.48 | 0.32 | 74,74,74,74                 | 0     |
| 56  | MG   | QG    | 202  | 1/1   | 0.48 | 0.17 | 133,133,133,133             | 0     |
| 56  | MG   | XA    | 1781 | 1/1   | 0.49 | 0.36 | 92,92,92,92                 | 0     |
| 56  | MG   | RA    | 3507 | 1/1   | 0.49 | 0.33 | 76,76,76,76                 | 0     |
| 56  | MG   | RA    | 3100 | 1/1   | 0.49 | 0.25 | 144,144,144,144             | 0     |
| 56  | MG   | RA    | 3484 | 1/1   | 0.49 | 0.26 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3673 | 1/1   | 0.49 | 0.49 | 91,91,91,91                 | 0     |
| 56  | MG   | QA    | 1695 | 1/1   | 0.50 | 0.23 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3138 | 1/1   | 0.50 | 0.27 | 96,96,96,96                 | 0     |
| 56  | MG   | RA    | 3382 | 1/1   | 0.50 | 0.21 | 57,57,57,57                 | 0     |
| 56  | MG   | XA    | 1670 | 1/1   | 0.51 | 0.22 | 90,90,90,90                 | 0     |
| 56  | MG   | QA    | 1762 | 1/1   | 0.52 | 0.13 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3482 | 1/1   | 0.52 | 0.76 | 127,127,127,127             | 0     |
| 56  | MG   | RA    | 3103 | 1/1   | 0.52 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3097 | 1/1   | 0.52 | 0.20 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3182 | 1/1   | 0.52 | 0.23 | 94,94,94,94                 | 0     |
| 56  | MG   | QV    | 102  | 1/1   | 0.52 | 0.19 | 92,92,92,92                 | 0     |
| 56  | MG   | RA    | 3093 | 1/1   | 0.53 | 0.29 | 92,92,92,92                 | 0     |
| 56  | MG   | RA    | 3326 | 1/1   | 0.53 | 0.22 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3175 | 1/1   | 0.53 | 0.45 | 79,79,79,79                 | 0     |
| 56  | MG   | QA    | 1618 | 1/1   | 0.53 | 0.28 | 86,86,86,86                 | 0     |
| 56  | MG   | RA    | 3049 | 1/1   | 0.53 | 0.24 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3405 | 1/1   | 0.54 | 0.16 | 71,71,71,71                 | 0     |
| 56  | MG   | Y1    | 101  | 1/1   | 0.54 | 0.19 | 76,76,76,76                 | 0     |
| 56  | MG   | RA    | 3682 | 1/1   | 0.54 | 0.27 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3376 | 1/1   | 0.54 | 0.21 | 98,98,98,98                 | 0     |
| 56  | MG   | RA    | 3104 | 1/1   | 0.54 | 0.46 | 89,89,89,89                 | 0     |
| 56  | MG   | XJ    | 201  | 1/1   | 0.54 | 0.20 | 81,81,81,81                 | 0     |
| 56  | MG   | RA    | 3178 | 1/1   | 0.55 | 0.20 | 97,97,97,97                 | 0     |
| 56  | MG   | RB    | 204  | 1/1   | 0.55 | 0.17 | 140,140,140,140             | 0     |
| 56  | MG   | QA    | 1813 | 1/1   | 0.55 | 0.14 | 86,86,86,86                 | 0     |
| 56  | MG   | RA    | 3458 | 1/1   | 0.55 | 0.23 | 97,97,97,97                 | 0     |
| 56  | MG   | RA    | 3571 | 1/1   | 0.55 | 0.15 | 89,89,89,89                 | 0     |
| 56  | MG   | RB    | 202  | 1/1   | 0.56 | 0.14 | 107,107,107,107             | 0     |
| 56  | MG   | RA    | 3110 | 1/1   | 0.56 | 0.12 | 83,83,83,83                 | 0     |
| 56  | MG   | RA    | 3347 | 1/1   | 0.56 | 0.26 | 99,99,99,99                 | 0     |
| 56  | MG   | RA    | 3403 | 1/1   | 0.57 | 0.36 | 84,84,84,84                 | 0     |
| 56  | MG   | XA    | 1778 | 1/1   | 0.57 | 0.74 | 127,127,127,127             | 0     |
| 56  | MG   | QA    | 1676 | 1/1   | 0.57 | 0.31 | 81,81,81,81                 | 0     |
| 56  | MG   | RA    | 3123 | 1/1   | 0.57 | 0.31 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3080 | 1/1   | 0.57 | 0.48 | 108,108,108,108             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3140 | 1/1   | 0.57 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | QA    | 1659 | 1/1   | 0.57 | 0.17 | 95,95,95,95                 | 0     |
| 56  | MG   | QA    | 1660 | 1/1   | 0.57 | 0.18 | 120,120,120,120             | 0     |
| 56  | MG   | RA    | 3631 | 1/1   | 0.57 | 0.35 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3654 | 1/1   | 0.57 | 0.55 | 90,90,90,90                 | 0     |
| 56  | MG   | YA    | 3668 | 1/1   | 0.57 | 0.29 | 109,109,109,109             | 0     |
| 56  | MG   | RA    | 3219 | 1/1   | 0.58 | 0.37 | 101,101,101,101             | 0     |
| 56  | MG   | RA    | 3072 | 1/1   | 0.58 | 0.82 | 109,109,109,109             | 0     |
| 56  | MG   | RA    | 3323 | 1/1   | 0.58 | 0.11 | 76,76,76,76                 | 0     |
| 56  | MG   | QA    | 1728 | 1/1   | 0.58 | 0.19 | 90,90,90,90                 | 0     |
| 56  | MG   | RA    | 3397 | 1/1   | 0.58 | 0.35 | 96,96,96,96                 | 0     |
| 56  | MG   | RA    | 3589 | 1/1   | 0.58 | 0.33 | 117,117,117,117             | 0     |
| 56  | MG   | RA    | 3469 | 1/1   | 0.58 | 0.74 | 114,114,114,114             | 0     |
| 56  | MG   | YA    | 3412 | 1/1   | 0.58 | 0.60 | 82,82,82,82                 | 0     |
| 56  | MG   | YA    | 3426 | 1/1   | 0.58 | 0.14 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3045 | 1/1   | 0.58 | 0.23 | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3647 | 1/1   | 0.58 | 0.70 | 121,121,121,121             | 0     |
| 56  | MG   | YA    | 3652 | 1/1   | 0.58 | 0.16 | 67,67,67,67                 | 0     |
| 56  | MG   | QA    | 1787 | 1/1   | 0.58 | 0.18 | 140,140,140,140             | 0     |
| 56  | MG   | RA    | 3009 | 1/1   | 0.59 | 0.34 | 98,98,98,98                 | 0     |
| 56  | MG   | QN    | 102  | 1/1   | 0.59 | 0.39 | 82,82,82,82                 | 0     |
| 56  | MG   | YA    | 3253 | 1/1   | 0.59 | 0.26 | 41,41,41,41                 | 0     |
| 56  | MG   | YG    | 201  | 1/1   | 0.59 | 0.15 | 111,111,111,111             | 0     |
| 56  | MG   | RA    | 3201 | 1/1   | 0.60 | 0.50 | 83,83,83,83                 | 0     |
| 56  | MG   | QA    | 1646 | 1/1   | 0.60 | 0.11 | 80,80,80,80                 | 0     |
| 56  | MG   | RA    | 3039 | 1/1   | 0.60 | 0.35 | 85,85,85,85                 | 0     |
| 56  | MG   | RA    | 3392 | 1/1   | 0.60 | 0.18 | 103,103,103,103             | 0     |
| 56  | MG   | RA    | 3091 | 1/1   | 0.60 | 0.14 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3134 | 1/1   | 0.61 | 0.21 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3374 | 1/1   | 0.61 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | QA    | 1770 | 1/1   | 0.61 | 0.21 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3606 | 1/1   | 0.61 | 0.22 | 77,77,77,77                 | 0     |
| 56  | MG   | RA    | 3060 | 1/1   | 0.61 | 0.23 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3161 | 1/1   | 0.61 | 0.16 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3143 | 1/1   | 0.61 | 0.20 | 94,94,94,94                 | 0     |
| 56  | MG   | RA    | 3064 | 1/1   | 0.61 | 0.27 | 80,80,80,80                 | 0     |
| 56  | MG   | RA    | 3481 | 1/1   | 0.62 | 0.38 | 102,102,102,102             | 0     |
| 56  | MG   | RA    | 3363 | 1/1   | 0.62 | 0.41 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3313 | 1/1   | 0.62 | 0.16 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3037 | 1/1   | 0.62 | 0.25 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3029 | 1/1   | 0.62 | 0.19 | 99,99,99,99                 | 0     |
| 56  | MG   | XA    | 1624 | 1/1   | 0.62 | 0.23 | 101,101,101,101             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | MG   | YA    | 3387 | 1/1   | 0.62 | 0.38 | 90,90,90,90                | 0     |
| 56  | MG   | RA    | 3461 | 1/1   | 0.63 | 0.39 | 104,104,104,104            | 0     |
| 56  | MG   | RA    | 3462 | 1/1   | 0.63 | 0.23 | 44,44,44,44                | 0     |
| 56  | MG   | RA    | 3173 | 1/1   | 0.63 | 0.52 | 142,142,142,142            | 0     |
| 56  | MG   | RA    | 3477 | 1/1   | 0.63 | 0.33 | 100,100,100,100            | 0     |
| 56  | MG   | RA    | 3059 | 1/1   | 0.63 | 0.15 | 61,61,61,61                | 0     |
| 56  | MG   | QA    | 1633 | 1/1   | 0.63 | 0.19 | 104,104,104,104            | 0     |
| 56  | MG   | QA    | 1601 | 1/1   | 0.63 | 0.25 | 94,94,94,94                | 0     |
| 56  | MG   | RA    | 3055 | 1/1   | 0.63 | 0.14 | 91,91,91,91                | 0     |
| 56  | MG   | RA    | 3224 | 1/1   | 0.63 | 0.16 | 111,111,111,111            | 0     |
| 56  | MG   | XA    | 1782 | 1/1   | 0.63 | 0.16 | 73,73,73,73                | 0     |
| 56  | MG   | RA    | 3250 | 1/1   | 0.63 | 0.37 | 97,97,97,97                | 0     |
| 56  | MG   | QA    | 1718 | 1/1   | 0.63 | 0.21 | 64,64,64,64                | 0     |
| 56  | MG   | RA    | 3454 | 1/1   | 0.64 | 0.11 | 51,51,51,51                | 0     |
| 56  | MG   | RA    | 3479 | 1/1   | 0.64 | 0.23 | 75,75,75,75                | 0     |
| 56  | MG   | XA    | 1700 | 1/1   | 0.64 | 0.26 | 90,90,90,90                | 0     |
| 56  | MG   | RA    | 3209 | 1/1   | 0.64 | 0.23 | 103,103,103,103            | 0     |
| 56  | MG   | QA    | 1694 | 1/1   | 0.64 | 0.23 | 87,87,87,87                | 0     |
| 56  | MG   | QA    | 1643 | 1/1   | 0.64 | 0.31 | 86,86,86,86                | 0     |
| 56  | MG   | RA    | 3497 | 1/1   | 0.64 | 0.13 | 56,56,56,56                | 0     |
| 56  | MG   | RA    | 3129 | 1/1   | 0.64 | 0.18 | 58,58,58,58                | 0     |
| 56  | MG   | RP    | 202  | 1/1   | 0.64 | 0.27 | 73,73,73,73                | 0     |
| 56  | MG   | RA    | 3015 | 1/1   | 0.64 | 0.28 | 70,70,70,70                | 0     |
| 56  | MG   | YB    | 207  | 1/1   | 0.64 | 0.34 | 77,77,77,77                | 0     |
| 56  | MG   | XA    | 1657 | 1/1   | 0.64 | 0.20 | 102,102,102,102            | 0     |
| 56  | MG   | QA    | 1662 | 1/1   | 0.65 | 0.15 | 42,42,42,42                | 0     |
| 56  | MG   | RA    | 3416 | 1/1   | 0.65 | 0.41 | 63,63,63,63                | 0     |
| 56  | MG   | RA    | 3330 | 1/1   | 0.65 | 0.16 | 57,57,57,57                | 0     |
| 56  | MG   | XA    | 1701 | 1/1   | 0.65 | 0.12 | 53,53,53,53                | 0     |
| 56  | MG   | QA    | 1688 | 1/1   | 0.65 | 0.30 | 98,98,98,98                | 0     |
| 56  | MG   | QA    | 1746 | 1/1   | 0.65 | 0.18 | 54,54,54,54                | 0     |
| 56  | MG   | RA    | 3237 | 1/1   | 0.65 | 0.19 | 111,111,111,111            | 0     |
| 56  | MG   | YA    | 3527 | 1/1   | 0.65 | 0.18 | 75,75,75,75                | 0     |
| 56  | MG   | QA    | 1791 | 1/1   | 0.65 | 0.11 | 83,83,83,83                | 0     |
| 56  | MG   | YA    | 3629 | 1/1   | 0.65 | 0.32 | 50,50,50,50                | 0     |
| 56  | MG   | XA    | 1607 | 1/1   | 0.65 | 0.19 | 95,95,95,95                | 0     |
| 56  | MG   | XA    | 1614 | 1/1   | 0.65 | 0.34 | 85,85,85,85                | 0     |
| 56  | MG   | RA    | 3401 | 1/1   | 0.65 | 0.52 | 124,124,124,124            | 0     |
| 56  | MG   | RA    | 3164 | 1/1   | 0.65 | 0.18 | 65,65,65,65                | 0     |
| 56  | MG   | RA    | 3677 | 1/1   | 0.66 | 0.14 | 47,47,47,47                | 0     |
| 56  | MG   | RA    | 3411 | 1/1   | 0.66 | 0.22 | 60,60,60,60                | 0     |
| 56  | MG   | QA    | 1673 | 1/1   | 0.66 | 0.16 | 95,95,95,95                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3601 | 1/1   | 0.66 | 0.30 | 88,88,88,88                 | 0     |
| 56  | MG   | RA    | 3417 | 1/1   | 0.66 | 0.94 | 125,125,125,125             | 0     |
| 56  | MG   | RA    | 3463 | 1/1   | 0.66 | 0.35 | 104,104,104,104             | 0     |
| 56  | MG   | QA    | 1808 | 1/1   | 0.66 | 0.23 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3128 | 1/1   | 0.66 | 0.13 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3616 | 1/1   | 0.66 | 0.15 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3665 | 1/1   | 0.66 | 0.24 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3643 | 1/1   | 0.66 | 0.25 | 67,67,67,67                 | 0     |
| 56  | MG   | XA    | 1634 | 1/1   | 0.66 | 0.17 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3160 | 1/1   | 0.66 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3226 | 1/1   | 0.66 | 0.17 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3052 | 1/1   | 0.66 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3471 | 1/1   | 0.67 | 0.21 | 98,98,98,98                 | 0     |
| 56  | MG   | RQ    | 201  | 1/1   | 0.67 | 0.38 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3218 | 1/1   | 0.67 | 0.15 | 79,79,79,79                 | 0     |
| 56  | MG   | QH    | 202  | 1/1   | 0.67 | 0.11 | 82,82,82,82                 | 0     |
| 56  | MG   | RA    | 3318 | 1/1   | 0.67 | 0.40 | 73,73,73,73                 | 0     |
| 56  | MG   | YA    | 3483 | 1/1   | 0.67 | 0.29 | 83,83,83,83                 | 0     |
| 56  | MG   | RA    | 3383 | 1/1   | 0.67 | 0.50 | 88,88,88,88                 | 0     |
| 56  | MG   | RA    | 3198 | 1/1   | 0.67 | 0.24 | 97,97,97,97                 | 0     |
| 56  | MG   | XY    | 101  | 1/1   | 0.67 | 0.25 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3066 | 1/1   | 0.67 | 0.37 | 98,98,98,98                 | 0     |
| 56  | MG   | RA    | 3421 | 1/1   | 0.67 | 0.26 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3204 | 1/1   | 0.67 | 0.38 | 97,97,97,97                 | 0     |
| 56  | MG   | RB    | 209  | 1/1   | 0.67 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3152 | 1/1   | 0.67 | 0.31 | 81,81,81,81                 | 0     |
| 56  | MG   | YA    | 3160 | 1/1   | 0.67 | 0.36 | 102,102,102,102             | 0     |
| 56  | MG   | XA    | 1649 | 1/1   | 0.68 | 0.26 | 96,96,96,96                 | 0     |
| 56  | MG   | XA    | 1653 | 1/1   | 0.68 | 0.21 | 93,93,93,93                 | 0     |
| 56  | MG   | RA    | 3483 | 1/1   | 0.68 | 0.25 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3547 | 1/1   | 0.68 | 0.44 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3192 | 1/1   | 0.68 | 0.48 | 85,85,85,85                 | 0     |
| 56  | MG   | QA    | 1616 | 1/1   | 0.68 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3514 | 1/1   | 0.69 | 0.42 | 108,108,108,108             | 0     |
| 56  | MG   | RA    | 3526 | 1/1   | 0.69 | 0.51 | 110,110,110,110             | 0     |
| 56  | MG   | RA    | 3113 | 1/1   | 0.69 | 0.26 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3657 | 1/1   | 0.69 | 0.32 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3027 | 1/1   | 0.69 | 0.17 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3395 | 1/1   | 0.69 | 0.41 | 85,85,85,85                 | 0     |
| 56  | MG   | RA    | 3026 | 1/1   | 0.69 | 0.15 | 63,63,63,63                 | 0     |
| 56  | MG   | QA    | 1665 | 1/1   | 0.69 | 0.10 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3499 | 1/1   | 0.69 | 0.53 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1754 | 1/1   | 0.69 | 0.23 | 89,89,89,89                 | 0     |
| 56  | MG   | YA    | 3310 | 1/1   | 0.69 | 0.13 | 5,5,5,5                     | 0     |
| 56  | MG   | RA    | 3706 | 1/1   | 0.69 | 0.23 | 94,94,94,94                 | 0     |
| 56  | MG   | QA    | 1792 | 1/1   | 0.69 | 0.20 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3391 | 1/1   | 0.70 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3360 | 1/1   | 0.70 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3592 | 1/1   | 0.70 | 0.22 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3444 | 1/1   | 0.70 | 0.30 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3474 | 1/1   | 0.70 | 0.26 | 71,71,71,71                 | 0     |
| 56  | MG   | QA    | 1627 | 1/1   | 0.70 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | QA    | 1804 | 1/1   | 0.70 | 0.21 | 85,85,85,85                 | 0     |
| 56  | MG   | RA    | 3075 | 1/1   | 0.70 | 0.33 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3119 | 1/1   | 0.71 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | RA    | 3707 | 1/1   | 0.71 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1623 | 1/1   | 0.71 | 0.12 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3170 | 1/1   | 0.71 | 0.20 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3184 | 1/1   | 0.71 | 0.22 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3448 | 1/1   | 0.71 | 0.19 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3186 | 1/1   | 0.71 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3348 | 1/1   | 0.71 | 0.21 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3642 | 1/1   | 0.71 | 0.16 | 84,84,84,84                 | 0     |
| 56  | MG   | RP    | 203  | 1/1   | 0.71 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3387 | 1/1   | 0.71 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | RV    | 201  | 1/1   | 0.71 | 0.13 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3186 | 1/1   | 0.72 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | XA    | 1673 | 1/1   | 0.72 | 0.22 | 77,77,77,77                 | 0     |
| 56  | MG   | RA    | 3057 | 1/1   | 0.72 | 0.23 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3051 | 1/1   | 0.72 | 0.10 | 109,109,109,109             | 0     |
| 56  | MG   | XA    | 1706 | 1/1   | 0.72 | 0.32 | 87,87,87,87                 | 0     |
| 56  | MG   | QA    | 1715 | 1/1   | 0.72 | 0.35 | 82,82,82,82                 | 0     |
| 56  | MG   | RA    | 3639 | 1/1   | 0.72 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3509 | 1/1   | 0.72 | 0.33 | 77,77,77,77                 | 0     |
| 56  | MG   | RA    | 3426 | 1/1   | 0.72 | 0.19 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3441 | 1/1   | 0.72 | 0.29 | 89,89,89,89                 | 0     |
| 56  | MG   | RA    | 3139 | 1/1   | 0.72 | 0.20 | 62,62,62,62                 | 0     |
| 56  | MG   | RA    | 3662 | 1/1   | 0.72 | 0.36 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3087 | 1/1   | 0.72 | 0.25 | 88,88,88,88                 | 0     |
| 56  | MG   | RA    | 3545 | 1/1   | 0.72 | 0.34 | 90,90,90,90                 | 0     |
| 56  | MG   | RA    | 3566 | 1/1   | 0.72 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3408 | 1/1   | 0.72 | 0.34 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3455 | 1/1   | 0.72 | 0.31 | 82,82,82,82                 | 0     |
| 56  | MG   | RA    | 3457 | 1/1   | 0.72 | 0.13 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1689 | 1/1   | 0.72 | 0.20 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3380 | 1/1   | 0.72 | 0.20 | 62,62,62,62                 | 0     |
| 56  | MG   | QA    | 1630 | 1/1   | 0.73 | 0.13 | 92,92,92,92                 | 0     |
| 56  | MG   | QA    | 1812 | 1/1   | 0.73 | 0.09 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3126 | 1/1   | 0.73 | 0.12 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3106 | 1/1   | 0.73 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3017 | 1/1   | 0.73 | 0.14 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3365 | 1/1   | 0.73 | 0.24 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3151 | 1/1   | 0.73 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1703 | 1/1   | 0.73 | 0.73 | 82,82,82,82                 | 0     |
| 56  | MG   | RA    | 3644 | 1/1   | 0.73 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3697 | 1/1   | 0.73 | 0.42 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3007 | 1/1   | 0.73 | 0.37 | 99,99,99,99                 | 0     |
| 56  | MG   | RA    | 3249 | 1/1   | 0.73 | 0.32 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3609 | 1/1   | 0.74 | 0.22 | 69,69,69,69                 | 0     |
| 56  | MG   | QA    | 1773 | 1/1   | 0.74 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3632 | 1/1   | 0.74 | 0.24 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3032 | 1/1   | 0.74 | 0.30 | 95,95,95,95                 | 0     |
| 56  | MG   | XA    | 1714 | 1/1   | 0.74 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3051 | 1/1   | 0.74 | 0.35 | 58,58,58,58                 | 0     |
| 56  | MG   | XA    | 1625 | 1/1   | 0.74 | 0.24 | 79,79,79,79                 | 0     |
| 56  | MG   | YA    | 3514 | 1/1   | 0.74 | 0.35 | 85,85,85,85                 | 0     |
| 56  | MG   | YA    | 3074 | 1/1   | 0.74 | 0.15 | 39,39,39,39                 | 0     |
| 56  | MG   | QA    | 1649 | 1/1   | 0.74 | 0.19 | 115,115,115,115             | 0     |
| 56  | MG   | YA    | 3131 | 1/1   | 0.74 | 0.28 | 87,87,87,87                 | 0     |
| 56  | MG   | XA    | 1770 | 1/1   | 0.74 | 0.26 | 87,87,87,87                 | 0     |
| 56  | MG   | YA    | 3159 | 1/1   | 0.74 | 0.18 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3560 | 1/1   | 0.74 | 0.26 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3165 | 1/1   | 0.74 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3414 | 1/1   | 0.74 | 0.40 | 91,91,91,91                 | 0     |
| 56  | MG   | YA    | 3678 | 1/1   | 0.74 | 0.16 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3689 | 1/1   | 0.74 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3377 | 1/1   | 0.74 | 0.24 | 73,73,73,73                 | 0     |
| 56  | MG   | YB    | 215  | 1/1   | 0.74 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | XA    | 1604 | 1/1   | 0.74 | 0.19 | 91,91,91,91                 | 0     |
| 56  | MG   | RA    | 3542 | 1/1   | 0.75 | 0.13 | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3242 | 1/1   | 0.75 | 0.15 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3246 | 1/1   | 0.75 | 0.38 | 65,65,65,65                 | 0     |
| 56  | MG   | QA    | 1655 | 1/1   | 0.75 | 0.22 | 90,90,90,90                 | 0     |
| 56  | MG   | XE    | 201  | 1/1   | 0.75 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3383 | 1/1   | 0.75 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3393 | 1/1   | 0.75 | 0.31 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3054 | 1/1   | 0.75 | 0.19 | 72,72,72,72                 | 0     |
| 56  | MG   | QE    | 203  | 1/1   | 0.75 | 0.17 | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3432 | 1/1   | 0.75 | 0.32 | 79,79,79,79                 | 0     |
| 56  | MG   | QA    | 1636 | 1/1   | 0.75 | 0.10 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3470 | 1/1   | 0.75 | 0.39 | 93,93,93,93                 | 0     |
| 56  | MG   | YA    | 3014 | 1/1   | 0.75 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3183 | 1/1   | 0.75 | 0.36 | 99,99,99,99                 | 0     |
| 56  | MG   | RA    | 3597 | 1/1   | 0.75 | 0.16 | 46,46,46,46                 | 0     |
| 56  | MG   | QA    | 1795 | 1/1   | 0.75 | 0.40 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3404 | 1/1   | 0.75 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3135 | 1/1   | 0.75 | 0.20 | 98,98,98,98                 | 0     |
| 56  | MG   | YA    | 3066 | 1/1   | 0.75 | 0.43 | 103,103,103,103             | 0     |
| 56  | MG   | QA    | 1632 | 1/1   | 0.75 | 0.11 | 81,81,81,81                 | 0     |
| 56  | MG   | YA    | 3633 | 1/1   | 0.75 | 0.31 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3410 | 1/1   | 0.75 | 0.32 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3111 | 1/1   | 0.75 | 0.22 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3119 | 1/1   | 0.75 | 0.43 | 90,90,90,90                 | 0     |
| 56  | MG   | XA    | 1702 | 1/1   | 0.75 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3085 | 1/1   | 0.75 | 0.14 | 81,81,81,81                 | 0     |
| 56  | MG   | RA    | 3518 | 1/1   | 0.75 | 0.23 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1820 | 1/1   | 0.75 | 0.13 | 81,81,81,81                 | 0     |
| 56  | MG   | RA    | 3027 | 1/1   | 0.75 | 0.68 | 92,92,92,92                 | 0     |
| 56  | MG   | YR    | 202  | 1/1   | 0.75 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1660 | 1/1   | 0.76 | 0.22 | 96,96,96,96                 | 0     |
| 56  | MG   | XA    | 1787 | 1/1   | 0.76 | 0.11 | 94,94,94,94                 | 0     |
| 56  | MG   | QA    | 1642 | 1/1   | 0.76 | 0.31 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3499 | 1/1   | 0.76 | 0.41 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3442 | 1/1   | 0.76 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | XA    | 1602 | 1/1   | 0.76 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | R5    | 103  | 1/1   | 0.76 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | QE    | 204  | 1/1   | 0.76 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3177 | 1/1   | 0.76 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3625 | 1/1   | 0.76 | 0.31 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3534 | 1/1   | 0.76 | 0.34 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3535 | 1/1   | 0.76 | 0.21 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3649 | 1/1   | 0.76 | 0.26 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3670 | 1/1   | 0.76 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3664 | 1/1   | 0.76 | 0.32 | 85,85,85,85                 | 0     |
| 56  | MG   | RF    | 304  | 1/1   | 0.76 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | XA    | 1745 | 1/1   | 0.76 | 0.35 | 74,74,74,74                 | 0     |
| 56  | MG   | RP    | 201  | 1/1   | 0.76 | 0.28 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3094 | 1/1   | 0.76 | 0.17 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YB    | 212  | 1/1   | 0.76 | 0.16 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3082 | 1/1   | 0.76 | 0.09 | 73,73,73,73                 | 0     |
| 56  | MG   | YA    | 3092 | 1/1   | 0.76 | 0.19 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3511 | 1/1   | 0.76 | 0.78 | 87,87,87,87                 | 0     |
| 56  | MG   | RA    | 3298 | 1/1   | 0.77 | 0.11 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3473 | 1/1   | 0.77 | 0.36 | 87,87,87,87                 | 0     |
| 56  | MG   | RA    | 3187 | 1/1   | 0.77 | 0.24 | 93,93,93,93                 | 0     |
| 56  | MG   | RA    | 3303 | 1/1   | 0.77 | 0.30 | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3220 | 1/1   | 0.77 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3480 | 1/1   | 0.77 | 0.29 | 65,65,65,65                 | 0     |
| 56  | MG   | QA    | 1771 | 1/1   | 0.77 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3063 | 1/1   | 0.77 | 0.41 | 101,101,101,101             | 0     |
| 56  | MG   | XA    | 1661 | 1/1   | 0.77 | 0.30 | 76,76,76,76                 | 0     |
| 56  | MG   | YA    | 3029 | 1/1   | 0.77 | 0.20 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3052 | 1/1   | 0.77 | 0.11 | 78,78,78,78                 | 0     |
| 56  | MG   | YA    | 3490 | 1/1   | 0.77 | 0.25 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3227 | 1/1   | 0.77 | 0.16 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3228 | 1/1   | 0.77 | 0.18 | 75,75,75,75                 | 0     |
| 56  | MG   | XA    | 1696 | 1/1   | 0.77 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | R9    | 102  | 1/1   | 0.77 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3555 | 1/1   | 0.77 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3239 | 1/1   | 0.77 | 0.21 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3620 | 1/1   | 0.77 | 0.31 | 33,33,33,33                 | 0     |
| 56  | MG   | QA    | 1656 | 1/1   | 0.77 | 0.27 | 134,134,134,134             | 0     |
| 56  | MG   | RA    | 3351 | 1/1   | 0.77 | 0.20 | 41,41,41,41                 | 0     |
| 56  | MG   | QK    | 201  | 1/1   | 0.77 | 0.11 | 73,73,73,73                 | 0     |
| 56  | MG   | YA    | 3648 | 1/1   | 0.77 | 0.39 | 80,80,80,80                 | 0     |
| 56  | MG   | YA    | 3151 | 1/1   | 0.77 | 0.18 | 70,70,70,70                 | 0     |
| 56  | MG   | QA    | 1617 | 1/1   | 0.77 | 0.12 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3640 | 1/1   | 0.77 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | XA    | 1758 | 1/1   | 0.77 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3077 | 1/1   | 0.77 | 0.16 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3373 | 1/1   | 0.77 | 0.24 | 73,73,73,73                 | 0     |
| 56  | MG   | QA    | 1608 | 1/1   | 0.77 | 0.12 | 87,87,87,87                 | 0     |
| 56  | MG   | YA    | 3211 | 1/1   | 0.77 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | YA    | 3247 | 1/1   | 0.77 | 0.33 | 77,77,77,77                 | 0     |
| 56  | MG   | RA    | 3468 | 1/1   | 0.77 | 0.22 | 39,39,39,39                 | 0     |
| 56  | MG   | QA    | 1740 | 1/1   | 0.77 | 0.30 | 100,100,100,100             | 0     |
| 56  | MG   | RA    | 3041 | 1/1   | 0.78 | 0.23 | 85,85,85,85                 | 0     |
| 56  | MG   | YA    | 3080 | 1/1   | 0.78 | 0.11 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3353 | 1/1   | 0.78 | 0.19 | 38,38,38,38                 | 0     |
| 56  | MG   | RH    | 202  | 1/1   | 0.78 | 0.13 | 136,136,136,136             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1772 | 1/1   | 0.78 | 0.20 | 71,71,71,71                 | 0     |
| 56  | MG   | XA    | 1656 | 1/1   | 0.78 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | RN    | 202  | 1/1   | 0.78 | 0.26 | 89,89,89,89                 | 0     |
| 56  | MG   | RA    | 3311 | 1/1   | 0.78 | 0.54 | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3147 | 1/1   | 0.78 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3611 | 1/1   | 0.78 | 0.31 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3208 | 1/1   | 0.78 | 0.12 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3472 | 1/1   | 0.78 | 0.16 | 77,77,77,77                 | 0     |
| 56  | MG   | R0    | 103  | 1/1   | 0.78 | 0.27 | 96,96,96,96                 | 0     |
| 56  | MG   | XA    | 1680 | 1/1   | 0.78 | 0.26 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3625 | 1/1   | 0.78 | 0.21 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1774 | 1/1   | 0.78 | 0.15 | 108,108,108,108             | 0     |
| 56  | MG   | Y7    | 101  | 1/1   | 0.78 | 0.26 | 81,81,81,81                 | 0     |
| 56  | MG   | YA    | 3201 | 1/1   | 0.78 | 0.44 | 89,89,89,89                 | 0     |
| 56  | MG   | RA    | 3259 | 1/1   | 0.78 | 0.11 | 102,102,102,102             | 0     |
| 56  | MG   | RA    | 3181 | 1/1   | 0.78 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3012 | 1/1   | 0.78 | 0.14 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3288 | 1/1   | 0.78 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | XA    | 1618 | 1/1   | 0.78 | 0.09 | 104,104,104,104             | 0     |
| 56  | MG   | QP    | 101  | 1/1   | 0.78 | 0.22 | 88,88,88,88                 | 0     |
| 56  | MG   | XA    | 1717 | 1/1   | 0.78 | 0.15 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3703 | 1/1   | 0.78 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | RA    | 3594 | 1/1   | 0.78 | 0.14 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3058 | 1/1   | 0.78 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | YB    | 214  | 1/1   | 0.78 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3396 | 1/1   | 0.78 | 0.16 | 74,74,74,74                 | 0     |
| 56  | MG   | YD    | 301  | 1/1   | 0.78 | 0.12 | 78,78,78,78                 | 0     |
| 56  | MG   | YA    | 3400 | 1/1   | 0.78 | 0.44 | 113,113,113,113             | 0     |
| 56  | MG   | YQ    | 201  | 1/1   | 0.78 | 0.40 | 65,65,65,65                 | 0     |
| 56  | MG   | QA    | 1631 | 1/1   | 0.78 | 0.08 | 122,122,122,122             | 0     |
| 56  | MG   | RA    | 3390 | 1/1   | 0.79 | 0.21 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3690 | 1/1   | 0.79 | 0.20 | 47,47,47,47                 | 0     |
| 56  | MG   | QA    | 1641 | 1/1   | 0.79 | 0.11 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3359 | 1/1   | 0.79 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | QA    | 1644 | 1/1   | 0.79 | 0.30 | 150,150,150,150             | 0     |
| 56  | MG   | QA    | 1698 | 1/1   | 0.79 | 0.21 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3365 | 1/1   | 0.79 | 0.13 | 66,66,66,66                 | 0     |
| 56  | MG   | QA    | 1805 | 1/1   | 0.79 | 0.23 | 70,70,70,70                 | 0     |
| 56  | MG   | RB    | 215  | 1/1   | 0.79 | 0.13 | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1747 | 1/1   | 0.79 | 0.22 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3641 | 1/1   | 0.79 | 0.47 | 110,110,110,110             | 0     |
| 56  | MG   | RA    | 3084 | 1/1   | 0.79 | 0.25 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3205 | 1/1   | 0.79 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1678 | 1/1   | 0.79 | 0.22 | 91,91,91,91                 | 0     |
| 56  | MG   | QA    | 1749 | 1/1   | 0.79 | 0.15 | 113,113,113,113             | 0     |
| 56  | MG   | XA    | 1682 | 1/1   | 0.79 | 0.29 | 85,85,85,85                 | 0     |
| 56  | MG   | XA    | 1685 | 1/1   | 0.79 | 0.12 | 77,77,77,77                 | 0     |
| 56  | MG   | YA    | 3657 | 1/1   | 0.79 | 0.30 | 76,76,76,76                 | 0     |
| 56  | MG   | XA    | 1689 | 1/1   | 0.79 | 0.23 | 59,59,59,59                 | 0     |
| 56  | MG   | QA    | 1675 | 1/1   | 0.79 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3485 | 1/1   | 0.79 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3378 | 1/1   | 0.79 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1736 | 1/1   | 0.79 | 0.25 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3503 | 1/1   | 0.79 | 0.17 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3073 | 1/1   | 0.79 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3222 | 1/1   | 0.79 | 0.12 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3414 | 1/1   | 0.79 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3596 | 1/1   | 0.79 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3269 | 1/1   | 0.79 | 0.50 | 80,80,80,80                 | 0     |
| 56  | MG   | RA    | 3120 | 1/1   | 0.79 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3070 | 1/1   | 0.79 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | QA    | 1640 | 1/1   | 0.80 | 0.19 | 104,104,104,104             | 0     |
| 56  | MG   | RA    | 3697 | 1/1   | 0.80 | 0.34 | 74,74,74,74                 | 0     |
| 56  | MG   | XA    | 1750 | 1/1   | 0.80 | 0.27 | 82,82,82,82                 | 0     |
| 56  | MG   | YA    | 3103 | 1/1   | 0.80 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3478 | 1/1   | 0.80 | 0.41 | 89,89,89,89                 | 0     |
| 56  | MG   | RA    | 3528 | 1/1   | 0.80 | 0.18 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3533 | 1/1   | 0.80 | 0.16 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3128 | 1/1   | 0.80 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3628 | 1/1   | 0.80 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3512 | 1/1   | 0.80 | 0.44 | 69,69,69,69                 | 0     |
| 56  | MG   | QA    | 1776 | 1/1   | 0.80 | 0.22 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3197 | 1/1   | 0.80 | 0.15 | 83,83,83,83                 | 0     |
| 56  | MG   | RB    | 207  | 1/1   | 0.80 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3034 | 1/1   | 0.80 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1668 | 1/1   | 0.80 | 0.30 | 87,87,87,87                 | 0     |
| 56  | MG   | RB    | 214  | 1/1   | 0.80 | 0.14 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3001 | 1/1   | 0.80 | 0.20 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3179 | 1/1   | 0.80 | 0.24 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3145 | 1/1   | 0.80 | 0.09 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3197 | 1/1   | 0.80 | 0.19 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3453 | 1/1   | 0.80 | 0.16 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3375 | 1/1   | 0.80 | 0.39 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3132 | 1/1   | 0.80 | 0.15 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3226 | 1/1   | 0.80 | 0.28 | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3268 | 1/1   | 0.80 | 0.18 | 80,80,80,80                 | 0     |
| 56  | MG   | YA    | 3666 | 1/1   | 0.80 | 0.28 | 86,86,86,86                 | 0     |
| 56  | MG   | RA    | 3333 | 1/1   | 0.80 | 0.17 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3265 | 1/1   | 0.80 | 0.36 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3406 | 1/1   | 0.80 | 0.20 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3379 | 1/1   | 0.80 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3341 | 1/1   | 0.80 | 0.20 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3185 | 1/1   | 0.80 | 0.23 | 70,70,70,70                 | 0     |
| 56  | MG   | QA    | 1693 | 1/1   | 0.80 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3210 | 1/1   | 0.80 | 0.25 | 115,115,115,115             | 0     |
| 56  | MG   | YA    | 3070 | 1/1   | 0.80 | 0.15 | 67,67,67,67                 | 0     |
| 56  | MG   | YF    | 301  | 1/1   | 0.80 | 0.23 | 62,62,62,62                 | 0     |
| 56  | MG   | RA    | 3229 | 1/1   | 0.80 | 0.19 | 77,77,77,77                 | 0     |
| 56  | MG   | YI    | 201  | 1/1   | 0.80 | 0.09 | 83,83,83,83                 | 0     |
| 56  | MG   | QA    | 1668 | 1/1   | 0.80 | 0.17 | 70,70,70,70                 | 0     |
| 56  | MG   | XA    | 1721 | 1/1   | 0.80 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | QA    | 1663 | 1/1   | 0.81 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3032 | 1/1   | 0.81 | 0.13 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3399 | 1/1   | 0.81 | 0.15 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3045 | 1/1   | 0.81 | 0.07 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3406 | 1/1   | 0.81 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3547 | 1/1   | 0.81 | 0.28 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3554 | 1/1   | 0.81 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3420 | 1/1   | 0.81 | 0.18 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3057 | 1/1   | 0.81 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1619 | 1/1   | 0.81 | 0.23 | 77,77,77,77                 | 0     |
| 56  | MG   | XA    | 1692 | 1/1   | 0.81 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3456 | 1/1   | 0.81 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | QA    | 1816 | 1/1   | 0.81 | 0.16 | 108,108,108,108             | 0     |
| 56  | MG   | QA    | 1605 | 1/1   | 0.81 | 0.13 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3174 | 1/1   | 0.81 | 0.16 | 102,102,102,102             | 0     |
| 56  | MG   | QD    | 303  | 1/1   | 0.81 | 0.22 | 90,90,90,90                 | 0     |
| 56  | MG   | RA    | 3024 | 1/1   | 0.81 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3498 | 1/1   | 0.81 | 0.10 | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3510 | 1/1   | 0.81 | 0.20 | 80,80,80,80                 | 0     |
| 56  | MG   | XA    | 1606 | 1/1   | 0.81 | 0.15 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3025 | 1/1   | 0.81 | 0.38 | 109,109,109,109             | 0     |
| 56  | MG   | RA    | 3671 | 1/1   | 0.81 | 0.32 | 79,79,79,79                 | 0     |
| 56  | MG   | QA    | 1786 | 1/1   | 0.81 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1740 | 1/1   | 0.81 | 0.33 | 69,69,69,69                 | 0     |
| 56  | MG   | XA    | 1621 | 1/1   | 0.81 | 0.12 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1622 | 1/1   | 0.81 | 0.38 | 88,88,88,88                 | 0     |
| 56  | MG   | RA    | 3429 | 1/1   | 0.81 | 0.15 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3438 | 1/1   | 0.81 | 0.31 | 91,91,91,91                 | 0     |
| 56  | MG   | RA    | 3245 | 1/1   | 0.81 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3642 | 1/1   | 0.81 | 0.22 | 54,54,54,54                 | 0     |
| 56  | MG   | XA    | 1628 | 1/1   | 0.81 | 0.34 | 111,111,111,111             | 0     |
| 56  | MG   | XA    | 1780 | 1/1   | 0.81 | 0.30 | 57,57,57,57                 | 0     |
| 56  | MG   | QA    | 1678 | 1/1   | 0.81 | 0.10 | 70,70,70,70                 | 0     |
| 56  | MG   | XA    | 1636 | 1/1   | 0.81 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3531 | 1/1   | 0.81 | 0.11 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3660 | 1/1   | 0.81 | 0.20 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3615 | 1/1   | 0.81 | 0.23 | 125,125,125,125             | 0     |
| 56  | MG   | XE    | 202  | 1/1   | 0.81 | 0.16 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3532 | 1/1   | 0.81 | 0.41 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3622 | 1/1   | 0.81 | 0.18 | 58,58,58,58                 | 0     |
| 56  | MG   | R3    | 101  | 1/1   | 0.81 | 0.12 | 78,78,78,78                 | 0     |
| 56  | MG   | R5    | 102  | 1/1   | 0.81 | 0.23 | 80,80,80,80                 | 0     |
| 56  | MG   | QA    | 1671 | 1/1   | 0.81 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3010 | 1/1   | 0.81 | 0.16 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3276 | 1/1   | 0.81 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3012 | 1/1   | 0.81 | 0.18 | 47,47,47,47                 | 0     |
| 56  | MG   | YB    | 219  | 1/1   | 0.81 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | QG    | 201  | 1/1   | 0.81 | 0.12 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3331 | 1/1   | 0.81 | 0.21 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3638 | 1/1   | 0.81 | 0.25 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3360 | 1/1   | 0.81 | 0.20 | 32,32,32,32                 | 0     |
| 56  | MG   | QA    | 1811 | 1/1   | 0.81 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | RE    | 301  | 1/1   | 0.81 | 0.38 | 95,95,95,95                 | 0     |
| 56  | MG   | YA    | 3068 | 1/1   | 0.82 | 0.51 | 98,98,98,98                 | 0     |
| 56  | MG   | XA    | 1615 | 1/1   | 0.82 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | QA    | 1803 | 1/1   | 0.82 | 0.17 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3399 | 1/1   | 0.82 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1652 | 1/1   | 0.82 | 0.41 | 115,115,115,115             | 0     |
| 56  | MG   | XA    | 1736 | 1/1   | 0.82 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3428 | 1/1   | 0.82 | 0.28 | 87,87,87,87                 | 0     |
| 56  | MG   | YA    | 3085 | 1/1   | 0.82 | 0.30 | 56,56,56,56                 | 0     |
| 56  | MG   | QA    | 1653 | 1/1   | 0.82 | 0.10 | 99,99,99,99                 | 0     |
| 56  | MG   | QA    | 1733 | 1/1   | 0.82 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3372 | 1/1   | 0.82 | 0.22 | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1627 | 1/1   | 0.82 | 0.19 | 61,61,61,61                 | 0     |
| 56  | MG   | QH    | 201  | 1/1   | 0.82 | 0.30 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3223 | 1/1   | 0.82 | 0.18 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1773 | 1/1   | 0.82 | 0.27 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3496 | 1/1   | 0.82 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | QA    | 1750 | 1/1   | 0.82 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1638 | 1/1   | 0.82 | 0.07 | 82,82,82,82                 | 0     |
| 56  | MG   | XA    | 1643 | 1/1   | 0.82 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3225 | 1/1   | 0.82 | 0.10 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3188 | 1/1   | 0.82 | 0.28 | 90,90,90,90                 | 0     |
| 56  | MG   | YA    | 3531 | 1/1   | 0.82 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3164 | 1/1   | 0.82 | 0.16 | 76,76,76,76                 | 0     |
| 56  | MG   | RA    | 3038 | 1/1   | 0.82 | 0.36 | 95,95,95,95                 | 0     |
| 56  | MG   | RA    | 3415 | 1/1   | 0.82 | 0.41 | 80,80,80,80                 | 0     |
| 56  | MG   | QA    | 1691 | 1/1   | 0.82 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3623 | 1/1   | 0.82 | 0.29 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3133 | 1/1   | 0.82 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3189 | 1/1   | 0.82 | 0.17 | 74,74,74,74                 | 0     |
| 56  | MG   | RD    | 306  | 1/1   | 0.82 | 0.15 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3420 | 1/1   | 0.82 | 0.40 | 116,116,116,116             | 0     |
| 56  | MG   | QA    | 1789 | 1/1   | 0.82 | 0.20 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3006 | 1/1   | 0.82 | 0.26 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3215 | 1/1   | 0.82 | 0.16 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3165 | 1/1   | 0.82 | 0.24 | 56,56,56,56                 | 0     |
| 56  | MG   | RN    | 201  | 1/1   | 0.82 | 0.10 | 86,86,86,86                 | 0     |
| 56  | MG   | XA    | 1679 | 1/1   | 0.82 | 0.27 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3168 | 1/1   | 0.82 | 0.18 | 71,71,71,71                 | 0     |
| 56  | MG   | QA    | 1761 | 1/1   | 0.82 | 0.31 | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3650 | 1/1   | 0.82 | 0.28 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3674 | 1/1   | 0.82 | 0.23 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3289 | 1/1   | 0.82 | 0.26 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3687 | 1/1   | 0.82 | 0.22 | 107,107,107,107             | 0     |
| 56  | MG   | YA    | 3689 | 1/1   | 0.82 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3653 | 1/1   | 0.82 | 0.25 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3702 | 1/1   | 0.82 | 0.20 | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3313 | 1/1   | 0.82 | 0.16 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3137 | 1/1   | 0.82 | 0.18 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3014 | 1/1   | 0.82 | 0.24 | 88,88,88,88                 | 0     |
| 56  | MG   | QA    | 1637 | 1/1   | 0.82 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3495 | 1/1   | 0.82 | 0.18 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3372 | 1/1   | 0.82 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3375 | 1/1   | 0.82 | 0.10 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3377 | 1/1   | 0.82 | 0.34 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3056 | 1/1   | 0.82 | 0.21 | 85,85,85,85                 | 0     |
| 56  | MG   | YG    | 202  | 1/1   | 0.82 | 0.15 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1602 | 1/1   | 0.82 | 0.44 | 84,84,84,84                 | 0     |
| 56  | MG   | QA    | 1741 | 1/1   | 0.82 | 0.09 | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3451 | 1/1   | 0.82 | 0.29 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3629 | 1/1   | 0.83 | 0.15 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3294 | 1/1   | 0.83 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3446 | 1/1   | 0.83 | 0.27 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3492 | 1/1   | 0.83 | 0.28 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3633 | 1/1   | 0.83 | 0.23 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3162 | 1/1   | 0.83 | 0.35 | 67,67,67,67                 | 0     |
| 56  | MG   | R7    | 103  | 1/1   | 0.83 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3056 | 1/1   | 0.83 | 0.11 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3452 | 1/1   | 0.83 | 0.29 | 107,107,107,107             | 0     |
| 56  | MG   | RA    | 3238 | 1/1   | 0.83 | 0.27 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3028 | 1/1   | 0.83 | 0.28 | 119,119,119,119             | 0     |
| 56  | MG   | YA    | 3064 | 1/1   | 0.83 | 0.13 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3074 | 1/1   | 0.83 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3648 | 1/1   | 0.83 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3586 | 1/1   | 0.83 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3149 | 1/1   | 0.83 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | RO    | 201  | 1/1   | 0.83 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | QA    | 1625 | 1/1   | 0.83 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3459 | 1/1   | 0.83 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3634 | 1/1   | 0.83 | 0.14 | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3084 | 1/1   | 0.83 | 0.28 | 87,87,87,87                 | 0     |
| 56  | MG   | YA    | 3354 | 1/1   | 0.83 | 0.30 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3358 | 1/1   | 0.83 | 0.19 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3195 | 1/1   | 0.83 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | QA    | 1685 | 1/1   | 0.83 | 0.22 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3656 | 1/1   | 0.83 | 0.22 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3251 | 1/1   | 0.83 | 0.15 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3373 | 1/1   | 0.83 | 0.26 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3254 | 1/1   | 0.83 | 0.26 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3104 | 1/1   | 0.83 | 0.21 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3106 | 1/1   | 0.83 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | QA    | 1677 | 1/1   | 0.83 | 0.19 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3388 | 1/1   | 0.83 | 0.27 | 86,86,86,86                 | 0     |
| 56  | MG   | YA    | 3684 | 1/1   | 0.83 | 0.28 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3115 | 1/1   | 0.83 | 0.11 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3061 | 1/1   | 0.83 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | XT    | 201  | 1/1   | 0.83 | 0.13 | 55,55,55,55                 | 0     |
| 56  | MG   | XA    | 1683 | 1/1   | 0.83 | 0.16 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3264 | 1/1   | 0.83 | 0.07 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3148 | 1/1   | 0.83 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | Y6    | 102  | 1/1   | 0.83 | 0.35 | 54,54,54,54                 | 0     |
| 56  | MG   | XA    | 1610 | 1/1   | 0.83 | 0.10 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3035 | 1/1   | 0.83 | 0.29 | 75,75,75,75                 | 0     |
| 56  | MG   | QD    | 305  | 1/1   | 0.83 | 0.15 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3436 | 1/1   | 0.83 | 0.31 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3439 | 1/1   | 0.83 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | QA    | 1815 | 1/1   | 0.83 | 0.07 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3285 | 1/1   | 0.83 | 0.12 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3457 | 1/1   | 0.83 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3174 | 1/1   | 0.83 | 0.07 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3290 | 1/1   | 0.83 | 0.10 | 59,59,59,59                 | 0     |
| 56  | MG   | RV    | 202  | 1/1   | 0.84 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3604 | 1/1   | 0.84 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3185 | 1/1   | 0.84 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3669 | 1/1   | 0.84 | 0.26 | 82,82,82,82                 | 0     |
| 56  | MG   | QA    | 1766 | 1/1   | 0.84 | 0.06 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3488 | 1/1   | 0.84 | 0.23 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3192 | 1/1   | 0.84 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3608 | 1/1   | 0.84 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3130 | 1/1   | 0.84 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3043 | 1/1   | 0.84 | 0.20 | 37,37,37,37                 | 0     |
| 56  | MG   | R3    | 102  | 1/1   | 0.84 | 0.19 | 83,83,83,83                 | 0     |
| 56  | MG   | XA    | 1710 | 1/1   | 0.84 | 0.20 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3221 | 1/1   | 0.84 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | QA    | 1680 | 1/1   | 0.84 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3686 | 1/1   | 0.84 | 0.10 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3619 | 1/1   | 0.84 | 0.22 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3315 | 1/1   | 0.84 | 0.19 | 74,74,74,74                 | 0     |
| 56  | MG   | YA    | 3271 | 1/1   | 0.84 | 0.08 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3018 | 1/1   | 0.84 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1724 | 1/1   | 0.84 | 0.25 | 55,55,55,55                 | 0     |
| 56  | MG   | QA    | 1782 | 1/1   | 0.84 | 0.58 | 80,80,80,80                 | 0     |
| 56  | MG   | YA    | 3307 | 1/1   | 0.84 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3252 | 1/1   | 0.84 | 0.21 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3708 | 1/1   | 0.84 | 0.41 | 56,56,56,56                 | 0     |
| 56  | MG   | RA    | 3105 | 1/1   | 0.84 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3336 | 1/1   | 0.84 | 0.15 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3343 | 1/1   | 0.84 | 0.17 | 32,32,32,32                 | 0     |
| 56  | MG   | QL    | 202  | 1/1   | 0.84 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3044 | 1/1   | 0.84 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3498 | 1/1   | 0.84 | 0.33 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3563 | 1/1   | 0.84 | 0.27 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1774 | 1/1   | 0.84 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1744 | 1/1   | 0.84 | 0.23 | 68,68,68,68                 | 0     |
| 56  | MG   | QA    | 1817 | 1/1   | 0.84 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3385 | 1/1   | 0.84 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3584 | 1/1   | 0.84 | 0.26 | 107,107,107,107             | 0     |
| 56  | MG   | QF    | 202  | 1/1   | 0.84 | 0.24 | 82,82,82,82                 | 0     |
| 56  | MG   | RG    | 204  | 1/1   | 0.84 | 0.07 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3588 | 1/1   | 0.84 | 0.15 | 40,40,40,40                 | 0     |
| 56  | MG   | XF    | 201  | 1/1   | 0.84 | 0.19 | 80,80,80,80                 | 0     |
| 56  | MG   | QA    | 1818 | 1/1   | 0.84 | 0.34 | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3146 | 1/1   | 0.84 | 0.09 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3177 | 1/1   | 0.84 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3408 | 1/1   | 0.84 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1672 | 1/1   | 0.84 | 0.20 | 108,108,108,108             | 0     |
| 56  | MG   | RA    | 3512 | 1/1   | 0.84 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3233 | 1/1   | 0.84 | 0.36 | 83,83,83,83                 | 0     |
| 56  | MG   | RA    | 3092 | 1/1   | 0.84 | 0.10 | 76,76,76,76                 | 0     |
| 56  | MG   | RA    | 3658 | 1/1   | 0.84 | 0.19 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3127 | 1/1   | 0.84 | 0.08 | 53,53,53,53                 | 0     |
| 56  | MG   | RU    | 202  | 1/1   | 0.84 | 0.53 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3169 | 1/1   | 0.84 | 0.22 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3170 | 1/1   | 0.84 | 0.14 | 77,77,77,77                 | 0     |
| 56  | MG   | YA    | 3451 | 1/1   | 0.84 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | QA    | 1614 | 1/1   | 0.84 | 0.09 | 82,82,82,82                 | 0     |
| 56  | MG   | YA    | 3244 | 1/1   | 0.85 | 0.24 | 47,47,47,47                 | 0     |
| 56  | MG   | RH    | 201  | 1/1   | 0.85 | 0.06 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3443 | 1/1   | 0.85 | 0.31 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3256 | 1/1   | 0.85 | 0.16 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3263 | 1/1   | 0.85 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1764 | 1/1   | 0.85 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3111 | 1/1   | 0.85 | 0.23 | 97,97,97,97                 | 0     |
| 56  | MG   | XA    | 1663 | 1/1   | 0.85 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3663 | 1/1   | 0.85 | 0.45 | 90,90,90,90                 | 0     |
| 56  | MG   | QV    | 105  | 1/1   | 0.85 | 0.19 | 80,80,80,80                 | 0     |
| 56  | MG   | YA    | 3301 | 1/1   | 0.85 | 0.38 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3262 | 1/1   | 0.85 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3096 | 1/1   | 0.85 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1783 | 1/1   | 0.85 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3321 | 1/1   | 0.85 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3031 | 1/1   | 0.85 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3265 | 1/1   | 0.85 | 0.18 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1677 | 1/1   | 0.85 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | QA    | 1650 | 1/1   | 0.85 | 0.07 | 60,60,60,60                 | 0     |
| 56  | MG   | QA    | 1711 | 1/1   | 0.85 | 0.25 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3546 | 1/1   | 0.85 | 0.30 | 81,81,81,81                 | 0     |
| 56  | MG   | YA    | 3639 | 1/1   | 0.85 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1681 | 1/1   | 0.85 | 0.29 | 43,43,43,43                 | 0     |
| 56  | MG   | XV    | 101  | 1/1   | 0.85 | 0.17 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3680 | 1/1   | 0.85 | 0.22 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3335 | 1/1   | 0.85 | 0.31 | 41,41,41,41                 | 0     |
| 56  | MG   | QA    | 1634 | 1/1   | 0.85 | 0.13 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3278 | 1/1   | 0.85 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | QA    | 1696 | 1/1   | 0.85 | 0.20 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3505 | 1/1   | 0.85 | 0.34 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3011 | 1/1   | 0.85 | 0.23 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3506 | 1/1   | 0.85 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3575 | 1/1   | 0.85 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3670 | 1/1   | 0.85 | 0.30 | 101,101,101,101             | 0     |
| 56  | MG   | XA    | 1620 | 1/1   | 0.85 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3635 | 1/1   | 0.85 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3407 | 1/1   | 0.85 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3171 | 1/1   | 0.85 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3288 | 1/1   | 0.85 | 0.20 | 74,74,74,74                 | 0     |
| 56  | MG   | RA    | 3581 | 1/1   | 0.85 | 0.20 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3418 | 1/1   | 0.85 | 0.26 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3389 | 1/1   | 0.85 | 0.27 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3423 | 1/1   | 0.85 | 0.21 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3585 | 1/1   | 0.85 | 0.23 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3243 | 1/1   | 0.85 | 0.24 | 51,51,51,51                 | 0     |
| 56  | MG   | RB    | 212  | 1/1   | 0.85 | 0.08 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1692 | 1/1   | 0.85 | 0.21 | 71,71,71,71                 | 0     |
| 56  | MG   | R7    | 101  | 1/1   | 0.85 | 0.20 | 68,68,68,68                 | 0     |
| 56  | MG   | YE    | 302  | 1/1   | 0.85 | 0.39 | 82,82,82,82                 | 0     |
| 56  | MG   | QA    | 1775 | 1/1   | 0.85 | 0.10 | 82,82,82,82                 | 0     |
| 56  | MG   | QA    | 1679 | 1/1   | 0.85 | 0.13 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3059 | 1/1   | 0.85 | 0.18 | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1801 | 1/1   | 0.85 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | YP    | 201  | 1/1   | 0.85 | 0.14 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3108 | 1/1   | 0.85 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | XA    | 1759 | 1/1   | 0.85 | 0.11 | 71,71,71,71                 | 0     |
| 56  | MG   | QA    | 1667 | 1/1   | 0.86 | 0.13 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3429 | 1/1   | 0.86 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3434 | 1/1   | 0.86 | 0.12 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3437 | 1/1   | 0.86 | 0.30 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3193 | 1/1   | 0.86 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3443 | 1/1   | 0.86 | 0.14 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3260 | 1/1   | 0.86 | 0.13 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3386 | 1/1   | 0.86 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3046 | 1/1   | 0.86 | 0.28 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3210 | 1/1   | 0.86 | 0.15 | 77,77,77,77                 | 0     |
| 56  | MG   | XA    | 1603 | 1/1   | 0.86 | 0.16 | 92,92,92,92                 | 0     |
| 56  | MG   | YA    | 3474 | 1/1   | 0.86 | 0.23 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3043 | 1/1   | 0.86 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3082 | 1/1   | 0.86 | 0.42 | 86,86,86,86                 | 0     |
| 56  | MG   | YA    | 3225 | 1/1   | 0.86 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3444 | 1/1   | 0.86 | 0.08 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3235 | 1/1   | 0.86 | 0.15 | 30,30,30,30                 | 0     |
| 56  | MG   | QD    | 301  | 1/1   | 0.86 | 0.23 | 56,56,56,56                 | 0     |
| 56  | MG   | QA    | 1806 | 1/1   | 0.86 | 0.31 | 85,85,85,85                 | 0     |
| 56  | MG   | YA    | 3252 | 1/1   | 0.86 | 0.19 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3046 | 1/1   | 0.86 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3507 | 1/1   | 0.86 | 0.20 | 81,81,81,81                 | 0     |
| 56  | MG   | YA    | 3508 | 1/1   | 0.86 | 0.18 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3254 | 1/1   | 0.86 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3598 | 1/1   | 0.86 | 0.13 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3522 | 1/1   | 0.86 | 0.30 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3048 | 1/1   | 0.86 | 0.11 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3357 | 1/1   | 0.86 | 0.22 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3542 | 1/1   | 0.86 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3546 | 1/1   | 0.86 | 0.31 | 73,73,73,73                 | 0     |
| 56  | MG   | YA    | 3267 | 1/1   | 0.86 | 0.22 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3169 | 1/1   | 0.86 | 0.15 | 93,93,93,93                 | 0     |
| 56  | MG   | YA    | 3577 | 1/1   | 0.86 | 0.17 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3595 | 1/1   | 0.86 | 0.16 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3398 | 1/1   | 0.86 | 0.41 | 97,97,97,97                 | 0     |
| 56  | MG   | RA    | 3199 | 1/1   | 0.86 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3622 | 1/1   | 0.86 | 0.12 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3699 | 1/1   | 0.86 | 0.31 | 96,96,96,96                 | 0     |
| 56  | MG   | XA    | 1762 | 1/1   | 0.86 | 0.29 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3627 | 1/1   | 0.86 | 0.19 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3306 | 1/1   | 0.86 | 0.25 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3700 | 1/1   | 0.86 | 0.17 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3704 | 1/1   | 0.86 | 0.18 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3456 | 1/1   | 0.86 | 0.31 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3115 | 1/1   | 0.86 | 0.08 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3364 | 1/1   | 0.86 | 0.20 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3203 | 1/1   | 0.86 | 0.41 | 95,95,95,95                 | 0     |
| 56  | MG   | YA    | 3338 | 1/1   | 0.86 | 0.29 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3529 | 1/1   | 0.86 | 0.23 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3367 | 1/1   | 0.86 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3118 | 1/1   | 0.86 | 0.23 | 98,98,98,98                 | 0     |
| 56  | MG   | RA    | 3371 | 1/1   | 0.86 | 0.29 | 117,117,117,117             | 0     |
| 56  | MG   | YA    | 3126 | 1/1   | 0.86 | 0.30 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3364 | 1/1   | 0.86 | 0.20 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3141 | 1/1   | 0.86 | 0.20 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3367 | 1/1   | 0.86 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3466 | 1/1   | 0.86 | 0.12 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3140 | 1/1   | 0.86 | 0.18 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3374 | 1/1   | 0.86 | 0.16 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3206 | 1/1   | 0.86 | 0.31 | 89,89,89,89                 | 0     |
| 56  | MG   | XA    | 1665 | 1/1   | 0.86 | 0.15 | 81,81,81,81                 | 0     |
| 56  | MG   | QD    | 304  | 1/1   | 0.86 | 0.13 | 73,73,73,73                 | 0     |
| 56  | MG   | RD    | 307  | 1/1   | 0.86 | 0.08 | 73,73,73,73                 | 0     |
| 56  | MG   | RD    | 308  | 1/1   | 0.86 | 0.19 | 75,75,75,75                 | 0     |
| 56  | MG   | QA    | 1726 | 1/1   | 0.86 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3122 | 1/1   | 0.86 | 0.16 | 90,90,90,90                 | 0     |
| 56  | MG   | RA    | 3212 | 1/1   | 0.86 | 0.27 | 70,70,70,70                 | 0     |
| 56  | MG   | QA    | 1727 | 1/1   | 0.86 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | YB    | 216  | 1/1   | 0.86 | 0.21 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3418 | 1/1   | 0.86 | 0.21 | 56,56,56,56                 | 0     |
| 56  | MG   | RA    | 3478 | 1/1   | 0.86 | 0.21 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3006 | 1/1   | 0.86 | 0.13 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3569 | 1/1   | 0.86 | 0.41 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3415 | 1/1   | 0.86 | 0.70 | 84,84,84,84                 | 0     |
| 56  | MG   | YA    | 3416 | 1/1   | 0.86 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | QE    | 202  | 1/1   | 0.86 | 0.21 | 109,109,109,109             | 0     |
| 56  | MG   | QA    | 1638 | 1/1   | 0.86 | 0.39 | 103,103,103,103             | 0     |
| 56  | MG   | YA    | 3181 | 1/1   | 0.86 | 0.15 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3040 | 1/1   | 0.86 | 0.10 | 40,40,40,40                 | 0     |
| 59  | ZN   | R4    | 101  | 1/1   | 0.86 | 0.11 | 285,285,285,285             | 0     |
| 56  | MG   | RA    | 3236 | 1/1   | 0.87 | 0.26 | 80,80,80,80                 | 0     |
| 56  | MG   | YA    | 3100 | 1/1   | 0.87 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3270 | 1/1   | 0.87 | 0.26 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3530 | 1/1   | 0.87 | 0.12 | 101,101,101,101             | 0     |
| 56  | MG   | XA    | 1792 | 1/1   | 0.87 | 0.16 | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3280 | 1/1   | 0.87 | 0.20 | 15,15,15,15                 | 0     |
| 56  | MG   | QA    | 1710 | 1/1   | 0.87 | 0.12 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3432 | 1/1   | 0.87 | 0.22 | 88,88,88,88                 | 0     |
| 56  | MG   | YA    | 3500 | 1/1   | 0.87 | 0.23 | 30,30,30,30                 | 0     |
| 56  | MG   | QA    | 1735 | 1/1   | 0.87 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3354 | 1/1   | 0.87 | 0.23 | 56,56,56,56                 | 0     |
| 56  | MG   | RR    | 201  | 1/1   | 0.87 | 0.22 | 74,74,74,74                 | 0     |
| 56  | MG   | YA    | 3129 | 1/1   | 0.87 | 0.16 | 47,47,47,47                 | 0     |
| 56  | MG   | RT    | 202  | 1/1   | 0.87 | 0.15 | 82,82,82,82                 | 0     |
| 56  | MG   | QA    | 1639 | 1/1   | 0.87 | 0.18 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3327 | 1/1   | 0.87 | 0.31 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3533 | 1/1   | 0.87 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3534 | 1/1   | 0.87 | 0.11 | 18,18,18,18                 | 0     |
| 56  | MG   | QA    | 1697 | 1/1   | 0.87 | 0.25 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3047 | 1/1   | 0.87 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | Y3    | 101  | 1/1   | 0.87 | 0.24 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3149 | 1/1   | 0.87 | 0.42 | 77,77,77,77                 | 0     |
| 56  | MG   | RA    | 3097 | 1/1   | 0.87 | 0.35 | 77,77,77,77                 | 0     |
| 56  | MG   | YA    | 3582 | 1/1   | 0.87 | 0.27 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3586 | 1/1   | 0.87 | 0.08 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3349 | 1/1   | 0.87 | 0.29 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3297 | 1/1   | 0.87 | 0.16 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3154 | 1/1   | 0.87 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3157 | 1/1   | 0.87 | 0.13 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3361 | 1/1   | 0.87 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3693 | 1/1   | 0.87 | 0.32 | 77,77,77,77                 | 0     |
| 56  | MG   | QA    | 1654 | 1/1   | 0.87 | 0.12 | 92,92,92,92                 | 0     |
| 56  | MG   | RA    | 3550 | 1/1   | 0.87 | 0.33 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3248 | 1/1   | 0.87 | 0.25 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3702 | 1/1   | 0.87 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3193 | 1/1   | 0.87 | 0.17 | 90,90,90,90                 | 0     |
| 56  | MG   | YA    | 3023 | 1/1   | 0.87 | 0.47 | 90,90,90,90                 | 0     |
| 56  | MG   | RA    | 3308 | 1/1   | 0.87 | 0.12 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3644 | 1/1   | 0.87 | 0.22 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3647 | 1/1   | 0.87 | 0.41 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3101 | 1/1   | 0.87 | 0.32 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3102 | 1/1   | 0.87 | 0.18 | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1701 | 1/1   | 0.87 | 0.17 | 67,67,67,67                 | 0     |
| 56  | MG   | QA    | 1622 | 1/1   | 0.87 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3398 | 1/1   | 0.87 | 0.13 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3658 | 1/1   | 0.87 | 0.24 | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1670 | 1/1   | 0.87 | 0.13 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3662 | 1/1   | 0.87 | 0.22 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3188 | 1/1   | 0.87 | 0.11 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1768 | 1/1   | 0.87 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3643 | 1/1   | 0.87 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3413 | 1/1   | 0.87 | 0.32 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3194 | 1/1   | 0.87 | 0.21 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3413 | 1/1   | 0.87 | 0.24 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3679 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1633 | 1/1   | 0.87 | 0.06 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1744 | 1/1   | 0.87 | 0.17 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3508 | 1/1   | 0.87 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | QA    | 1769 | 1/1   | 0.87 | 0.12 | 68,68,68,68                 | 0     |
| 56  | MG   | XA    | 1752 | 1/1   | 0.87 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3214 | 1/1   | 0.87 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | YB    | 202  | 1/1   | 0.87 | 0.14 | 91,91,91,91                 | 0     |
| 56  | MG   | YB    | 204  | 1/1   | 0.87 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3424 | 1/1   | 0.87 | 0.30 | 70,70,70,70                 | 0     |
| 56  | MG   | YB    | 210  | 1/1   | 0.87 | 0.20 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1755 | 1/1   | 0.87 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3216 | 1/1   | 0.87 | 0.07 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3156 | 1/1   | 0.87 | 0.14 | 76,76,76,76                 | 0     |
| 56  | MG   | RA    | 3328 | 1/1   | 0.87 | 0.25 | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1646 | 1/1   | 0.87 | 0.21 | 92,92,92,92                 | 0     |
| 56  | MG   | YA    | 3234 | 1/1   | 0.87 | 0.12 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3158 | 1/1   | 0.87 | 0.05 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3243 | 1/1   | 0.87 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3231 | 1/1   | 0.87 | 0.30 | 91,91,91,91                 | 0     |
| 56  | MG   | RA    | 3464 | 1/1   | 0.87 | 0.35 | 118,118,118,118             | 0     |
| 56  | MG   | RG    | 201  | 1/1   | 0.87 | 0.07 | 79,79,79,79                 | 0     |
| 56  | MG   | YA    | 3460 | 1/1   | 0.87 | 0.24 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3660 | 1/1   | 0.87 | 0.39 | 62,62,62,62                 | 0     |
| 56  | MG   | RA    | 3267 | 1/1   | 0.87 | 0.26 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3089 | 1/1   | 0.87 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3316 | 1/1   | 0.88 | 0.31 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3510 | 1/1   | 0.88 | 0.21 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3026 | 1/1   | 0.88 | 0.14 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3513 | 1/1   | 0.88 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | QA    | 1651 | 1/1   | 0.88 | 0.26 | 91,91,91,91                 | 0     |
| 56  | MG   | YA    | 3519 | 1/1   | 0.88 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | XA    | 1650 | 1/1   | 0.88 | 0.08 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3031 | 1/1   | 0.88 | 0.24 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3528 | 1/1   | 0.88 | 0.16 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3161 | 1/1   | 0.88 | 0.13 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3445 | 1/1   | 0.88 | 0.12 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3034 | 1/1   | 0.88 | 0.19 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3167 | 1/1   | 0.88 | 0.33 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1664 | 1/1   | 0.88 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3261 | 1/1   | 0.88 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3552 | 1/1   | 0.88 | 0.19 | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3307 | 1/1   | 0.88 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3131 | 1/1   | 0.88 | 0.23 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3579 | 1/1   | 0.88 | 0.13 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3645 | 1/1   | 0.88 | 0.20 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3585 | 1/1   | 0.88 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3202 | 1/1   | 0.88 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3180 | 1/1   | 0.88 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | RW    | 201  | 1/1   | 0.88 | 0.07 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3611 | 1/1   | 0.88 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3065 | 1/1   | 0.88 | 0.15 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3709 | 1/1   | 0.88 | 0.37 | 120,120,120,120             | 0     |
| 56  | MG   | QA    | 1729 | 1/1   | 0.88 | 0.27 | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1788 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3378 | 1/1   | 0.88 | 0.12 | 95,95,95,95                 | 0     |
| 56  | MG   | QA    | 1763 | 1/1   | 0.88 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1608 | 1/1   | 0.88 | 0.40 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3321 | 1/1   | 0.88 | 0.23 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3196 | 1/1   | 0.88 | 0.14 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3366 | 1/1   | 0.88 | 0.68 | 98,98,98,98                 | 0     |
| 56  | MG   | YA    | 3077 | 1/1   | 0.88 | 0.21 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3422 | 1/1   | 0.88 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3206 | 1/1   | 0.88 | 0.26 | 77,77,77,77                 | 0     |
| 56  | MG   | QA    | 1748 | 1/1   | 0.88 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3073 | 1/1   | 0.88 | 0.26 | 104,104,104,104             | 0     |
| 56  | MG   | R3    | 103  | 1/1   | 0.88 | 0.41 | 111,111,111,111             | 0     |
| 56  | MG   | RA    | 3327 | 1/1   | 0.88 | 0.29 | 68,68,68,68                 | 0     |
| 56  | MG   | XA    | 1691 | 1/1   | 0.88 | 0.32 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1730 | 1/1   | 0.88 | 0.30 | 73,73,73,73                 | 0     |
| 56  | MG   | YA    | 3659 | 1/1   | 0.88 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3564 | 1/1   | 0.88 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3230 | 1/1   | 0.88 | 0.27 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3228 | 1/1   | 0.88 | 0.28 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3467 | 1/1   | 0.88 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | QA    | 1714 | 1/1   | 0.88 | 0.19 | 76,76,76,76                 | 0     |
| 56  | MG   | YA    | 3669 | 1/1   | 0.88 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3109 | 1/1   | 0.88 | 0.06 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3427 | 1/1   | 0.88 | 0.16 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1703 | 1/1   | 0.88 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | XA    | 1705 | 1/1   | 0.88 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3680 | 1/1   | 0.88 | 0.20 | 133,133,133,133             | 0     |
| 56  | MG   | YA    | 3248 | 1/1   | 0.88 | 0.32 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3118 | 1/1   | 0.88 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3688 | 1/1   | 0.88 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | XA    | 1629 | 1/1   | 0.88 | 0.23 | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3002 | 1/1   | 0.88 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3255 | 1/1   | 0.88 | 0.29 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3447 | 1/1   | 0.88 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3706 | 1/1   | 0.88 | 0.19 | 82,82,82,82                 | 0     |
| 56  | MG   | YA    | 3259 | 1/1   | 0.88 | 0.06 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3262 | 1/1   | 0.88 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3008 | 1/1   | 0.88 | 0.07 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3130 | 1/1   | 0.88 | 0.07 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3470 | 1/1   | 0.88 | 0.31 | 88,88,88,88                 | 0     |
| 56  | MG   | YA    | 3473 | 1/1   | 0.88 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3179 | 1/1   | 0.88 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3475 | 1/1   | 0.88 | 0.27 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3142 | 1/1   | 0.88 | 0.14 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3687 | 1/1   | 0.88 | 0.38 | 148,148,148,148             | 0     |
| 56  | MG   | YD    | 307  | 1/1   | 0.88 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3583 | 1/1   | 0.88 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1645 | 1/1   | 0.88 | 0.16 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3296 | 1/1   | 0.88 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3019 | 1/1   | 0.88 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3150 | 1/1   | 0.88 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3344 | 1/1   | 0.88 | 0.24 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1648 | 1/1   | 0.88 | 0.08 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3311 | 1/1   | 0.88 | 0.22 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3153 | 1/1   | 0.88 | 0.10 | 52,52,52,52                 | 0     |
| 59  | ZN   | Y4    | 101  | 1/1   | 0.88 | 0.07 | 284,284,284,284             | 0     |
| 56  | MG   | YA    | 3342 | 1/1   | 0.89 | 0.29 | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1819 | 1/1   | 0.89 | 0.19 | 46,46,46,46                 | 0     |
| 56  | MG   | RQ    | 202  | 1/1   | 0.89 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1756 | 1/1   | 0.89 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | RQ    | 204  | 1/1   | 0.89 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1659 | 1/1   | 0.89 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3359 | 1/1   | 0.89 | 0.28 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3183 | 1/1   | 0.89 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3296 | 1/1   | 0.89 | 0.21 | 45,45,45,45                 | 0     |
| 56  | MG   | QI    | 201  | 1/1   | 0.89 | 0.11 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RT    | 204  | 1/1   | 0.89 | 0.08 | 57,57,57,57                 | 0     |
| 56  | MG   | RU    | 201  | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3565 | 1/1   | 0.89 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3191 | 1/1   | 0.89 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1666 | 1/1   | 0.89 | 0.07 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3099 | 1/1   | 0.89 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3425 | 1/1   | 0.89 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1778 | 1/1   | 0.89 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3588 | 1/1   | 0.89 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | RV    | 203  | 1/1   | 0.89 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3596 | 1/1   | 0.89 | 0.24 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3605 | 1/1   | 0.89 | 0.23 | 74,74,74,74                 | 0     |
| 56  | MG   | YA    | 3198 | 1/1   | 0.89 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3385 | 1/1   | 0.89 | 0.35 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3199 | 1/1   | 0.89 | 0.19 | 84,84,84,84                 | 0     |
| 56  | MG   | RA    | 3427 | 1/1   | 0.89 | 0.16 | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1784 | 1/1   | 0.89 | 0.20 | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1785 | 1/1   | 0.89 | 0.20 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1674 | 1/1   | 0.89 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3346 | 1/1   | 0.89 | 0.20 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3401 | 1/1   | 0.89 | 0.16 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3403 | 1/1   | 0.89 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1780 | 1/1   | 0.89 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3537 | 1/1   | 0.89 | 0.10 | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3539 | 1/1   | 0.89 | 0.13 | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3541 | 1/1   | 0.89 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3223 | 1/1   | 0.89 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | RB    | 203  | 1/1   | 0.89 | 0.07 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3602 | 1/1   | 0.89 | 0.37 | 66,66,66,66                 | 0     |
| 56  | MG   | YA    | 3651 | 1/1   | 0.89 | 0.27 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3656 | 1/1   | 0.89 | 0.27 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3113 | 1/1   | 0.89 | 0.25 | 72,72,72,72                 | 0     |
| 56  | MG   | XV    | 103  | 1/1   | 0.89 | 0.11 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1687 | 1/1   | 0.89 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3501 | 1/1   | 0.89 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3247 | 1/1   | 0.89 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3088 | 1/1   | 0.89 | 0.08 | 77,77,77,77                 | 0     |
| 56  | MG   | QA    | 1623 | 1/1   | 0.89 | 0.54 | 86,86,86,86                 | 0     |
| 56  | MG   | RA    | 3407 | 1/1   | 0.89 | 0.11 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3090 | 1/1   | 0.89 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3135 | 1/1   | 0.89 | 0.27 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3139 | 1/1   | 0.89 | 0.08 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3261 | 1/1   | 0.89 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3076 | 1/1   | 0.89 | 0.18 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3445 | 1/1   | 0.89 | 0.06 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3141 | 1/1   | 0.89 | 0.10 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3232 | 1/1   | 0.89 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | RF    | 301  | 1/1   | 0.89 | 0.23 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3268 | 1/1   | 0.89 | 0.25 | 77,77,77,77                 | 0     |
| 56  | MG   | RA    | 3282 | 1/1   | 0.89 | 0.24 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3691 | 1/1   | 0.89 | 0.20 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1711 | 1/1   | 0.89 | 0.16 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3472 | 1/1   | 0.89 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1632 | 1/1   | 0.89 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3705 | 1/1   | 0.89 | 0.13 | 77,77,77,77                 | 0     |
| 56  | MG   | YA    | 3284 | 1/1   | 0.89 | 0.25 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3672 | 1/1   | 0.89 | 0.18 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3283 | 1/1   | 0.89 | 0.21 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3676 | 1/1   | 0.89 | 0.41 | 108,108,108,108             | 0     |
| 56  | MG   | YA    | 3298 | 1/1   | 0.89 | 0.20 | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3484 | 1/1   | 0.89 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1722 | 1/1   | 0.89 | 0.32 | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1669 | 1/1   | 0.89 | 0.19 | 74,74,74,74                 | 0     |
| 56  | MG   | YA    | 3491 | 1/1   | 0.89 | 0.20 | 28,28,28,28                 | 0     |
| 56  | MG   | YB    | 218  | 1/1   | 0.89 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3287 | 1/1   | 0.89 | 0.18 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3030 | 1/1   | 0.89 | 0.18 | 48,48,48,48                 | 0     |
| 56  | MG   | YD    | 303  | 1/1   | 0.89 | 0.23 | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1743 | 1/1   | 0.89 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3685 | 1/1   | 0.89 | 0.09 | 58,58,58,58                 | 0     |
| 56  | MG   | XA    | 1741 | 1/1   | 0.89 | 0.08 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3320 | 1/1   | 0.89 | 0.27 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3040 | 1/1   | 0.89 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3509 | 1/1   | 0.89 | 0.07 | 3,3,3,3                     | 0     |
| 56  | MG   | YN    | 201  | 1/1   | 0.89 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3042 | 1/1   | 0.89 | 0.21 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3511 | 1/1   | 0.89 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3524 | 1/1   | 0.89 | 0.21 | 41,41,41,41                 | 0     |
| 56  | MG   | YW    | 201  | 1/1   | 0.89 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3081 | 1/1   | 0.89 | 0.05 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3637 | 1/1   | 0.89 | 0.20 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3569 | 1/1   | 0.90 | 0.26 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3571 | 1/1   | 0.90 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1720 | 1/1   | 0.90 | 0.20 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3242 | 1/1   | 0.90 | 0.23 | 43,43,43,43                 | 0     |
| 56  | MG   | QV    | 104  | 1/1   | 0.90 | 0.17 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3167 | 1/1   | 0.90 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3684 | 1/1   | 0.90 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3217 | 1/1   | 0.90 | 0.10 | 86,86,86,86                 | 0     |
| 56  | MG   | YA    | 3591 | 1/1   | 0.90 | 0.21 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3593 | 1/1   | 0.90 | 0.21 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3020 | 1/1   | 0.90 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1647 | 1/1   | 0.90 | 0.06 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3142 | 1/1   | 0.90 | 0.28 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3606 | 1/1   | 0.90 | 0.09 | 9,9,9,9                     | 0     |
| 56  | MG   | QA    | 1681 | 1/1   | 0.90 | 0.23 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3258 | 1/1   | 0.90 | 0.12 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3143 | 1/1   | 0.90 | 0.20 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1752 | 1/1   | 0.90 | 0.05 | 51,51,51,51                 | 0     |
| 56  | MG   | RQ    | 203  | 1/1   | 0.90 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3421 | 1/1   | 0.90 | 0.12 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3626 | 1/1   | 0.90 | 0.12 | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3196 | 1/1   | 0.90 | 0.08 | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1682 | 1/1   | 0.90 | 0.15 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3578 | 1/1   | 0.90 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3368 | 1/1   | 0.90 | 0.31 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3636 | 1/1   | 0.90 | 0.07 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3269 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3640 | 1/1   | 0.90 | 0.15 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3641 | 1/1   | 0.90 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3067 | 1/1   | 0.90 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3516 | 1/1   | 0.90 | 0.13 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3277 | 1/1   | 0.90 | 0.22 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3703 | 1/1   | 0.90 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | XA    | 1769 | 1/1   | 0.90 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | QA    | 1809 | 1/1   | 0.90 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3520 | 1/1   | 0.90 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1777 | 1/1   | 0.90 | 0.22 | 46,46,46,46                 | 0     |
| 56  | MG   | RZ    | 301  | 1/1   | 0.90 | 0.05 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3452 | 1/1   | 0.90 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3525 | 1/1   | 0.90 | 0.14 | 83,83,83,83                 | 0     |
| 56  | MG   | RA    | 3286 | 1/1   | 0.90 | 0.25 | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1759 | 1/1   | 0.90 | 0.07 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3462 | 1/1   | 0.90 | 0.18 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3060 | 1/1   | 0.90 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3016 | 1/1   | 0.90 | 0.25 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1725 | 1/1   | 0.90 | 0.08 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3293 | 1/1   | 0.90 | 0.17 | 15,15,15,15                 | 0     |
| 56  | MG   | QA    | 1781 | 1/1   | 0.90 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | XA    | 1613 | 1/1   | 0.90 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3479 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3324 | 1/1   | 0.90 | 0.26 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3482 | 1/1   | 0.90 | 0.16 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3681 | 1/1   | 0.90 | 0.17 | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1790 | 1/1   | 0.90 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3685 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 56  | MG   | XA    | 1791 | 1/1   | 0.90 | 0.34 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3295 | 1/1   | 0.90 | 0.21 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3659 | 1/1   | 0.90 | 0.41 | 81,81,81,81                 | 0     |
| 56  | MG   | XA    | 1617 | 1/1   | 0.90 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3696 | 1/1   | 0.90 | 0.25 | 145,145,145,145             | 0     |
| 56  | MG   | RA    | 3412 | 1/1   | 0.90 | 0.10 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3493 | 1/1   | 0.90 | 0.15 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3344 | 1/1   | 0.90 | 0.18 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3088 | 1/1   | 0.90 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1619 | 1/1   | 0.90 | 0.06 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3093 | 1/1   | 0.90 | 0.15 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3501 | 1/1   | 0.90 | 0.21 | 57,57,57,57                 | 0     |
| 56  | MG   | YB    | 206  | 1/1   | 0.90 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3095 | 1/1   | 0.90 | 0.14 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3345 | 1/1   | 0.90 | 0.10 | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3114 | 1/1   | 0.90 | 0.29 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3493 | 1/1   | 0.90 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MG   | R7    | 102  | 1/1   | 0.90 | 0.32 | 92,92,92,92                 | 0     |
| 56  | MG   | QA    | 1657 | 1/1   | 0.90 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3384 | 1/1   | 0.90 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3369 | 1/1   | 0.90 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3108 | 1/1   | 0.90 | 0.11 | 67,67,67,67                 | 0     |
| 56  | MG   | RF    | 302  | 1/1   | 0.90 | 0.23 | 107,107,107,107             | 0     |
| 56  | MG   | RA    | 3544 | 1/1   | 0.90 | 0.09 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3112 | 1/1   | 0.90 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1784 | 1/1   | 0.90 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3500 | 1/1   | 0.90 | 0.28 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3117 | 1/1   | 0.90 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | QA    | 1606 | 1/1   | 0.90 | 0.06 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3305 | 1/1   | 0.90 | 0.17 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3123 | 1/1   | 0.90 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3551 | 1/1   | 0.90 | 0.09 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3395 | 1/1   | 0.90 | 0.29 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3679 | 1/1   | 0.90 | 0.19 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3564 | 1/1   | 0.90 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3127 | 1/1   | 0.90 | 0.21 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3630 | 1/1   | 0.91 | 0.20 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3575 | 1/1   | 0.91 | 0.15 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3570 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3245 | 1/1   | 0.91 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | QA    | 1798 | 1/1   | 0.91 | 0.24 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3572 | 1/1   | 0.91 | 0.12 | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3138 | 1/1   | 0.91 | 0.22 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3587 | 1/1   | 0.91 | 0.13 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3125 | 1/1   | 0.91 | 0.27 | 94,94,94,94                 | 0     |
| 56  | MG   | XA    | 1654 | 1/1   | 0.91 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3692 | 1/1   | 0.91 | 0.29 | 56,56,56,56                 | 0     |
| 56  | MG   | QA    | 1717 | 1/1   | 0.91 | 0.33 | 45,45,45,45                 | 0     |
| 56  | MG   | RT    | 203  | 1/1   | 0.91 | 0.09 | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3598 | 1/1   | 0.91 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3417 | 1/1   | 0.91 | 0.20 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3144 | 1/1   | 0.91 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3036 | 1/1   | 0.91 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | QA    | 1802 | 1/1   | 0.91 | 0.30 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3580 | 1/1   | 0.91 | 0.14 | 87,87,87,87                 | 0     |
| 56  | MG   | QA    | 1757 | 1/1   | 0.91 | 0.05 | 54,54,54,54                 | 0     |
| 56  | MG   | QA    | 1745 | 1/1   | 0.91 | 0.06 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3349 | 1/1   | 0.91 | 0.14 | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3147 | 1/1   | 0.91 | 0.09 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3095 | 1/1   | 0.91 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3054 | 1/1   | 0.91 | 0.23 | 65,65,65,65                 | 0     |
| 56  | MG   | R0    | 101  | 1/1   | 0.91 | 0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3438 | 1/1   | 0.91 | 0.15 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3436 | 1/1   | 0.91 | 0.29 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3590 | 1/1   | 0.91 | 0.12 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3649 | 1/1   | 0.91 | 0.25 | 98,98,98,98                 | 0     |
| 56  | MG   | YA    | 3163 | 1/1   | 0.91 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | QA    | 1604 | 1/1   | 0.91 | 0.08 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3062 | 1/1   | 0.91 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3356 | 1/1   | 0.91 | 0.21 | 39,39,39,39                 | 0     |
| 56  | MG   | QL    | 203  | 1/1   | 0.91 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | XA    | 1609 | 1/1   | 0.91 | 0.28 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3069 | 1/1   | 0.91 | 0.37 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3173 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3358 | 1/1   | 0.91 | 0.32 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3471 | 1/1   | 0.91 | 0.24 | 84,84,84,84                 | 0     |
| 56  | MG   | YA    | 3319 | 1/1   | 0.91 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | XA    | 1789 | 1/1   | 0.91 | 0.16 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3154 | 1/1   | 0.91 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3322 | 1/1   | 0.91 | 0.12 | 21,21,21,21                 | 0     |
| 56  | MG   | RA    | 3289 | 1/1   | 0.91 | 0.19 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3663 | 1/1   | 0.91 | 0.26 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3599 | 1/1   | 0.91 | 0.25 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3086 | 1/1   | 0.91 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3481 | 1/1   | 0.91 | 0.29 | 80,80,80,80                 | 0     |
| 56  | MG   | RB    | 216  | 1/1   | 0.91 | 0.09 | 74,74,74,74                 | 0     |
| 56  | MG   | RD    | 301  | 1/1   | 0.91 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | XA    | 1695 | 1/1   | 0.91 | 0.15 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3019 | 1/1   | 0.91 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3548 | 1/1   | 0.91 | 0.24 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3347 | 1/1   | 0.91 | 0.14 | 8,8,8,8                     | 0     |
| 56  | MG   | RA    | 3036 | 1/1   | 0.91 | 0.42 | 80,80,80,80                 | 0     |
| 56  | MG   | RA    | 3553 | 1/1   | 0.91 | 0.20 | 22,22,22,22                 | 0     |
| 56  | MG   | RE    | 302  | 1/1   | 0.91 | 0.16 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3475 | 1/1   | 0.91 | 0.13 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3449 | 1/1   | 0.91 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3612 | 1/1   | 0.91 | 0.25 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3562 | 1/1   | 0.91 | 0.15 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3107 | 1/1   | 0.91 | 0.26 | 80,80,80,80                 | 0     |
| 56  | MG   | YA    | 3202 | 1/1   | 0.91 | 0.24 | 48,48,48,48                 | 0     |
| 56  | MG   | Y7    | 102  | 1/1   | 0.91 | 0.08 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3368 | 1/1   | 0.91 | 0.14 | 21,21,21,21                 | 0     |
| 56  | MG   | RA    | 3263 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3370 | 1/1   | 0.91 | 0.20 | 30,30,30,30                 | 0     |
| 56  | MG   | YB    | 201  | 1/1   | 0.91 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3209 | 1/1   | 0.91 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3110 | 1/1   | 0.91 | 0.29 | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1739 | 1/1   | 0.91 | 0.17 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3007 | 1/1   | 0.91 | 0.07 | 66,66,66,66                 | 0     |
| 56  | MG   | YB    | 208  | 1/1   | 0.91 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | YB    | 209  | 1/1   | 0.91 | 0.15 | 92,92,92,92                 | 0     |
| 56  | MG   | YA    | 3525 | 1/1   | 0.91 | 0.18 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3376 | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3565 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3530 | 1/1   | 0.91 | 0.16 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3678 | 1/1   | 0.91 | 0.27 | 98,98,98,98                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3380 | 1/1   | 0.91 | 0.33 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3116 | 1/1   | 0.91 | 0.11 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3537 | 1/1   | 0.91 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | YD    | 302  | 1/1   | 0.91 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3540 | 1/1   | 0.91 | 0.14 | 33,33,33,33                 | 0     |
| 56  | MG   | YD    | 305  | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3384 | 1/1   | 0.91 | 0.07 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3543 | 1/1   | 0.91 | 0.12 | 16,16,16,16                 | 0     |
| 56  | MG   | YE    | 303  | 1/1   | 0.91 | 0.27 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3623 | 1/1   | 0.91 | 0.28 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3180 | 1/1   | 0.91 | 0.11 | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3568 | 1/1   | 0.91 | 0.10 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3393 | 1/1   | 0.91 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3016 | 1/1   | 0.91 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3557 | 1/1   | 0.91 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3419 | 1/1   | 0.91 | 0.24 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1728 | 1/1   | 0.91 | 0.26 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3566 | 1/1   | 0.91 | 0.10 | 25,25,25,25                 | 0     |
| 57  | PAR  | QA    | 1821 | 42/42 | 0.91 | 0.13 | 52,66,86,95                 | 0     |
| 57  | PAR  | XA    | 1794 | 42/42 | 0.91 | 0.10 | 52,63,76,81                 | 0     |
| 56  | MG   | XA    | 1735 | 1/1   | 0.91 | 0.08 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3570 | 1/1   | 0.91 | 0.13 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3231 | 1/1   | 0.92 | 0.13 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3194 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3567 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |
| 56  | MG   | XA    | 1715 | 1/1   | 0.92 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3237 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3238 | 1/1   | 0.92 | 0.18 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3574 | 1/1   | 0.92 | 0.17 | 24,24,24,24                 | 0     |
| 56  | MG   | QA    | 1707 | 1/1   | 0.92 | 0.07 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3576 | 1/1   | 0.92 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3404 | 1/1   | 0.92 | 0.05 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3120 | 1/1   | 0.92 | 0.32 | 102,102,102,102             | 0     |
| 56  | MG   | YA    | 3580 | 1/1   | 0.92 | 0.20 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3581 | 1/1   | 0.92 | 0.31 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3361 | 1/1   | 0.92 | 0.22 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3013 | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3411 | 1/1   | 0.92 | 0.19 | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1719 | 1/1   | 0.92 | 0.08 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3402 | 1/1   | 0.92 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3590 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3250 | 1/1   | 0.92 | 0.22 | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3030 | 1/1   | 0.92 | 0.13 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3603 | 1/1   | 0.92 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | RA    | 3667 | 1/1   | 0.92 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3255 | 1/1   | 0.92 | 0.13 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3419 | 1/1   | 0.92 | 0.25 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3132 | 1/1   | 0.92 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1760 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3136 | 1/1   | 0.92 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3613 | 1/1   | 0.92 | 0.21 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3615 | 1/1   | 0.92 | 0.14 | 22,22,22,22                 | 0     |
| 56  | MG   | XA    | 1726 | 1/1   | 0.92 | 0.06 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3425 | 1/1   | 0.92 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | QA    | 1708 | 1/1   | 0.92 | 0.22 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3624 | 1/1   | 0.92 | 0.14 | 17,17,17,17                 | 0     |
| 56  | MG   | XA    | 1642 | 1/1   | 0.92 | 0.05 | 77,77,77,77                 | 0     |
| 56  | MG   | YA    | 3264 | 1/1   | 0.92 | 0.15 | 21,21,21,21                 | 0     |
| 56  | MG   | RG    | 203  | 1/1   | 0.92 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | RA    | 3607 | 1/1   | 0.92 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3631 | 1/1   | 0.92 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3033 | 1/1   | 0.92 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | QA    | 1779 | 1/1   | 0.92 | 0.18 | 38,38,38,38                 | 0     |
| 56  | MG   | QA    | 1603 | 1/1   | 0.92 | 0.05 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3442 | 1/1   | 0.92 | 0.23 | 86,86,86,86                 | 0     |
| 56  | MG   | XA    | 1746 | 1/1   | 0.92 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3037 | 1/1   | 0.92 | 0.21 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1747 | 1/1   | 0.92 | 0.08 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3446 | 1/1   | 0.92 | 0.08 | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3320 | 1/1   | 0.92 | 0.50 | 93,93,93,93                 | 0     |
| 56  | MG   | YA    | 3449 | 1/1   | 0.92 | 0.22 | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3450 | 1/1   | 0.92 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1615 | 1/1   | 0.92 | 0.16 | 47,47,47,47                 | 0     |
| 56  | MG   | QV    | 101  | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3454 | 1/1   | 0.92 | 0.06 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3655 | 1/1   | 0.92 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1629 | 1/1   | 0.92 | 0.08 | 75,75,75,75                 | 0     |
| 56  | MG   | YA    | 3047 | 1/1   | 0.92 | 0.09 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3281 | 1/1   | 0.92 | 0.14 | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3117 | 1/1   | 0.92 | 0.35 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3467 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3053 | 1/1   | 0.92 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3309 | 1/1   | 0.92 | 0.32 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3624 | 1/1   | 0.92 | 0.32 | 77,77,77,77                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1764 | 1/1   | 0.92 | 0.23 | 25,25,25,25                 | 0     |
| 56  | MG   | XA    | 1765 | 1/1   | 0.92 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | QA    | 1731 | 1/1   | 0.92 | 0.26 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3477 | 1/1   | 0.92 | 0.29 | 98,98,98,98                 | 0     |
| 56  | MG   | YA    | 3671 | 1/1   | 0.92 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3672 | 1/1   | 0.92 | 0.18 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3626 | 1/1   | 0.92 | 0.28 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3675 | 1/1   | 0.92 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3676 | 1/1   | 0.92 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3168 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3688 | 1/1   | 0.92 | 0.20 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3146 | 1/1   | 0.92 | 0.08 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3331 | 1/1   | 0.92 | 0.21 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3683 | 1/1   | 0.92 | 0.12 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3325 | 1/1   | 0.92 | 0.21 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3332 | 1/1   | 0.92 | 0.20 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3686 | 1/1   | 0.92 | 0.07 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3329 | 1/1   | 0.92 | 0.28 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3465 | 1/1   | 0.92 | 0.34 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3696 | 1/1   | 0.92 | 0.25 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3178 | 1/1   | 0.92 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3339 | 1/1   | 0.92 | 0.18 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3495 | 1/1   | 0.92 | 0.13 | 30,30,30,30                 | 0     |
| 56  | MG   | QA    | 1621 | 1/1   | 0.92 | 0.36 | 100,100,100,100             | 0     |
| 56  | MG   | YA    | 3071 | 1/1   | 0.92 | 0.09 | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3704 | 1/1   | 0.92 | 0.27 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3698 | 1/1   | 0.92 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3182 | 1/1   | 0.92 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3573 | 1/1   | 0.92 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3504 | 1/1   | 0.92 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1674 | 1/1   | 0.92 | 0.25 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3078 | 1/1   | 0.92 | 0.06 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3701 | 1/1   | 0.92 | 0.16 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3576 | 1/1   | 0.92 | 0.12 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3519 | 1/1   | 0.92 | 0.17 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3150 | 1/1   | 0.92 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3087 | 1/1   | 0.92 | 0.05 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3121 | 1/1   | 0.92 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3515 | 1/1   | 0.92 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | R0    | 102  | 1/1   | 0.92 | 0.07 | 65,65,65,65                 | 0     |
| 56  | MG   | RA    | 3582 | 1/1   | 0.92 | 0.32 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3291 | 1/1   | 0.92 | 0.14 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RB    | 201  | 1/1   | 0.92 | 0.25 | 98,98,98,98                 | 0     |
| 56  | MG   | QA    | 1609 | 1/1   | 0.92 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3348 | 1/1   | 0.92 | 0.10 | 2,2,2,2                     | 0     |
| 56  | MG   | QA    | 1719 | 1/1   | 0.92 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3022 | 1/1   | 0.92 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | QA    | 1720 | 1/1   | 0.92 | 0.08 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3536 | 1/1   | 0.92 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | QA    | 1814 | 1/1   | 0.92 | 0.32 | 64,64,64,64                 | 0     |
| 56  | MG   | YF    | 302  | 1/1   | 0.92 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3538 | 1/1   | 0.92 | 0.13 | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1755 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3299 | 1/1   | 0.92 | 0.10 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3382 | 1/1   | 0.92 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3544 | 1/1   | 0.92 | 0.39 | 34,34,34,34                 | 0     |
| 56  | MG   | YP    | 202  | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3593 | 1/1   | 0.92 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1707 | 1/1   | 0.92 | 0.07 | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1709 | 1/1   | 0.92 | 0.19 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3005 | 1/1   | 0.92 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3114 | 1/1   | 0.92 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | QA    | 1793 | 1/1   | 0.92 | 0.21 | 64,64,64,64                 | 0     |
| 56  | MG   | QA    | 1612 | 1/1   | 0.92 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3041 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3257 | 1/1   | 0.93 | 0.05 | 38,38,38,38                 | 0     |
| 56  | MG   | QA    | 1767 | 1/1   | 0.93 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1675 | 1/1   | 0.93 | 0.17 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3215 | 1/1   | 0.93 | 0.28 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3486 | 1/1   | 0.93 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3491 | 1/1   | 0.93 | 0.20 | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1766 | 1/1   | 0.93 | 0.23 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3492 | 1/1   | 0.93 | 0.17 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3266 | 1/1   | 0.93 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3423 | 1/1   | 0.93 | 0.16 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3216 | 1/1   | 0.93 | 0.24 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3592 | 1/1   | 0.93 | 0.19 | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3496 | 1/1   | 0.93 | 0.19 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3155 | 1/1   | 0.93 | 0.15 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3274 | 1/1   | 0.93 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3587 | 1/1   | 0.93 | 0.27 | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3604 | 1/1   | 0.93 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1775 | 1/1   | 0.93 | 0.13 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3430 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3431 | 1/1   | 0.93 | 0.19 | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1686 | 1/1   | 0.93 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3612 | 1/1   | 0.93 | 0.24 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3434 | 1/1   | 0.93 | 0.14 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3281 | 1/1   | 0.93 | 0.16 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3437 | 1/1   | 0.93 | 0.23 | 29,29,29,29                 | 0     |
| 56  | MG   | XA    | 1779 | 1/1   | 0.93 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3162 | 1/1   | 0.93 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | XA    | 1688 | 1/1   | 0.93 | 0.28 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3292 | 1/1   | 0.93 | 0.06 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3157 | 1/1   | 0.93 | 0.10 | 59,59,59,59                 | 0     |
| 56  | MG   | XA    | 1690 | 1/1   | 0.93 | 0.20 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3299 | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3300 | 1/1   | 0.93 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3071 | 1/1   | 0.93 | 0.38 | 102,102,102,102             | 0     |
| 56  | MG   | QF    | 201  | 1/1   | 0.93 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3635 | 1/1   | 0.93 | 0.14 | 18,18,18,18                 | 0     |
| 56  | MG   | XA    | 1694 | 1/1   | 0.93 | 0.08 | 27,27,27,27                 | 0     |
| 56  | MG   | QA    | 1753 | 1/1   | 0.93 | 0.21 | 83,83,83,83                 | 0     |
| 56  | MG   | YA    | 3072 | 1/1   | 0.93 | 0.12 | 7,7,7,7                     | 0     |
| 56  | MG   | YA    | 3455 | 1/1   | 0.93 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1788 | 1/1   | 0.93 | 0.05 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3543 | 1/1   | 0.93 | 0.14 | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3175 | 1/1   | 0.93 | 0.13 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3317 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3464 | 1/1   | 0.93 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3176 | 1/1   | 0.93 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3468 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | XA    | 1699 | 1/1   | 0.93 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3694 | 1/1   | 0.93 | 0.35 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3302 | 1/1   | 0.93 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3502 | 1/1   | 0.93 | 0.10 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3433 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1684 | 1/1   | 0.93 | 0.33 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3328 | 1/1   | 0.93 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1641 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3435 | 1/1   | 0.93 | 0.16 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3335 | 1/1   | 0.93 | 0.05 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3089 | 1/1   | 0.93 | 0.07 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3667 | 1/1   | 0.93 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3091 | 1/1   | 0.93 | 0.18 | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1708 | 1/1   | 0.93 | 0.24 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1635 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3487 | 1/1   | 0.93 | 0.25 | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1644 | 1/1   | 0.93 | 0.10 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3273 | 1/1   | 0.93 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3345 | 1/1   | 0.93 | 0.07 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3651 | 1/1   | 0.93 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3195 | 1/1   | 0.93 | 0.09 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3275 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3350 | 1/1   | 0.93 | 0.12 | 24,24,24,24                 | 0     |
| 56  | MG   | QA    | 1756 | 1/1   | 0.93 | 0.05 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3682 | 1/1   | 0.93 | 0.21 | 63,63,63,63                 | 0     |
| 56  | MG   | RA    | 3017 | 1/1   | 0.93 | 0.07 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1772 | 1/1   | 0.93 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3001 | 1/1   | 0.93 | 0.13 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3502 | 1/1   | 0.93 | 0.24 | 60,60,60,60                 | 0     |
| 56  | MG   | XA    | 1651 | 1/1   | 0.93 | 0.05 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3505 | 1/1   | 0.93 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3203 | 1/1   | 0.93 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3003 | 1/1   | 0.93 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3693 | 1/1   | 0.93 | 0.39 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3694 | 1/1   | 0.93 | 0.30 | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3366 | 1/1   | 0.93 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | XA    | 1652 | 1/1   | 0.93 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1713 | 1/1   | 0.93 | 0.15 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3317 | 1/1   | 0.93 | 0.13 | 7,7,7,7                     | 0     |
| 56  | MG   | QA    | 1645 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3610 | 1/1   | 0.93 | 0.10 | 62,62,62,62                 | 0     |
| 56  | MG   | XA    | 1727 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3516 | 1/1   | 0.93 | 0.13 | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3517 | 1/1   | 0.93 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1730 | 1/1   | 0.93 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1733 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3224 | 1/1   | 0.93 | 0.16 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3253 | 1/1   | 0.93 | 0.23 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3379 | 1/1   | 0.93 | 0.19 | 37,37,37,37                 | 0     |
| 56  | MG   | RB    | 206  | 1/1   | 0.93 | 0.21 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3121 | 1/1   | 0.93 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3230 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3535 | 1/1   | 0.93 | 0.23 | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1738 | 1/1   | 0.93 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1662 | 1/1   | 0.93 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3613 | 1/1   | 0.93 | 0.15 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1742 | 1/1   | 0.93 | 0.34 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3389 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3391 | 1/1   | 0.93 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3392 | 1/1   | 0.93 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | YD    | 306  | 1/1   | 0.93 | 0.17 | 84,84,84,84                 | 0     |
| 56  | MG   | XA    | 1743 | 1/1   | 0.93 | 0.15 | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3394 | 1/1   | 0.93 | 0.21 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3239 | 1/1   | 0.93 | 0.08 | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3207 | 1/1   | 0.93 | 0.21 | 107,107,107,107             | 0     |
| 56  | MG   | YA    | 3554 | 1/1   | 0.93 | 0.15 | 7,7,7,7                     | 0     |
| 56  | MG   | QL    | 201  | 1/1   | 0.93 | 0.16 | 103,103,103,103             | 0     |
| 56  | MG   | XA    | 1667 | 1/1   | 0.93 | 0.14 | 81,81,81,81                 | 0     |
| 56  | MG   | YA    | 3134 | 1/1   | 0.93 | 0.08 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3523 | 1/1   | 0.93 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | YO    | 201  | 1/1   | 0.93 | 0.39 | 88,88,88,88                 | 0     |
| 56  | MG   | QA    | 1783 | 1/1   | 0.93 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | XA    | 1751 | 1/1   | 0.93 | 0.26 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3405 | 1/1   | 0.93 | 0.33 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3190 | 1/1   | 0.93 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | YT    | 202  | 1/1   | 0.93 | 0.17 | 85,85,85,85                 | 0     |
| 56  | MG   | YV    | 201  | 1/1   | 0.93 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3068 | 1/1   | 0.93 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3572 | 1/1   | 0.93 | 0.15 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3573 | 1/1   | 0.93 | 0.10 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3039 | 1/1   | 0.93 | 0.11 | 65,65,65,65                 | 0     |
| 56  | MG   | R1    | 101  | 1/1   | 0.93 | 0.37 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3610 | 1/1   | 0.94 | 0.19 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3465 | 1/1   | 0.94 | 0.25 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3212 | 1/1   | 0.94 | 0.18 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3213 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | RD    | 302  | 1/1   | 0.94 | 0.22 | 82,82,82,82                 | 0     |
| 56  | MG   | YA    | 3028 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3617 | 1/1   | 0.94 | 0.12 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3620 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 56  | MG   | RD    | 303  | 1/1   | 0.94 | 0.23 | 91,91,91,91                 | 0     |
| 56  | MG   | YA    | 3352 | 1/1   | 0.94 | 0.21 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3219 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3675 | 1/1   | 0.94 | 0.07 | 10,10,10,10                 | 0     |
| 56  | MG   | RA    | 3021 | 1/1   | 0.94 | 0.14 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3125 | 1/1   | 0.94 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3487 | 1/1   | 0.94 | 0.09 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3363 | 1/1   | 0.94 | 0.12 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3632 | 1/1   | 0.94 | 0.12 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3003 | 1/1   | 0.94 | 0.18 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3035 | 1/1   | 0.94 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3229 | 1/1   | 0.94 | 0.20 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3171 | 1/1   | 0.94 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3486 | 1/1   | 0.94 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3023 | 1/1   | 0.94 | 0.20 | 105,105,105,105             | 0     |
| 56  | MG   | YA    | 3233 | 1/1   | 0.94 | 0.11 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3489 | 1/1   | 0.94 | 0.17 | 36,36,36,36                 | 0     |
| 56  | MG   | XA    | 1626 | 1/1   | 0.94 | 0.06 | 31,31,31,31                 | 0     |
| 56  | MG   | QA    | 1610 | 1/1   | 0.94 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3645 | 1/1   | 0.94 | 0.09 | 36,36,36,36                 | 0     |
| 56  | MG   | XA    | 1771 | 1/1   | 0.94 | 0.15 | 44,44,44,44                 | 0     |
| 56  | MG   | RF    | 303  | 1/1   | 0.94 | 0.24 | 102,102,102,102             | 0     |
| 56  | MG   | RA    | 3109 | 1/1   | 0.94 | 0.16 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3044 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1630 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3654 | 1/1   | 0.94 | 0.23 | 15,15,15,15                 | 0     |
| 56  | MG   | QA    | 1704 | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1698 | 1/1   | 0.94 | 0.11 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3049 | 1/1   | 0.94 | 0.25 | 48,48,48,48                 | 0     |
| 56  | MG   | RG    | 202  | 1/1   | 0.94 | 0.05 | 56,56,56,56                 | 0     |
| 56  | MG   | RA    | 3310 | 1/1   | 0.94 | 0.33 | 77,77,77,77                 | 0     |
| 56  | MG   | XA    | 1635 | 1/1   | 0.94 | 0.05 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3506 | 1/1   | 0.94 | 0.15 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3540 | 1/1   | 0.94 | 0.23 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3055 | 1/1   | 0.94 | 0.11 | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1637 | 1/1   | 0.94 | 0.21 | 78,78,78,78                 | 0     |
| 56  | MG   | QA    | 1807 | 1/1   | 0.94 | 0.06 | 63,63,63,63                 | 0     |
| 56  | MG   | QA    | 1797 | 1/1   | 0.94 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3388 | 1/1   | 0.94 | 0.16 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3314 | 1/1   | 0.94 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3061 | 1/1   | 0.94 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1723 | 1/1   | 0.94 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3284 | 1/1   | 0.94 | 0.20 | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3397 | 1/1   | 0.94 | 0.21 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3520 | 1/1   | 0.94 | 0.12 | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3158 | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3695 | 1/1   | 0.94 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3067 | 1/1   | 0.94 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1712 | 1/1   | 0.94 | 0.18 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3013 | 1/1   | 0.94 | 0.11 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3078 | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3394 | 1/1   | 0.94 | 0.18 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3079 | 1/1   | 0.94 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3166 | 1/1   | 0.94 | 0.07 | 60,60,60,60                 | 0     |
| 56  | MG   | XL    | 202  | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3409 | 1/1   | 0.94 | 0.13 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3279 | 1/1   | 0.94 | 0.21 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3690 | 1/1   | 0.94 | 0.24 | 126,126,126,126             | 0     |
| 56  | MG   | QA    | 1799 | 1/1   | 0.94 | 0.05 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3075 | 1/1   | 0.94 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3283 | 1/1   | 0.94 | 0.17 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3555 | 1/1   | 0.94 | 0.37 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3286 | 1/1   | 0.94 | 0.18 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3699 | 1/1   | 0.94 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3557 | 1/1   | 0.94 | 0.11 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3550 | 1/1   | 0.94 | 0.20 | 21,21,21,21                 | 0     |
| 56  | MG   | RA    | 3098 | 1/1   | 0.94 | 0.09 | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3081 | 1/1   | 0.94 | 0.21 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3293 | 1/1   | 0.94 | 0.21 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3707 | 1/1   | 0.94 | 0.25 | 98,98,98,98                 | 0     |
| 56  | MG   | YA    | 3295 | 1/1   | 0.94 | 0.12 | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3605 | 1/1   | 0.94 | 0.16 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3562 | 1/1   | 0.94 | 0.18 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3563 | 1/1   | 0.94 | 0.22 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3083 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3705 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3258 | 1/1   | 0.94 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | YA    | 3086 | 1/1   | 0.94 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | QA    | 1800 | 1/1   | 0.94 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3292 | 1/1   | 0.94 | 0.22 | 56,56,56,56                 | 0     |
| 56  | MG   | XA    | 1729 | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1790 | 1/1   | 0.94 | 0.06 | 73,73,73,73                 | 0     |
| 56  | MG   | XA    | 1731 | 1/1   | 0.94 | 0.19 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3312 | 1/1   | 0.94 | 0.22 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3440 | 1/1   | 0.94 | 0.14 | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3661 | 1/1   | 0.94 | 0.28 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3370 | 1/1   | 0.94 | 0.27 | 117,117,117,117             | 0     |
| 56  | MG   | YD    | 304  | 1/1   | 0.94 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3318 | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 56  | MG   | QA    | 1611 | 1/1   | 0.94 | 0.05 | 31,31,31,31                 | 0     |
| 56  | MG   | XA    | 1739 | 1/1   | 0.94 | 0.27 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3664 | 1/1   | 0.94 | 0.05 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3584 | 1/1   | 0.94 | 0.07 | 58,58,58,58                 | 0     |
| 56  | MG   | YE    | 305  | 1/1   | 0.94 | 0.05 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3234 | 1/1   | 0.94 | 0.13 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3105 | 1/1   | 0.94 | 0.13 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3235 | 1/1   | 0.94 | 0.16 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3616 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3334 | 1/1   | 0.94 | 0.19 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3015 | 1/1   | 0.94 | 0.07 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3166 | 1/1   | 0.94 | 0.12 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3453 | 1/1   | 0.94 | 0.24 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3594 | 1/1   | 0.94 | 0.12 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3409 | 1/1   | 0.94 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | XA    | 1676 | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | YT    | 201  | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3597 | 1/1   | 0.94 | 0.14 | 30,30,30,30                 | 0     |
| 56  | MG   | YT    | 203  | 1/1   | 0.94 | 0.30 | 97,97,97,97                 | 0     |
| 56  | MG   | QA    | 1738 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3603 | 1/1   | 0.94 | 0.27 | 51,51,51,51                 | 0     |
| 56  | MG   | RB    | 217  | 1/1   | 0.94 | 0.07 | 62,62,62,62                 | 0     |
| 56  | MG   | QA    | 1648 | 1/1   | 0.94 | 0.08 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3025 | 1/1   | 0.94 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1753 | 1/1   | 0.94 | 0.16 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1777 | 1/1   | 0.95 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3200 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3340 | 1/1   | 0.95 | 0.05 | 31,31,31,31                 | 0     |
| 56  | MG   | XA    | 1669 | 1/1   | 0.95 | 0.05 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3653 | 1/1   | 0.95 | 0.17 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3002 | 1/1   | 0.95 | 0.04 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3094 | 1/1   | 0.95 | 0.15 | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3342 | 1/1   | 0.95 | 0.15 | 19,19,19,19                 | 0     |
| 56  | MG   | QO    | 102  | 1/1   | 0.95 | 0.14 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3004 | 1/1   | 0.95 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3440 | 1/1   | 0.95 | 0.17 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3441 | 1/1   | 0.95 | 0.08 | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3098 | 1/1   | 0.95 | 0.26 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3548 | 1/1   | 0.95 | 0.28 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3351 | 1/1   | 0.95 | 0.15 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3099 | 1/1   | 0.95 | 0.21 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1725 | 1/1   | 0.95 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3355 | 1/1   | 0.95 | 0.19 | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1786 | 1/1   | 0.95 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3556 | 1/1   | 0.95 | 0.28 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1686 | 1/1   | 0.95 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3561 | 1/1   | 0.95 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3038 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | QA    | 1702 | 1/1   | 0.95 | 0.05 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3362 | 1/1   | 0.95 | 0.19 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3677 | 1/1   | 0.95 | 0.08 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3244 | 1/1   | 0.95 | 0.06 | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3428 | 1/1   | 0.95 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3668 | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3551 | 1/1   | 0.95 | 0.14 | 11,11,11,11                 | 0     |
| 56  | MG   | QA    | 1628 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 56  | MG   | QA    | 1613 | 1/1   | 0.95 | 0.05 | 97,97,97,97                 | 0     |
| 56  | MG   | RA    | 3490 | 1/1   | 0.95 | 0.15 | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3556 | 1/1   | 0.95 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3048 | 1/1   | 0.95 | 0.05 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3319 | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3050 | 1/1   | 0.95 | 0.05 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3469 | 1/1   | 0.95 | 0.18 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3578 | 1/1   | 0.95 | 0.20 | 20,20,20,20                 | 0     |
| 56  | MG   | R6    | 102  | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3278 | 1/1   | 0.95 | 0.19 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3561 | 1/1   | 0.95 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | RB    | 208  | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3583 | 1/1   | 0.95 | 0.19 | 39,39,39,39                 | 0     |
| 56  | MG   | XV    | 102  | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3700 | 1/1   | 0.95 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3282 | 1/1   | 0.95 | 0.12 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3476 | 1/1   | 0.95 | 0.28 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3124 | 1/1   | 0.95 | 0.18 | 90,90,90,90                 | 0     |
| 56  | MG   | QA    | 1810 | 1/1   | 0.95 | 0.21 | 59,59,59,59                 | 0     |
| 56  | MG   | Y0    | 101  | 1/1   | 0.95 | 0.07 | 14,14,14,14                 | 0     |
| 56  | MG   | RB    | 213  | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3386 | 1/1   | 0.95 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3211 | 1/1   | 0.95 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | YB    | 203  | 1/1   | 0.95 | 0.04 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3291 | 1/1   | 0.95 | 0.16 | 2,2,2,2                     | 0     |
| 56  | MG   | YB    | 205  | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3200 | 1/1   | 0.95 | 0.08 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3390 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | QA    | 1721 | 1/1   | 0.95 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | XA    | 1748 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | XA    | 1749 | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YB    | 211  | 1/1   | 0.95 | 0.21 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3297 | 1/1   | 0.95 | 0.18 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3063 | 1/1   | 0.95 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1661 | 1/1   | 0.95 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3300 | 1/1   | 0.95 | 0.14 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3608 | 1/1   | 0.95 | 0.19 | 32,32,32,32                 | 0     |
| 56  | MG   | XA    | 1601 | 1/1   | 0.95 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3302 | 1/1   | 0.95 | 0.11 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3303 | 1/1   | 0.95 | 0.17 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3137 | 1/1   | 0.95 | 0.08 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3329 | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3308 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3646 | 1/1   | 0.95 | 0.26 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3112 | 1/1   | 0.95 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3621 | 1/1   | 0.95 | 0.18 | 11,11,11,11                 | 0     |
| 56  | MG   | RD    | 305  | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1724 | 1/1   | 0.95 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1655 | 1/1   | 0.95 | 0.05 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1763 | 1/1   | 0.95 | 0.27 | 40,40,40,40                 | 0     |
| 56  | MG   | YF    | 303  | 1/1   | 0.95 | 0.05 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3145 | 1/1   | 0.95 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | QA    | 1699 | 1/1   | 0.95 | 0.20 | 41,41,41,41                 | 0     |
| 56  | MG   | YG    | 203  | 1/1   | 0.95 | 0.05 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3628 | 1/1   | 0.95 | 0.10 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3076 | 1/1   | 0.95 | 0.22 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3691 | 1/1   | 0.95 | 0.22 | 89,89,89,89                 | 0     |
| 56  | MG   | RA    | 3504 | 1/1   | 0.95 | 0.08 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3079 | 1/1   | 0.95 | 0.23 | 64,64,64,64                 | 0     |
| 56  | MG   | XA    | 1611 | 1/1   | 0.95 | 0.08 | 52,52,52,52                 | 0     |
| 56  | MG   | YQ    | 202  | 1/1   | 0.95 | 0.08 | 30,30,30,30                 | 0     |
| 56  | MG   | YR    | 201  | 1/1   | 0.95 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3148 | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3517 | 1/1   | 0.95 | 0.12 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3538 | 1/1   | 0.95 | 0.24 | 53,53,53,53                 | 0     |
| 56  | MG   | XA    | 1713 | 1/1   | 0.95 | 0.18 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3022 | 1/1   | 0.95 | 0.04 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3330 | 1/1   | 0.95 | 0.19 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3577 | 1/1   | 0.95 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3332 | 1/1   | 0.95 | 0.18 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3257 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 59  | ZN   | RY    | 201  | 1/1   | 0.95 | 0.10 | 197,197,197,197             | 0     |
| 56  | MG   | RA    | 3614 | 1/1   | 0.95 | 0.15 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1761 | 1/1   | 0.96 | 0.17 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1605 | 1/1   | 0.96 | 0.05 | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3560 | 1/1   | 0.96 | 0.05 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3459 | 1/1   | 0.96 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3287 | 1/1   | 0.96 | 0.16 | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3461 | 1/1   | 0.96 | 0.08 | 46,46,46,46                 | 0     |
| 56  | MG   | QA    | 1647 | 1/1   | 0.96 | 0.04 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3274 | 1/1   | 0.96 | 0.13 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3290 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3466 | 1/1   | 0.96 | 0.10 | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3673 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 56  | MG   | QA    | 1666 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3208 | 1/1   | 0.96 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3324 | 1/1   | 0.96 | 0.18 | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1767 | 1/1   | 0.96 | 0.04 | 46,46,46,46                 | 0     |
| 56  | MG   | XA    | 1768 | 1/1   | 0.96 | 0.18 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3574 | 1/1   | 0.96 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3277 | 1/1   | 0.96 | 0.14 | 32,32,32,32                 | 0     |
| 56  | MG   | XA    | 1612 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 56  | MG   | RE    | 303  | 1/1   | 0.96 | 0.06 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3008 | 1/1   | 0.96 | 0.05 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3218 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1664 | 1/1   | 0.96 | 0.21 | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3220 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 56  | MG   | XA    | 1716 | 1/1   | 0.96 | 0.18 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3222 | 1/1   | 0.96 | 0.09 | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3655 | 1/1   | 0.96 | 0.11 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3279 | 1/1   | 0.96 | 0.13 | 31,31,31,31                 | 0     |
| 56  | MG   | QA    | 1700 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3692 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3172 | 1/1   | 0.96 | 0.18 | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3476 | 1/1   | 0.96 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3695 | 1/1   | 0.96 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3589 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3617 | 1/1   | 0.96 | 0.10 | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3698 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3156 | 1/1   | 0.96 | 0.18 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3402 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3116 | 1/1   | 0.96 | 0.09 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3306 | 1/1   | 0.96 | 0.16 | 11,11,11,11                 | 0     |
| 56  | MG   | RA    | 3050 | 1/1   | 0.96 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3494 | 1/1   | 0.96 | 0.12 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3191 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3010 | 1/1   | 0.96 | 0.13 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3336 | 1/1   | 0.96 | 0.05 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3515 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3337 | 1/1   | 0.96 | 0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3101 | 1/1   | 0.96 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3102 | 1/1   | 0.96 | 0.06 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3503 | 1/1   | 0.96 | 0.05 | 13,13,13,13                 | 0     |
| 56  | MG   | RA    | 3552 | 1/1   | 0.96 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3339 | 1/1   | 0.96 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3176 | 1/1   | 0.96 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3249 | 1/1   | 0.96 | 0.18 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3614 | 1/1   | 0.96 | 0.18 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3062 | 1/1   | 0.96 | 0.19 | 46,46,46,46                 | 0     |
| 56  | MG   | YB    | 213  | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3337 | 1/1   | 0.96 | 0.11 | 7,7,7,7                     | 0     |
| 56  | MG   | XA    | 1737 | 1/1   | 0.96 | 0.04 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3618 | 1/1   | 0.96 | 0.09 | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3107 | 1/1   | 0.96 | 0.26 | 83,83,83,83                 | 0     |
| 56  | MG   | YA    | 3422 | 1/1   | 0.96 | 0.17 | 29,29,29,29                 | 0     |
| 56  | MG   | XA    | 1684 | 1/1   | 0.96 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3634 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3343 | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 56  | MG   | XA    | 1687 | 1/1   | 0.96 | 0.28 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3595 | 1/1   | 0.96 | 0.11 | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1640 | 1/1   | 0.96 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3042 | 1/1   | 0.96 | 0.04 | 45,45,45,45                 | 0     |
| 56  | MG   | RB    | 210  | 1/1   | 0.96 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3630 | 1/1   | 0.96 | 0.24 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3523 | 1/1   | 0.96 | 0.17 | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3430 | 1/1   | 0.96 | 0.05 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3526 | 1/1   | 0.96 | 0.12 | 18,18,18,18                 | 0     |
| 56  | MG   | XA    | 1693 | 1/1   | 0.96 | 0.24 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3433 | 1/1   | 0.96 | 0.09 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3353 | 1/1   | 0.96 | 0.17 | 3,3,3,3                     | 0     |
| 56  | MG   | YA    | 3184 | 1/1   | 0.96 | 0.10 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3532 | 1/1   | 0.96 | 0.10 | 22,22,22,22                 | 0     |
| 56  | MG   | QA    | 1716 | 1/1   | 0.96 | 0.05 | 73,73,73,73                 | 0     |
| 56  | MG   | YA    | 3356 | 1/1   | 0.96 | 0.15 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3357 | 1/1   | 0.96 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3527 | 1/1   | 0.96 | 0.30 | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3683 | 1/1   | 0.96 | 0.06 | 103,103,103,103             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | Y8    | 101  | 1/1   | 0.96 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3270 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3124 | 1/1   | 0.96 | 0.13 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3494 | 1/1   | 0.96 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3136 | 1/1   | 0.96 | 0.03 | 45,45,45,45                 | 0     |
| 56  | MG   | QV    | 103  | 1/1   | 0.96 | 0.08 | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3065 | 1/1   | 0.96 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3004 | 1/1   | 0.96 | 0.29 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3271 | 1/1   | 0.96 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1757 | 1/1   | 0.96 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3020 | 1/1   | 0.96 | 0.07 | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3371 | 1/1   | 0.96 | 0.20 | 29,29,29,29                 | 0     |
| 56  | MG   | RD    | 304  | 1/1   | 0.96 | 0.26 | 131,131,131,131             | 0     |
| 56  | MG   | YA    | 3458 | 1/1   | 0.97 | 0.08 | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1706 | 1/1   | 0.97 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3529 | 1/1   | 0.97 | 0.14 | 5,5,5,5                     | 0     |
| 56  | MG   | YA    | 3326 | 1/1   | 0.97 | 0.11 | 11,11,11,11                 | 0     |
| 56  | MG   | Y5    | 102  | 1/1   | 0.97 | 0.21 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3355 | 1/1   | 0.97 | 0.19 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3463 | 1/1   | 0.97 | 0.16 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3652 | 1/1   | 0.97 | 0.10 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3621 | 1/1   | 0.97 | 0.04 | 7,7,7,7                     | 0     |
| 56  | MG   | QT    | 201  | 1/1   | 0.97 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3266 | 1/1   | 0.97 | 0.17 | 31,31,31,31                 | 0     |
| 56  | MG   | QA    | 1690 | 1/1   | 0.97 | 0.09 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3539 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 56  | MG   | XA    | 1616 | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3144 | 1/1   | 0.97 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3312 | 1/1   | 0.97 | 0.13 | 7,7,7,7                     | 0     |
| 56  | MG   | YA    | 3207 | 1/1   | 0.97 | 0.14 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3701 | 1/1   | 0.97 | 0.07 | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3627 | 1/1   | 0.97 | 0.18 | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1732 | 1/1   | 0.97 | 0.11 | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1624 | 1/1   | 0.97 | 0.06 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3272 | 1/1   | 0.97 | 0.11 | 6,6,6,6                     | 0     |
| 56  | MG   | YA    | 3273 | 1/1   | 0.97 | 0.07 | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3009 | 1/1   | 0.97 | 0.08 | 8,8,8,8                     | 0     |
| 56  | MG   | XA    | 1734 | 1/1   | 0.97 | 0.18 | 46,46,46,46                 | 0     |
| 56  | MG   | QA    | 1709 | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1658 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | QA    | 1751 | 1/1   | 0.97 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1697 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3217 | 1/1   | 0.97 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3637 | 1/1   | 0.97 | 0.11 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3638 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 56  | MG   | RR    | 202  | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | RT    | 201  | 1/1   | 0.97 | 0.13 | 47,47,47,47                 | 0     |
| 56  | MG   | QA    | 1732 | 1/1   | 0.97 | 0.11 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3488 | 1/1   | 0.97 | 0.15 | 24,24,24,24                 | 0     |
| 56  | MG   | QA    | 1765 | 1/1   | 0.97 | 0.06 | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3021 | 1/1   | 0.97 | 0.18 | 87,87,87,87                 | 0     |
| 56  | MG   | QB    | 301  | 1/1   | 0.97 | 0.06 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3646 | 1/1   | 0.97 | 0.13 | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1704 | 1/1   | 0.97 | 0.08 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3172 | 1/1   | 0.97 | 0.10 | 88,88,88,88                 | 0     |
| 56  | MG   | YB    | 220  | 1/1   | 0.97 | 0.15 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3227 | 1/1   | 0.97 | 0.10 | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3650 | 1/1   | 0.97 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1742 | 1/1   | 0.97 | 0.14 | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3497 | 1/1   | 0.97 | 0.14 | 17,17,17,17                 | 0     |
| 56  | MG   | QA    | 1794 | 1/1   | 0.97 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1631 | 1/1   | 0.97 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1793 | 1/1   | 0.97 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | QA    | 1672 | 1/1   | 0.97 | 0.05 | 54,54,54,54                 | 0     |
| 56  | MG   | QA    | 1734 | 1/1   | 0.97 | 0.05 | 46,46,46,46                 | 0     |
| 56  | MG   | YE    | 304  | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3521 | 1/1   | 0.97 | 0.24 | 42,42,42,42                 | 0     |
| 56  | MG   | XF    | 202  | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3549 | 1/1   | 0.97 | 0.15 | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3661 | 1/1   | 0.97 | 0.24 | 38,38,38,38                 | 0     |
| 56  | MG   | XL    | 201  | 1/1   | 0.97 | 0.04 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3240 | 1/1   | 0.97 | 0.15 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3241 | 1/1   | 0.97 | 0.05 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3665 | 1/1   | 0.97 | 0.10 | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3522 | 1/1   | 0.97 | 0.12 | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3240 | 1/1   | 0.97 | 0.11 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3396 | 1/1   | 0.97 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | XA    | 1639 | 1/1   | 0.97 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3246 | 1/1   | 0.97 | 0.19 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3187 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3315 | 1/1   | 0.97 | 0.18 | 3,3,3,3                     | 0     |
| 56  | MG   | RA    | 3325 | 1/1   | 0.97 | 0.11 | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3241 | 1/1   | 0.97 | 0.14 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3190 | 1/1   | 0.97 | 0.17 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3251 | 1/1   | 0.97 | 0.14 | 16,16,16,16                 | 0     |
| 56  | MG   | QA    | 1683 | 1/1   | 0.97 | 0.17 | 37,37,37,37                 | 0     |
| 56  | MG   | QA    | 1712 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | YW    | 202  | 1/1   | 0.97 | 0.04 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3599 | 1/1   | 0.97 | 0.32 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3600 | 1/1   | 0.97 | 0.19 | 2,2,2,2                     | 0     |
| 58  | SF4  | QD    | 302  | 8/8   | 0.97 | 0.08 | 54,93,149,174               | 0     |
| 56  | MG   | YA    | 3524 | 1/1   | 0.97 | 0.08 | 6,6,6,6                     | 0     |
| 56  | MG   | QA    | 1758 | 1/1   | 0.97 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | Y1    | 102  | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 59  | ZN   | YY    | 201  | 1/1   | 0.97 | 0.05 | 99,99,99,99                 | 0     |
| 56  | MG   | YA    | 3260 | 1/1   | 0.98 | 0.06 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3553 | 1/1   | 0.98 | 0.07 | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3204 | 1/1   | 0.98 | 0.07 | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3609 | 1/1   | 0.98 | 0.11 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3294 | 1/1   | 0.98 | 0.10 | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3232 | 1/1   | 0.98 | 0.10 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3333 | 1/1   | 0.98 | 0.10 | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3558 | 1/1   | 0.98 | 0.11 | 9,9,9,9                     | 0     |
| 56  | MG   | YA    | 3334 | 1/1   | 0.98 | 0.08 | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3304 | 1/1   | 0.98 | 0.06 | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3489 | 1/1   | 0.98 | 0.05 | 4,4,4,4                     | 0     |
| 56  | MG   | YB    | 217  | 1/1   | 0.98 | 0.10 | 8,8,8,8                     | 0     |
| 56  | MG   | RA    | 3280 | 1/1   | 0.98 | 0.10 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3236 | 1/1   | 0.98 | 0.15 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1620 | 1/1   | 0.98 | 0.03 | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3340 | 1/1   | 0.98 | 0.10 | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3341 | 1/1   | 0.98 | 0.09 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3568 | 1/1   | 0.98 | 0.09 | 21,21,21,21                 | 0     |
| 56  | MG   | XA    | 1776 | 1/1   | 0.98 | 0.25 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3439 | 1/1   | 0.98 | 0.12 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3033 | 1/1   | 0.98 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3305 | 1/1   | 0.98 | 0.06 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3346 | 1/1   | 0.98 | 0.08 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3521 | 1/1   | 0.98 | 0.10 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3133 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | XA    | 1754 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3338 | 1/1   | 0.98 | 0.08 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3276 | 1/1   | 0.98 | 0.16 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3435 | 1/1   | 0.98 | 0.08 | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3275 | 1/1   | 0.98 | 0.09 | 8,8,8,8                     | 0     |
| 56  | MG   | RA    | 3600 | 1/1   | 0.98 | 0.12 | 13,13,13,13                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3674 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3636 | 1/1   | 0.98 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3314 | 1/1   | 0.98 | 0.14 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3485 | 1/1   | 0.98 | 0.12 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3618 | 1/1   | 0.98 | 0.10 | 21,21,21,21                 | 0     |
| 56  | MG   | QA    | 1722 | 1/1   | 0.98 | 0.14 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3090 | 1/1   | 0.98 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3431 | 1/1   | 0.98 | 0.25 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3316 | 1/1   | 0.98 | 0.18 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3005 | 1/1   | 0.98 | 0.21 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3285 | 1/1   | 0.98 | 0.09 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3448 | 1/1   | 0.98 | 0.13 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3541 | 1/1   | 0.98 | 0.12 | 11,11,11,11                 | 0     |
| 56  | MG   | RA    | 3681 | 1/1   | 0.98 | 0.05 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3323 | 1/1   | 0.98 | 0.12 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3352 | 1/1   | 0.98 | 0.04 | 20,20,20,20                 | 0     |
| 56  | MG   | YA    | 3545 | 1/1   | 0.98 | 0.04 | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3447 | 1/1   | 0.98 | 0.13 | 11,11,11,11                 | 0     |
| 56  | MG   | QA    | 1785 | 1/1   | 0.98 | 0.06 | 74,74,74,74                 | 0     |
| 58  | SF4  | XD    | 301  | 8/8   | 0.98 | 0.07 | 64,74,104,108               | 0     |
| 59  | ZN   | QN    | 101  | 1/1   | 0.98 | 0.07 | 200,200,200,200             | 0     |
| 56  | MG   | YA    | 3602 | 1/1   | 0.98 | 0.26 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3410 | 1/1   | 0.98 | 0.08 | 37,37,37,37                 | 0     |
| 59  | ZN   | XN    | 101  | 1/1   | 0.98 | 0.06 | 114,114,114,114             | 0     |
| 56  | MG   | RA    | 3558 | 1/1   | 0.98 | 0.06 | 32,32,32,32                 | 0     |
| 59  | ZN   | Y5    | 101  | 1/1   | 0.98 | 0.04 | 88,88,88,88                 | 0     |
| 59  | ZN   | Y9    | 101  | 1/1   | 0.98 | 0.03 | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3559 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3018 | 1/1   | 0.99 | 0.05 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3304 | 1/1   | 0.99 | 0.21 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3518 | 1/1   | 0.99 | 0.03 | 10,10,10,10                 | 0     |
| 56  | MG   | RB    | 211  | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 56  | MG   | QA    | 1822 | 1/1   | 0.99 | 0.03 | 62,62,62,62                 | 0     |
| 56  | MG   | QA    | 1626 | 1/1   | 0.99 | 0.10 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3601 | 1/1   | 0.99 | 0.19 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3559 | 1/1   | 0.99 | 0.04 | 9,9,9,9                     | 0     |
| 56  | MG   | RE    | 304  | 1/1   | 0.99 | 0.07 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3619 | 1/1   | 0.99 | 0.05 | 9,9,9,9                     | 0     |
| 56  | MG   | XA    | 1760 | 1/1   | 0.99 | 0.25 | 35,35,35,35                 | 0     |
| 59  | ZN   | R5    | 101  | 1/1   | 0.99 | 0.05 | 126,126,126,126             | 0     |
| 59  | ZN   | R6    | 101  | 1/1   | 0.99 | 0.03 | 71,71,71,71                 | 0     |
| 56  | MG   | RA    | 3362 | 1/1   | 0.99 | 0.06 | 17,17,17,17                 | 0     |

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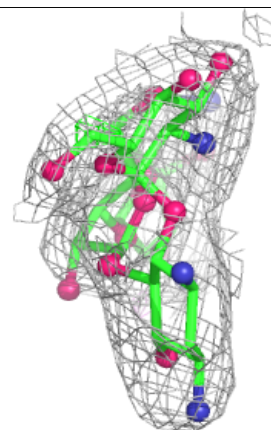
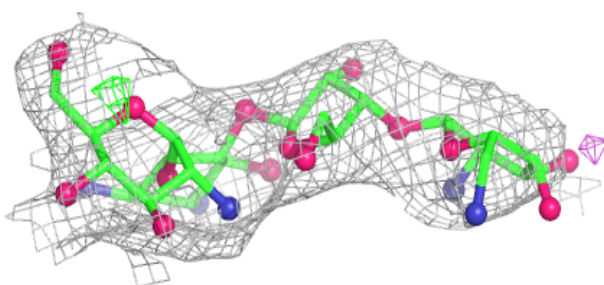
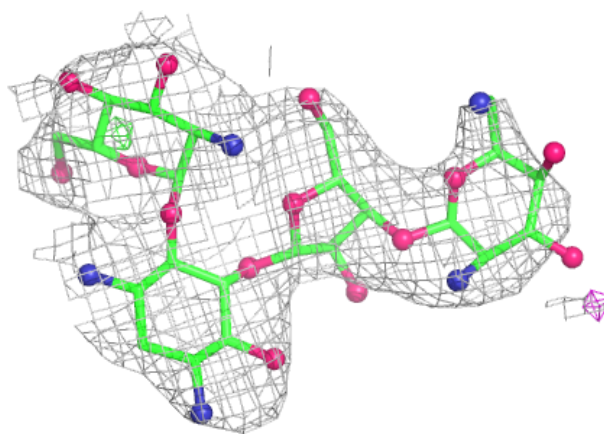
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3549 | 1/1   | 0.99 | 0.31 | 44,44,44,44                 | 0     |
| 56  | MG   | YE    | 301  | 1/1   | 0.99 | 0.11 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3381 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 59  | ZN   | Y6    | 101  | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3567 | 1/1   | 0.99 | 0.10 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3122 | 1/1   | 0.99 | 0.04 | 36,36,36,36                 | 0     |
| 59  | ZN   | R9    | 101  | 1/1   | 1.00 | 0.02 | 90,90,90,90                 | 0     |

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

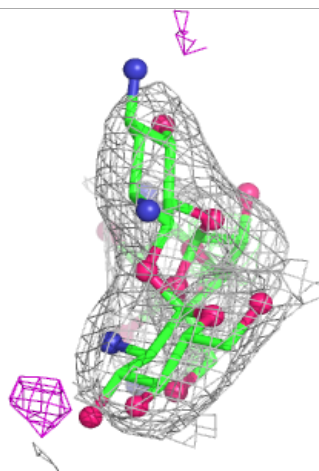
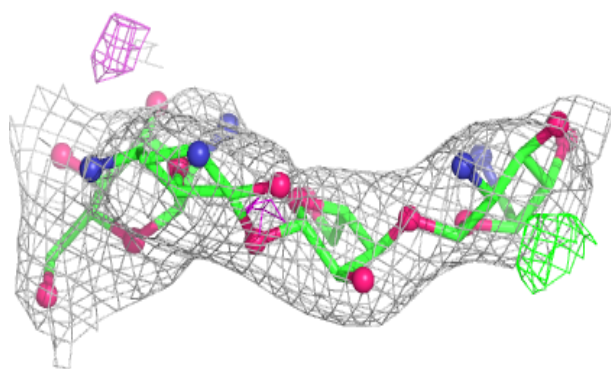
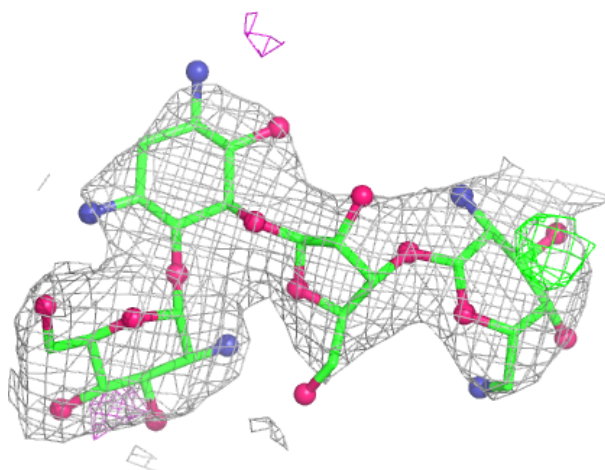
**Electron density around PAR QA 1821:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR XA 1794:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.