



## Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 06:00 PM JST

PDB ID : 8JDJ / pdb\_00008j dj  
EMDB ID : EMD-36178  
Title : Structure of the Human cytoplasmic Ribosome with human tRNA Asp(Q34) and mRNA(GAU)  
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.  
Deposited on : 2023-05-14  
Resolution : 2.50 Å(reported)  
Based on initial model : 6Y0G

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

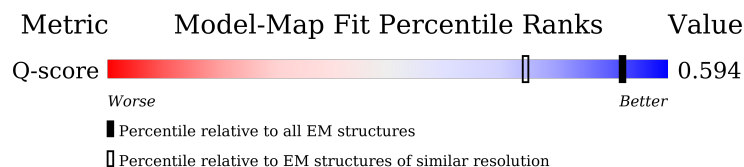
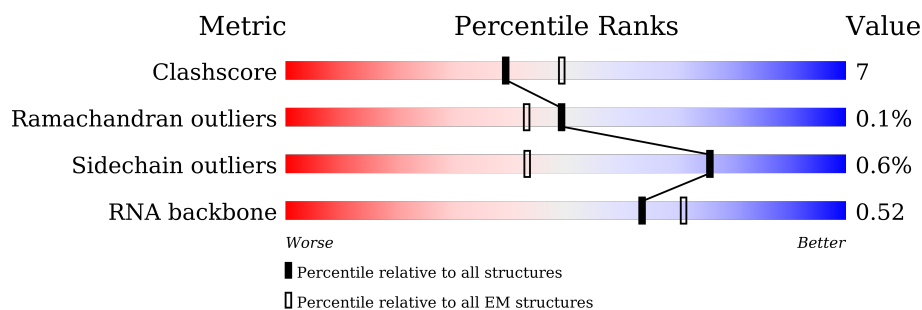
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 7115 ( 2.00 - 3.00 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 14     |                  |
| 2   | B     | 75     |                  |
| 2   | C     | 75     |                  |

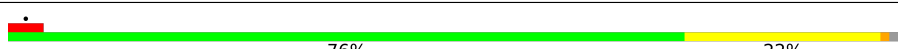
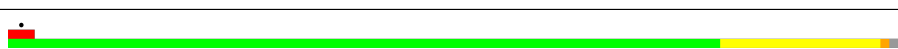
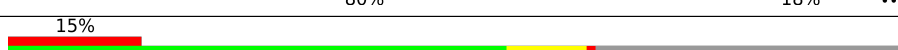
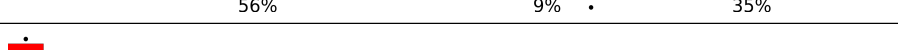
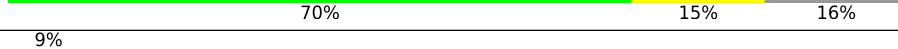
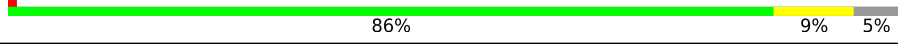
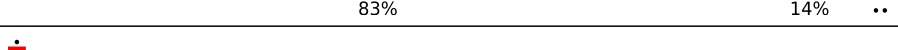
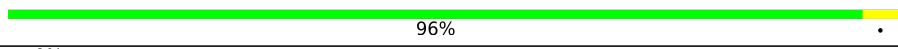
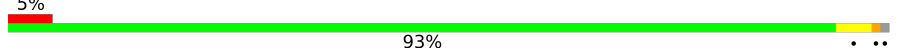
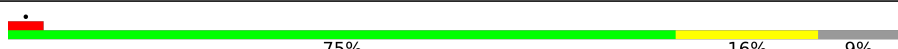
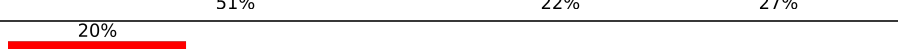
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | D     | 5070   |                  |
| 4   | E     | 120    |                  |
| 5   | F     | 156    |                  |
| 6   | G     | 257    |                  |
| 7   | H     | 403    |                  |
| 8   | I     | 427    |                  |
| 9   | J     | 297    |                  |
| 10  | K     | 288    |                  |
| 11  | L     | 248    |                  |
| 12  | M     | 266    |                  |
| 13  | N     | 192    |                  |
| 14  | O     | 214    |                  |
| 15  | P     | 178    |                  |
| 16  | Q     | 211    |                  |
| 17  | R     | 215    |                  |
| 18  | S     | 204    |                  |
| 19  | T     | 203    |                  |
| 20  | U     | 184    |                  |
| 21  | V     | 188    |                  |
| 22  | W     | 196    |                  |
| 23  | X     | 176    |                  |
| 24  | Y     | 160    |                  |
| 25  | Z     | 128    |                  |
| 26  | a     | 140    |                  |
| 27  | b     | 157    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | c     | 156    |    |
| 29  | d     | 145    |    |
| 30  | e     | 136    |    |
| 31  | f     | 148    |    |
| 32  | g     | 159    |    |
| 33  | h     | 115    |    |
| 34  | i     | 125    |    |
| 35  | j     | 135    |    |
| 36  | k     | 110    |    |
| 37  | l     | 117    |    |
| 38  | m     | 123    |    |
| 39  | n     | 105    |    |
| 40  | o     | 97     |   |
| 41  | p     | 70     |  |
| 42  | q     | 51     |  |
| 43  | r     | 128    |  |
| 44  | s     | 25     |  |
| 45  | t     | 106    |  |
| 46  | u     | 92     |  |
| 47  | v     | 137    |  |
| 48  | w     | 1869   |  |
| 49  | x     | 295    |  |
| 50  | y     | 264    |  |
| 51  | z     | 293    |  |
| 52  | 0     | 243    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | 1     | 263    |                  |
| 54  | 2     | 204    |                  |
| 55  | 3     | 249    |                  |
| 56  | 4     | 194    |                  |
| 57  | 5     | 208    |                  |
| 58  | 6     | 194    |                  |
| 59  | 7     | 165    |                  |
| 60  | 8     | 158    |                  |
| 61  | 9     | 151    |                  |
| 62  | AA    | 151    |                  |
| 63  | AB    | 145    |                  |
| 64  | AC    | 146    |                  |
| 65  | AD    | 135    |                  |
| 66  | AE    | 152    |                  |
| 67  | AF    | 145    |                  |
| 68  | AG    | 119    |                  |
| 69  | AH    | 83     |                  |
| 70  | AI    | 130    |                  |
| 71  | AJ    | 143    |                  |
| 72  | AK    | 133    |                  |
| 73  | AL    | 125    |                  |
| 74  | AM    | 115    |                  |
| 75  | AN    | 84     |                  |
| 76  | AO    | 69     |                  |
| 77  | AP    | 56     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                               |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------|
| 78  | AQ    | 59     | <div><div></div><div>73%</div><div></div><div>76%</div><div></div><div>20%</div><div></div><div>.</div></div>  |
| 79  | AR    | 317    | <div><div></div><div>87%</div><div></div><div>56%</div><div></div><div>43%</div><div></div><div>..</div></div> |

## 2 Entry composition [i](#)

There are 81 unique types of molecules in this entry. The entry contains 209545 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 1   | A     | 14       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 303   | 135 | 55 | 99 | 14 |         |       |

- Molecule 2 is a RNA chain called tRNA(Asp).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | B     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1612  | 726 | 283 | 529 | 74 |         |       |
| 2   | C     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1612  | 726 | 283 | 529 | 74 |         |       |

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | D     | 3512     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 75336 | 33585 | 13757 | 24482 | 3512 |         |       |

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | E     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 5 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5   | F     | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3315  | 1481 | 585 | 1094 | 155 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | G     | 247      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1891  | 1185 | 388 | 312 | 6 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | H     | 398      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3211  | 2045 | 604 | 548 | 14 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | I     | 363      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2884  | 1815 | 577 | 478 | 14 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | J     | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2379  | 1506 | 434 | 425 | 14 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | K     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1751  | 1128 | 332 | 287 | 4 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | L     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | M     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1832  | 1168 | 352 | 308 | 4 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | N     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L10-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | O     | 206      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1660  | 1053 | 319 | 275 | 13 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | P     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1362  | 861 | 254 | 241 | 6 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | Q     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1052 | 348 | 278 | 4 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | R     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1120  | 719 | 215 | 179 | 7 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | S     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | T     | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1641  | 1058 | 320 | 258 | 5 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | U     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1273  | 797 | 246 | 221 | 9 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | V     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | W     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 933 | 328 | 238 | 9 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | X     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Y     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Z     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 526 | 143 | 150 | 2 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | a     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | b     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 528   | 337 | 103 | 85 | 3 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 628 | 185 | 167 | 1 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 515 | 182 | 132 | 3 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 755   | 479 | 133 | 137 | 6 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | j     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | k     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | l     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 555 | 183 | 144 | 6 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | m     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1010  | 638 | 204 | 167 | 1 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | n     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 41  | p     | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | q     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | r     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | s     | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | t     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | u     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | v     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 48  | w     | 1634     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 34933 | 15622 | 6267 | 11411 | 1633 |         |       |

- Molecule 49 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | x     | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1077 | 297 | 313 | 8 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | y     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1096 | 308 | 307 | 14 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | z     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1633  | 1059 | 279 | 285 | 10 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | 0     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1646  | 1050 | 299 | 290 | 7 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | 1     | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2070  | 1321 | 383 | 358 | 8 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | 2     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1464  | 916 | 276 | 265 | 7 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | 3     | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1917  | 1197 | 384 | 329 | 7 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | 4     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1510  | 963 | 278 | 268 | 1 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | 5     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1674  | 1049 | 329 | 291 | 5 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | 6     | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 959 | 300 | 245 | 2 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | 7     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 530 | 143 | 131 | 6 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | 8     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1150  | 732 | 215 | 197 | 6 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | 9     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | AA    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 612 | 197 | 187 | 6 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | AB    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1103  | 703 | 208 | 185 | 7 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | AC    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 717 | 213 | 195 | 3 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | AD    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1057  | 665 | 197 | 191 | 4 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | AE    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1169  | 731 | 236 | 201 | 1 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | AF    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 696 | 213 | 198 | 4 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | AG    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 501 | 153 | 141 | 4 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | AH    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | AI    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | AJ    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | AK    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 634 | 196 | 167 | 5 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | AL    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 680   | 436 | 127 | 116 | 1 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | AM    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | AN    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 402 | 119 | 115 | 7 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 76  | AO    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 479   | 292 | 95 | 90 | 2 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 77  | AP    | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 370   | 228 | 77 | 60 | 5 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78  | AQ    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 279 | 99 | 73 | 1 |         |       |

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 79  | AR    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 80  | A     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 80  | D     | 398      | Total | Mg  | 0       |
|     |       |          | 398   | 398 |         |
| 80  | E     | 10       | Total | Mg  | 0       |
|     |       |          | 10    | 10  |         |
| 80  | F     | 6        | Total | Mg  | 0       |
|     |       |          | 6     | 6   |         |
| 80  | G     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 80  | H     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 80  | I     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 80  | N     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 80  | O     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |

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| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 80  | S     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | U     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 80  | V     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 80  | X     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | a     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | g     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | j     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | k     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | l     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | u     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | w     | 103      | Total<br>103 | Mg<br>103 | 0       |
| 80  | AA    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 80  | AF    | 1        | Total<br>1   | Mg<br>1   | 0       |

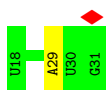
- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 81  | o     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 81  | r     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 81  | t     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 81  | u     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 81  | AM    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 81  | AP    | 1        | Total<br>1 | Zn<br>1 | 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

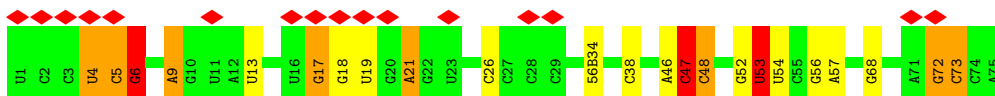
- Molecule 1: mRNA



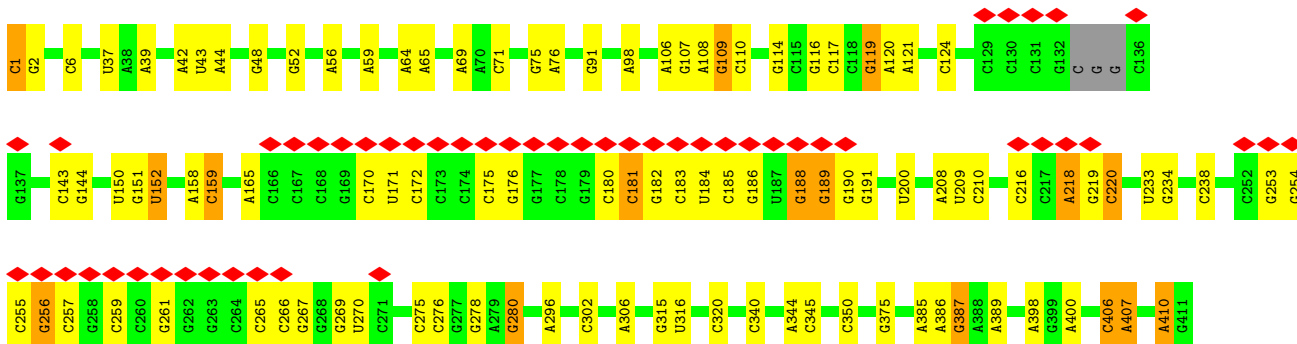
- Molecule 2: tRNA(Asp)

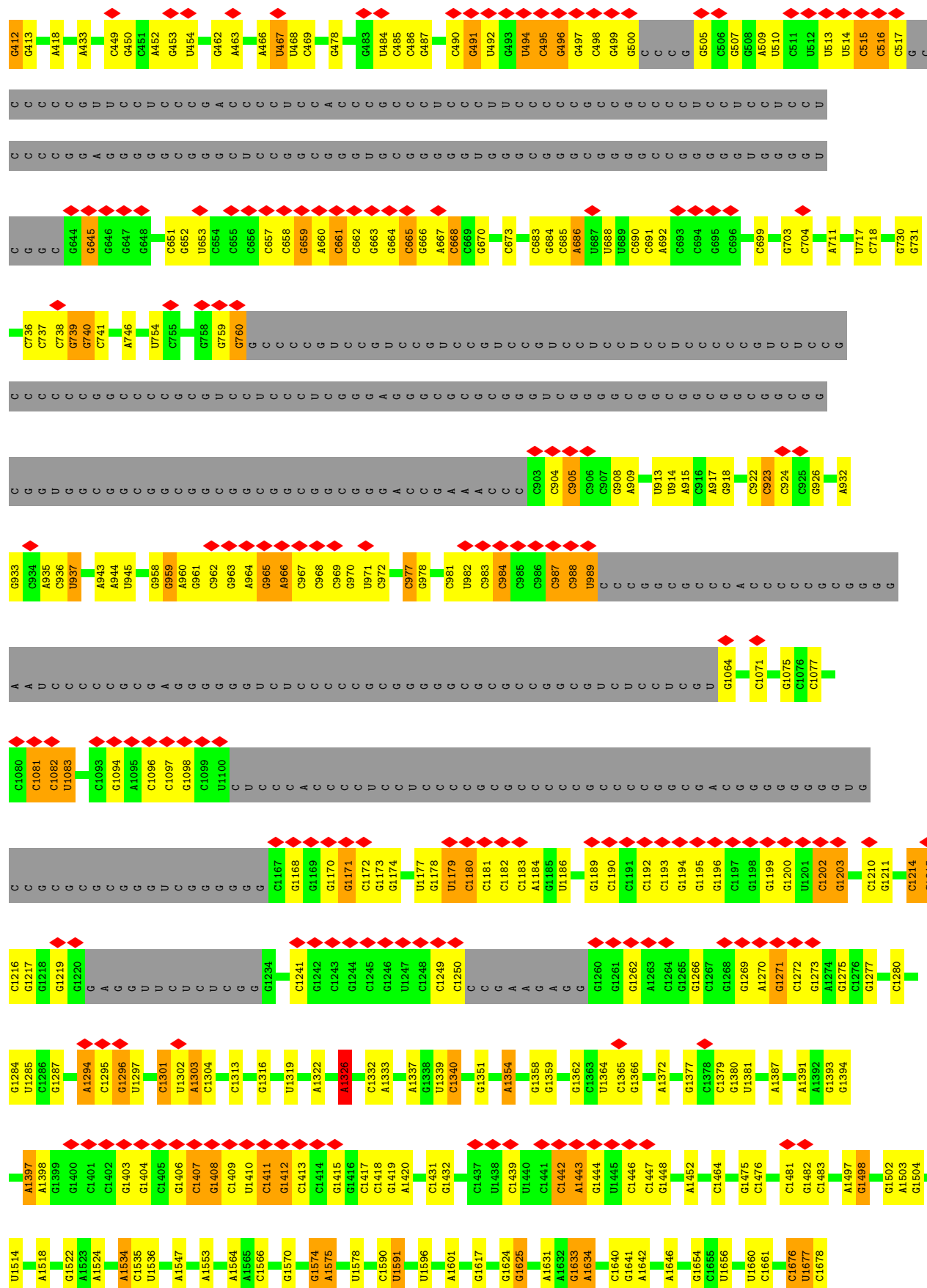


- Molecule 2: tRNA(Asp)



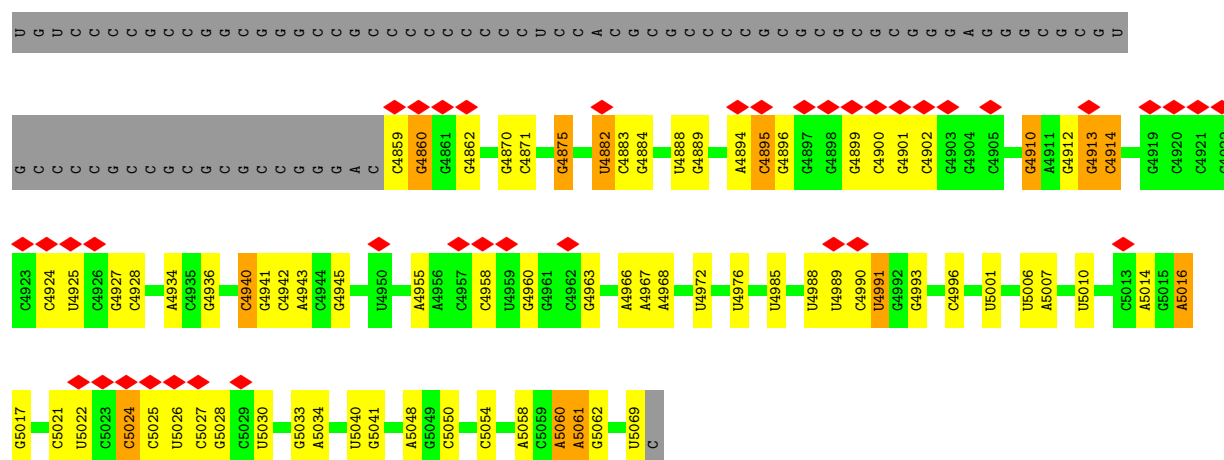
- Molecule 3: 28S ribosomal RNA



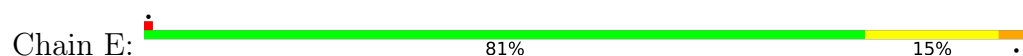




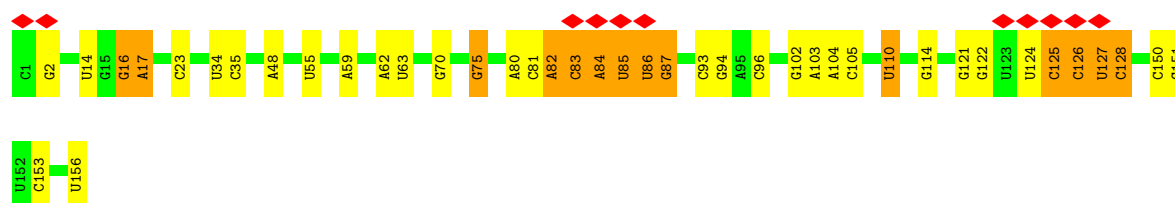




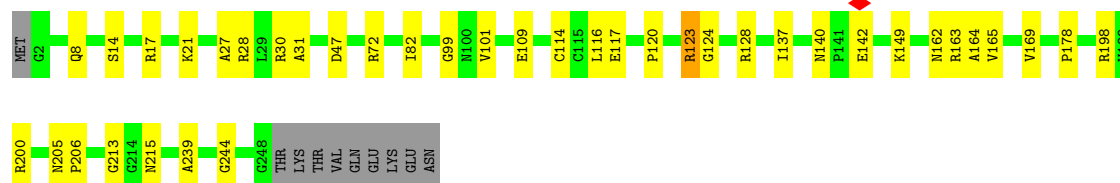
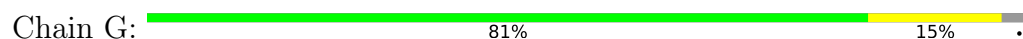
• Molecule 4: 5S ribosomal RNA



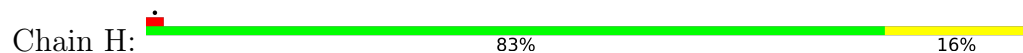
• Molecule 5: 5.8S ribosomal RNA

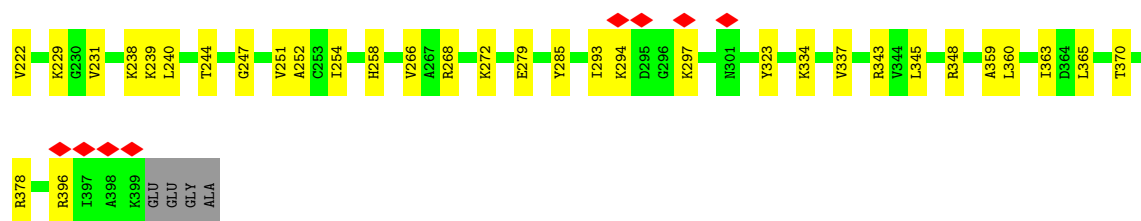


• Molecule 6: 60S ribosomal protein L8



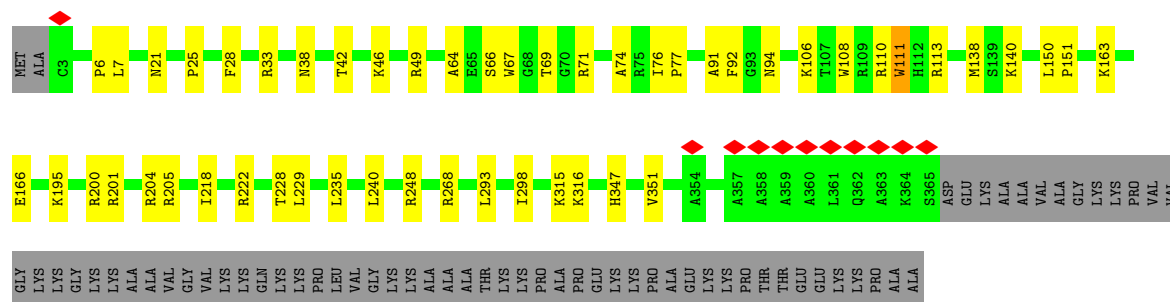
• Molecule 7: 60S ribosomal protein L3





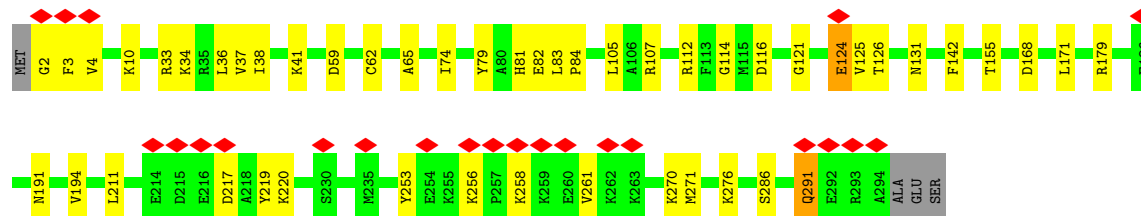
• Molecule 8: 60S ribosomal protein L4

Chain I: 73% 12% 15%



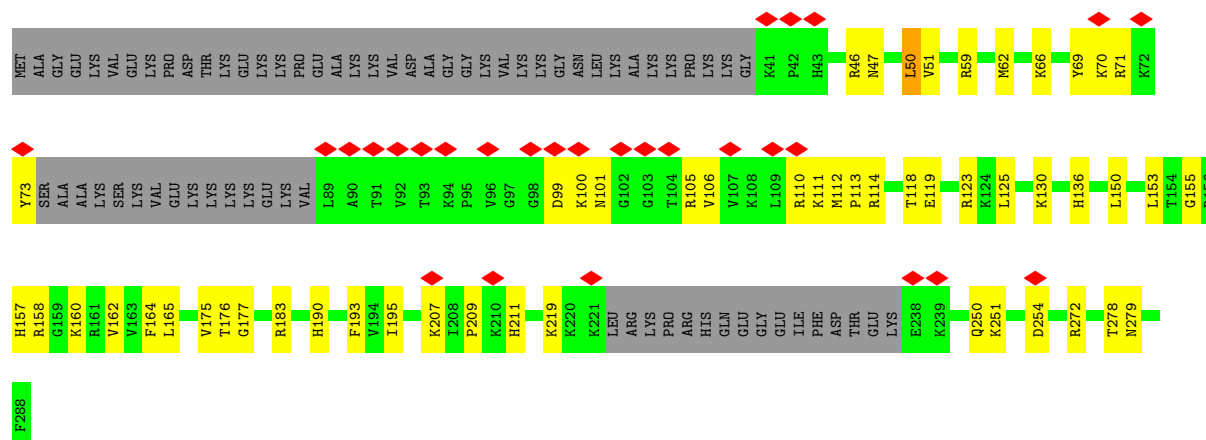
• Molecule 9: 60S ribosomal protein L5

Chain J: 8% 82% 16% ..

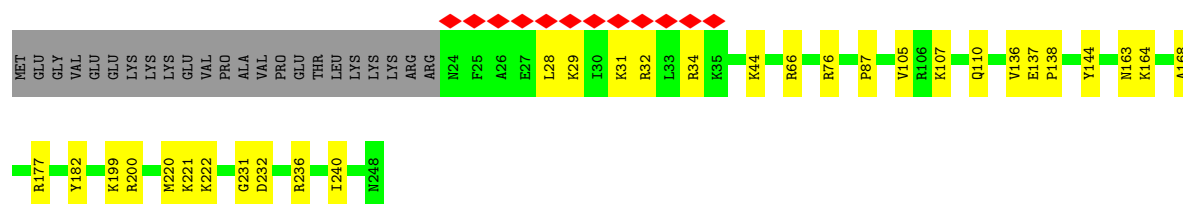
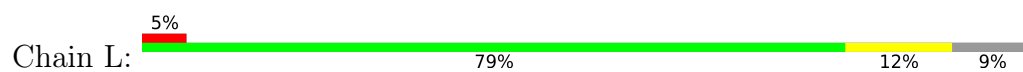


• Molecule 10: 60S ribosomal protein L6

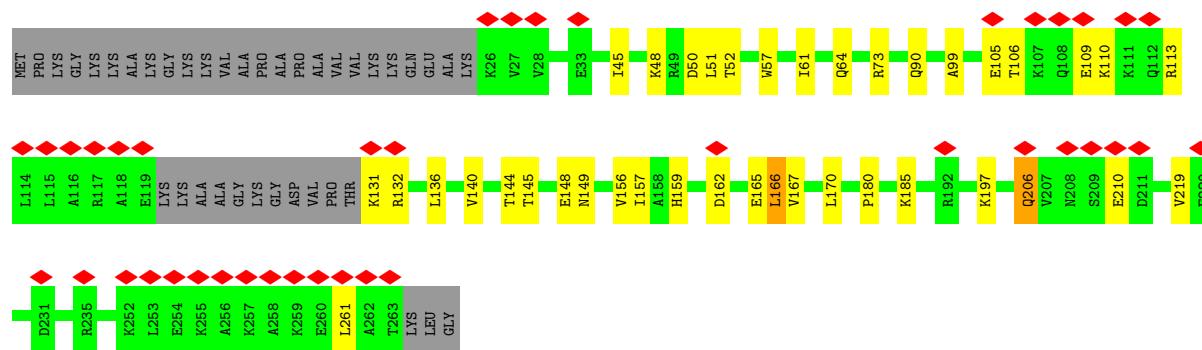
Chain K: 10% 57% 18% 25%



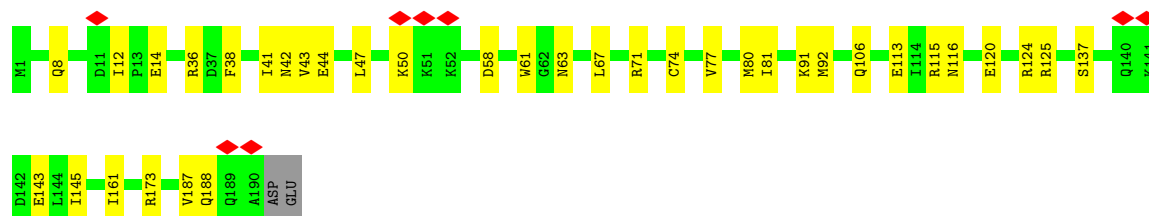
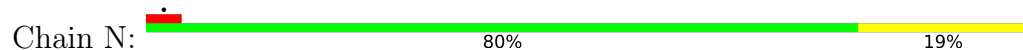
• Molecule 11: 60S ribosomal protein L7



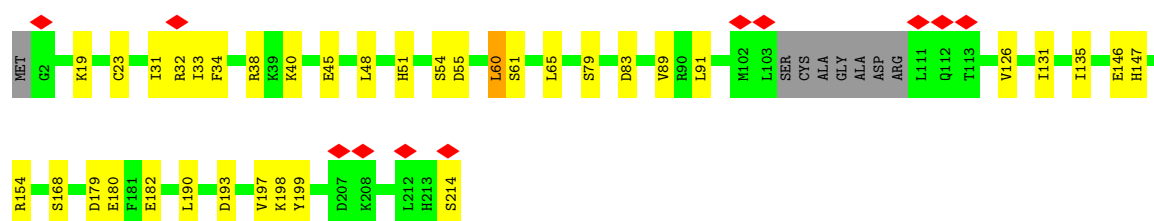
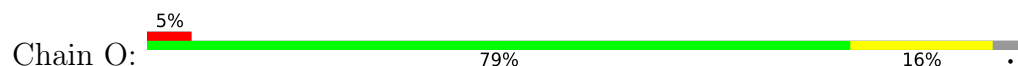
- Molecule 12: 60S ribosomal protein L7a



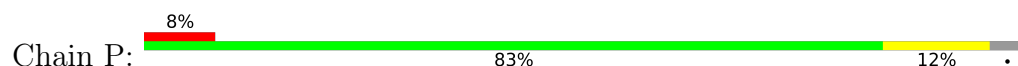
- Molecule 13: 60S ribosomal protein L9

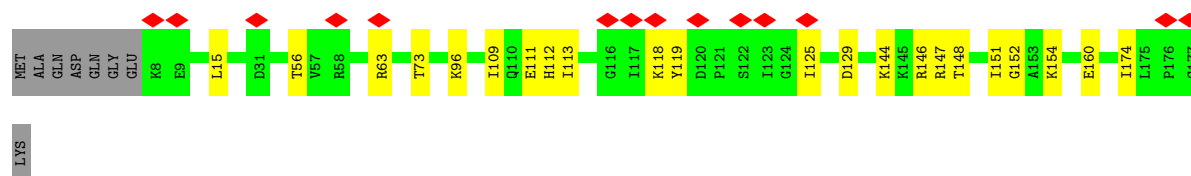


- Molecule 14: 60S ribosomal protein L10-like

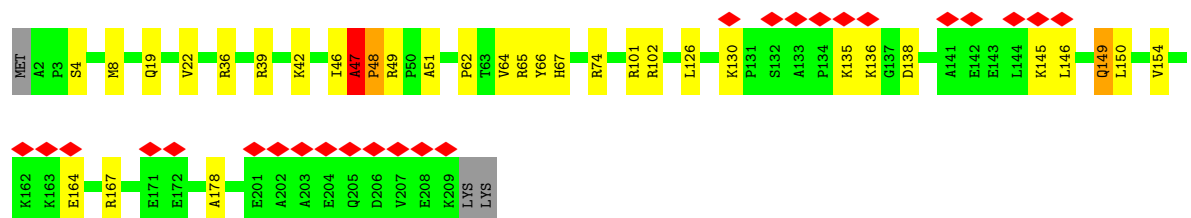
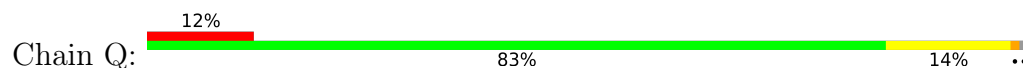


- Molecule 15: 60S ribosomal protein L11

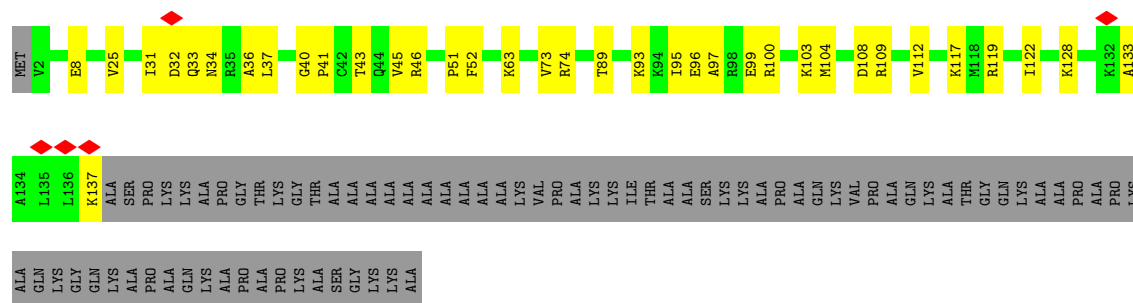




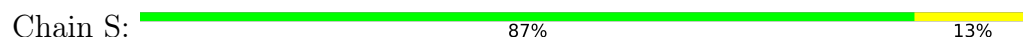
- Molecule 16: 60S ribosomal protein L13



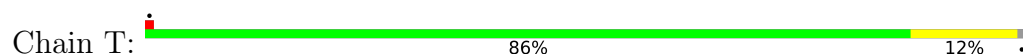
- Molecule 17: 60S ribosomal protein L14



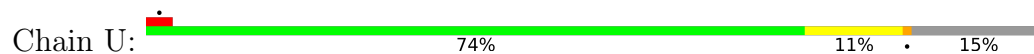
- Molecule 18: 60S ribosomal protein L15

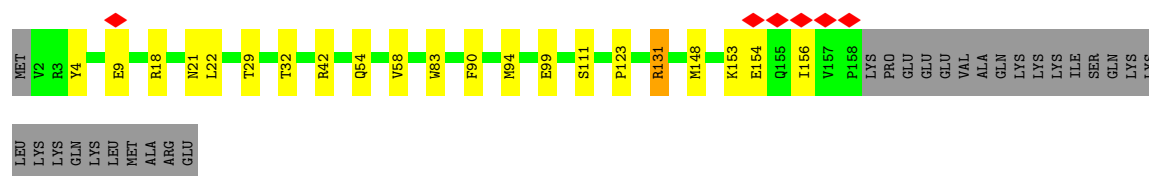


- Molecule 19: 60S ribosomal protein L13a

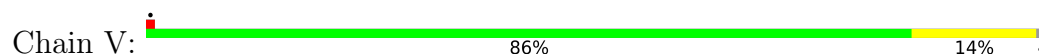


- Molecule 20: 60S ribosomal protein L17

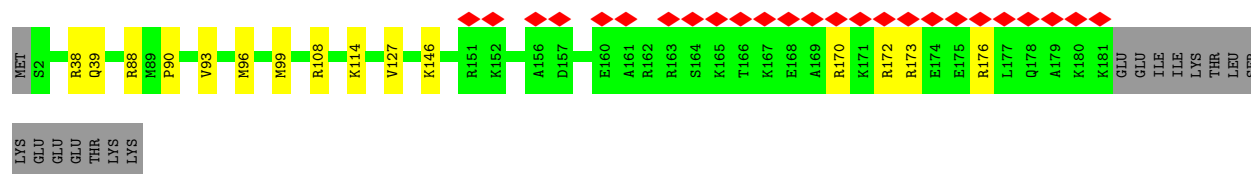
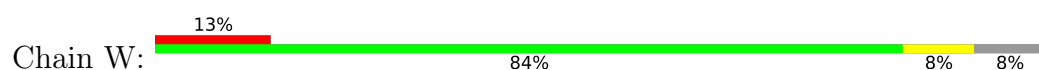




- Molecule 21: 60S ribosomal protein L18



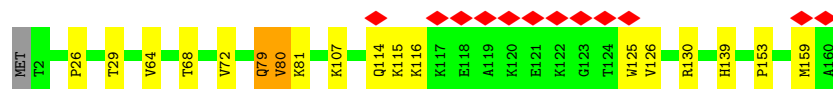
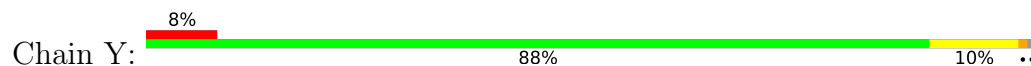
- Molecule 22: 60S ribosomal protein L19



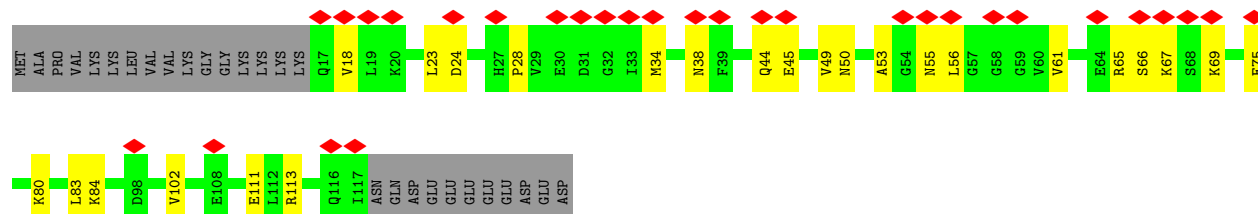
- Molecule 23: 60S ribosomal protein L18a



- Molecule 24: 60S ribosomal protein L21



- Molecule 25: 60S ribosomal protein L22



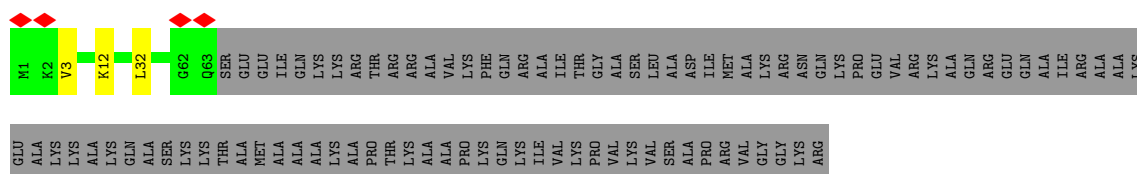
- Molecule 26: 60S ribosomal protein L23

Chain a:  86% 7% 6%



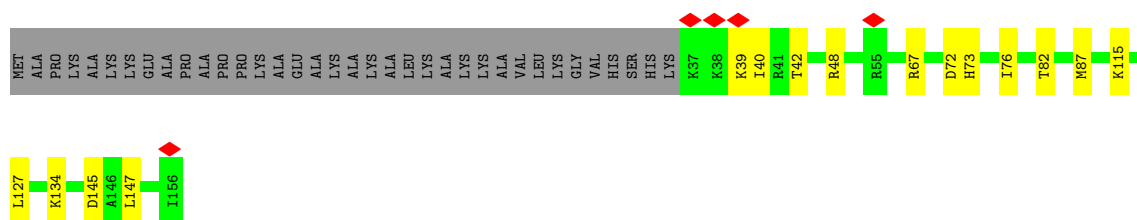
- Molecule 27: 60S ribosomal protein L24

Chain b:  38% 60%



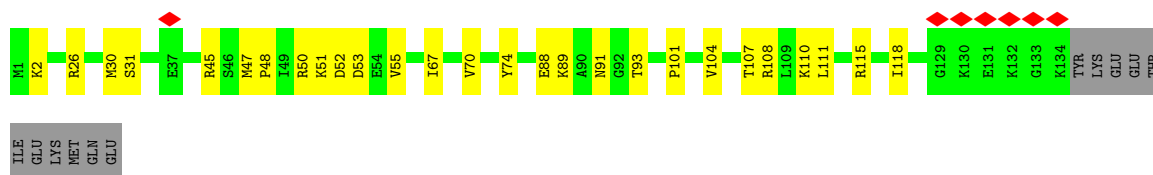
- Molecule 28: 60S ribosomal protein L23a

Chain c:  67% 10% 23%



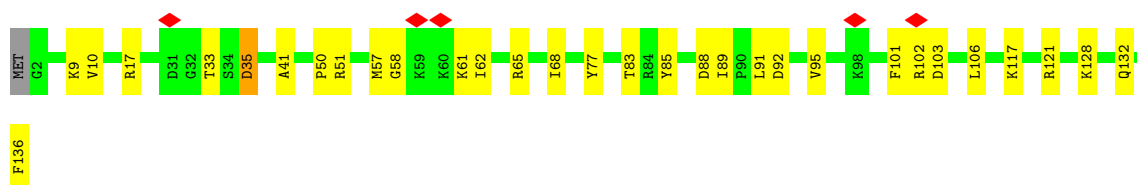
- Molecule 29: 60S ribosomal protein L26

Chain d:  5% 74% 19% 8%



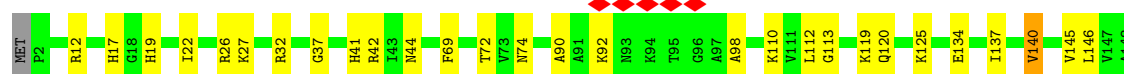
- Molecule 30: 60S ribosomal protein L27

Chain e:  76% 22% ..



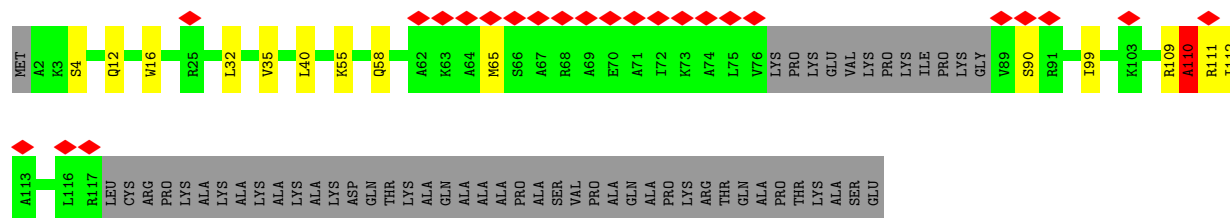
- Molecule 31: 60S ribosomal protein L27a

Chain f:  80% 18% ..



- Molecule 32: 60S ribosomal protein L29

Chain g:  15% 56% 9% . 35%



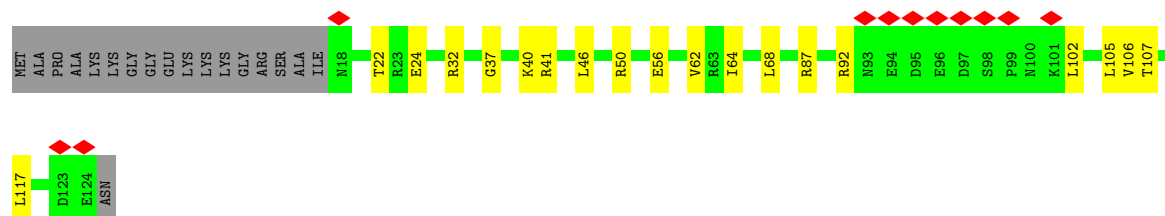
- Molecule 33: 60S ribosomal protein L30

Chain h:  70% 15% 16%



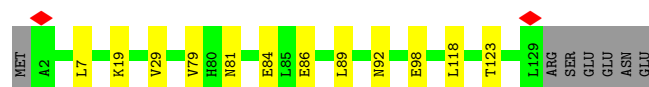
- Molecule 34: 60S ribosomal protein L31

Chain i:  9% 70% 15% 14%



- Molecule 35: 60S ribosomal protein L32

Chain j:  86% 9% 5%

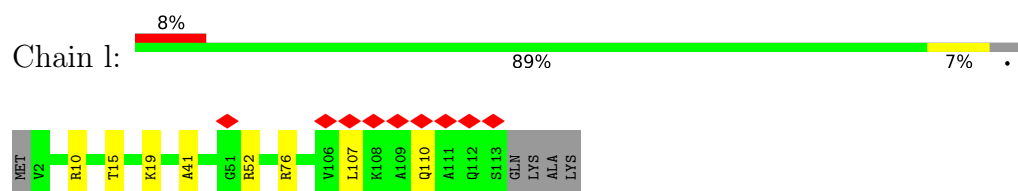


- Molecule 36: 60S ribosomal protein L35a

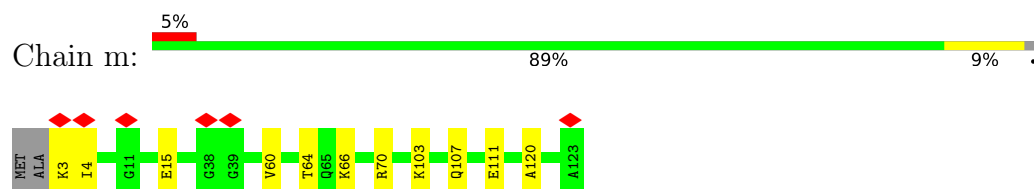
Chain k:  82% 17% .



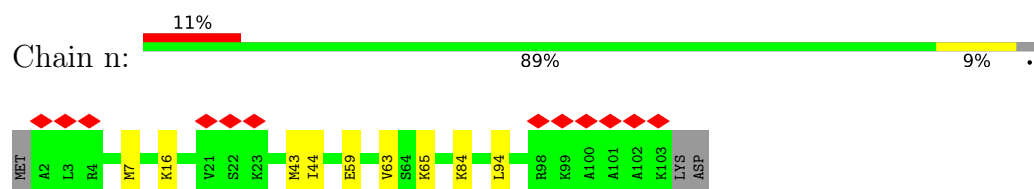
- Molecule 37: 60S ribosomal protein L34



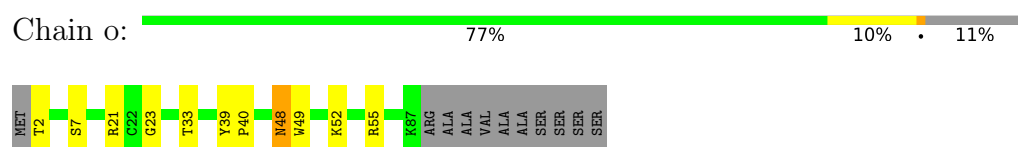
- Molecule 38: 60S ribosomal protein L35



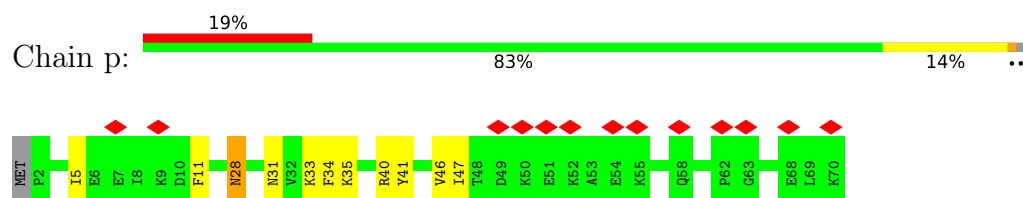
- Molecule 39: 60S ribosomal protein L36



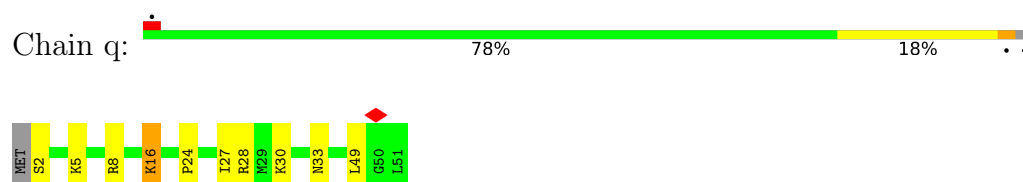
- Molecule 40: 60S ribosomal protein L37



- Molecule 41: 60S ribosomal protein L38

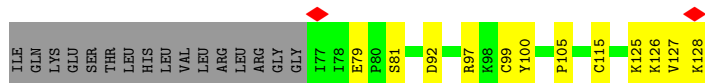


- Molecule 42: 60S ribosomal protein L39

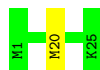


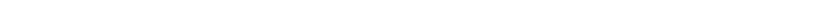
- Molecule 43: Ubiquitin-60S ribosomal protein L40

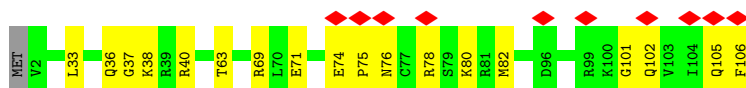




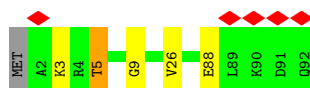
- Chain s:  96% .



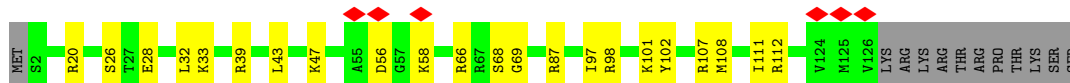
- Chain t: 



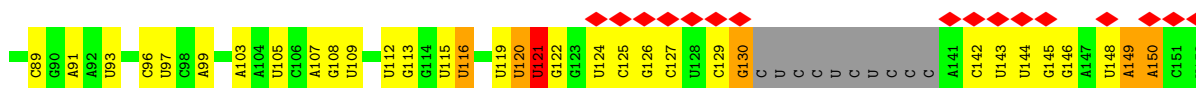
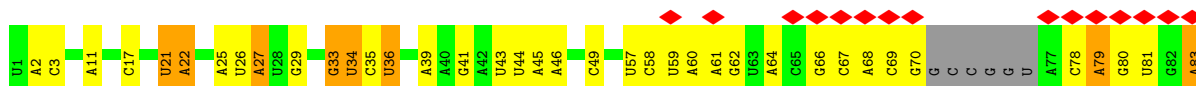
- Chain u:  5% 93% ...



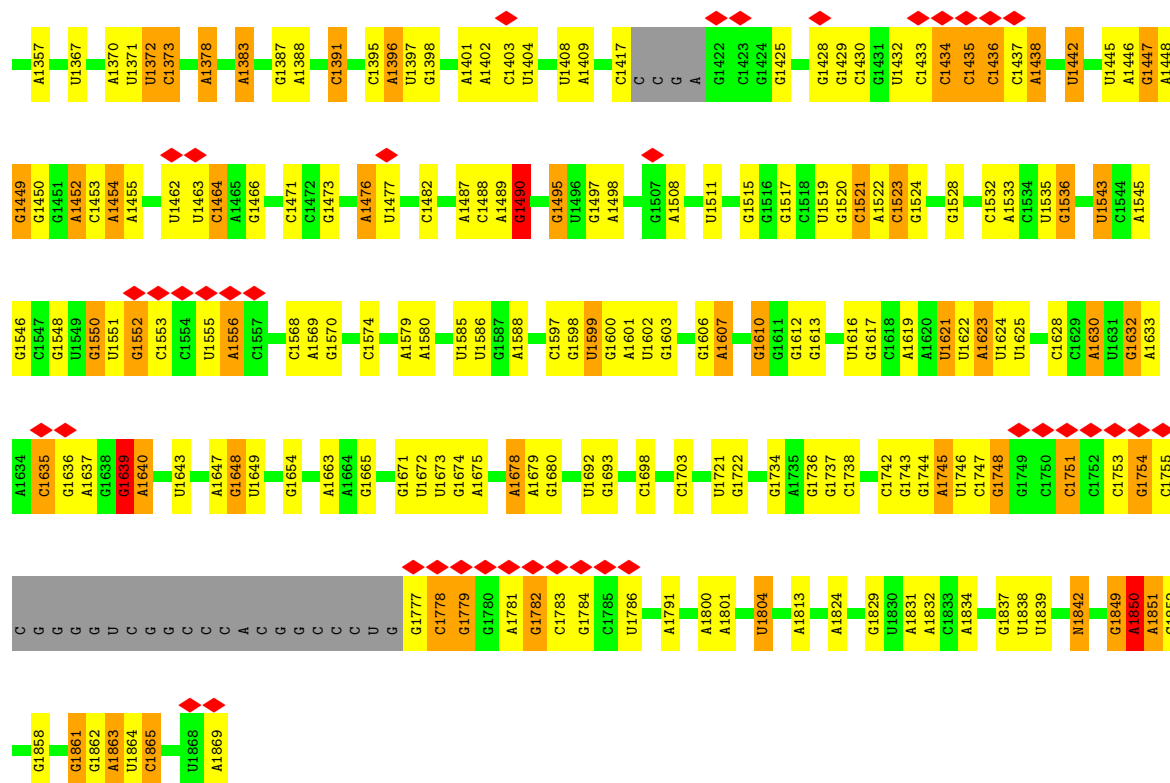
- Chain v:  75% 16% 9%



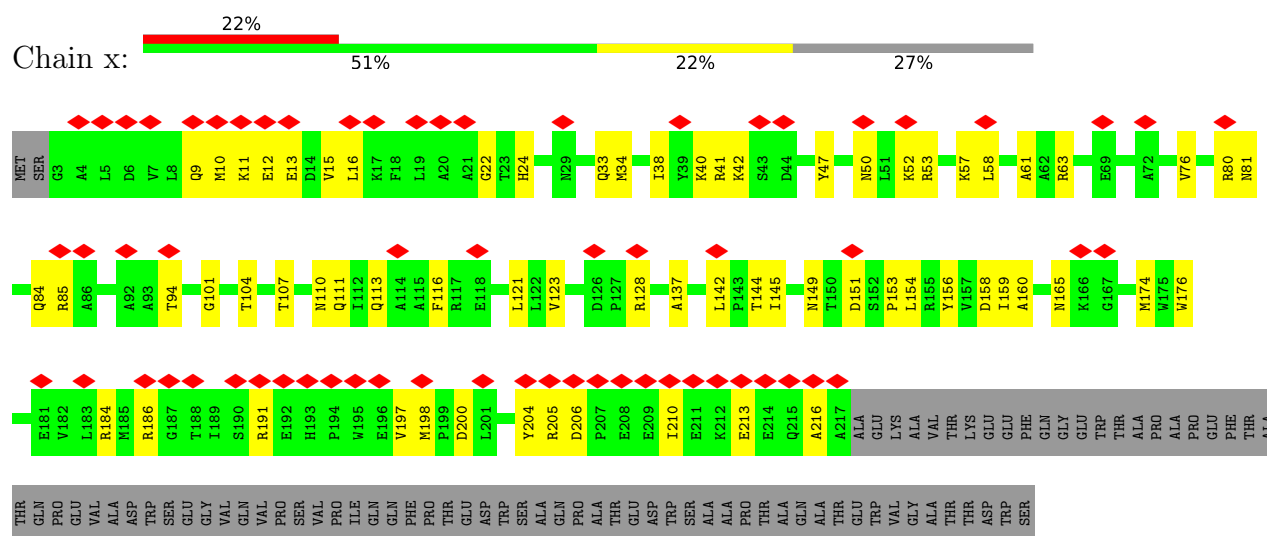
- Chain w: 17% 49% 29% 8% 13%



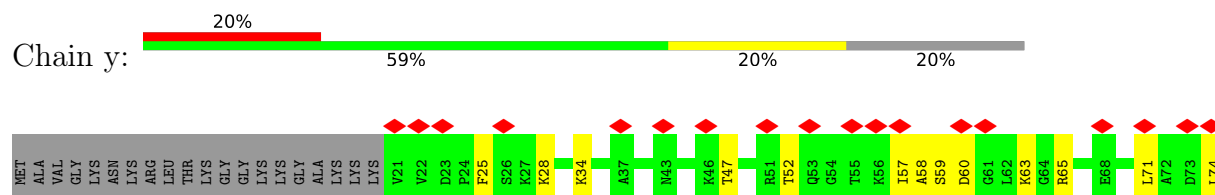




• Molecule 49: 40S ribosomal protein SA



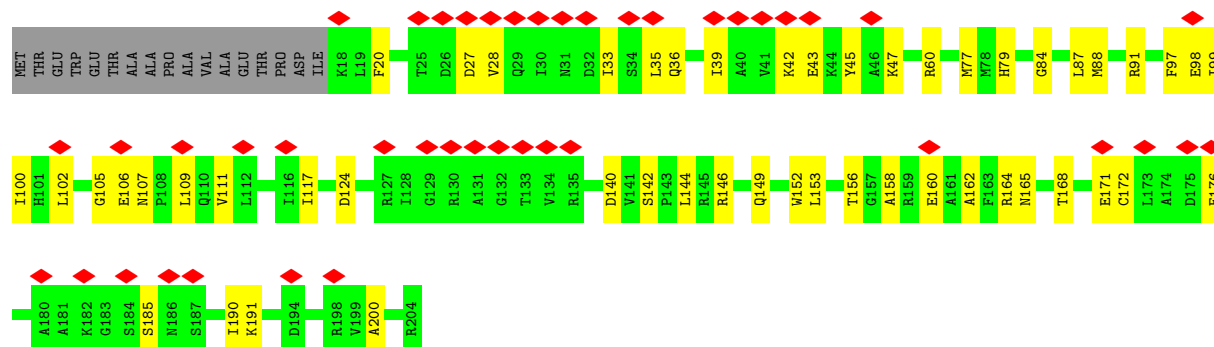
• Molecule 50: 40S ribosomal protein S3a



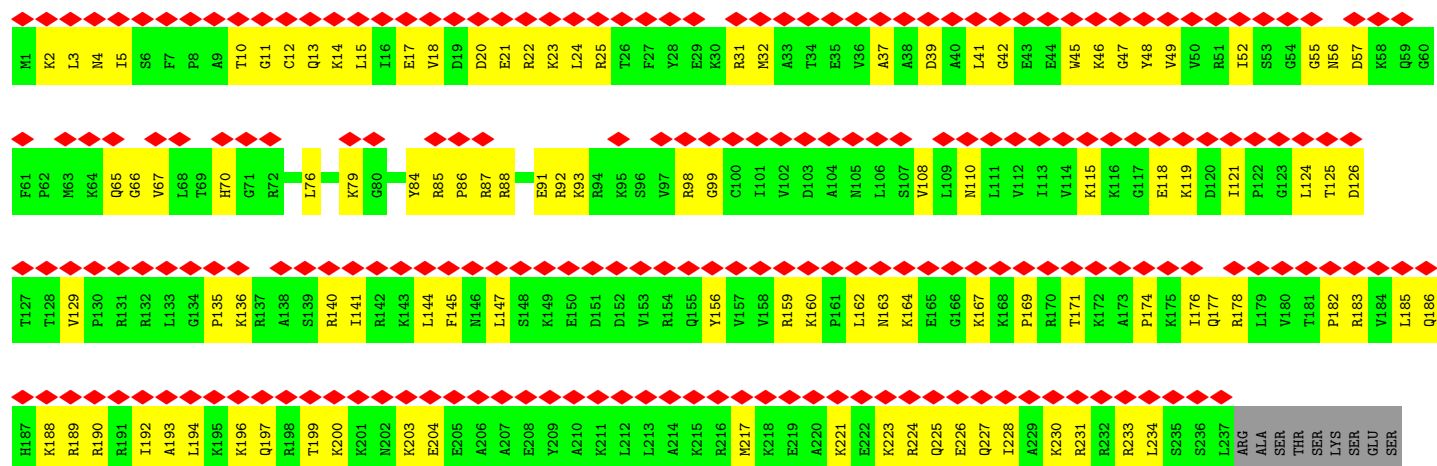
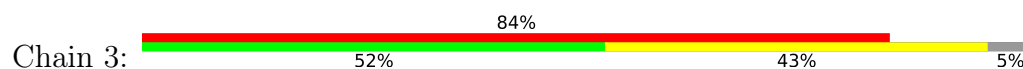




• Molecule 54: 40S ribosomal protein S5

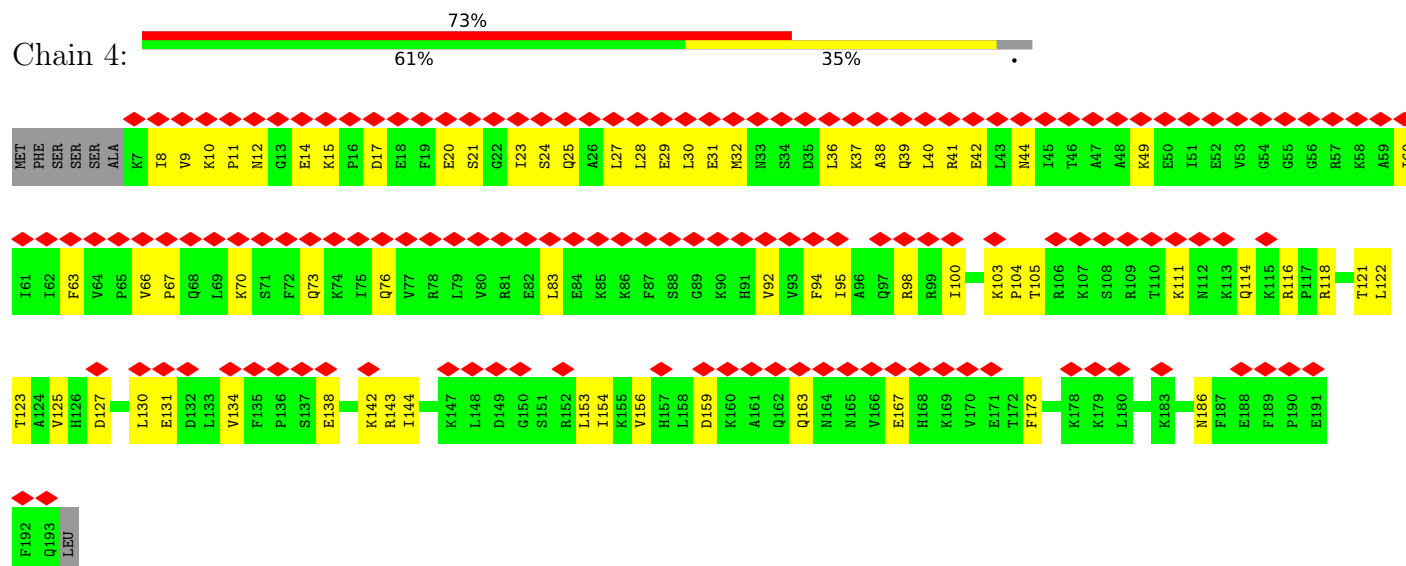


• Molecule 55: 40S ribosomal protein S6

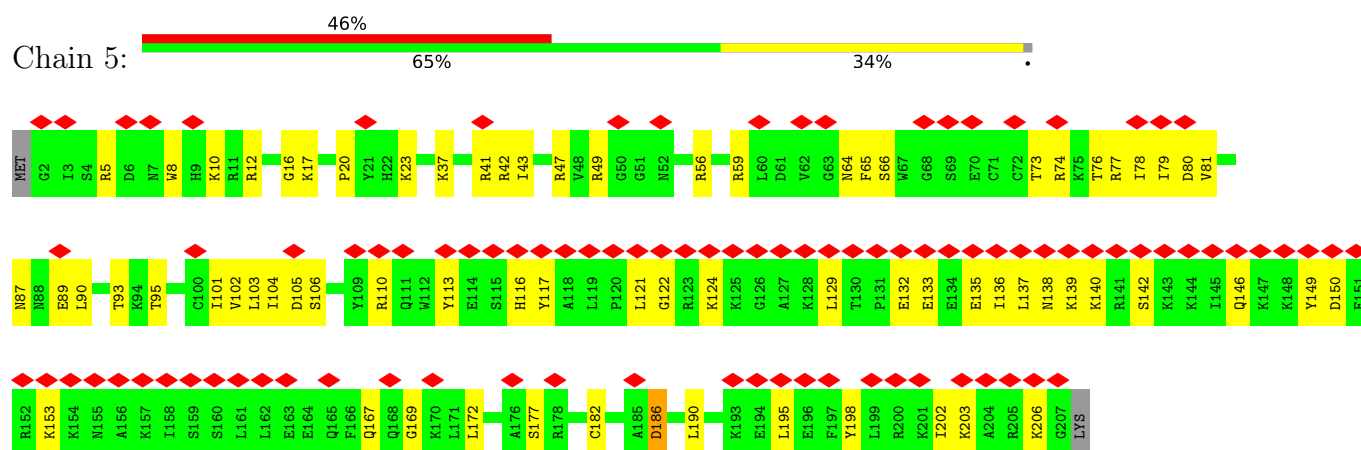


SER  
GLN  
LYS

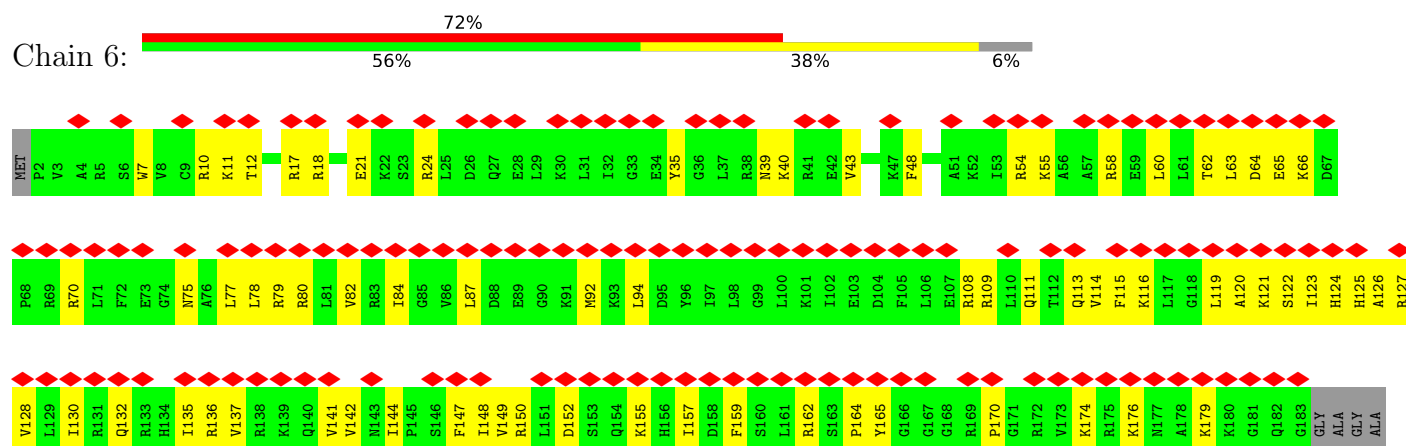
• Molecule 56: 40S ribosomal protein S7



• Molecule 57: 40S ribosomal protein S8

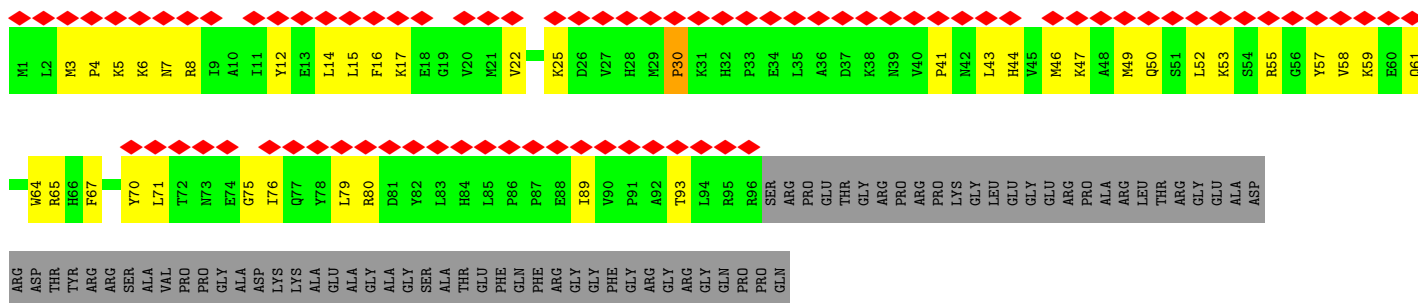
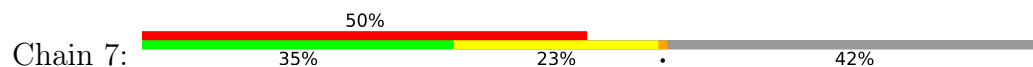


• Molecule 58: 40S ribosomal protein S9

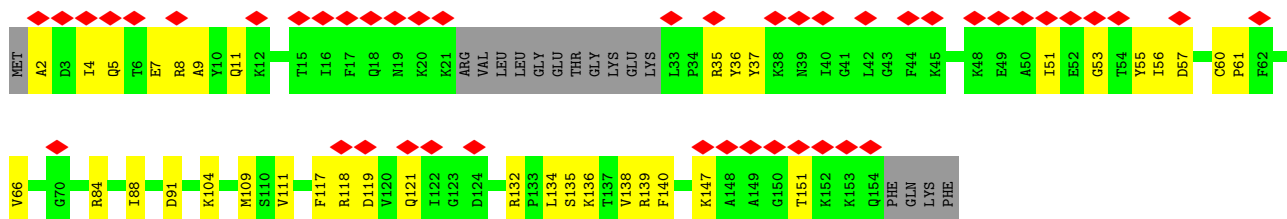


GLY  
ASP  
ASP  
GLU  
GLU  
GLU  
ASP

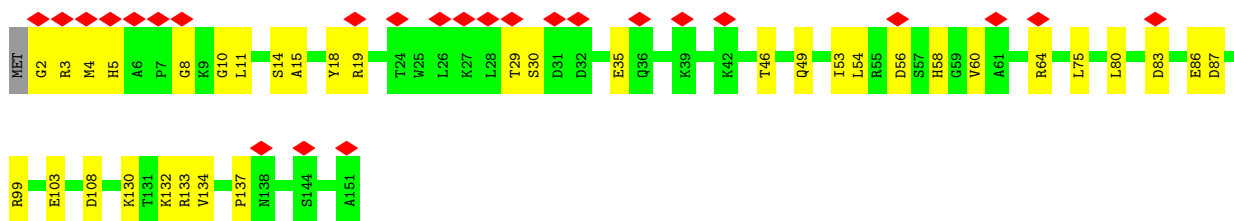
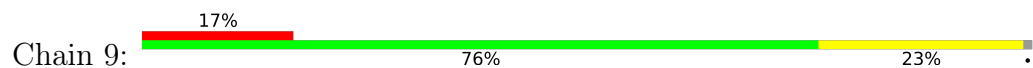
• Molecule 59: 40S ribosomal protein S10



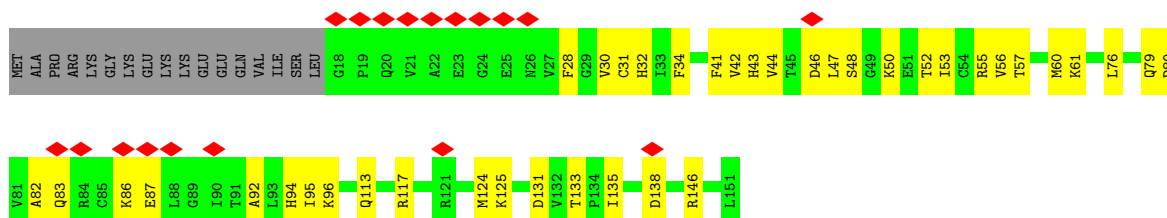
• Molecule 60: 40S ribosomal protein S11



• Molecule 61: 40S ribosomal protein S13

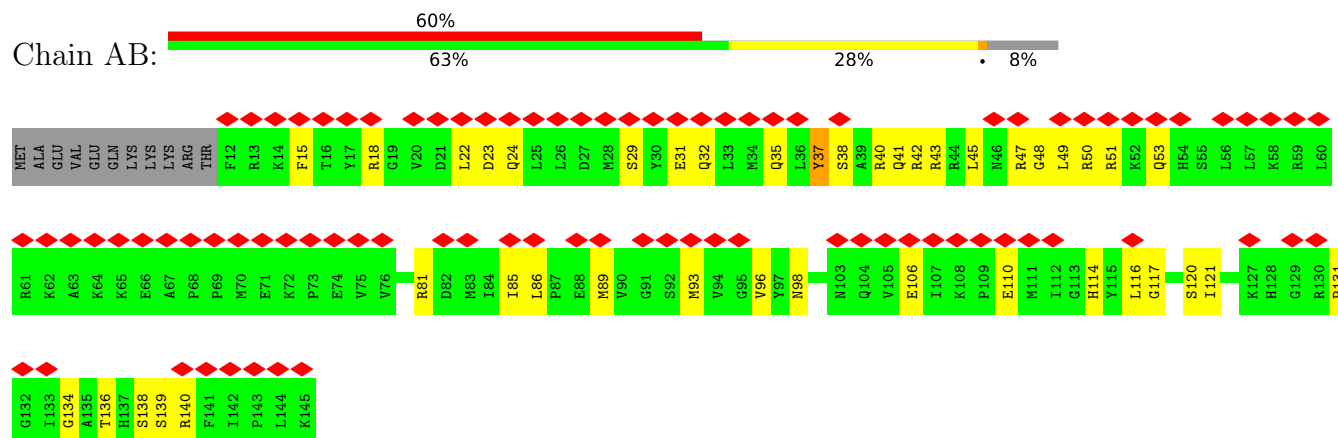


• Molecule 62: 40S ribosomal protein S14



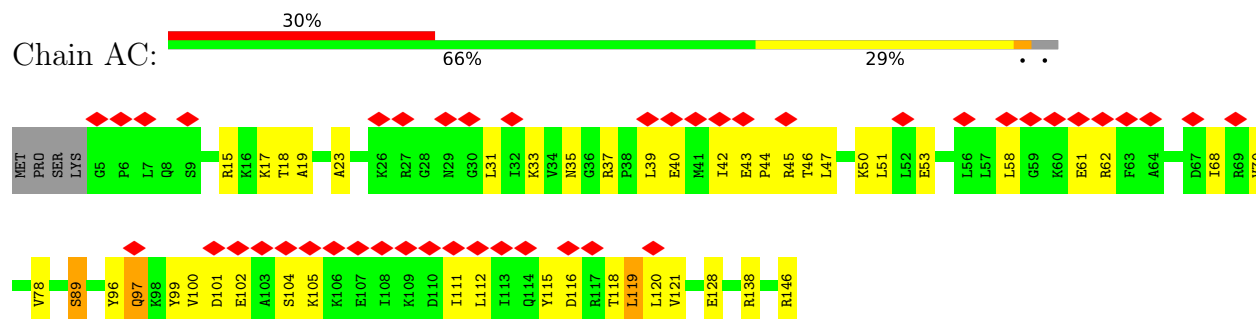
- Molecule 63: 40S ribosomal protein S15

Chain AB:



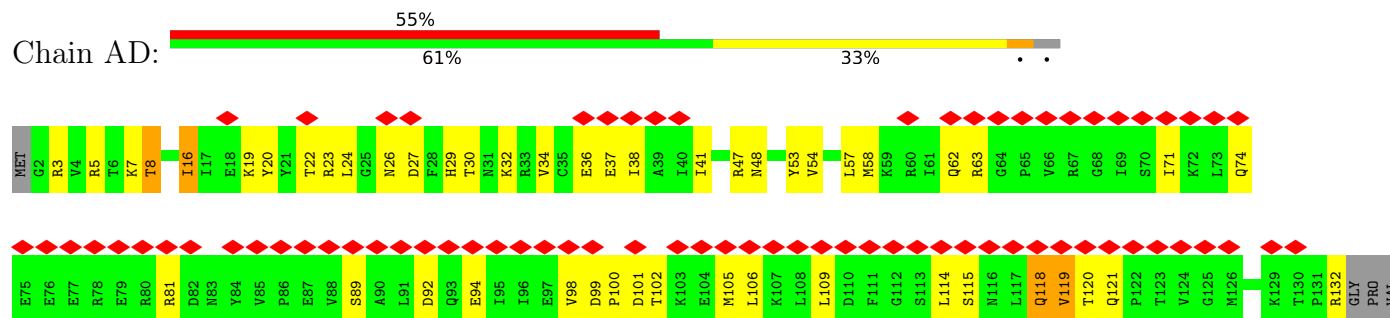
- Molecule 64: 40S ribosomal protein S16

Chain AC:



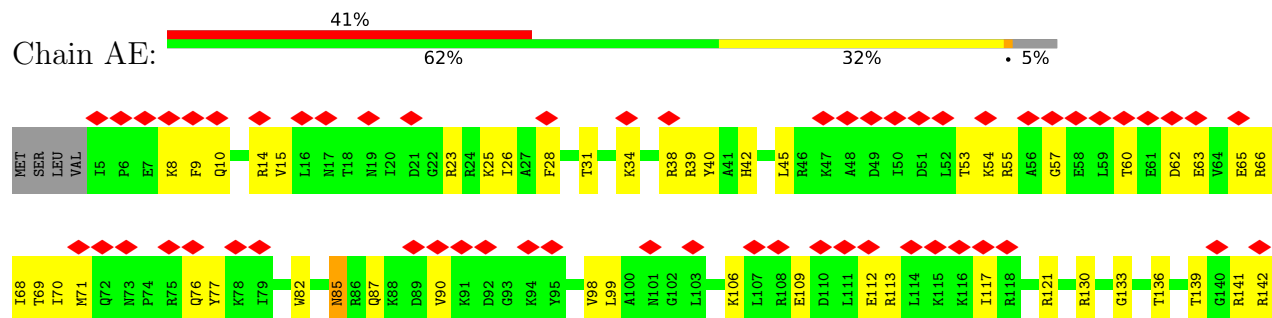
- Molecule 65: 40S ribosomal protein S17

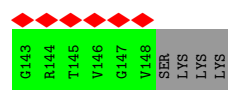
Chain AD:



- Molecule 66: 40S ribosomal protein S18

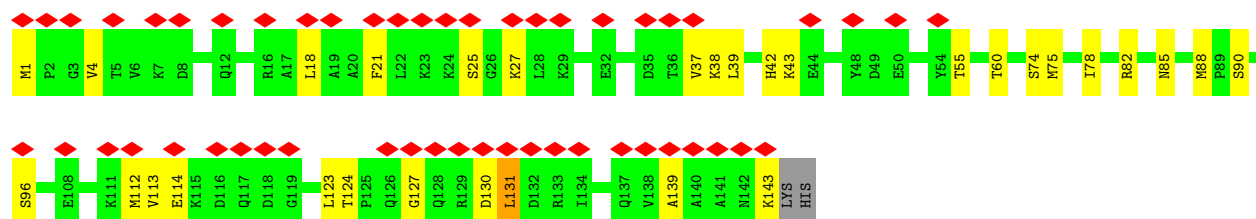
Chain AE:





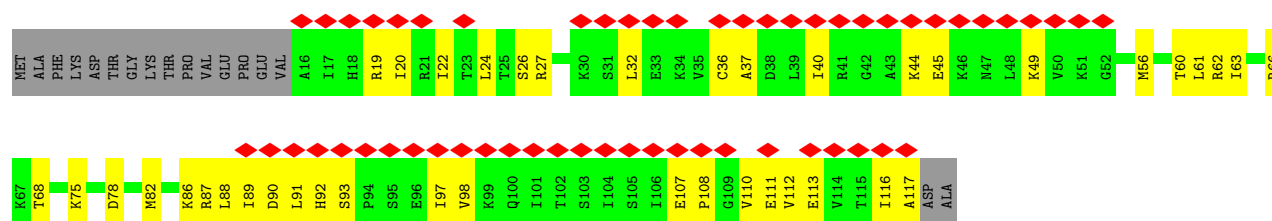
- Molecule 67: 40S ribosomal protein S19

Chain AF: 35% 77% 21% ..



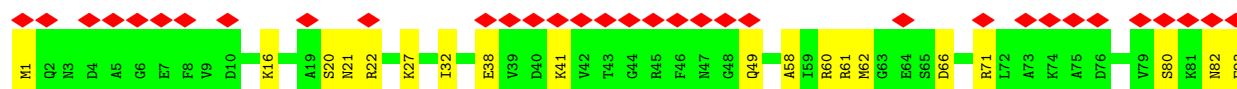
- Molecule 68: 40S ribosomal protein S20

Chain AG: 47% 51% 34% 14%



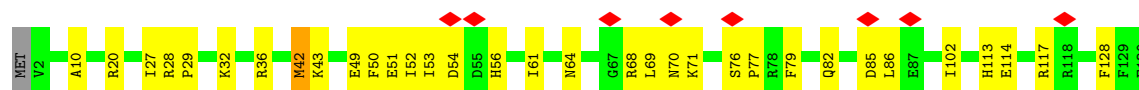
- Molecule 69: 40S ribosomal protein S21

Chain AH: 40% 77% 23%



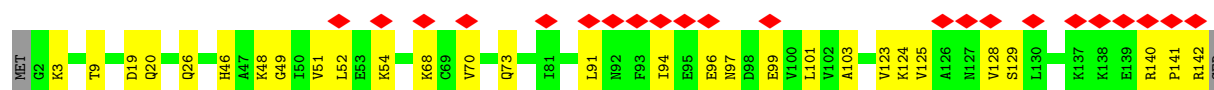
- Molecule 70: 40S ribosomal protein S15a

Chain AI: 6% 74% 25% ..

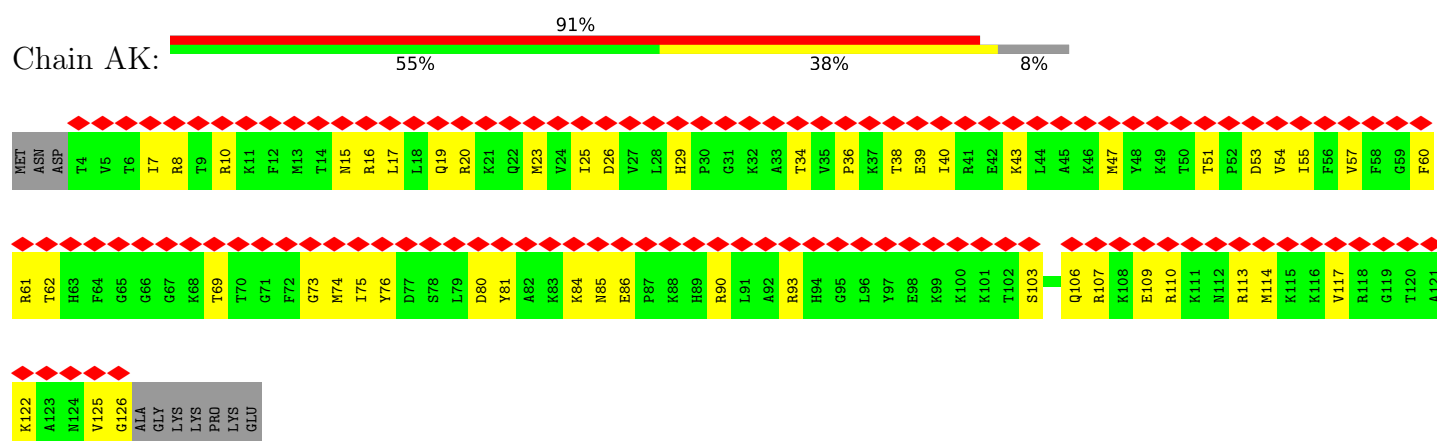


- Molecule 71: 40S ribosomal protein S23

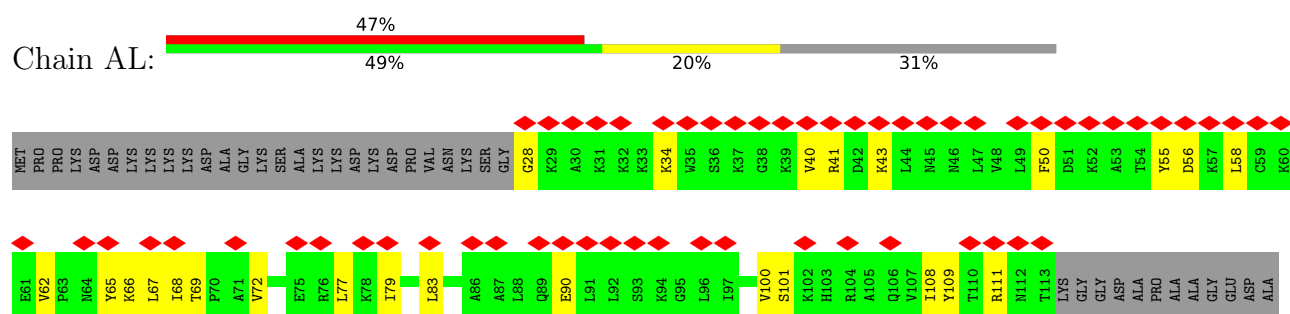
Chain AJ: 15% 78% 20%



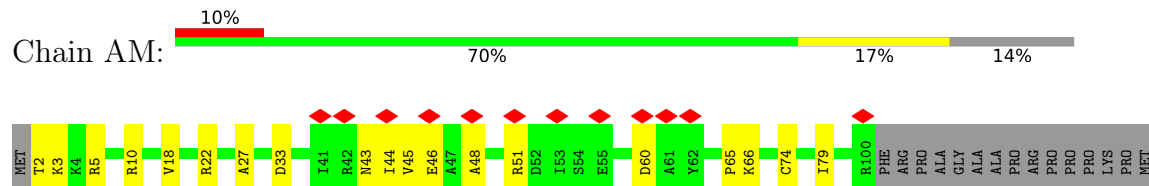
- Molecule 72: 40S ribosomal protein S24



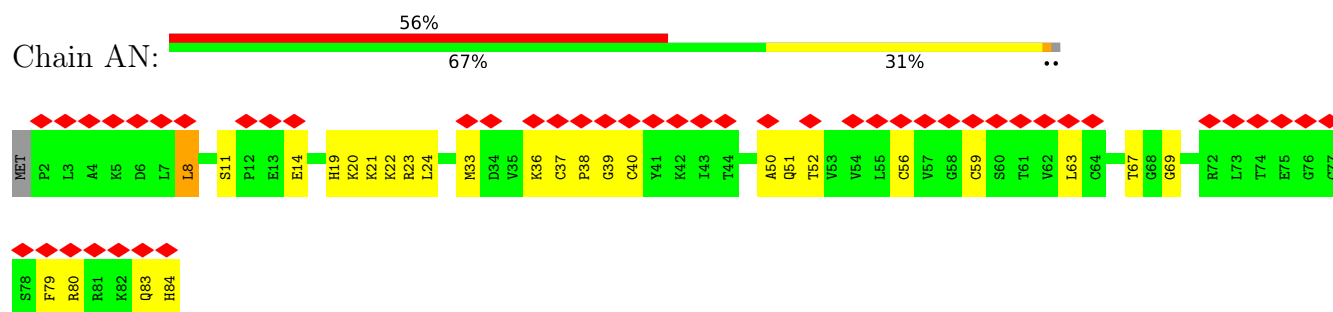
- Molecule 73: 40S ribosomal protein S25



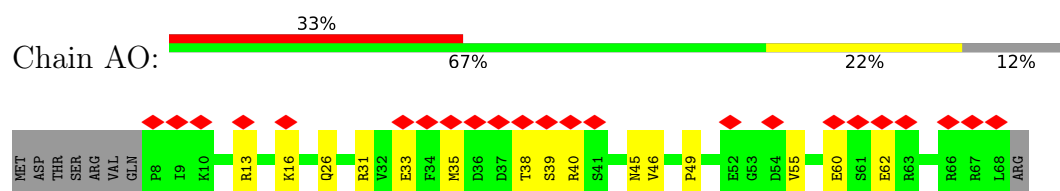
- Molecule 74: 40S ribosomal protein S26



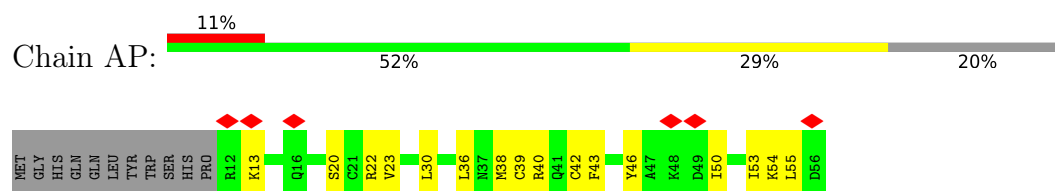
- Molecule 75: 40S ribosomal protein S27



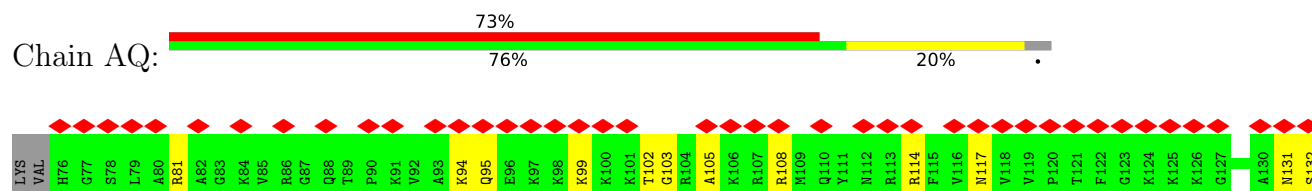
- Molecule 76: 40S ribosomal protein S28



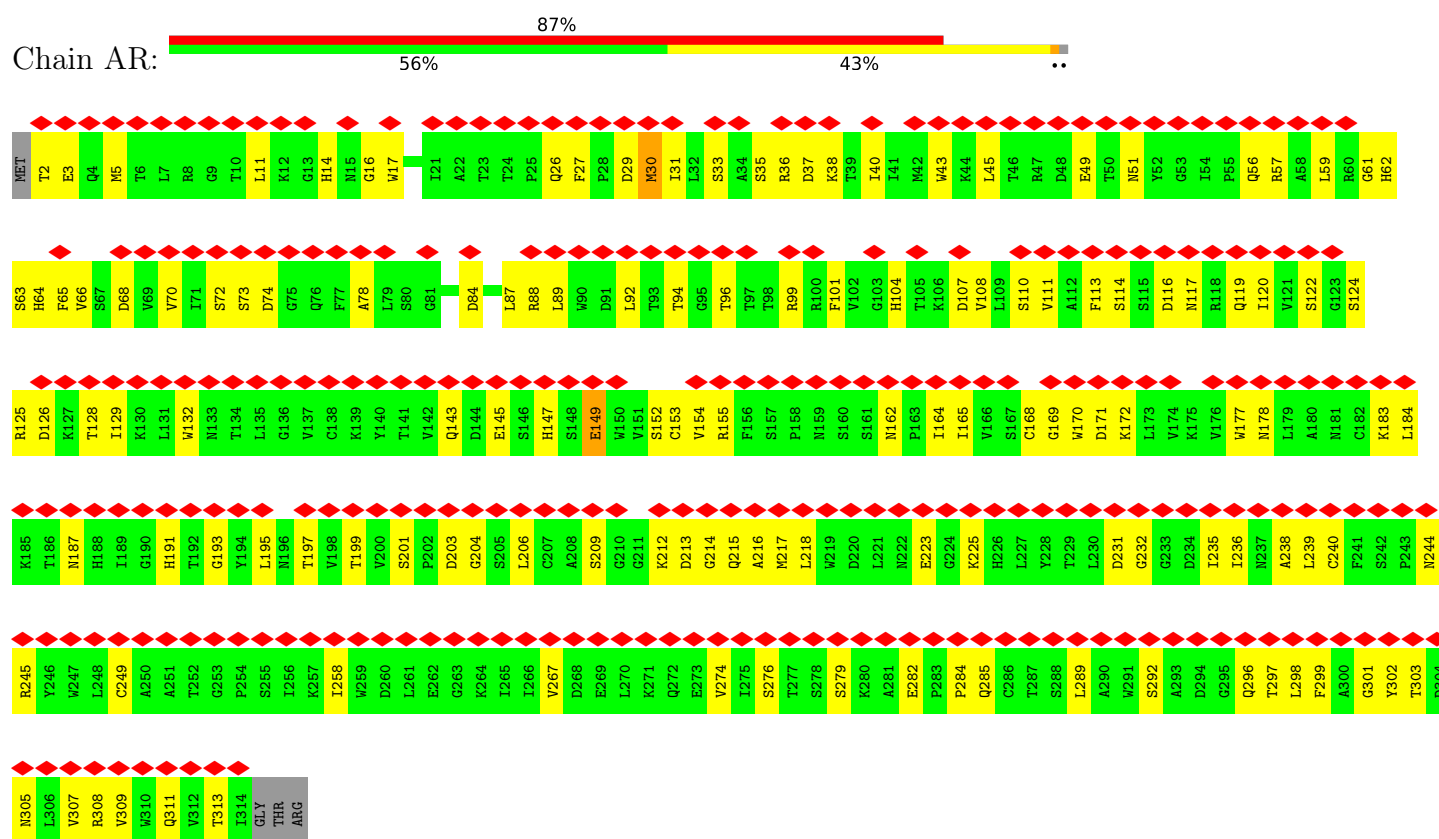
- Molecule 77: 40S ribosomal protein S29



- Molecule 78: 40S ribosomal protein S30



- Molecule 79: Receptor of activated protein C kinase 1



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 128240                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.163                                   | Depositor |
| Minimum map value                    | -0.047                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.0204                                  | Depositor |
| Map size (Å)                         | 439.9, 439.9, 439.9                     | wwPDB     |
| Map dimensions                       | 530, 530, 530                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.83, 0.83, 0.83                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 56B, 6MZ, 1MA, PSU, A2M, OMU, 4AC, G7M, MG, 5MC, MA6, H2U, UY1, OMG, B8N, ZN, UR3, OMC, 5MU

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   | A     | 0.20         | 0/339   | 0.20        | 0/527           |
| 2   | B     | 0.18         | 0/1525  | 0.21        | 0/2375          |
| 2   | C     | 0.14         | 0/1525  | 0.21        | 0/2375          |
| 3   | D     | 0.31         | 0/81567 | 0.27        | 6/127232 (0.0%) |
| 4   | E     | 0.30         | 0/2858  | 0.23        | 0/4455          |
| 5   | F     | 0.29         | 0/3675  | 0.25        | 0/5725          |
| 6   | G     | 0.30         | 0/1929  | 0.46        | 0/2586          |
| 7   | H     | 0.29         | 0/3279  | 0.44        | 0/4388          |
| 8   | I     | 0.29         | 0/2938  | 0.44        | 2/3946 (0.1%)   |
| 9   | J     | 0.25         | 0/2425  | 0.38        | 0/3248          |
| 10  | K     | 0.24         | 0/1785  | 0.45        | 0/2394          |
| 11  | L     | 0.30         | 0/1905  | 0.43        | 0/2539          |
| 12  | M     | 0.24         | 0/1863  | 0.45        | 1/2510 (0.0%)   |
| 13  | N     | 0.26         | 0/1537  | 0.43        | 0/2066          |
| 14  | O     | 0.27         | 0/1699  | 0.42        | 0/2270          |
| 15  | P     | 0.22         | 0/1385  | 0.39        | 0/1852          |
| 16  | Q     | 0.27         | 0/1713  | 0.45        | 0/2293          |
| 17  | R     | 0.26         | 0/1142  | 0.40        | 0/1527          |
| 18  | S     | 0.31         | 0/1746  | 0.40        | 0/2338          |
| 19  | T     | 0.30         | 0/1673  | 0.39        | 0/2238          |
| 20  | U     | 0.30         | 0/1300  | 0.42        | 0/1746          |
| 21  | V     | 0.31         | 0/1537  | 0.46        | 0/2052          |
| 22  | W     | 0.26         | 0/1524  | 0.42        | 0/2013          |
| 23  | X     | 0.29         | 0/1493  | 0.40        | 0/2003          |
| 24  | Y     | 0.28         | 0/1326  | 0.43        | 0/1770          |
| 25  | Z     | 0.21         | 0/835   | 0.43        | 0/1122          |
| 26  | a     | 0.27         | 0/993   | 0.41        | 0/1332          |
| 27  | b     | 0.26         | 0/541   | 0.36        | 0/720           |
| 28  | c     | 0.25         | 0/998   | 0.40        | 0/1340          |
| 29  | d     | 0.27         | 0/1132  | 0.39        | 0/1504          |
| 30  | e     | 0.25         | 0/1130  | 0.39        | 0/1507          |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 31  | f     | 0.30         | 0/1191  | 0.40        | 0/1591        |
| 32  | g     | 0.25         | 0/844   | 0.49        | 0/1115        |
| 33  | h     | 0.25         | 0/765   | 0.37        | 0/1027        |
| 34  | i     | 0.27         | 0/903   | 0.41        | 0/1216        |
| 35  | j     | 0.30         | 0/1071  | 0.39        | 0/1429        |
| 36  | k     | 0.32         | 0/895   | 0.51        | 0/1198        |
| 37  | l     | 0.27         | 0/898   | 0.46        | 0/1197        |
| 38  | m     | 0.25         | 0/1018  | 0.36        | 0/1344        |
| 39  | n     | 0.21         | 0/843   | 0.38        | 0/1115        |
| 40  | o     | 0.31         | 0/720   | 0.47        | 0/952         |
| 41  | p     | 0.23         | 0/575   | 0.42        | 0/761         |
| 42  | q     | 0.29         | 0/454   | 0.40        | 0/599         |
| 43  | r     | 0.25         | 0/435   | 0.40        | 0/575         |
| 44  | s     | 0.29         | 0/240   | 0.41        | 0/305         |
| 45  | t     | 0.27         | 0/876   | 0.48        | 0/1156        |
| 46  | u     | 0.27         | 0/718   | 0.37        | 0/953         |
| 47  | v     | 0.29         | 0/1017  | 0.44        | 0/1364        |
| 48  | w     | 0.24         | 0/37158 | 0.25        | 0/57908       |
| 49  | x     | 0.18         | 0/1732  | 0.40        | 0/2355        |
| 50  | y     | 0.18         | 0/1752  | 0.39        | 0/2345        |
| 51  | z     | 0.20         | 0/1668  | 0.41        | 0/2254        |
| 52  | 0     | 0.17         | 0/1672  | 0.37        | 0/2250        |
| 53  | 1     | 0.14         | 0/2112  | 0.35        | 0/2842        |
| 54  | 2     | 0.19         | 0/1485  | 0.40        | 0/1998        |
| 55  | 3     | 0.15         | 0/1940  | 0.42        | 0/2583        |
| 56  | 4     | 0.16         | 0/1533  | 0.43        | 0/2053        |
| 57  | 5     | 0.16         | 0/1703  | 0.38        | 0/2275        |
| 58  | 6     | 0.15         | 0/1531  | 0.37        | 0/2045        |
| 59  | 7     | 0.23         | 0/834   | 0.63        | 2/1125 (0.2%) |
| 60  | 8     | 0.18         | 0/1170  | 0.40        | 0/1568        |
| 61  | 9     | 0.19         | 0/1232  | 0.38        | 0/1656        |
| 62  | AA    | 0.23         | 0/1015  | 0.45        | 0/1361        |
| 63  | AB    | 0.16         | 0/1126  | 0.40        | 0/1505        |
| 64  | AC    | 0.21         | 0/1146  | 0.50        | 0/1534        |
| 65  | AD    | 0.18         | 0/1071  | 0.48        | 0/1438        |
| 66  | AE    | 0.22         | 0/1187  | 0.54        | 0/1593        |
| 67  | AF    | 0.19         | 0/1130  | 0.43        | 0/1515        |
| 68  | AG    | 0.19         | 0/809   | 0.42        | 0/1087        |
| 69  | AH    | 0.20         | 0/643   | 0.45        | 0/860         |
| 70  | AI    | 0.20         | 0/1051  | 0.38        | 0/1406        |
| 71  | AJ    | 0.17         | 0/1116  | 0.35        | 0/1490        |
| 72  | AK    | 0.16         | 0/1019  | 0.45        | 0/1355        |
| 73  | AL    | 0.17         | 0/688   | 0.41        | 0/921         |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5          |
| 74  | AM    | 0.24         | 0/805    | 0.44        | 0/1079           |
| 75  | AN    | 0.18         | 0/657    | 0.44        | 0/883            |
| 76  | AO    | 0.21         | 0/481    | 0.54        | 0/643            |
| 77  | AP    | 0.23         | 0/375    | 0.46        | 0/492            |
| 78  | AQ    | 0.16         | 0/458    | 0.44        | 0/602            |
| 79  | AR    | 0.16         | 0/2493   | 0.46        | 1/3394 (0.0%)    |
| All | All   | 0.27         | 0/219572 | 0.33        | 12/322305 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | G     | 0                   | 2                   |
| 7   | H     | 0                   | 2                   |
| 8   | I     | 0                   | 1                   |
| 9   | J     | 0                   | 1                   |
| 10  | K     | 0                   | 1                   |
| 11  | L     | 0                   | 1                   |
| 16  | Q     | 0                   | 1                   |
| 20  | U     | 0                   | 1                   |
| 21  | V     | 0                   | 1                   |
| 24  | Y     | 0                   | 1                   |
| 29  | d     | 0                   | 1                   |
| 32  | g     | 0                   | 1                   |
| 40  | o     | 0                   | 1                   |
| 54  | 2     | 0                   | 1                   |
| 65  | AD    | 0                   | 1                   |
| 79  | AR    | 0                   | 1                   |
| All | All   | 0                   | 18                  |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 3   | D     | 2101 | C    | OP1-P-OP2 | -13.28 | 79.75       | 119.60   |
| 59  | 7     | 30   | PRO  | CA-N-CD   | -12.70 | 94.22       | 112.00   |
| 3   | D     | 2100 | A    | OP2-P-O3' | -12.27 | 71.19       | 108.00   |
| 3   | D     | 2101 | C    | O5'-P-OP1 | -10.00 | 78.00       | 108.00   |
| 3   | D     | 2100 | A    | OP1-P-O3' | 9.41   | 136.24      | 108.00   |
| 3   | D     | 2101 | C    | O5'-P-OP2 | 7.34   | 130.01      | 108.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | I     | 316  | LYS  | CA-C-N    | -6.18 | 100.71      | 122.15   |
| 8   | I     | 316  | LYS  | C-N-CA    | -6.18 | 100.71      | 122.15   |
| 12  | M     | 206  | GLN  | CA-CB-CG  | 5.70  | 125.50      | 114.10   |
| 59  | 7     | 30   | PRO  | N-CD-CG   | -5.35 | 95.18       | 103.20   |
| 79  | AR    | 30   | MET  | CB-CG-SD  | 5.25  | 128.47      | 112.70   |
| 3   | D     | 2100 | A    | O3'-P-O5' | -5.20 | 96.20       | 104.00   |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 54  | 2     | 79  | HIS  | Peptide |
| 65  | AD    | 118 | GLN  | Peptide |
| 79  | AR    | 149 | GLU  | Peptide |
| 6   | G     | 123 | ARG  | Peptide |
| 6   | G     | 239 | ALA  | Peptide |
| 7   | H     | 16  | PHE  | Peptide |
| 7   | H     | 258 | HIS  | Peptide |
| 8   | I     | 91  | ALA  | Peptide |
| 9   | J     | 124 | GLU  | Peptide |
| 10  | K     | 130 | LYS  | Peptide |
| 11  | L     | 163 | ASN  | Peptide |
| 16  | Q     | 47  | ALA  | Peptide |
| 20  | U     | 131 | ARG  | Peptide |
| 21  | V     | 159 | PRO  | Peptide |
| 24  | Y     | 80  | VAL  | Peptide |
| 29  | d     | 108 | ARG  | Peptide |
| 32  | g     | 110 | ALA  | Peptide |
| 40  | o     | 39  | TYR  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 303   | 0        | 150      | 0       | 0            |
| 2   | B     | 1612  | 0        | 814      | 14      | 0            |
| 2   | C     | 1612  | 0        | 814      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 75336 | 0        | 38155    | 437     | 0            |
| 4   | E     | 2558  | 0        | 1296     | 9       | 0            |
| 5   | F     | 3315  | 0        | 1685     | 23      | 0            |
| 6   | G     | 1891  | 0        | 1986     | 28      | 0            |
| 7   | H     | 3211  | 0        | 3356     | 46      | 0            |
| 8   | I     | 2884  | 0        | 3060     | 35      | 0            |
| 9   | J     | 2379  | 0        | 2408     | 35      | 0            |
| 10  | K     | 1751  | 0        | 1905     | 44      | 0            |
| 11  | L     | 1870  | 0        | 1996     | 28      | 0            |
| 12  | M     | 1832  | 0        | 1962     | 31      | 0            |
| 13  | N     | 1518  | 0        | 1601     | 23      | 0            |
| 14  | O     | 1660  | 0        | 1692     | 27      | 0            |
| 15  | P     | 1362  | 0        | 1399     | 16      | 0            |
| 16  | Q     | 1682  | 0        | 1792     | 33      | 0            |
| 17  | R     | 1120  | 0        | 1187     | 25      | 0            |
| 18  | S     | 1701  | 0        | 1749     | 23      | 0            |
| 19  | T     | 1641  | 0        | 1788     | 17      | 0            |
| 20  | U     | 1273  | 0        | 1304     | 16      | 0            |
| 21  | V     | 1513  | 0        | 1628     | 18      | 0            |
| 22  | W     | 1508  | 0        | 1664     | 13      | 0            |
| 23  | X     | 1453  | 0        | 1490     | 13      | 0            |
| 24  | Y     | 1298  | 0        | 1366     | 17      | 0            |
| 25  | Z     | 821   | 0        | 839      | 20      | 0            |
| 26  | a     | 979   | 0        | 1039     | 7       | 0            |
| 27  | b     | 528   | 0        | 541      | 2       | 0            |
| 28  | c     | 981   | 0        | 1062     | 10      | 0            |
| 29  | d     | 1115  | 0        | 1205     | 20      | 0            |
| 30  | e     | 1107  | 0        | 1182     | 22      | 0            |
| 31  | f     | 1162  | 0        | 1213     | 23      | 0            |
| 32  | g     | 832   | 0        | 883      | 10      | 0            |
| 33  | h     | 755   | 0        | 791      | 10      | 0            |
| 34  | i     | 888   | 0        | 930      | 11      | 0            |
| 35  | j     | 1053  | 0        | 1147     | 10      | 0            |
| 36  | k     | 876   | 0        | 912      | 12      | 0            |
| 37  | l     | 888   | 0        | 981      | 6       | 0            |
| 38  | m     | 1010  | 0        | 1143     | 9       | 0            |
| 39  | n     | 832   | 0        | 917      | 8       | 0            |
| 40  | o     | 705   | 0        | 737      | 8       | 0            |
| 41  | p     | 569   | 0        | 637      | 6       | 0            |
| 42  | q     | 444   | 0        | 483      | 8       | 0            |
| 43  | r     | 429   | 0        | 466      | 10      | 0            |
| 44  | s     | 239   | 0        | 289      | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45  | t     | 862   | 0        | 930      | 14      | 0            |
| 46  | u     | 708   | 0        | 756      | 3       | 0            |
| 47  | v     | 1002  | 0        | 1068     | 14      | 0            |
| 48  | w     | 34933 | 0        | 17694    | 393     | 0            |
| 49  | x     | 1695  | 0        | 1690     | 52      | 0            |
| 50  | y     | 1725  | 0        | 1800     | 41      | 0            |
| 51  | z     | 1633  | 0        | 1716     | 33      | 0            |
| 52  | 0     | 1646  | 0        | 1734     | 49      | 0            |
| 53  | 1     | 2070  | 0        | 2166     | 76      | 0            |
| 54  | 2     | 1464  | 0        | 1505     | 39      | 0            |
| 55  | 3     | 1917  | 0        | 2078     | 93      | 0            |
| 56  | 4     | 1510  | 0        | 1606     | 54      | 0            |
| 57  | 5     | 1674  | 0        | 1739     | 52      | 0            |
| 58  | 6     | 1506  | 0        | 1618     | 62      | 0            |
| 59  | 7     | 810   | 0        | 836      | 36      | 0            |
| 60  | 8     | 1150  | 0        | 1199     | 27      | 0            |
| 61  | 9     | 1208  | 0        | 1294     | 31      | 0            |
| 62  | AA    | 1002  | 0        | 1023     | 30      | 0            |
| 63  | AB    | 1103  | 0        | 1156     | 34      | 0            |
| 64  | AC    | 1128  | 0        | 1195     | 36      | 0            |
| 65  | AD    | 1057  | 0        | 1110     | 42      | 0            |
| 66  | AE    | 1169  | 0        | 1198     | 40      | 0            |
| 67  | AF    | 1111  | 0        | 1144     | 23      | 0            |
| 68  | AG    | 799   | 0        | 850      | 36      | 0            |
| 69  | AH    | 636   | 0        | 637      | 19      | 0            |
| 70  | AI    | 1034  | 0        | 1080     | 28      | 0            |
| 71  | AJ    | 1098  | 0        | 1167     | 20      | 0            |
| 72  | AK    | 1002  | 0        | 1067     | 45      | 0            |
| 73  | AL    | 680   | 0        | 744      | 21      | 0            |
| 74  | AM    | 792   | 0        | 842      | 16      | 0            |
| 75  | AN    | 643   | 0        | 650      | 22      | 0            |
| 76  | AO    | 479   | 0        | 507      | 17      | 0            |
| 77  | AP    | 370   | 0        | 373      | 18      | 0            |
| 78  | AQ    | 452   | 0        | 494      | 11      | 0            |
| 79  | AR    | 2436  | 0        | 2393     | 107     | 0            |
| 80  | A     | 1     | 0        | 0        | 0       | 0            |
| 80  | AA    | 1     | 0        | 0        | 0       | 0            |
| 80  | AF    | 1     | 0        | 0        | 0       | 0            |
| 80  | D     | 398   | 0        | 0        | 0       | 0            |
| 80  | E     | 10    | 0        | 0        | 0       | 0            |
| 80  | F     | 6     | 0        | 0        | 0       | 0            |
| 80  | G     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 80  | H     | 1      | 0        | 0        | 0       | 0            |
| 80  | I     | 1      | 0        | 0        | 0       | 0            |
| 80  | N     | 1      | 0        | 0        | 0       | 0            |
| 80  | O     | 2      | 0        | 0        | 0       | 0            |
| 80  | S     | 1      | 0        | 0        | 0       | 0            |
| 80  | U     | 2      | 0        | 0        | 0       | 0            |
| 80  | V     | 2      | 0        | 0        | 0       | 0            |
| 80  | X     | 1      | 0        | 0        | 0       | 0            |
| 80  | a     | 1      | 0        | 0        | 0       | 0            |
| 80  | g     | 1      | 0        | 0        | 0       | 0            |
| 80  | j     | 1      | 0        | 0        | 0       | 0            |
| 80  | k     | 1      | 0        | 0        | 0       | 0            |
| 80  | l     | 1      | 0        | 0        | 0       | 0            |
| 80  | u     | 1      | 0        | 0        | 0       | 0            |
| 80  | w     | 103    | 0        | 0        | 0       | 0            |
| 81  | AM    | 1      | 0        | 0        | 0       | 0            |
| 81  | AP    | 1      | 0        | 0        | 0       | 0            |
| 81  | o     | 1      | 0        | 0        | 0       | 0            |
| 81  | r     | 1      | 0        | 0        | 0       | 0            |
| 81  | t     | 1      | 0        | 0        | 0       | 0            |
| 81  | u     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 209545 | 0        | 154703   | 2380    | 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 7.

All (2380) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:4092:G:H21   | 3:D:4093:G:H1     | 1.12                     | 0.95              |
| 3:D:1271:G:H1'   | 11:L:34:ARG:HH12  | 1.35                     | 0.90              |
| 3:D:1303:A:N6    | 3:D:2316:G:N7     | 2.20                     | 0.89              |
| 5:F:110:U:H5''   | 42:q:8:ARG:HH22   | 1.41                     | 0.85              |
| 48:w:1745:A:H1'  | 55:3:66:GLY:HA2   | 1.59                     | 0.85              |
| 55:3:194:LEU:HA  | 55:3:197:GLN:HE22 | 1.42                     | 0.84              |
| 3:D:3751:G:H21   | 3:D:3775:A:H8     | 1.22                     | 0.84              |
| 3:D:1656:U:OP2   | 31:f:26:ARG:NH2   | 2.11                     | 0.82              |
| 36:k:109:ARG:HG3 | 36:k:110:ILE:HD12 | 1.62                     | 0.82              |
| 6:G:117:GLU:HB2  | 6:G:162:ASN:HB2   | 1.61                     | 0.81              |
| 24:Y:79:GLN:O    | 24:Y:79:GLN:NE2   | 2.14                     | 0.81              |
| 48:w:925:G:H1    | 48:w:1017:U:H3    | 1.27                     | 0.81              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:w:1834:A:H2     | 48:w:1837:G:H1    | 1.29                     | 0.81              |
| 48:w:570:C:H4'     | 72:AK:36:PRO:HG3  | 1.63                     | 0.81              |
| 3:D:1:C:H42        | 5:F:156:U:H3      | 1.28                     | 0.80              |
| 3:D:496:G:N2       | 3:D:658:C:O2      | 2.10                     | 0.80              |
| 36:k:33:VAL:HG23   | 36:k:38:GLU:HG3   | 1.62                     | 0.80              |
| 48:w:1060:A:O2'    | 48:w:1062:A:N7    | 2.13                     | 0.79              |
| 79:AR:14:HIS:CE1   | 79:AR:35:SER:HB2  | 2.16                     | 0.79              |
| 30:e:57:MET:HG2    | 30:e:61:LYS:HD3   | 1.65                     | 0.79              |
| 52:0:101:GLN:HG3   | 52:0:126:ILE:HD11 | 1.65                     | 0.79              |
| 3:D:184:U:O2       | 3:D:253:G:N2      | 2.16                     | 0.79              |
| 56:4:15:LYS:H      | 56:4:15:LYS:HE2   | 1.45                     | 0.79              |
| 47:v:26:SER:OG     | 47:v:28:GLU:OE1   | 2.02                     | 0.78              |
| 48:w:1396:A:O2'    | 48:w:1398:G:N7    | 2.16                     | 0.78              |
| 67:AF:1:MET:SD     | 67:AF:143:LYS:NZ  | 2.56                     | 0.78              |
| 48:w:1003:U:H5''   | 50:y:165:ARG:HH22 | 1.49                     | 0.78              |
| 72:AK:7:ILE:HD13   | 72:AK:43:LYS:HG2  | 1.65                     | 0.78              |
| 48:w:1488:C:O2'    | 48:w:1490:OMG:OP2 | 2.02                     | 0.77              |
| 48:w:830:A:OP2     | 48:w:846:G:N2     | 2.15                     | 0.77              |
| 32:g:110:ALA:O     | 32:g:112:ILE:N    | 2.14                     | 0.77              |
| 48:w:1649:U:H3     | 48:w:1675:A:H2    | 1.29                     | 0.77              |
| 60:8:7:GLU:OE2     | 60:8:11:GLN:NE2   | 2.18                     | 0.77              |
| 3:D:3937:C:H1'     | 18:S:125:SER:HB2  | 1.65                     | 0.76              |
| 57:5:87:ASN:HB3    | 57:5:90:LEU:HG    | 1.66                     | 0.76              |
| 6:G:30:ARG:O       | 6:G:163:ARG:NH2   | 2.18                     | 0.76              |
| 68:AG:26:SER:HB3   | 68:AG:32:LEU:HD21 | 1.66                     | 0.76              |
| 3:D:2487:G:H22     | 3:D:2492:C:H1'    | 1.50                     | 0.76              |
| 79:AR:26:GLN:NE2   | 79:AR:73:SER:O    | 2.19                     | 0.75              |
| 3:D:4742:G:N2      | 3:D:4958:C:O2     | 2.17                     | 0.75              |
| 48:w:594:A:H61     | 48:w:643:A:H5''   | 1.49                     | 0.75              |
| 62:AA:92:ALA:HB2   | 62:AA:125:LYS:HB2 | 1.68                     | 0.75              |
| 46:u:5:THR:HG21    | 46:u:9:GLY:H      | 1.48                     | 0.75              |
| 48:w:884:C:O2      | 48:w:902:G:N2     | 2.19                     | 0.75              |
| 48:w:928:G:H1      | 48:w:1013:U:H3    | 1.33                     | 0.75              |
| 64:AC:118:THR:HG23 | 64:AC:119:LEU:H   | 1.51                     | 0.75              |
| 48:w:1612:G:H1'    | 66:AE:87:GLN:HE21 | 1.51                     | 0.74              |
| 3:D:2474:G:N2      | 3:D:2502:G:O2'    | 2.21                     | 0.74              |
| 8:I:110:ARG:O      | 8:I:113:ARG:NH1   | 2.20                     | 0.74              |
| 72:AK:90:ARG:HA    | 72:AK:93:ARG:HD2  | 1.68                     | 0.74              |
| 59:7:8:ARG:NH2     | 59:7:12:TYR:OH    | 2.20                     | 0.74              |
| 55:3:20:ASP:OD1    | 55:3:22:ARG:NH1   | 2.20                     | 0.74              |
| 48:w:483:C:H5''    | 71:AJ:48:LYS:HD2  | 1.68                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1171:G:N2     | 3:D:1190:C:O2     | 2.16                     | 0.73              |
| 48:w:345:U:O2     | 53:l:33:THR:OG1   | 2.05                     | 0.73              |
| 69:AH:41:LYS:HE2  | 69:AH:41:LYS:H    | 1.52                     | 0.73              |
| 7:H:254:ILE:HG23  | 7:H:266:VAL:HG11  | 1.70                     | 0.73              |
| 53:l:94:LYS:NZ    | 72:AK:19:GLN:OE1  | 2.21                     | 0.73              |
| 54:2:100:ILE:HG21 | 54:2:111:VAL:HG11 | 1.70                     | 0.73              |
| 3:D:3689:G:O2'    | 3:D:3818:UY1:OP2  | 2.07                     | 0.73              |
| 62:AA:113:GLN:NE2 | 74:AM:44:ILE:O    | 2.22                     | 0.73              |
| 3:D:4882:U:OP1    | 17:R:117:LYS:NZ   | 2.21                     | 0.73              |
| 51:z:108:LYS:HE3  | 51:z:110:MET:HB3  | 1.70                     | 0.73              |
| 79:AR:35:SER:OG   | 79:AR:37:ASP:OD1  | 2.03                     | 0.73              |
| 48:w:560:A:N6     | 48:w:588:G:O6     | 2.22                     | 0.73              |
| 3:D:5022:U:O2'    | 3:D:5024:C:OP2    | 2.06                     | 0.72              |
| 72:AK:20:ARG:NH1  | 72:AK:85:ASN:O    | 2.22                     | 0.72              |
| 3:D:2658:G:N2     | 3:D:2676:A:OP2    | 2.20                     | 0.72              |
| 57:5:64:ASN:HB3   | 57:5:186:ASP:HB3  | 1.70                     | 0.72              |
| 31:f:17:HIS:O     | 31:f:19:HIS:N     | 2.19                     | 0.72              |
| 63:AB:93:MET:HE1  | 63:AB:106:GLU:HG3 | 1.70                     | 0.72              |
| 64:AC:118:THR:C   | 64:AC:120:LEU:H   | 1.98                     | 0.72              |
| 48:w:579:C:N3     | 72:AK:61:ARG:NH2  | 2.38                     | 0.72              |
| 3:D:1351:G:OP1    | 8:I:33:ARG:NH1    | 2.21                     | 0.72              |
| 41:p:28:ASN:ND2   | 41:p:31:ASN:OD1   | 2.22                     | 0.72              |
| 48:w:1858:G:OP2   | 62:AA:146:ARG:NH2 | 2.22                     | 0.72              |
| 50:y:57:ILE:HG13  | 50:y:58:ALA:H     | 1.53                     | 0.72              |
| 48:w:446:G:OP2    | 57:5:47:ARG:NH2   | 2.22                     | 0.72              |
| 72:AK:23:MET:HE1  | 72:AK:25:ILE:HG13 | 1.72                     | 0.72              |
| 3:D:1364:U:OP2    | 16:Q:36:ARG:NH2   | 2.23                     | 0.71              |
| 58:6:111:GLN:OE1  | 58:6:127:ARG:NH1  | 2.23                     | 0.71              |
| 3:D:4635:A:H2     | 3:D:4663:G:H21    | 1.38                     | 0.71              |
| 70:AI:51:GLU:HG2  | 75:AN:8:LEU:HD11  | 1.72                     | 0.71              |
| 64:AC:43:GLU:HG2  | 64:AC:44:PRO:HD3  | 1.72                     | 0.71              |
| 3:D:1391:A:OP1    | 21:V:181:ARG:NH1  | 2.20                     | 0.71              |
| 11:L:222:LYS:HB3  | 11:L:231:GLY:HA2  | 1.72                     | 0.71              |
| 59:7:3:MET:HE3    | 59:7:8:ARG:HH11   | 1.54                     | 0.71              |
| 3:D:516:C:N4      | 3:D:645:G:O6      | 2.19                     | 0.71              |
| 48:w:165:G:H1'    | 55:3:110:ASN:HD22 | 1.55                     | 0.71              |
| 48:w:807:G:H1     | 48:w:856:C:H5     | 1.37                     | 0.71              |
| 48:w:918:U:OP2    | 61:9:64:ARG:NH1   | 2.20                     | 0.71              |
| 3:D:2469:C:H5     | 3:D:2471:G:H1     | 1.39                     | 0.71              |
| 37:l:107:LEU:O    | 37:l:110:GLN:NE2  | 2.24                     | 0.71              |
| 66:AE:54:LYS:HA   | 66:AE:54:LYS:HE3  | 1.73                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:F:55:U:H3       | 5:F:62:A:H2        | 1.39                     | 0.71              |
| 57:5:139:LYS:HE3  | 57:5:146:GLN:HB2   | 1.73                     | 0.71              |
| 48:w:489:A:OP2    | 48:w:507:G:N2      | 2.23                     | 0.70              |
| 59:7:4:PRO:HB2    | 59:7:6:LYS:HE3     | 1.73                     | 0.70              |
| 25:Z:66:SER:HB3   | 25:Z:69:LYS:HB2    | 1.72                     | 0.70              |
| 49:x:128:ARG:NH2  | 49:x:151:ASP:O     | 2.25                     | 0.70              |
| 64:AC:31:LEU:HD11 | 64:AC:33:LYS:HE2   | 1.73                     | 0.70              |
| 3:D:188:G:N2      | 3:D:190:G:O6       | 2.24                     | 0.70              |
| 3:D:2755:A:OP1    | 30:e:65:ARG:NH1    | 2.20                     | 0.70              |
| 48:w:851:C:H5''   | 48:w:852:G:H5'     | 1.72                     | 0.70              |
| 56:4:144:ILE:HG13 | 70:AI:52:ILE:HB    | 1.73                     | 0.70              |
| 48:w:561:A:H61    | 48:w:590:A2M:H2    | 1.55                     | 0.70              |
| 59:7:80:ARG:NH1   | 59:7:89:ILE:O      | 2.25                     | 0.70              |
| 73:AL:50:PHE:HE2  | 73:AL:55:TYR:HA    | 1.57                     | 0.70              |
| 3:D:4094:G:N1     | 3:D:4114:C:O2      | 2.17                     | 0.69              |
| 3:D:4494:OMG:HM21 | 26:a:22:VAL:HG11   | 1.74                     | 0.69              |
| 79:AR:120:ILE:HB  | 79:AR:132:TRP:HB2  | 1.72                     | 0.69              |
| 5:F:82:A:N7       | 29:d:50:ARG:NH2    | 2.40                     | 0.69              |
| 25:Z:44:GLN:OE1   | 25:Z:44:GLN:N      | 2.25                     | 0.69              |
| 70:AI:42:MET:HE2  | 70:AI:49:GLU:HA    | 1.72                     | 0.69              |
| 76:AO:40:ARG:HH21 | 76:AO:40:ARG:HG3   | 1.56                     | 0.69              |
| 48:w:1543:U:OP1   | 64:AC:37:ARG:NH1   | 2.25                     | 0.69              |
| 79:AR:249:CYS:HA  | 79:AR:258:ILE:HA   | 1.74                     | 0.69              |
| 60:8:35:ARG:NH2   | 60:8:55:TYR:O      | 2.25                     | 0.69              |
| 72:AK:55:ILE:HG22 | 72:AK:75:ILE:HA    | 1.72                     | 0.69              |
| 63:AB:134:GLY:HA2 | 63:AB:140:ARG:HG3  | 1.73                     | 0.69              |
| 64:AC:118:THR:O   | 64:AC:120:LEU:N    | 2.24                     | 0.69              |
| 66:AE:98:VAL:HG11 | 66:AE:106:LYS:HD2  | 1.75                     | 0.69              |
| 10:K:47:ASN:HB2   | 10:K:62:MET:HE2    | 1.74                     | 0.69              |
| 79:AR:5:MET:HE1   | 79:AR:258:ILE:HD13 | 1.75                     | 0.69              |
| 3:D:964:A:OP2     | 11:L:29:LYS:NZ     | 2.26                     | 0.69              |
| 48:w:153:G:N3     | 55:3:13:GLN:NE2    | 2.41                     | 0.69              |
| 3:D:4141:G:H5''   | 3:D:4142:C:H5'     | 1.74                     | 0.68              |
| 48:w:429:C:O2'    | 48:w:811:A:N1      | 2.26                     | 0.68              |
| 48:w:1452:A:H5''  | 65:AD:48:ASN:HD22  | 1.58                     | 0.68              |
| 48:w:96:C:O2      | 48:w:473:A:O2'     | 2.11                     | 0.68              |
| 61:9:46:THR:OG1   | 61:9:49:GLN:OE1    | 2.11                     | 0.68              |
| 62:AA:61:LYS:NZ   | 62:AA:80:ASP:OD2   | 2.17                     | 0.68              |
| 59:7:47:LYS:HE2   | 59:7:50:GLN:HE21   | 1.57                     | 0.68              |
| 79:AR:108:VAL:HA  | 79:AR:124:SER:HA   | 1.75                     | 0.68              |
| 48:w:57:U:O2'     | 48:w:499:G:N3      | 2.27                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:x:10:MET:HE3    | 49:x:15:VAL:HG12   | 1.76                     | 0.68              |
| 55:3:183:ARG:HA    | 55:3:186:GLN:HE22  | 1.57                     | 0.68              |
| 13:N:106:GLN:NE2   | 13:N:113:GLU:OE2   | 2.26                     | 0.68              |
| 14:O:79:SER:OG     | 14:O:147:HIS:ND1   | 2.24                     | 0.68              |
| 56:4:27:LEU:HA     | 56:4:30:LEU:HD23   | 1.76                     | 0.68              |
| 8:I:201:ARG:HH11   | 8:I:201:ARG:HG2    | 1.58                     | 0.68              |
| 65:AD:27:ASP:OD2   | 65:AD:30:THR:OG1   | 2.10                     | 0.68              |
| 66:AE:10:GLN:HB2   | 66:AE:57:GLY:HA2   | 1.76                     | 0.68              |
| 73:AL:50:PHE:HZ    | 73:AL:58:LEU:HD13  | 1.58                     | 0.68              |
| 51:z:257:LYS:O     | 69:AH:16:LYS:NZ    | 2.27                     | 0.67              |
| 52:0:67:ARG:NE     | 59:7:93:THR:O      | 2.23                     | 0.67              |
| 79:AR:129:ILE:HD13 | 79:AR:154:VAL:HG11 | 1.74                     | 0.67              |
| 50:y:107:ARG:NH2   | 62:AA:133:THR:O    | 2.27                     | 0.67              |
| 7:H:231:VAL:HG11   | 7:H:251:VAL:HG23   | 1.76                     | 0.67              |
| 55:3:136:LYS:HG3   | 55:3:174:PRO:HB2   | 1.76                     | 0.67              |
| 48:w:571:U:O2'     | 72:AK:60:PHE:O     | 2.13                     | 0.67              |
| 48:w:317:C:OP2     | 55:3:183:ARG:NH2   | 2.23                     | 0.67              |
| 48:w:894:G:H3'     | 48:w:895:G:H5''    | 1.75                     | 0.67              |
| 3:D:4694:G:O2'     | 13:N:71:ARG:NH2    | 2.28                     | 0.67              |
| 14:O:38:ARG:HD3    | 14:O:83:ASP:HB2    | 1.76                     | 0.67              |
| 10:K:101:ASN:OD1   | 10:K:105:ARG:NH2   | 2.27                     | 0.67              |
| 4:E:110:G:OP1      | 9:J:270:LYS:NZ     | 2.28                     | 0.66              |
| 64:AC:100:VAL:O    | 79:AR:57:ARG:NH2   | 2.28                     | 0.66              |
| 79:AR:107:ASP:OD2  | 79:AR:125:ARG:NH1  | 2.27                     | 0.66              |
| 13:N:92:MET:HE1    | 13:N:161:ILE:HG13  | 1.76                     | 0.66              |
| 49:x:38:ILE:HD11   | 49:x:47:TYR:HB3    | 1.78                     | 0.66              |
| 58:6:152:ASP:O     | 58:6:155:LYS:NZ    | 2.28                     | 0.66              |
| 3:D:5027:C:OP2     | 57:5:77:ARG:NH1    | 2.28                     | 0.66              |
| 48:w:616:A:H4'     | 78:AQ:81:ARG:NH1   | 2.09                     | 0.66              |
| 55:3:88:ARG:HB3    | 55:3:91:GLU:HB2    | 1.76                     | 0.66              |
| 16:Q:47:ALA:O      | 16:Q:49:ARG:N      | 2.28                     | 0.66              |
| 25:Z:65:ARG:HD3    | 25:Z:66:SER:O      | 1.95                     | 0.66              |
| 45:t:75:PRO:HA     | 45:t:78:ARG:HH22   | 1.59                     | 0.66              |
| 3:D:977:C:OP2      | 10:K:59:ARG:NH1    | 2.29                     | 0.66              |
| 61:9:130:LYS:NZ    | 61:9:137:PRO:O     | 2.27                     | 0.66              |
| 48:w:511:U:H2'     | 48:w:512:A2M:H8    | 1.77                     | 0.66              |
| 59:7:59:LYS:HG2    | 59:7:70:TYR:HB2    | 1.77                     | 0.66              |
| 3:D:4884:G:N7      | 10:K:272:ARG:NH2   | 2.44                     | 0.66              |
| 7:H:222:VAL:O      | 7:H:343:ARG:NH1    | 2.29                     | 0.66              |
| 25:Z:111:GLU:OE1   | 25:Z:113:ARG:NH2   | 2.28                     | 0.66              |
| 48:w:1236:G:O2'    | 63:AB:131:PRO:O    | 2.14                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:AB:48:GLY:O     | 63:AB:50:ARG:NH1   | 2.28                     | 0.66              |
| 3:D:182:G:N2       | 3:D:255:C:O2       | 2.29                     | 0.66              |
| 3:D:1676:C:O2'     | 3:D:3914:U:N3      | 2.28                     | 0.66              |
| 3:D:1962:A:OP2     | 3:D:2024:G:N1      | 2.26                     | 0.66              |
| 8:I:46:LYS:HD2     | 8:I:113:ARG:HD3    | 1.79                     | 0.66              |
| 48:w:1616:U:OP2    | 63:AB:43:ARG:NH2   | 2.28                     | 0.66              |
| 56:4:144:ILE:HG22  | 56:4:154:ILE:HG12  | 1.76                     | 0.66              |
| 48:w:120:U:H2'     | 48:w:121:OMU:H6    | 1.79                     | 0.65              |
| 62:AA:117:ARG:HH21 | 76:AO:40:ARG:HH12  | 1.43                     | 0.65              |
| 3:D:76:A:N7        | 16:Q:74:ARG:NH2    | 2.44                     | 0.65              |
| 3:D:1761:G:N2      | 3:D:1771:U:O2      | 2.27                     | 0.65              |
| 3:D:4875:G:H2'     | 23:X:169:THR:HG22  | 1.79                     | 0.65              |
| 26:a:45:ILE:HG21   | 26:a:53:PRO:HB3    | 1.78                     | 0.65              |
| 48:w:568:C:H42     | 48:w:582:C:H42     | 1.43                     | 0.65              |
| 48:w:1354:G:N2     | 48:w:1357:A:OP2    | 2.27                     | 0.65              |
| 24:Y:115:LYS:HG2   | 24:Y:126:VAL:HG11  | 1.78                     | 0.65              |
| 50:y:165:ARG:HA    | 50:y:168:MET:HB2   | 1.78                     | 0.65              |
| 48:w:29:G:OP1      | 71:AJ:124:LYS:NZ   | 2.25                     | 0.65              |
| 74:AM:43:ASN:HA    | 74:AM:66:LYS:HA    | 1.78                     | 0.65              |
| 48:w:525:A:H2'     | 48:w:526:A:H8      | 1.62                     | 0.65              |
| 50:y:175:GLU:OE1   | 50:y:175:GLU:N     | 2.29                     | 0.65              |
| 71:AJ:52:LEU:HD11  | 71:AJ:73:GLN:HB2   | 1.78                     | 0.65              |
| 3:D:491:G:H5'      | 8:I:268:ARG:HH12   | 1.62                     | 0.65              |
| 61:9:19:ARG:NH1    | 75:AN:84:HIS:OXT   | 2.30                     | 0.65              |
| 79:AR:2:THR:OG1    | 79:AR:313:THR:O    | 2.12                     | 0.65              |
| 79:AR:199:THR:HG21 | 79:AR:240:CYS:HA   | 1.79                     | 0.65              |
| 7:H:107:ALA:HB2    | 7:H:201:LEU:HD22   | 1.79                     | 0.65              |
| 48:w:1628:C:OP1    | 67:AF:38:LYS:NZ    | 2.26                     | 0.65              |
| 52:0:23:GLU:OE2    | 52:0:27:ARG:NH2    | 2.30                     | 0.65              |
| 54:2:27:ASP:OD2    | 54:2:107:ASN:ND2   | 2.30                     | 0.65              |
| 66:AE:136:THR:HA   | 66:AE:139:THR:HG23 | 1.79                     | 0.65              |
| 79:AR:184:LEU:HD21 | 79:AR:187:ASN:HD21 | 1.62                     | 0.65              |
| 48:w:291:G:H1'     | 48:w:292:A:H2'     | 1.78                     | 0.65              |
| 3:D:1447:C:H2'     | 3:D:1448:G:H8      | 1.62                     | 0.65              |
| 3:D:2562:G:O2'     | 3:D:2565:A:N6      | 2.30                     | 0.65              |
| 48:w:1373:C:OP1    | 65:AD:7:LYS:N      | 2.30                     | 0.64              |
| 56:4:31:GLU:HB2    | 56:4:41:ARG:NH1    | 2.12                     | 0.64              |
| 3:D:1699:A:H3'     | 3:D:1700:G:H5''    | 1.79                     | 0.64              |
| 18:S:138:PHE:HA    | 18:S:143:ARG:HD2   | 1.79                     | 0.64              |
| 55:3:37:ALA:HA     | 55:3:49:VAL:HG23   | 1.79                     | 0.64              |
| 73:AL:100:VAL:HB   | 73:AL:108:ILE:HG13 | 1.77                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:492:U:O2      | 3:D:663:G:N2      | 2.29                     | 0.64              |
| 3:D:2562:G:N2     | 3:D:2565:A:OP2    | 2.31                     | 0.64              |
| 3:D:4092:G:N3     | 3:D:4093:G:N2     | 2.36                     | 0.64              |
| 3:D:2703:G:OP1    | 25:Z:113:ARG:NH1  | 2.31                     | 0.64              |
| 15:P:118:LYS:HG3  | 15:P:119:TYR:H    | 1.61                     | 0.64              |
| 31:f:146:LEU:HD11 | 39:n:7:MET:HG2    | 1.79                     | 0.64              |
| 3:D:3651:A:OP2    | 6:G:200:ARG:NH1   | 2.31                     | 0.64              |
| 48:w:332:G:N7     | 55:3:189:ARG:NH2  | 2.42                     | 0.64              |
| 62:AA:30:VAL:HG12 | 62:AA:94:HIS:HB2  | 1.79                     | 0.64              |
| 67:AF:113:VAL:HA  | 67:AF:123:LEU:HA  | 1.80                     | 0.64              |
| 8:I:140:LYS:O     | 8:I:204:ARG:NH1   | 2.30                     | 0.64              |
| 56:4:29:GLU:HA    | 56:4:32:MET:HE1   | 1.80                     | 0.64              |
| 73:AL:40:VAL:HG23 | 73:AL:41:ARG:H    | 1.62                     | 0.64              |
| 3:D:184:U:O2      | 3:D:254:G:N2      | 2.30                     | 0.64              |
| 5:F:14:U:H5''     | 20:U:123:PRO:HD3  | 1.80                     | 0.64              |
| 56:4:36:LEU:HD21  | 56:4:40:LEU:HD23  | 1.79                     | 0.64              |
| 56:4:127:ASP:OD1  | 56:4:142:LYS:NZ   | 2.30                     | 0.64              |
| 64:AC:118:THR:OG1 | 64:AC:121:VAL:O   | 2.14                     | 0.64              |
| 3:D:1096:C:O2     | 3:D:1200:G:N2     | 2.31                     | 0.64              |
| 3:D:3681:G:OP2    | 6:G:128:ARG:NH1   | 2.31                     | 0.64              |
| 63:AB:96:VAL:HG11 | 63:AB:116:LEU:HG  | 1.80                     | 0.64              |
| 65:AD:37:GLU:OE2  | 65:AD:37:GLU:N    | 2.17                     | 0.64              |
| 16:Q:4:SER:O      | 31:f:44:ASN:ND2   | 2.31                     | 0.63              |
| 19:T:47:PHE:HZ    | 19:T:144:GLU:HG3  | 1.63                     | 0.63              |
| 58:6:75:ASN:OD1   | 58:6:79:ARG:NH1   | 2.31                     | 0.63              |
| 34:i:24:GLU:OE2   | 34:i:87:ARG:NH2   | 2.29                     | 0.63              |
| 51:z:166:ARG:HB3  | 51:z:247:THR:HG22 | 1.79                     | 0.63              |
| 3:D:2262:G:OP2    | 47:v:98:ARG:NH2   | 2.30                     | 0.63              |
| 48:w:643:A:OP1    | 58:6:39:ASN:ND2   | 2.31                     | 0.63              |
| 48:w:1289:U:H3    | 48:w:1310:U:H3    | 1.46                     | 0.63              |
| 60:8:88:ILE:HD11  | 60:8:109:MET:HE2  | 1.81                     | 0.63              |
| 67:AF:85:ASN:HB3  | 67:AF:88:MET:HB2  | 1.81                     | 0.63              |
| 3:D:1362:G:OP1    | 16:Q:39:ARG:NH2   | 2.31                     | 0.63              |
| 8:I:49:ARG:HH11   | 8:I:111:TRP:HB3   | 1.64                     | 0.63              |
| 48:w:383:G:H4'    | 60:8:132:ARG:HD2  | 1.81                     | 0.63              |
| 54:2:35:LEU:HD12  | 54:2:117:ILE:HD13 | 1.79                     | 0.63              |
| 3:D:967:C:O2'     | 3:D:969:C:OP2     | 2.16                     | 0.63              |
| 14:O:38:ARG:NH2   | 14:O:45:GLU:OE2   | 2.28                     | 0.63              |
| 9:J:271:MET:HE2   | 9:J:276:LYS:HG3   | 1.79                     | 0.63              |
| 41:p:40:ARG:NH1   | 41:p:41:TYR:OH    | 2.31                     | 0.63              |
| 54:2:47:LYS:NZ    | 64:AC:115:TYR:O   | 2.32                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:2601:A:N6     | 3:D:2744:A:OP2    | 2.31                     | 0.63              |
| 6:G:47:ASP:N      | 6:G:47:ASP:OD1    | 2.32                     | 0.63              |
| 11:L:105:VAL:HG13 | 11:L:136:VAL:HG12 | 1.81                     | 0.63              |
| 16:Q:46:ILE:HD11  | 16:Q:51:ALA:HA    | 1.80                     | 0.63              |
| 48:w:1003:U:H5''  | 50:y:165:ARG:NH2  | 2.14                     | 0.63              |
| 48:w:1619:A:OP2   | 63:AB:47:ARG:NH2  | 2.31                     | 0.63              |
| 54:2:87:LEU:HD11  | 64:AC:47:LEU:HD22 | 1.80                     | 0.63              |
| 56:4:32:MET:H     | 56:4:32:MET:HE3   | 1.62                     | 0.63              |
| 48:w:447:A:OP1    | 57:5:49:ARG:NH1   | 2.32                     | 0.63              |
| 3:D:4092:G:H1'    | 3:D:4093:G:H21    | 1.64                     | 0.62              |
| 3:D:515:C:H4'     | 3:D:516:C:OP1     | 1.97                     | 0.62              |
| 19:T:37:ARG:HD2   | 19:T:108:ILE:HD11 | 1.80                     | 0.62              |
| 25:Z:66:SER:OG    | 25:Z:67:LYS:N     | 2.32                     | 0.62              |
| 48:w:952:G:H21    | 62:AA:52:THR:HG21 | 1.64                     | 0.62              |
| 56:4:25:GLN:HA    | 56:4:28:LEU:HD22  | 1.81                     | 0.62              |
| 3:D:375:G:OP2     | 40:o:52:LYS:NZ    | 2.28                     | 0.62              |
| 3:D:1177:U:HO2'   | 9:J:286:SER:HG    | 1.46                     | 0.62              |
| 48:w:509:OMG:HM22 | 48:w:510:G:H5'    | 1.80                     | 0.62              |
| 3:D:4940:C:OP2    | 10:K:219:LYS:NZ   | 2.28                     | 0.62              |
| 48:w:570:C:O2'    | 72:AK:34:THR:O    | 2.17                     | 0.62              |
| 55:3:118:GLU:OE2  | 55:3:119:LYS:NZ   | 2.31                     | 0.62              |
| 79:AR:110:SER:OG  | 79:AR:155:ARG:NH2 | 2.32                     | 0.62              |
| 3:D:3612:C:H1'    | 3:D:5016:A:C8     | 2.34                     | 0.62              |
| 3:D:5016:A:H2     | 3:D:5033:G:H21    | 1.48                     | 0.62              |
| 9:J:256:LYS:H     | 9:J:256:LYS:HD2   | 1.64                     | 0.62              |
| 52:0:69:LEU:HA    | 52:0:72:VAL:HG12  | 1.81                     | 0.62              |
| 53:1:183:VAL:HG11 | 53:1:188:ASN:HB2  | 1.81                     | 0.62              |
| 58:6:55:LYS:HA    | 58:6:58:ARG:HG3   | 1.82                     | 0.62              |
| 51:z:77:SER:O     | 51:z:79:GLU:N     | 2.31                     | 0.62              |
| 53:1:230:LYS:H    | 53:1:235:TRP:HE1  | 1.46                     | 0.62              |
| 57:5:76:THR:OG1   | 57:5:105:ASP:OD1  | 2.17                     | 0.62              |
| 4:E:12:U:O3'      | 4:E:109:U:O2'     | 2.17                     | 0.62              |
| 48:w:568:C:H2'    | 48:w:569:A:C8     | 2.35                     | 0.62              |
| 65:AD:22:THR:O    | 79:AR:212:LYS:NZ  | 2.33                     | 0.62              |
| 53:1:63:LYS:NZ    | 72:AK:84:LYS:O    | 2.33                     | 0.62              |
| 3:D:496:G:H2'     | 3:D:497:G:C8      | 2.34                     | 0.62              |
| 12:M:131:LYS:NZ   | 12:M:132:ARG:O    | 2.33                     | 0.62              |
| 57:5:177:SER:OG   | 57:5:182:CYS:SG   | 2.57                     | 0.62              |
| 75:AN:67:THR:HG22 | 75:AN:69:GLY:H    | 1.64                     | 0.62              |
| 48:w:919:A:O2'    | 48:w:1020:A:N1    | 2.29                     | 0.61              |
| 54:2:168:THR:OG1  | 54:2:171:GLU:OE1  | 2.17                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4:37:LYS:O      | 56:4:39:GLN:NE2    | 2.33                     | 0.61              |
| 79:AR:111:VAL:HG12 | 79:AR:122:SER:HA   | 1.82                     | 0.61              |
| 15:P:56:THR:HG23   | 15:P:63:ARG:HA     | 1.82                     | 0.61              |
| 48:w:1155:U:OP1    | 51:z:185:THR:OG1   | 2.15                     | 0.61              |
| 55:3:186:GLN:O     | 55:3:190:ARG:N     | 2.22                     | 0.61              |
| 59:7:41:PRO:HD2    | 59:7:44:HIS:ND1    | 2.15                     | 0.61              |
| 67:AF:27:LYS:H     | 67:AF:27:LYS:HD3   | 1.65                     | 0.61              |
| 57:5:139:LYS:NZ    | 57:5:140:LYS:O     | 2.33                     | 0.61              |
| 64:AC:58:LEU:HB3   | 64:AC:62:ARG:HD2   | 1.82                     | 0.61              |
| 3:D:664:G:H2'      | 3:D:666:G:C8       | 2.35                     | 0.61              |
| 3:D:5040:U:OP2     | 7:H:396:ARG:NH2    | 2.33                     | 0.61              |
| 48:w:453:C:O2'     | 55:3:92:ARG:O      | 2.17                     | 0.61              |
| 3:D:1172:C:O2'     | 3:D:1189:G:N2      | 2.33                     | 0.61              |
| 35:j:89:LEU:HD13   | 35:j:118:LEU:HD22  | 1.83                     | 0.61              |
| 48:w:1630:A:OP1    | 66:AE:40:TYR:HB2   | 2.00                     | 0.61              |
| 60:8:91:ASP:OD1    | 60:8:104:LYS:NZ    | 2.26                     | 0.61              |
| 73:AL:69:THR:HB    | 73:AL:72:VAL:HG12  | 1.83                     | 0.61              |
| 48:w:165:G:N2      | 48:w:165:G:OP2     | 2.34                     | 0.61              |
| 54:2:140:ASP:HB2   | 76:AO:46:VAL:HG12  | 1.83                     | 0.61              |
| 59:7:76:ILE:H      | 59:7:76:ILE:HD12   | 1.66                     | 0.61              |
| 3:D:505:G:H1       | 3:D:653:U:H3       | 1.49                     | 0.61              |
| 3:D:736:C:OP1      | 17:R:74:ARG:NH1    | 2.33                     | 0.61              |
| 9:J:142:PHE:HE1    | 9:J:171:LEU:HD22   | 1.66                     | 0.61              |
| 11:L:28:LEU:HD23   | 11:L:32:ARG:HH12   | 1.65                     | 0.61              |
| 48:w:1139:C:H5     | 48:w:1149:A:H62    | 1.48                     | 0.61              |
| 48:w:1300:U:H3'    | 63:AB:51:ARG:HH12  | 1.66                     | 0.61              |
| 48:w:1673:U:H5''   | 64:AC:78:VAL:HG12  | 1.81                     | 0.61              |
| 55:3:49:VAL:HG12   | 55:3:115:LYS:HB3   | 1.81                     | 0.61              |
| 79:AR:296:GLN:HG2  | 79:AR:311:GLN:HE22 | 1.65                     | 0.61              |
| 25:Z:28:PRO:HB2    | 25:Z:34:MET:HG2    | 1.82                     | 0.60              |
| 48:w:1372:U:O2'    | 48:w:1373:C:O5'    | 2.18                     | 0.60              |
| 49:x:16:LEU:HD11   | 65:AD:114:LEU:HD12 | 1.82                     | 0.60              |
| 62:AA:42:VAL:HG23  | 62:AA:43:HIS:H     | 1.66                     | 0.60              |
| 79:AR:223:GLU:HB2  | 79:AR:225:LYS:HE3  | 1.82                     | 0.60              |
| 3:D:52:G:OP2       | 40:o:48:ASN:ND2    | 2.34                     | 0.60              |
| 3:D:1772:C:H2'     | 3:D:1773:OMU:H6    | 1.82                     | 0.60              |
| 23:X:127:MET:HB3   | 24:Y:153:PRO:HG2   | 1.81                     | 0.60              |
| 72:AK:106:GLN:NE2  | 72:AK:109:GLU:OE2  | 2.33                     | 0.60              |
| 3:D:4942:C:H5''    | 10:K:155:GLY:HA2   | 1.83                     | 0.60              |
| 6:G:27:ALA:O       | 6:G:128:ARG:NH2    | 2.33                     | 0.60              |
| 9:J:142:PHE:CE1    | 9:J:171:LEU:HD22   | 2.36                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:w:382:C:H2'    | 48:w:383:G:H8     | 1.67                     | 0.60              |
| 51:z:121:ARG:HH22 | 51:z:123:ARG:HD3  | 1.66                     | 0.60              |
| 3:D:2621:A:OP1    | 25:Z:80:LYS:NZ    | 2.33                     | 0.60              |
| 3:D:4993:G:H1     | 3:D:5058:A:H61    | 1.50                     | 0.60              |
| 48:w:616:A:H4'    | 78:AQ:81:ARG:CZ   | 2.31                     | 0.60              |
| 52:0:37:VAL:HG12  | 52:0:50:ILE:HA    | 1.82                     | 0.60              |
| 52:0:55:THR:HA    | 52:0:58:VAL:HG22  | 1.84                     | 0.60              |
| 3:D:2083:C:OP2    | 21:V:14:ARG:NH1   | 2.31                     | 0.60              |
| 27:b:3:VAL:HG11   | 27:b:12:LYS:HE3   | 1.83                     | 0.60              |
| 32:g:110:ALA:C    | 32:g:112:ILE:H    | 2.07                     | 0.60              |
| 62:AA:46:ASP:OD1  | 62:AA:48:SER:N    | 2.34                     | 0.60              |
| 14:O:146:GLU:CD   | 14:O:146:GLU:H    | 2.08                     | 0.60              |
| 48:w:1287:A:C5    | 48:w:1288:OMU:H1' | 2.37                     | 0.60              |
| 58:6:113:GLN:HG3  | 58:6:149:VAL:HG21 | 1.83                     | 0.60              |
| 3:D:1761:G:H1     | 3:D:1771:U:H3     | 1.48                     | 0.60              |
| 3:D:3710:G:H4'    | 3:D:3711:A:C8     | 2.36                     | 0.60              |
| 3:D:4125:C:H4'    | 12:M:45:ILE:HD11  | 1.83                     | 0.60              |
| 3:D:4635:A:H8     | 3:D:5048:A:H61    | 1.48                     | 0.60              |
| 48:w:1158:G:H5''  | 70:AI:76:SER:HB2  | 1.82                     | 0.60              |
| 58:6:136:ARG:NH1  | 58:6:159:PHE:O    | 2.34                     | 0.60              |
| 59:7:5:LYS:HA     | 59:7:8:ARG:HB2    | 1.83                     | 0.60              |
| 8:I:204:ARG:NH2   | 8:I:205:ARG:O     | 2.35                     | 0.60              |
| 48:w:943:U:OP1    | 50:y:214:LYS:NZ   | 2.33                     | 0.60              |
| 79:AR:72:SER:OG   | 79:AR:74:ASP:O    | 2.18                     | 0.60              |
| 3:D:1700:G:OP1    | 3:D:1704:C:N4     | 2.34                     | 0.60              |
| 48:w:291:G:N2     | 48:w:293:C:OP2    | 2.30                     | 0.60              |
| 48:w:1613:G:OP1   | 63:AB:42:ARG:NH1  | 2.32                     | 0.60              |
| 79:AR:104:HIS:CE1 | 79:AR:124:SER:HB3 | 2.37                     | 0.60              |
| 13:N:44:GLU:HB3   | 13:N:58:ASP:HB2   | 1.84                     | 0.60              |
| 48:w:496:C:OP2    | 53:1:49:ARG:NH1   | 2.35                     | 0.60              |
| 51:z:72:ASP:OD2   | 51:z:74:LYS:HG3   | 2.02                     | 0.60              |
| 55:3:45:TRP:HA    | 55:3:48:TYR:HE2   | 1.66                     | 0.60              |
| 68:AG:78:ASP:HB2  | 77:AP:54:LYS:HD2  | 1.84                     | 0.60              |
| 3:D:937:U:OP1     | 17:R:46:ARG:NH1   | 2.35                     | 0.59              |
| 14:O:33:ILE:HD12  | 14:O:33:ILE:O     | 2.03                     | 0.59              |
| 63:AB:110:GLU:OE2 | 63:AB:110:GLU:N   | 2.23                     | 0.59              |
| 66:AE:141:ARG:O   | 73:AL:28:GLY:N    | 2.35                     | 0.59              |
| 3:D:469:C:N3      | 10:K:105:ARG:NH1  | 2.50                     | 0.59              |
| 9:J:3:PHE:HD2     | 9:J:4:VAL:HG22    | 1.66                     | 0.59              |
| 53:1:106:LYS:HG3  | 53:1:108:ARG:H    | 1.66                     | 0.59              |
| 61:9:56:ASP:OD1   | 61:9:56:ASP:N     | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:AA:31:CYS:HB3  | 62:AA:95:ILE:HG22 | 1.84                     | 0.59              |
| 3:D:4474:A:H5''   | 43:r:125:LYS:HD2  | 1.83                     | 0.59              |
| 7:H:293:ILE:HG23  | 7:H:294:LYS:H     | 1.66                     | 0.59              |
| 49:x:80:ARG:NH2   | 49:x:165:ASN:O    | 2.35                     | 0.59              |
| 50:y:112:SER:O    | 50:y:115:LYS:NZ   | 2.33                     | 0.59              |
| 68:AG:93:SER:HB3  | 68:AG:97:ILE:HD11 | 1.84                     | 0.59              |
| 73:AL:62:VAL:O    | 73:AL:65:TYR:HB2  | 2.02                     | 0.59              |
| 3:D:491:G:H1      | 3:D:663:G:H1      | 1.49                     | 0.59              |
| 3:D:963:G:O6      | 3:D:2095:A:N6     | 2.35                     | 0.59              |
| 61:9:3:ARG:HG3    | 61:9:8:GLY:HA3    | 1.85                     | 0.59              |
| 69:AH:38:GLU:N    | 69:AH:38:GLU:OE2  | 2.35                     | 0.59              |
| 3:D:4754:G:N7     | 10:K:279:ASN:HB2  | 2.16                     | 0.59              |
| 20:U:9:GLU:OE1    | 20:U:9:GLU:N      | 2.26                     | 0.59              |
| 29:d:67:ILE:HD13  | 29:d:107:THR:HG21 | 1.83                     | 0.59              |
| 48:w:496:C:H5'    | 53:l:29:PRO:HG3   | 1.83                     | 0.59              |
| 48:w:927:C:O2     | 75:AN:51:GLN:NE2  | 2.35                     | 0.59              |
| 48:w:1550:G:H3'   | 48:w:1579:A:H61   | 1.68                     | 0.59              |
| 73:AL:50:PHE:CE2  | 73:AL:55:TYR:HA   | 2.36                     | 0.59              |
| 52:0:25:LEU:HD13  | 52:0:37:VAL:HG11  | 1.85                     | 0.59              |
| 6:G:137:ILE:HD11  | 6:G:149:LYS:HB2   | 1.85                     | 0.59              |
| 3:D:4894:A:H3'    | 3:D:4895:C:H5'    | 1.85                     | 0.59              |
| 35:j:79:VAL:HG23  | 35:j:84:GLU:HB2   | 1.85                     | 0.59              |
| 55:3:45:TRP:HA    | 55:3:48:TYR:CE2   | 2.38                     | 0.59              |
| 79:AR:61:GLY:O    | 79:AR:88:ARG:NH1  | 2.34                     | 0.59              |
| 3:D:662:C:H2'     | 3:D:663:G:C4      | 2.37                     | 0.59              |
| 3:D:1077:C:H4'    | 3:D:1215:C:N4     | 2.17                     | 0.59              |
| 3:D:1518:A:OP1    | 31:f:27:LYS:NZ    | 2.26                     | 0.59              |
| 53:l:44:LEU:HD21  | 53:l:72:ILE:HD11  | 1.85                     | 0.59              |
| 30:e:101:PHE:O    | 30:e:102:ARG:HD3  | 2.02                     | 0.59              |
| 48:w:172:OMU:N3   | 48:w:337:C:O2'    | 2.33                     | 0.59              |
| 56:4:31:GLU:HA    | 56:4:36:LEU:HD23  | 1.85                     | 0.59              |
| 6:G:101:VAL:HG22  | 6:G:165:VAL:HG22  | 1.84                     | 0.58              |
| 13:N:137:SER:HB3  | 13:N:143:GLU:HB3  | 1.85                     | 0.58              |
| 48:w:579:C:O2     | 72:AK:61:ARG:NH1  | 2.36                     | 0.58              |
| 3:D:2901:G:H1     | 3:D:3598:C:H42    | 1.49                     | 0.58              |
| 8:I:195:LYS:HB2   | 8:I:200:ARG:HD2   | 1.85                     | 0.58              |
| 33:h:34:THR:HG23  | 33:h:95:ALA:HB2   | 1.84                     | 0.58              |
| 48:w:525:A:OP2    | 78:AQ:99:LYS:NZ   | 2.35                     | 0.58              |
| 50:y:71:LEU:HD22  | 50:y:82:ARG:HB3   | 1.85                     | 0.58              |
| 72:AK:109:GLU:OE2 | 72:AK:113:ARG:NH2 | 2.36                     | 0.58              |
| 3:D:2557:G:H1     | 3:D:2570:U:H3     | 1.50                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:N:187:VAL:HG12  | 13:N:188:GLN:H     | 1.68                     | 0.58              |
| 48:w:493:A:H1'     | 48:w:574:A:H5'     | 1.85                     | 0.58              |
| 56:4:20:GLU:HA     | 56:4:23:ILE:HD13   | 1.85                     | 0.58              |
| 57:5:129:LEU:HG    | 57:5:132:GLU:HB2   | 1.84                     | 0.58              |
| 72:AK:29:HIS:ND1   | 72:AK:29:HIS:O     | 2.37                     | 0.58              |
| 48:w:1736:G:H2'    | 48:w:1737:G:C8     | 2.38                     | 0.58              |
| 72:AK:86:GLU:OE2   | 72:AK:90:ARG:NH1   | 2.36                     | 0.58              |
| 79:AR:87:LEU:HB2   | 79:AR:101:PHE:HB2  | 1.85                     | 0.58              |
| 79:AR:274:VAL:HG13 | 79:AR:276:SER:H    | 1.69                     | 0.58              |
| 3:D:1837:A:OP2     | 24:Y:130:ARG:NH2   | 2.35                     | 0.58              |
| 65:AD:106:LEU:HD23 | 65:AD:109:LEU:HD12 | 1.85                     | 0.58              |
| 30:e:50:PRO:HD3    | 30:e:68:ILE:HG12   | 1.85                     | 0.58              |
| 49:x:176:TRP:HE1   | 49:x:197:VAL:HG23  | 1.68                     | 0.58              |
| 20:U:111:SER:HB3   | 20:U:156:ILE:HD13  | 1.84                     | 0.58              |
| 53:1:185:GLY:N     | 53:1:189:LEU:HD13  | 2.19                     | 0.58              |
| 64:AC:40:GLU:H     | 64:AC:40:GLU:CD    | 2.12                     | 0.58              |
| 75:AN:11:SER:N     | 75:AN:14:GLU:OE2   | 2.36                     | 0.58              |
| 11:L:199:LYS:HE2   | 11:L:200:ARG:HD3   | 1.85                     | 0.58              |
| 48:w:600:G:H1      | 48:w:622:C:H5      | 1.50                     | 0.58              |
| 49:x:213:GLU:HA    | 49:x:216:ALA:HB3   | 1.85                     | 0.58              |
| 56:4:36:LEU:HG     | 56:4:39:GLN:HB2    | 1.84                     | 0.58              |
| 74:AM:43:ASN:OD1   | 74:AM:46:GLU:HG3   | 2.03                     | 0.58              |
| 76:AO:35:MET:HA    | 76:AO:38:THR:HG22  | 1.85                     | 0.58              |
| 79:AR:279:SER:HB2  | 79:AR:282:GLU:HB2  | 1.86                     | 0.58              |
| 55:3:186:GLN:HA    | 55:3:189:ARG:HB2   | 1.85                     | 0.58              |
| 58:6:115:PHE:HA    | 58:6:120:ALA:HB3   | 1.85                     | 0.58              |
| 68:AG:19:ARG:HB2   | 68:AG:117:ALA:HB2  | 1.85                     | 0.58              |
| 72:AK:110:ARG:HE   | 72:AK:126:GLY:HA3  | 1.69                     | 0.58              |
| 9:J:217:ASP:HA     | 9:J:220:LYS:HD3    | 1.85                     | 0.58              |
| 48:w:531:A:N6      | 48:w:552:G:O6      | 2.36                     | 0.58              |
| 48:w:566:U:H3      | 48:w:584:G:H1      | 1.52                     | 0.58              |
| 53:1:208:VAL:HB    | 53:1:225:ILE:HD11  | 1.84                     | 0.58              |
| 72:AK:40:ILE:H     | 72:AK:40:ILE:HD12  | 1.68                     | 0.58              |
| 5:F:110:U:H5''     | 42:q:8:ARG:NH2     | 2.16                     | 0.57              |
| 67:AF:60:THR:HG23  | 67:AF:75:MET:HE3   | 1.86                     | 0.57              |
| 12:M:90:GLN:OE1    | 12:M:90:GLN:N      | 2.35                     | 0.57              |
| 16:Q:64:VAL:HA     | 16:Q:67:HIS:CD2    | 2.38                     | 0.57              |
| 49:x:85:ARG:NH1    | 65:AD:81:ARG:O     | 2.37                     | 0.57              |
| 54:2:28:VAL:HG23   | 54:2:42:LYS:HE2    | 1.85                     | 0.57              |
| 55:3:135:PRO:HG2   | 55:3:141:ILE:HD12  | 1.86                     | 0.57              |
| 75:AN:83:GLN:NE2   | 75:AN:84:HIS:OXT   | 2.37                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:AR:197:THR:HG21 | 79:AR:238:ALA:HA   | 1.87                     | 0.57              |
| 3:D:2351:OMC:HM22  | 3:D:2352:U:H5'     | 1.86                     | 0.57              |
| 3:D:4546:A:N7      | 6:G:215:ASN:ND2    | 2.53                     | 0.57              |
| 52:0:40:ARG:NH1    | 68:AG:107:GLU:O    | 2.37                     | 0.57              |
| 60:8:119:ASP:O     | 60:8:147:LYS:NZ    | 2.37                     | 0.57              |
| 68:AG:40:ILE:HD11  | 68:AG:89:ILE:HG13  | 1.86                     | 0.57              |
| 74:AM:43:ASN:HB3   | 74:AM:66:LYS:HG2   | 1.86                     | 0.57              |
| 79:AR:244:ASN:HB3  | 79:AR:245:ARG:HE   | 1.68                     | 0.57              |
| 21:V:157:GLY:O     | 21:V:188:ASN:ND2   | 2.37                     | 0.57              |
| 43:r:127:VAL:HG13  | 43:r:128:LYS:HG2   | 1.86                     | 0.57              |
| 48:w:1434:C:H4'    | 48:w:1435:C:O5'    | 2.03                     | 0.57              |
| 61:9:56:ASP:OD2    | 75:AN:52:THR:OG1   | 2.21                     | 0.57              |
| 3:D:496:G:H2'      | 3:D:497:G:H8       | 1.68                     | 0.57              |
| 3:D:2838:G:H5'     | 7:H:247:GLY:HA2    | 1.87                     | 0.57              |
| 3:D:4740:G:H1'     | 3:D:4742:G:H5''    | 1.86                     | 0.57              |
| 48:w:824:C:C2      | 58:6:144:ILE:HD13  | 2.38                     | 0.57              |
| 56:4:10:LYS:HE3    | 56:4:20:GLU:HG3    | 1.86                     | 0.57              |
| 3:D:1498:G:OP1     | 21:V:150:ARG:NH1   | 2.37                     | 0.57              |
| 12:M:50:ASP:OD2    | 12:M:52:THR:HG23   | 2.05                     | 0.57              |
| 14:O:19:LYS:HA     | 14:O:23:CYS:SG     | 2.44                     | 0.57              |
| 3:D:3614:G:O2'     | 3:D:3615:G:OP1     | 2.18                     | 0.57              |
| 56:4:143:ARG:HB3   | 70:AI:51:GLU:OE1   | 2.05                     | 0.57              |
| 68:AG:24:LEU:O     | 68:AG:32:LEU:HD11  | 2.05                     | 0.57              |
| 3:D:4691:A:H5'     | 13:N:71:ARG:HH11   | 1.69                     | 0.57              |
| 48:w:1271:C:H42    | 48:w:1511:U:H3     | 1.51                     | 0.57              |
| 79:AR:214:GLY:HA2  | 79:AR:236:ILE:HG12 | 1.87                     | 0.57              |
| 3:D:2611:A:H5'     | 3:D:2688:G:H4'     | 1.85                     | 0.57              |
| 14:O:190:LEU:HB3   | 14:O:197:VAL:HG22  | 1.87                     | 0.57              |
| 20:U:9:GLU:H       | 20:U:9:GLU:CD      | 2.11                     | 0.57              |
| 55:3:136:LYS:HG2   | 55:3:176:ILE:HA    | 1.85                     | 0.57              |
| 3:D:478:G:OP1      | 47:v:66:ARG:NH2    | 2.24                     | 0.57              |
| 3:D:1202:C:N3      | 3:D:1203:G:O2'     | 2.36                     | 0.57              |
| 55:3:45:TRP:O      | 55:3:46:LYS:NZ     | 2.31                     | 0.57              |
| 3:D:320:C:OP1      | 39:n:84:LYS:NZ     | 2.35                     | 0.56              |
| 3:D:4092:G:H1'     | 3:D:4093:G:N2      | 2.20                     | 0.56              |
| 13:N:173:ARG:HB3   | 43:r:127:VAL:HB    | 1.85                     | 0.56              |
| 48:w:799:OMU:H5''  | 56:4:111:LYS:HE2   | 1.87                     | 0.56              |
| 53:1:107:GLY:HA2   | 53:1:189:LEU:HG    | 1.87                     | 0.56              |
| 58:6:124:HIS:CD2   | 78:AQ:108:ARG:HG3  | 2.40                     | 0.56              |
| 3:D:418:A:N6       | 5:F:16:G:H1'       | 2.20                     | 0.56              |
| 3:D:684:G:OP1      | 10:K:100:LYS:NZ    | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:66:SER:O      | 8:I:66:SER:OG     | 2.18                     | 0.56              |
| 15:P:113:ILE:HG12 | 15:P:125:ILE:HD11 | 1.87                     | 0.56              |
| 45:t:36:GLN:OE1   | 45:t:40:ARG:NH1   | 2.38                     | 0.56              |
| 48:w:122:G:H21    | 53:l:146:THR:HG21 | 1.69                     | 0.56              |
| 48:w:492:C:OP2    | 72:AK:107:ARG:NH2 | 2.38                     | 0.56              |
| 48:w:525:A:H5''   | 78:AQ:105:ALA:HB2 | 1.86                     | 0.56              |
| 49:x:81:ASN:HA    | 49:x:84:GLN:HG3   | 1.86                     | 0.56              |
| 51:z:121:ARG:HH12 | 51:z:123:ARG:HH21 | 1.52                     | 0.56              |
| 70:AI:28:ARG:HB3  | 70:AI:29:PRO:HD3  | 1.86                     | 0.56              |
| 79:AR:126:ASP:OD1 | 79:AR:128:THR:OG1 | 2.23                     | 0.56              |
| 3:D:4076:G:OP1    | 12:M:73:ARG:NE    | 2.28                     | 0.56              |
| 29:d:50:ARG:HG2   | 29:d:51:LYS:H     | 1.69                     | 0.56              |
| 29:d:88:GLU:N     | 29:d:88:GLU:OE2   | 2.37                     | 0.56              |
| 30:e:51:ARG:HB2   | 30:e:65:ARG:HG2   | 1.87                     | 0.56              |
| 47:v:97:ILE:HG21  | 47:v:107:ARG:HB3  | 1.87                     | 0.56              |
| 48:w:1568:C:OP1   | 67:AF:96:SER:OG   | 2.20                     | 0.56              |
| 48:w:1751:C:H42   | 48:w:1782:G:H1    | 1.54                     | 0.56              |
| 51:z:168:GLY:HA2  | 69:AH:1:MET:HE1   | 1.87                     | 0.56              |
| 59:7:16:PHE:CD2   | 59:7:79:LEU:HD11  | 2.40                     | 0.56              |
| 66:AE:53:THR:HG23 | 66:AE:54:LYS:HD2  | 1.86                     | 0.56              |
| 3:D:4378:A:O2'    | 3:D:4379:A:H2'    | 2.06                     | 0.56              |
| 6:G:28:ARG:HB2    | 6:G:123:ARG:HB3   | 1.86                     | 0.56              |
| 7:H:378:ARG:HG2   | 27:b:32:LEU:HD21  | 1.87                     | 0.56              |
| 22:W:170:ARG:HH21 | 22:W:173:ARG:HE   | 1.54                     | 0.56              |
| 52:0:28:GLU:OE2   | 52:0:65:ARG:NH2   | 2.36                     | 0.56              |
| 3:D:466:A:O2'     | 3:D:467:U:O4'     | 2.24                     | 0.56              |
| 3:D:2710:C:H2'    | 3:D:2712:G:H5'    | 1.86                     | 0.56              |
| 9:J:62:CYS:HB3    | 9:J:105:LEU:HD22  | 1.87                     | 0.56              |
| 25:Z:84:LYS:NZ    | 25:Z:102:VAL:O    | 2.38                     | 0.56              |
| 72:AK:7:ILE:HG23  | 72:AK:25:ILE:HG23 | 1.88                     | 0.56              |
| 29:d:26:ARG:O     | 29:d:30:MET:HG3   | 2.06                     | 0.56              |
| 55:3:57:ASP:OD2   | 55:3:98:ARG:HG3   | 2.05                     | 0.56              |
| 60:8:7:GLU:OE1    | 60:8:9:ALA:N      | 2.34                     | 0.56              |
| 60:8:136:LYS:O    | 60:8:139:ARG:NH1  | 2.37                     | 0.56              |
| 64:AC:101:ASP:O   | 64:AC:104:SER:OG  | 2.23                     | 0.56              |
| 73:AL:56:ASP:N    | 73:AL:56:ASP:OD1  | 2.39                     | 0.56              |
| 2:B:17:G:O2'      | 2:B:56:G:N2       | 2.30                     | 0.56              |
| 3:D:989:U:H3      | 3:D:1064:G:H1     | 1.52                     | 0.56              |
| 47:v:47:LYS:HB2   | 47:v:102:TYR:CZ   | 2.41                     | 0.56              |
| 48:w:148:U:H2'    | 48:w:149:A:H5''   | 1.87                     | 0.56              |
| 64:AC:99:TYR:O    | 79:AR:57:ARG:NH1  | 2.38                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 72:AK:29:HIS:O    | 72:AK:29:HIS:CG    | 2.59                     | 0.56              |
| 79:AR:11:LEU:HD13 | 79:AR:307:VAL:HG23 | 1.86                     | 0.56              |
| 14:O:31:ILE:HD12  | 14:O:65:LEU:HB3    | 1.88                     | 0.56              |
| 16:Q:65:ARG:HG3   | 31:f:69:PHE:CG     | 2.40                     | 0.56              |
| 48:w:913:A:N6     | 56:4:98:ARG:O      | 2.36                     | 0.56              |
| 48:w:1473:G:N2    | 48:w:1476:A:OP2    | 2.28                     | 0.56              |
| 48:w:1834:A:H2    | 48:w:1837:G:N1     | 2.01                     | 0.56              |
| 52:0:79:PHE:HE2   | 52:0:84:VAL:HB     | 1.70                     | 0.56              |
| 57:5:124:LYS:H    | 57:5:124:LYS:HD2   | 1.71                     | 0.56              |
| 65:AD:100:PRO:HD3 | 65:AD:119:VAL:HB   | 1.87                     | 0.56              |
| 68:AG:32:LEU:HD12 | 68:AG:87:ARG:HG3   | 1.87                     | 0.56              |
| 73:AL:68:ILE:HB   | 73:AL:109:TYR:HB2  | 1.87                     | 0.56              |
| 2:B:33:U:OP2      | 64:AC:146:ARG:NH1  | 2.39                     | 0.56              |
| 3:D:4093:G:H3'    | 3:D:4094:G:H8      | 1.71                     | 0.56              |
| 12:M:166:LEU:HD23 | 18:S:7:ILE:HG12    | 1.87                     | 0.56              |
| 48:w:1274:G:H4'   | 59:7:47:LYS:HZ2    | 1.71                     | 0.56              |
| 53:1:229:GLY:HA2  | 53:1:235:TRP:CD1   | 2.41                     | 0.56              |
| 55:3:2:LYS:HG2    | 55:3:17:GLU:HG3    | 1.88                     | 0.56              |
| 60:8:35:ARG:NE    | 60:8:53:GLY:O      | 2.38                     | 0.56              |
| 3:D:1777:C:O2'    | 9:J:2:GLY:HA2      | 2.06                     | 0.56              |
| 3:D:3641:U:H5     | 3:D:3646:A:N7      | 2.04                     | 0.56              |
| 9:J:124:GLU:O     | 9:J:126:THR:HG23   | 2.06                     | 0.56              |
| 68:AG:61:LEU:HB2  | 68:AG:82:MET:HB3   | 1.88                     | 0.56              |
| 3:D:2475:G:O6     | 28:c:48:ARG:NH2    | 2.39                     | 0.55              |
| 11:L:29:LYS:HD2   | 11:L:32:ARG:HH11   | 1.71                     | 0.55              |
| 31:f:90:ALA:HB3   | 31:f:120:GLN:HE21  | 1.72                     | 0.55              |
| 48:w:1520:G:O2'   | 48:w:1521:C:OP1    | 2.21                     | 0.55              |
| 48:w:1597:C:H4'   | 48:w:1603:G:C6     | 2.41                     | 0.55              |
| 48:w:1849:G:O2'   | 48:w:1850:MA6:H8   | 2.06                     | 0.55              |
| 53:1:92:ILE:HD11  | 72:AK:17:LEU:HD11  | 1.88                     | 0.55              |
| 55:3:70:HIS:HA    | 55:3:98:ARG:HH12   | 1.70                     | 0.55              |
| 79:AR:114:SER:OG  | 79:AR:116:ASP:OD1  | 2.23                     | 0.55              |
| 48:w:594:A:N6     | 48:w:643:A:H5''    | 2.19                     | 0.55              |
| 63:AB:81:ARG:HH12 | 63:AB:120:SER:HG   | 1.53                     | 0.55              |
| 66:AE:142:ARG:HA  | 73:AL:28:GLY:HA3   | 1.88                     | 0.55              |
| 79:AR:299:PHE:HD1 | 79:AR:309:VAL:HG12 | 1.71                     | 0.55              |
| 48:w:921:G:C6     | 70:AI:28:ARG:HD2   | 2.40                     | 0.55              |
| 51:z:200:ARG:O    | 58:6:58:ARG:NH2    | 2.39                     | 0.55              |
| 3:D:2485:U:H2'    | 3:D:2486:G:H8      | 1.71                     | 0.55              |
| 10:K:162:VAL:HG22 | 10:K:175:VAL:HG22  | 1.88                     | 0.55              |
| 48:w:1464:C:OP1   | 65:AD:63:ARG:NH2   | 2.36                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:3:39:ASP:OD1   | 55:3:47:GLY:N      | 2.40                     | 0.55              |
| 79:AR:285:GLN:HB3 | 79:AR:303:THR:HB   | 1.88                     | 0.55              |
| 10:K:162:VAL:HG23 | 10:K:177:GLY:H     | 1.71                     | 0.55              |
| 50:y:140:VAL:HG13 | 50:y:213:ARG:HB2   | 1.89                     | 0.55              |
| 79:AR:292:SER:HB2 | 79:AR:297:THR:HB   | 1.88                     | 0.55              |
| 3:D:165:A:H61     | 3:D:270:U:H3       | 1.55                     | 0.55              |
| 8:I:76:ILE:HD12   | 8:I:77:PRO:HD2     | 1.87                     | 0.55              |
| 8:I:218:ILE:HA    | 8:I:229:LEU:HD22   | 1.89                     | 0.55              |
| 16:Q:150:LEU:HD23 | 16:Q:154:VAL:HG12  | 1.88                     | 0.55              |
| 29:d:91:ASN:OD1   | 29:d:93:THR:HG23   | 2.07                     | 0.55              |
| 48:w:124:U:OP1    | 53:1:148:ARG:NH2   | 2.39                     | 0.55              |
| 53:1:198:ARG:HE   | 53:1:200:ARG:HE    | 1.52                     | 0.55              |
| 55:3:85:ARG:O     | 55:3:87:ARG:NH1    | 2.40                     | 0.55              |
| 79:AR:178:ASN:HB3 | 79:AR:183:LYS:H    | 1.72                     | 0.55              |
| 3:D:4717:A:OP2    | 7:H:30:LYS:NZ      | 2.36                     | 0.55              |
| 7:H:229:LYS:HG3   | 7:H:272:LYS:HD3    | 1.88                     | 0.55              |
| 79:AR:113:PHE:HE2 | 79:AR:117:ASN:HD22 | 1.54                     | 0.55              |
| 3:D:2743:A:O2'    | 6:G:21:LYS:NZ      | 2.40                     | 0.55              |
| 9:J:155:THR:OG1   | 9:J:179:ARG:NH2    | 2.39                     | 0.55              |
| 48:w:26:U:H2'     | 48:w:27:A2M:H8     | 1.87                     | 0.55              |
| 48:w:289:G:OP1    | 53:1:155:LYS:NZ    | 2.38                     | 0.55              |
| 53:1:189:LEU:O    | 53:1:245:ARG:NH2   | 2.39                     | 0.55              |
| 74:AM:18:VAL:HG21 | 74:AM:33:ASP:OD1   | 2.06                     | 0.55              |
| 77:AP:30:LEU:HA   | 77:AP:39:CYS:HA    | 1.89                     | 0.55              |
| 3:D:491:G:O6      | 3:D:662:C:N4       | 2.40                     | 0.55              |
| 18:S:68:ARG:NH1   | 18:S:124:ASP:O     | 2.35                     | 0.55              |
| 67:AF:112:MET:HE2 | 67:AF:112:MET:HA   | 1.88                     | 0.55              |
| 68:AG:22:ILE:HG13 | 68:AG:89:ILE:HB    | 1.88                     | 0.55              |
| 68:AG:107:GLU:HG2 | 68:AG:108:PRO:HD3  | 1.87                     | 0.55              |
| 65:AD:100:PRO:HG2 | 65:AD:121:GLN:HB3  | 1.90                     | 0.55              |
| 67:AF:18:LEU:HD11 | 67:AF:131:LEU:HD22 | 1.88                     | 0.55              |
| 79:AR:201:SER:OG  | 79:AR:203:ASP:OD1  | 2.16                     | 0.55              |
| 3:D:1574:G:O2'    | 3:D:1575:A:O5'     | 2.22                     | 0.54              |
| 3:D:2472:A:H1'    | 28:c:48:ARG:HB3    | 1.88                     | 0.54              |
| 48:w:436:OMG:OP2  | 48:w:471:G:O2'     | 2.25                     | 0.54              |
| 55:3:12:CYS:HB3   | 55:3:124:LEU:HD22  | 1.89                     | 0.54              |
| 56:4:21:SER:O     | 56:4:24:SER:OG     | 2.17                     | 0.54              |
| 79:AR:147:HIS:HB2 | 79:AR:171:ASP:HB2  | 1.88                     | 0.54              |
| 3:D:1194:G:H2'    | 3:D:1195:G:C8      | 2.42                     | 0.54              |
| 3:D:1408:G:H1'    | 3:D:1411:C:H42     | 1.72                     | 0.54              |
| 3:D:2899:C:OP1    | 22:W:108:ARG:NH2   | 2.35                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:Z:23:LEU:HD11  | 25:Z:83:LEU:HD12  | 1.89                     | 0.54              |
| 48:w:155:G:N2     | 55:3:56:ASN:OD1   | 2.35                     | 0.54              |
| 48:w:505:G:O2'    | 48:w:506:G:O5'    | 2.23                     | 0.54              |
| 56:4:8:ILE:HG22   | 56:4:9:VAL:HG23   | 1.88                     | 0.54              |
| 56:4:12:ASN:ND2   | 56:4:14:GLU:O     | 2.40                     | 0.54              |
| 3:D:1319:U:OP2    | 31:f:22:ILE:HG22  | 2.07                     | 0.54              |
| 48:w:1552:G:H8    | 52:0:3:VAL:HG11   | 1.72                     | 0.54              |
| 63:AB:38:SER:OG   | 63:AB:41:GLN:OE1  | 2.25                     | 0.54              |
| 21:V:39:THR:HG22  | 21:V:41:SER:H     | 1.72                     | 0.54              |
| 29:d:30:MET:HB3   | 29:d:101:PRO:HG2  | 1.90                     | 0.54              |
| 52:0:79:PHE:CE2   | 52:0:84:VAL:HB    | 2.42                     | 0.54              |
| 53:1:100:ARG:NH2  | 53:1:121:TYR:O    | 2.41                     | 0.54              |
| 58:6:114:VAL:HG13 | 58:6:126:ALA:HB1  | 1.89                     | 0.54              |
| 69:AH:80:SER:O    | 69:AH:83:PHE:N    | 2.39                     | 0.54              |
| 3:D:1372:A:OP1    | 18:S:202:ARG:NH2  | 2.38                     | 0.54              |
| 3:D:1771:U:H2'    | 3:D:1772:C:C6     | 2.43                     | 0.54              |
| 43:r:99:CYS:HB2   | 43:r:115:CYS:HB3  | 1.90                     | 0.54              |
| 48:w:974:C:O2     | 62:AA:55:ARG:NH1  | 2.41                     | 0.54              |
| 52:0:210:ILE:HD13 | 65:AD:16:ILE:HG22 | 1.89                     | 0.54              |
| 65:AD:23:ARG:HB2  | 79:AR:170:TRP:HZ3 | 1.72                     | 0.54              |
| 3:D:3811:G:O2'    | 3:D:3814:U:OP2    | 2.25                     | 0.54              |
| 3:D:4472:G:O2'    | 43:r:100:TYR:O    | 2.23                     | 0.54              |
| 48:w:294:U:OP1    | 60:8:36:TYR:OH    | 2.18                     | 0.54              |
| 50:y:47:THR:OG1   | 50:y:65:ARG:NH1   | 2.40                     | 0.54              |
| 56:4:100:ILE:HG12 | 56:4:125:VAL:HG21 | 1.90                     | 0.54              |
| 58:6:70:ARG:HH22  | 58:6:94:LEU:HD21  | 1.73                     | 0.54              |
| 3:D:114:G:N2      | 3:D:158:A:H61     | 2.06                     | 0.54              |
| 48:w:11:A:H8      | 48:w:1357:A:O2'   | 1.90                     | 0.54              |
| 48:w:372:U:OP1    | 60:8:136:LYS:NZ   | 2.29                     | 0.54              |
| 54:2:102:LEU:HD11 | 73:AL:67:LEU:HD13 | 1.90                     | 0.54              |
| 73:AL:50:PHE:CE1  | 73:AL:83:LEU:HD21 | 2.43                     | 0.54              |
| 3:D:1759:G:H1     | 3:D:1773:OMU:C2   | 2.20                     | 0.54              |
| 12:M:90:GLN:CD    | 12:M:90:GLN:H     | 2.16                     | 0.54              |
| 20:U:22:LEU:HD13  | 20:U:90:PHE:CD2   | 2.42                     | 0.54              |
| 48:w:379:C:OP1    | 57:5:56:ARG:NH1   | 2.41                     | 0.54              |
| 48:w:884:C:N3     | 48:w:902:G:N1     | 2.43                     | 0.54              |
| 49:x:85:ARG:HD2   | 65:AD:81:ARG:HD2  | 1.89                     | 0.54              |
| 79:AR:16:GLY:C    | 79:AR:305:ASN:HB3 | 2.33                     | 0.54              |
| 79:AR:35:SER:OG   | 79:AR:36:ARG:N    | 2.40                     | 0.54              |
| 31:f:72:THR:HG22  | 31:f:110:LYS:HB3  | 1.90                     | 0.54              |
| 36:k:78:HIS:HB3   | 36:k:83:MET:O     | 2.08                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:3:87:ARG:N      | 55:3:91:GLU:OE1   | 2.38                     | 0.54              |
| 62:AA:117:ARG:HH12 | 74:AM:48:ALA:HB3  | 1.73                     | 0.54              |
| 68:AG:56:MET:HA    | 68:AG:56:MET:HE2  | 1.89                     | 0.54              |
| 2:C:17:G:O2'       | 2:C:56:G:N2       | 2.27                     | 0.54              |
| 3:D:2578:G:N7      | 30:e:17:ARG:NH1   | 2.56                     | 0.54              |
| 48:w:39:A:H62      | 48:w:515:G:H21    | 1.56                     | 0.54              |
| 48:w:371:A:OP2     | 57:5:10:LYS:HB2   | 2.08                     | 0.54              |
| 5:F:127:U:O2'      | 5:F:128:C:H6      | 1.90                     | 0.53              |
| 8:I:7:LEU:HG       | 8:I:21:ASN:HB3    | 1.90                     | 0.53              |
| 17:R:96:GLU:OE2    | 17:R:100:ARG:NH2  | 2.40                     | 0.53              |
| 50:y:230:GLU:N     | 50:y:230:GLU:OE2  | 2.39                     | 0.53              |
| 56:4:153:LEU:HD11  | 56:4:186:ASN:OD1  | 2.07                     | 0.53              |
| 57:5:81:VAL:HG12   | 57:5:102:VAL:HG12 | 1.90                     | 0.53              |
| 59:7:52:LEU:HD22   | 59:7:55:ARG:HH21  | 1.73                     | 0.53              |
| 72:AK:38:THR:OG1   | 72:AK:39:GLU:OE1  | 2.26                     | 0.53              |
| 79:AR:56:GLN:HG2   | 79:AR:57:ARG:H    | 1.71                     | 0.53              |
| 2:B:52:G:H2'       | 2:B:53:5MU:C6     | 2.44                     | 0.53              |
| 48:w:1161:U:O4     | 71:AJ:3:LYS:NZ    | 2.41                     | 0.53              |
| 51:z:196:ILE:HB    | 51:z:223:TYR:HB2  | 1.90                     | 0.53              |
| 53:1:73:ASP:HB3    | 53:1:164:LEU:HD22 | 1.90                     | 0.53              |
| 72:AK:51:THR:HG22  | 72:AK:53:ASP:H    | 1.72                     | 0.53              |
| 3:D:4424:A:OP2     | 43:r:97:ARG:NH2   | 2.41                     | 0.53              |
| 17:R:8:GLU:HB3     | 23:X:151:LYS:HG3  | 1.91                     | 0.53              |
| 48:w:1648:G:N7     | 64:AC:17:LYS:HD3  | 2.23                     | 0.53              |
| 49:x:104:THR:O     | 49:x:107:THR:OG1  | 2.23                     | 0.53              |
| 64:AC:61:GLU:OE1   | 64:AC:61:GLU:N    | 2.42                     | 0.53              |
| 3:D:2814:C:H5'     | 3:D:2815:A2M:OP2  | 2.09                     | 0.53              |
| 48:w:838:G:N2      | 48:w:840:C:O2'    | 2.41                     | 0.53              |
| 48:w:1597:C:O2'    | 48:w:1598:G:O4'   | 2.27                     | 0.53              |
| 48:w:1672:U:OP1    | 64:AC:18:THR:OG1  | 2.23                     | 0.53              |
| 51:z:229:CYS:O     | 51:z:232:THR:HG22 | 2.08                     | 0.53              |
| 57:5:89:GLU:O      | 57:5:93:THR:HG22  | 2.09                     | 0.53              |
| 59:7:14:LEU:HA     | 59:7:17:LYS:HE3   | 1.90                     | 0.53              |
| 3:D:4084:G:O6      | 6:G:72:ARG:NH2    | 2.37                     | 0.53              |
| 33:h:105:ILE:HG13  | 33:h:106:ARG:HD3  | 1.91                     | 0.53              |
| 48:w:885:U:H3      | 48:w:901:G:H1     | 1.57                     | 0.53              |
| 48:w:1274:G:H4'    | 59:7:47:LYS:NZ    | 2.23                     | 0.53              |
| 48:w:1519:U:O2'    | 48:w:1520:G:H5'   | 2.08                     | 0.53              |
| 53:1:103:TYR:HD2   | 53:1:182:MET:HE2  | 1.73                     | 0.53              |
| 3:D:968:C:OP2      | 10:K:110:ARG:NH2  | 2.41                     | 0.53              |
| 3:D:1447:C:H2'     | 3:D:1448:G:C8     | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1553:A:N6     | 3:D:1574:G:H1'    | 2.23                     | 0.53              |
| 5:F:96:C:H5''     | 38:m:66:LYS:HD2   | 1.89                     | 0.53              |
| 20:U:22:LEU:HD13  | 20:U:90:PHE:HD2   | 1.74                     | 0.53              |
| 48:w:1693:G:H21   | 48:w:1834:A:H8    | 1.57                     | 0.53              |
| 61:9:18:TYR:OH    | 70:AI:54:ASP:OD1  | 2.22                     | 0.53              |
| 3:D:121:A:OP1     | 12:M:110:LYS:NZ   | 2.41                     | 0.53              |
| 21:V:63:LEU:HB2   | 21:V:88:ASP:HA    | 1.91                     | 0.53              |
| 48:w:681:PSU:H4'  | 71:AJ:9:THR:HG22  | 1.91                     | 0.53              |
| 48:w:918:U:P      | 61:9:64:ARG:HH12  | 2.32                     | 0.53              |
| 48:w:1674:G:H4'   | 54:2:77:MET:HE1   | 1.90                     | 0.53              |
| 48:w:1734:G:H21   | 48:w:1800:A:H2    | 1.55                     | 0.53              |
| 55:3:182:PRO:HA   | 55:3:185:LEU:HD12 | 1.91                     | 0.53              |
| 55:3:193:ALA:HA   | 55:3:196:LYS:HE3  | 1.89                     | 0.53              |
| 58:6:94:LEU:HD23  | 58:6:94:LEU:H     | 1.74                     | 0.53              |
| 72:AK:54:VAL:HG22 | 72:AK:76:TYR:HB2  | 1.91                     | 0.53              |
| 76:AO:40:ARG:HG3  | 76:AO:40:ARG:NH2  | 2.24                     | 0.53              |
| 3:D:37:U:H4'      | 31:f:32:ARG:HD2   | 1.91                     | 0.53              |
| 5:F:75:OMG:OP2    | 29:d:74:TYR:OH    | 2.23                     | 0.53              |
| 9:J:291:GLN:CA    | 9:J:291:GLN:HE21  | 2.22                     | 0.53              |
| 38:m:107:GLN:NE2  | 38:m:111:GLU:OE1  | 2.39                     | 0.53              |
| 48:w:1471:C:H42   | 48:w:1476:A:H62   | 1.56                     | 0.53              |
| 53:1:160:ILE:HD12 | 53:1:169:ILE:HG22 | 1.91                     | 0.53              |
| 55:3:18:VAL:HG11  | 55:3:24:LEU:HD21  | 1.91                     | 0.53              |
| 55:3:217:MET:HE2  | 55:3:217:MET:C    | 2.34                     | 0.53              |
| 79:AR:14:HIS:HE1  | 79:AR:35:SER:HB2  | 1.71                     | 0.53              |
| 3:D:1821:G:N3     | 3:D:1821:G:H2'    | 2.24                     | 0.53              |
| 3:D:2415:OMU:H3'  | 3:D:2416:G:N2     | 2.24                     | 0.53              |
| 19:T:5:GLN:HG3    | 19:T:6:VAL:HG23   | 1.91                     | 0.53              |
| 48:w:935:G:O2'    | 61:9:108:ASP:OD1  | 2.23                     | 0.53              |
| 48:w:1425:G:O3'   | 64:AC:33:LYS:NZ   | 2.29                     | 0.53              |
| 49:x:12:GLU:O     | 49:x:15:VAL:HG22  | 2.09                     | 0.53              |
| 53:1:180:LEU:HG   | 53:1:232:ASN:HA   | 1.91                     | 0.53              |
| 7:H:28:LYS:HG3    | 7:H:30:LYS:HG3    | 1.91                     | 0.53              |
| 48:w:144:U:O4     | 55:3:178:ARG:NH2  | 2.42                     | 0.53              |
| 48:w:1291:A:OP2   | 48:w:1302:G:O2'   | 2.27                     | 0.53              |
| 55:3:4:ASN:HB3    | 55:3:110:ASN:HA   | 1.91                     | 0.53              |
| 55:3:194:LEU:CA   | 55:3:197:GLN:HE22 | 2.20                     | 0.53              |
| 55:3:159:ARG:HB2  | 55:3:171:THR:HG22 | 1.91                     | 0.52              |
| 59:7:64:TRP:CD2   | 77:AP:23:VAL:HG12 | 2.43                     | 0.52              |
| 71:AJ:49:GLY:N    | 71:AJ:99:GLU:OE1  | 2.42                     | 0.52              |
| 3:D:661:C:H2'     | 3:D:662:C:C6      | 2.43                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D:4093:G:H3'     | 3:D:4094:G:C8      | 2.44                     | 0.52              |
| 22:W:170:ARG:CZ    | 22:W:170:ARG:HA    | 2.39                     | 0.52              |
| 23:X:99:ASP:OD1    | 23:X:100:LEU:N     | 2.39                     | 0.52              |
| 48:w:290:U:O2'     | 48:w:292:A:N7      | 2.34                     | 0.52              |
| 50:y:139:CYS:SG    | 50:y:172:MET:HE2   | 2.50                     | 0.52              |
| 56:4:60:ILE:HD11   | 56:4:92:VAL:HG12   | 1.90                     | 0.52              |
| 58:6:84:ILE:HA     | 58:6:150:ARG:HA    | 1.90                     | 0.52              |
| 59:7:25:LYS:HB3    | 59:7:67:PHE:HE2    | 1.74                     | 0.52              |
| 75:AN:37:CYS:HB3   | 75:AN:63:LEU:HD11  | 1.91                     | 0.52              |
| 2:B:17:G:HO2'      | 2:B:56:G:H22       | 1.55                     | 0.52              |
| 3:D:699:C:O2'      | 3:D:968:C:O2       | 2.27                     | 0.52              |
| 3:D:1406:G:H2'     | 3:D:1407:C:C5      | 2.45                     | 0.52              |
| 3:D:1697:G:H22     | 3:D:2084:C:P       | 2.32                     | 0.52              |
| 14:O:214:SER:OXT   | 14:O:214:SER:OG    | 2.26                     | 0.52              |
| 48:w:603:C:N4      | 48:w:620:G:O6      | 2.41                     | 0.52              |
| 51:z:256:TRP:CD2   | 70:AI:68:ARG:HD3   | 2.45                     | 0.52              |
| 70:AI:27:ILE:HB    | 70:AI:61:ILE:CG2   | 2.39                     | 0.52              |
| 79:AR:152:SER:H    | 79:AR:169:GLY:HA2  | 1.74                     | 0.52              |
| 9:J:59:ASP:OD2     | 9:J:81:HIS:ND1     | 2.34                     | 0.52              |
| 12:M:140:VAL:HG21  | 12:M:166:LEU:O     | 2.10                     | 0.52              |
| 49:x:137:ALA:HB1   | 49:x:142:LEU:HB3   | 1.91                     | 0.52              |
| 57:5:41:ARG:HD3    | 57:5:43:ILE:HD12   | 1.91                     | 0.52              |
| 57:5:116:HIS:HD1   | 57:5:117:TYR:HD1   | 1.56                     | 0.52              |
| 79:AR:199:THR:OG1  | 79:AR:239:LEU:O    | 2.22                     | 0.52              |
| 3:D:150:U:H3       | 12:M:162:ASP:HB2   | 1.74                     | 0.52              |
| 3:D:2485:U:H2'     | 3:D:2486:G:C8      | 2.44                     | 0.52              |
| 3:D:730:G:OP2      | 11:L:76:ARG:NE     | 2.41                     | 0.52              |
| 17:R:41:PRO:HG3    | 17:R:73:VAL:HG23   | 1.91                     | 0.52              |
| 26:a:107:ASN:OD1   | 26:a:108:ASN:N     | 2.42                     | 0.52              |
| 33:h:47:ILE:HD12   | 33:h:94:LEU:HD11   | 1.91                     | 0.52              |
| 48:w:165:G:H2'     | 48:w:166:A2M:H8    | 1.92                     | 0.52              |
| 48:w:1597:C:OP1    | 66:AE:25:LYS:NZ    | 2.33                     | 0.52              |
| 66:AE:65:GLU:O     | 66:AE:69:THR:HG22  | 2.10                     | 0.52              |
| 79:AR:289:LEU:HD22 | 79:AR:298:LEU:HD21 | 1.92                     | 0.52              |
| 3:D:3612:C:H1'     | 3:D:5016:A:H8      | 1.74                     | 0.52              |
| 48:w:25:A:HO2'     | 48:w:26:U:H6       | 1.58                     | 0.52              |
| 48:w:33:G:H1       | 48:w:522:A:H8      | 1.56                     | 0.52              |
| 54:2:168:THR:N     | 54:2:171:GLU:OE2   | 2.33                     | 0.52              |
| 55:3:136:LYS:HA    | 55:3:176:ILE:HG22  | 1.91                     | 0.52              |
| 3:D:1408:G:O2'     | 3:D:1411:C:N4      | 2.43                     | 0.52              |
| 48:w:198:U:O2'     | 48:w:202:G:O6      | 2.26                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:w:465:A:H4'    | 48:w:466:G:O5'     | 2.10                     | 0.52              |
| 52:0:64:ARG:O     | 52:0:68:GLU:HB2    | 2.10                     | 0.52              |
| 58:6:75:ASN:HA    | 58:6:78:LEU:HB2    | 1.92                     | 0.52              |
| 61:9:75:LEU:HD22  | 61:9:80:LEU:HD11   | 1.92                     | 0.52              |
| 3:D:4988:U:H1'    | 3:D:4991:U:O2      | 2.10                     | 0.52              |
| 7:H:47:LEU:HD11   | 7:H:181:MET:SD     | 2.49                     | 0.52              |
| 8:I:106:LYS:HD3   | 8:I:108:TRP:CZ2    | 2.45                     | 0.52              |
| 10:K:250:GLN:NE2  | 10:K:254:ASP:OD2   | 2.41                     | 0.52              |
| 13:N:120:GLU:OE2  | 13:N:124:ARG:NH1   | 2.36                     | 0.52              |
| 20:U:4:TYR:OH     | 20:U:18:ARG:HG3    | 2.10                     | 0.52              |
| 53:1:56:LEU:N     | 53:1:60:GLU:OE2    | 2.41                     | 0.52              |
| 65:AD:106:LEU:HA  | 65:AD:109:LEU:HB2  | 1.91                     | 0.52              |
| 66:AE:60:THR:OG1  | 66:AE:62:ASP:OD1   | 2.28                     | 0.52              |
| 3:D:505:G:H22     | 3:D:653:U:H3       | 1.58                     | 0.52              |
| 48:w:91:A:OP1     | 53:1:7:LYS:NZ      | 2.43                     | 0.52              |
| 48:w:826:A:O2'    | 58:6:11:LYS:NZ     | 2.41                     | 0.52              |
| 49:x:200:ASP:OD1  | 49:x:200:ASP:N     | 2.43                     | 0.52              |
| 55:3:147:LEU:HD21 | 55:3:156:TYR:CZ    | 2.45                     | 0.52              |
| 56:4:31:GLU:HB2   | 56:4:41:ARG:HH11   | 1.75                     | 0.52              |
| 67:AF:1:MET:HE1   | 67:AF:139:ALA:HB3  | 1.92                     | 0.52              |
| 79:AR:73:SER:H    | 79:AR:117:ASN:HD21 | 1.58                     | 0.52              |
| 3:D:1271:G:O2'    | 11:L:34:ARG:NH2    | 2.35                     | 0.51              |
| 6:G:120:PRO:HA    | 6:G:162:ASN:HB3    | 1.91                     | 0.51              |
| 7:H:396:ARG:NH1   | 7:H:396:ARG:HB3    | 2.25                     | 0.51              |
| 17:R:25:VAL:HG12  | 17:R:45:VAL:HG21   | 1.92                     | 0.51              |
| 21:V:16:LYS:O     | 21:V:33:ARG:NH2    | 2.41                     | 0.51              |
| 36:k:78:HIS:HB2   | 36:k:85:ARG:HG3    | 1.92                     | 0.51              |
| 48:w:551:U:O2'    | 78:AQ:117:ASN:ND2  | 2.37                     | 0.51              |
| 48:w:1351:G:O2'   | 48:w:1378:A:N1     | 2.39                     | 0.51              |
| 48:w:1395:C:O2'   | 48:w:1396:A:OP1    | 2.25                     | 0.51              |
| 48:w:1409:A:H61   | 48:w:1432:U:H3     | 1.58                     | 0.51              |
| 52:0:22:ASN:O     | 52:0:26:THR:HG22   | 2.10                     | 0.51              |
| 53:1:116:PRO:O    | 53:1:120:LYS:NZ    | 2.39                     | 0.51              |
| 79:AR:49:GLU:C    | 79:AR:51:ASN:H     | 2.18                     | 0.51              |
| 2:B:52:G:H2'      | 2:B:53:5MU:H6      | 1.75                     | 0.51              |
| 3:D:967:C:H2'     | 10:K:110:ARG:HH12  | 1.74                     | 0.51              |
| 12:M:159:HIS:ND1  | 12:M:185:LYS:HA    | 2.25                     | 0.51              |
| 12:M:165:GLU:C    | 12:M:167:VAL:H     | 2.19                     | 0.51              |
| 48:w:1861:G:H5''  | 74:AM:3:LYS:HA     | 1.93                     | 0.51              |
| 79:AR:27:PHE:HB3  | 79:AR:30:MET:HB3   | 1.91                     | 0.51              |
| 3:D:4537:C:H2'    | 3:D:4538:G:C8      | 2.45                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:R:112:VAL:HG11 | 19:T:201:LEU:HD21  | 1.93                     | 0.51              |
| 41:p:5:ILE:HD11   | 41:p:11:PHE:HD1    | 1.75                     | 0.51              |
| 48:w:3:C:O2       | 58:6:18:ARG:NH1    | 2.30                     | 0.51              |
| 53:1:204:SER:OG   | 53:1:205:PHE:N     | 2.41                     | 0.51              |
| 79:AR:68:ASP:HB2  | 79:AR:110:SER:HA   | 1.92                     | 0.51              |
| 79:AR:143:GLN:NE2 | 79:AR:145:GLU:OE2  | 2.43                     | 0.51              |
| 3:D:490:C:H2'     | 3:D:491:G:C8       | 2.45                     | 0.51              |
| 3:D:1082:C:O2'    | 3:D:1083:U:O5'     | 2.27                     | 0.51              |
| 3:D:2095:A:H4'    | 3:D:2096:G:N7      | 2.26                     | 0.51              |
| 3:D:2724:G:O2'    | 3:D:2726:G:OP2     | 2.25                     | 0.51              |
| 25:Z:38:ASN:OD1   | 25:Z:38:ASN:N      | 2.41                     | 0.51              |
| 25:Z:45:GLU:CD    | 25:Z:45:GLU:H      | 2.18                     | 0.51              |
| 48:w:1751:C:N4    | 48:w:1782:G:H1     | 2.08                     | 0.51              |
| 63:AB:23:ASP:OD1  | 63:AB:24:GLN:N     | 2.44                     | 0.51              |
| 72:AK:23:MET:C    | 72:AK:23:MET:HE2   | 2.36                     | 0.51              |
| 79:AR:149:GLU:N   | 79:AR:171:ASP:OD2  | 2.37                     | 0.51              |
| 3:D:1754:U:H3     | 3:D:1776:A:H61     | 1.58                     | 0.51              |
| 21:V:53:MET:O     | 21:V:58:ARG:NH1    | 2.43                     | 0.51              |
| 48:w:1232:PSU:H2' | 48:w:1233:G:H8     | 1.75                     | 0.51              |
| 48:w:1755:C:O2    | 48:w:1777:G:N2     | 2.43                     | 0.51              |
| 65:AD:34:VAL:HG22 | 65:AD:38:ILE:HD13  | 1.93                     | 0.51              |
| 71:AJ:46:HIS:HB3  | 71:AJ:101:LEU:HD11 | 1.93                     | 0.51              |
| 2:B:52:G:O2'      | 2:B:53:5MU:OP1     | 2.27                     | 0.51              |
| 48:w:900:C:H3'    | 48:w:901:G:H8      | 1.76                     | 0.51              |
| 52:0:213:PRO:HD3  | 65:AD:19:LYS:HD3   | 1.91                     | 0.51              |
| 53:1:79:ASP:HB3   | 53:1:82:TYR:HB2    | 1.92                     | 0.51              |
| 53:1:143:ASP:N    | 53:1:143:ASP:OD1   | 2.44                     | 0.51              |
| 62:AA:131:ASP:OD1 | 62:AA:131:ASP:N    | 2.44                     | 0.51              |
| 66:AE:66:ARG:O    | 66:AE:70:ILE:HG12  | 2.11                     | 0.51              |
| 67:AF:42:HIS:NE2  | 67:AF:43:LYS:HE3   | 2.25                     | 0.51              |
| 2:C:52:G:H2'      | 2:C:53:5MU:C6      | 2.46                     | 0.51              |
| 7:H:29:VAL:HG12   | 7:H:31:SER:H       | 1.75                     | 0.51              |
| 9:J:291:GLN:HE21  | 9:J:291:GLN:HA     | 1.74                     | 0.51              |
| 43:r:79:GLU:OE2   | 43:r:81:SER:OG     | 2.25                     | 0.51              |
| 48:w:428:OMU:HM22 | 58:6:7:TRP:HZ3     | 1.75                     | 0.51              |
| 48:w:591:U:H4'    | 48:w:592:C:O5'     | 2.10                     | 0.51              |
| 52:0:27:ARG:HG2   | 59:7:61:GLN:HE21   | 1.76                     | 0.51              |
| 53:1:42:LEU:HD11  | 53:1:46:ILE:HD11   | 1.92                     | 0.51              |
| 65:AD:26:ASN:OD1  | 65:AD:26:ASN:N     | 2.39                     | 0.51              |
| 68:AG:26:SER:OG   | 68:AG:27:ARG:N     | 2.41                     | 0.51              |
| 3:D:2318:G:O6     | 35:j:19:LYS:NZ     | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:31:ALA:HB2    | 6:G:123:ARG:HH21  | 1.76                     | 0.51              |
| 14:O:31:ILE:HG12  | 14:O:32:ARG:H     | 1.75                     | 0.51              |
| 16:Q:48:PRO:HA    | 16:Q:149:GLN:HG2  | 1.93                     | 0.51              |
| 33:h:23:LYS:NZ    | 33:h:23:LYS:HB3   | 2.26                     | 0.51              |
| 48:w:36:PSU:HN3   | 48:w:519:A:H61    | 1.58                     | 0.51              |
| 48:w:1743:G:H21   | 48:w:1791:A:H62   | 1.58                     | 0.51              |
| 50:y:167:LYS:O    | 50:y:171:ILE:HG12 | 2.10                     | 0.51              |
| 53:1:198:ARG:HH22 | 53:1:222:LEU:HD12 | 1.76                     | 0.51              |
| 55:3:225:GLN:HA   | 55:3:228:ILE:HG22 | 1.92                     | 0.51              |
| 61:9:54:LEU:HD12  | 61:9:58:HIS:ND1   | 2.25                     | 0.51              |
| 68:AG:20:ILE:HD11 | 68:AG:98:VAL:HG11 | 1.92                     | 0.51              |
| 14:O:182:GLU:HA   | 14:O:182:GLU:OE1  | 2.10                     | 0.51              |
| 48:w:837:A:H62    | 72:AK:8:ARG:HG3   | 1.75                     | 0.51              |
| 48:w:1447:G:OP1   | 68:AG:87:ARG:NH1  | 2.40                     | 0.51              |
| 51:z:187:ARG:HD3  | 51:z:192:LEU:HD12 | 1.91                     | 0.51              |
| 59:7:3:MET:HE3    | 59:7:8:ARG:NH1    | 2.23                     | 0.51              |
| 71:AJ:96:GLU:HG3  | 71:AJ:97:ASN:OD1  | 2.11                     | 0.51              |
| 79:AR:107:ASP:HB2 | 79:AR:125:ARG:HD2 | 1.92                     | 0.51              |
| 48:w:1606:G:O2'   | 48:w:1607:A:O5'   | 2.26                     | 0.51              |
| 60:8:4:ILE:HG23   | 60:8:5:GLN:HG2    | 1.93                     | 0.51              |
| 63:AB:81:ARG:NH1  | 63:AB:120:SER:OG  | 2.40                     | 0.51              |
| 3:D:71:C:H1'      | 16:Q:62:PRO:O     | 2.10                     | 0.50              |
| 3:D:2096:G:N3     | 3:D:2096:G:H2'    | 2.26                     | 0.50              |
| 3:D:2097:U:O3'    | 3:D:2098:G:H4'    | 2.11                     | 0.50              |
| 3:D:3906:A:H2'    | 8:I:69:THR:HG23   | 1.92                     | 0.50              |
| 8:I:38:ASN:O      | 8:I:42:THR:HG23   | 2.10                     | 0.50              |
| 12:M:57:TRP:HB3   | 12:M:61:ILE:HD11  | 1.93                     | 0.50              |
| 13:N:41:ILE:HG22  | 13:N:43:VAL:HG13  | 1.94                     | 0.50              |
| 52:0:51:LEU:HD12  | 52:0:91:VAL:HG12  | 1.92                     | 0.50              |
| 55:3:186:GLN:H    | 55:3:186:GLN:CD   | 2.20                     | 0.50              |
| 57:5:79:ILE:HG13  | 57:5:80:ASP:OD1   | 2.11                     | 0.50              |
| 65:AD:41:ILE:HD11 | 65:AD:47:ARG:HG2  | 1.93                     | 0.50              |
| 69:AH:41:LYS:H    | 69:AH:41:LYS:CE   | 2.22                     | 0.50              |
| 76:AO:13:ARG:N    | 76:AO:33:GLU:O    | 2.44                     | 0.50              |
| 3:D:1174:G:H1     | 3:D:1186:U:H3     | 1.58                     | 0.50              |
| 42:q:16:LYS:HD3   | 42:q:49:LEU:HD22  | 1.92                     | 0.50              |
| 56:4:122:LEU:HA   | 56:4:125:VAL:HG22 | 1.93                     | 0.50              |
| 71:AJ:140:ARG:HD2 | 71:AJ:141:PRO:HD2 | 1.93                     | 0.50              |
| 72:AK:76:TYR:OH   | 72:AK:86:GLU:OE1  | 2.17                     | 0.50              |
| 75:AN:36:LYS:HE2  | 75:AN:36:LYS:HA   | 1.93                     | 0.50              |
| 79:AR:62:HIS:CD2  | 79:AR:88:ARG:HG3  | 2.46                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:16:U:O2'       | 2:B:17:G:O5'      | 2.28                     | 0.50              |
| 3:D:181:C:N4       | 3:D:254:G:O6      | 2.44                     | 0.50              |
| 3:D:1194:G:H2'     | 3:D:1195:G:H8     | 1.77                     | 0.50              |
| 5:F:70:G:N2        | 5:F:87:G:O2'      | 2.37                     | 0.50              |
| 7:H:218:ASP:OD2    | 7:H:348:ARG:NH1   | 2.44                     | 0.50              |
| 28:c:73:HIS:CD2    | 28:c:115:LYS:HE3  | 2.46                     | 0.50              |
| 50:y:34:LYS:O      | 50:y:98:THR:OG1   | 2.27                     | 0.50              |
| 68:AG:56:MET:HG3   | 68:AG:86:LYS:HD2  | 1.92                     | 0.50              |
| 74:AM:45:VAL:HG23  | 74:AM:46:GLU:H    | 1.74                     | 0.50              |
| 3:D:4392:OMG:H2'   | 3:D:4447:5MC:HM51 | 1.94                     | 0.50              |
| 3:D:4455:G:H5''    | 7:H:5:LYS:HE2     | 1.94                     | 0.50              |
| 7:H:47:LEU:H       | 7:H:84:MET:HE2    | 1.77                     | 0.50              |
| 8:I:201:ARG:HG2    | 8:I:201:ARG:NH1   | 2.25                     | 0.50              |
| 17:R:99:GLU:O      | 17:R:103:LYS:HG2  | 2.12                     | 0.50              |
| 19:T:190:ASP:OD1   | 19:T:191:LYS:N    | 2.45                     | 0.50              |
| 42:q:24:PRO:HG2    | 42:q:27:ILE:HG12  | 1.93                     | 0.50              |
| 49:x:156:TYR:OH    | 69:AH:61:ARG:NH1  | 2.44                     | 0.50              |
| 52:0:81:GLU:N      | 52:0:81:GLU:OE1   | 2.42                     | 0.50              |
| 62:AA:44:VAL:HG13  | 62:AA:53:ILE:HB   | 1.94                     | 0.50              |
| 68:AG:66:ARG:HG3   | 68:AG:68:THR:HG22 | 1.92                     | 0.50              |
| 68:AG:116:ILE:HD12 | 68:AG:117:ALA:H   | 1.75                     | 0.50              |
| 3:D:151:G:OP2      | 18:S:4:TYR:OH     | 2.24                     | 0.50              |
| 10:K:190:HIS:HB3   | 10:K:193:PHE:HD2  | 1.77                     | 0.50              |
| 12:M:99:ALA:HB1    | 12:M:136:LEU:HD11 | 1.93                     | 0.50              |
| 19:T:61:ARG:HA     | 19:T:70:PRO:HD2   | 1.94                     | 0.50              |
| 33:h:11:LEU:O      | 33:h:14:ILE:HG22  | 2.11                     | 0.50              |
| 47:v:56:ASP:O      | 47:v:58:LYS:NZ    | 2.44                     | 0.50              |
| 48:w:811:A:O2'     | 48:w:812:A:OP1    | 2.26                     | 0.50              |
| 48:w:987:A:C6      | 50:y:120:MET:HE1  | 2.46                     | 0.50              |
| 64:AC:50:LYS:HA    | 64:AC:53:GLU:HG3  | 1.94                     | 0.50              |
| 79:AR:244:ASN:HB3  | 79:AR:245:ARG:NE  | 2.26                     | 0.50              |
| 3:D:208:A:H2       | 3:D:233:U:H5''    | 1.77                     | 0.50              |
| 39:n:59:GLU:OE1    | 39:n:59:GLU:HA    | 2.12                     | 0.50              |
| 48:w:379:C:O2      | 57:5:5:ARG:NE     | 2.44                     | 0.50              |
| 48:w:502:C:OP2     | 53:1:66:MET:HE1   | 2.12                     | 0.50              |
| 63:AB:98:ASN:ND2   | 63:AB:121:ILE:O   | 2.43                     | 0.50              |
| 7:H:396:ARG:HB3    | 7:H:396:ARG:HH11  | 1.77                     | 0.50              |
| 56:4:36:LEU:O      | 56:4:41:ARG:NH2   | 2.41                     | 0.50              |
| 61:9:46:THR:HB     | 61:9:86:GLU:OE2   | 2.12                     | 0.50              |
| 3:D:4623:OMG:OP1   | 7:H:19:ARG:NH2    | 2.45                     | 0.50              |
| 3:D:4913:G:H4'     | 3:D:4914:C:O5'    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:83:LEU:N      | 9:J:84:PRO:HD2    | 2.26                     | 0.50              |
| 19:T:54:TYR:OH    | 19:T:73:PHE:O     | 2.30                     | 0.50              |
| 48:w:519:A:O2'    | 58:6:11:LYS:HE2   | 2.12                     | 0.50              |
| 49:x:9:GLN:H      | 49:x:11:LYS:HZ1   | 1.60                     | 0.50              |
| 55:3:183:ARG:CA   | 55:3:186:GLN:HE22 | 2.24                     | 0.50              |
| 55:3:199:THR:O    | 55:3:203:LYS:HG2  | 2.12                     | 0.50              |
| 66:AE:28:PHE:O    | 66:AE:31:THR:OG1  | 2.30                     | 0.50              |
| 3:D:406:C:O2'     | 3:D:407:A:OP1     | 2.29                     | 0.50              |
| 3:D:1199:G:H2'    | 3:D:1200:G:C8     | 2.46                     | 0.50              |
| 48:w:844:U:H2'    | 48:w:845:G:C8     | 2.47                     | 0.50              |
| 57:5:124:LYS:O    | 57:5:124:LYS:HG2  | 2.12                     | 0.50              |
| 58:6:137:VAL:HG22 | 58:6:157:ILE:HG13 | 1.94                     | 0.50              |
| 59:7:16:PHE:HD2   | 59:7:79:LEU:HD11  | 1.77                     | 0.50              |
| 73:AL:50:PHE:CD1  | 73:AL:83:LEU:HD21 | 2.47                     | 0.50              |
| 4:E:11:A:O2'      | 4:E:13:A:OP2      | 2.27                     | 0.49              |
| 8:I:67:TRP:HB2    | 8:I:71:ARG:NH1    | 2.26                     | 0.49              |
| 24:Y:80:VAL:HG22  | 24:Y:81:LYS:H     | 1.77                     | 0.49              |
| 48:w:494:C:N4     | 48:w:509:OMG:HN22 | 2.09                     | 0.49              |
| 49:x:81:ASN:HA    | 49:x:84:GLN:HE21  | 1.76                     | 0.49              |
| 60:8:57:ASP:OD2   | 60:8:60:CYS:N     | 2.45                     | 0.49              |
| 64:AC:43:GLU:HG2  | 64:AC:44:PRO:CD   | 2.41                     | 0.49              |
| 3:D:492:U:P       | 8:I:268:ARG:HH11  | 2.35                     | 0.49              |
| 3:D:3896:C:O2'    | 7:H:268:ARG:NH2   | 2.43                     | 0.49              |
| 32:g:99:ILE:O     | 32:g:109:ARG:NH1  | 2.45                     | 0.49              |
| 48:w:834:C:N4     | 48:w:835:C:N3     | 2.61                     | 0.49              |
| 48:w:1647:A:OP1   | 64:AC:138:ARG:NH1 | 2.40                     | 0.49              |
| 66:AE:109:GLU:O   | 66:AE:113:ARG:NH1 | 2.45                     | 0.49              |
| 68:AG:63:ILE:HD11 | 77:AP:43:PHE:CE2  | 2.46                     | 0.49              |
| 9:J:107:ARG:NH2   | 9:J:116:ASP:OD1   | 2.46                     | 0.49              |
| 12:M:61:ILE:HA    | 12:M:64:GLN:HG2   | 1.93                     | 0.49              |
| 48:w:203:G:H2'    | 48:w:204:G:C8     | 2.46                     | 0.49              |
| 48:w:1388:A:N6    | 52:0:161:GLY:HA3  | 2.28                     | 0.49              |
| 49:x:63:ARG:NH1   | 69:AH:38:GLU:HA   | 2.26                     | 0.49              |
| 61:9:15:ALA:HB2   | 75:AN:20:LYS:HD3  | 1.94                     | 0.49              |
| 78:AQ:94:LYS:NZ   | 78:AQ:95:GLN:O    | 2.44                     | 0.49              |
| 79:AR:104:HIS:HD2 | 79:AR:108:VAL:HB  | 1.77                     | 0.49              |
| 3:D:1633:G:H5'    | 3:D:1634:A:OP1    | 2.13                     | 0.49              |
| 3:D:2096:G:H4'    | 3:D:2099:G:H4'    | 1.95                     | 0.49              |
| 3:D:2693:G:OP1    | 41:p:35:LYS:NZ    | 2.40                     | 0.49              |
| 12:M:144:THR:O    | 12:M:148:GLU:HG3  | 2.11                     | 0.49              |
| 20:U:32:THR:HA    | 20:U:58:VAL:HG21  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:k:50:VAL:HG22  | 36:k:69:VAL:HG12   | 1.94                     | 0.49              |
| 48:w:492:C:H42    | 48:w:508:A:H62     | 1.60                     | 0.49              |
| 48:w:1158:G:O3'   | 70:AI:76:SER:OG    | 2.29                     | 0.49              |
| 48:w:1610:G:P     | 66:AE:121:ARG:HH21 | 2.35                     | 0.49              |
| 61:9:18:TYR:O     | 70:AI:56:HIS:ND1   | 2.44                     | 0.49              |
| 76:AO:31:ARG:HH11 | 76:AO:31:ARG:HG3   | 1.77                     | 0.49              |
| 3:D:958:G:H21     | 10:K:125:LEU:H     | 1.61                     | 0.49              |
| 3:D:1214:C:N4     | 32:g:90:SER:OG     | 2.40                     | 0.49              |
| 3:D:4492:U:O2'    | 3:D:4512:U:O2      | 2.24                     | 0.49              |
| 14:O:54:SER:HB2   | 14:O:135:ILE:HD11  | 1.94                     | 0.49              |
| 15:P:129:ASP:N    | 15:P:129:ASP:OD1   | 2.41                     | 0.49              |
| 20:U:21:ASN:O     | 20:U:21:ASN:ND2    | 2.43                     | 0.49              |
| 25:Z:56:LEU:HD23  | 25:Z:61:VAL:O      | 2.13                     | 0.49              |
| 48:w:191:A:H5''   | 57:5:140:LYS:HE2   | 1.93                     | 0.49              |
| 51:z:213:LEU:HD21 | 51:z:241:PHE:HB2   | 1.95                     | 0.49              |
| 52:0:186:VAL:O    | 52:0:188:ILE:HG13  | 2.13                     | 0.49              |
| 52:0:192:TRP:CD2  | 52:0:194:PRO:HD3   | 2.48                     | 0.49              |
| 54:2:142:SER:OG   | 76:AO:49:PRO:O     | 2.26                     | 0.49              |
| 55:3:46:LYS:O     | 55:3:118:GLU:HG2   | 2.12                     | 0.49              |
| 58:6:119:LEU:H    | 58:6:119:LEU:HD23  | 1.78                     | 0.49              |
| 66:AE:34:LYS:NZ   | 66:AE:34:LYS:HB3   | 2.27                     | 0.49              |
| 67:AF:21:PHE:O    | 67:AF:25:SER:OG    | 2.22                     | 0.49              |
| 68:AG:49:LYS:HB2  | 68:AG:92:HIS:ND1   | 2.28                     | 0.49              |
| 72:AK:10:ARG:NH1  | 72:AK:26:ASP:OD1   | 2.45                     | 0.49              |
| 72:AK:16:ARG:H    | 72:AK:16:ARG:HD3   | 1.77                     | 0.49              |
| 79:AR:70:VAL:HG11 | 79:AR:113:PHE:HB2  | 1.93                     | 0.49              |
| 4:E:119:U:H2'     | 9:J:261:VAL:HG11   | 1.95                     | 0.49              |
| 5:F:102:G:OP2     | 5:F:104:A:O2'      | 2.26                     | 0.49              |
| 17:R:95:ILE:O     | 17:R:96:GLU:HB3    | 2.12                     | 0.49              |
| 48:w:455:A:H2'    | 48:w:456:C:C6      | 2.47                     | 0.49              |
| 48:w:554:A:H2'    | 48:w:555:A:C8      | 2.47                     | 0.49              |
| 48:w:917:U:O4'    | 56:4:118:ARG:HD2   | 2.12                     | 0.49              |
| 48:w:1452:A:H5''  | 65:AD:48:ASN:ND2   | 2.27                     | 0.49              |
| 53:1:139:LEU:O    | 53:1:146:THR:HA    | 2.12                     | 0.49              |
| 58:6:79:ARG:HA    | 58:6:82:VAL:HG12   | 1.95                     | 0.49              |
| 65:AD:94:GLU:OE1  | 65:AD:115:SER:OG   | 2.27                     | 0.49              |
| 69:AH:49:GLN:OE1  | 69:AH:49:GLN:HA    | 2.12                     | 0.49              |
| 79:AR:89:LEU:HB2  | 79:AR:99:ARG:HB3   | 1.95                     | 0.49              |
| 3:D:987:C:O2'     | 3:D:988:C:OP1      | 2.30                     | 0.49              |
| 3:D:1769:G:H2'    | 3:D:1770:A:C8      | 2.48                     | 0.49              |
| 48:w:921:G:C5     | 70:AI:28:ARG:HD2   | 2.48                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:w:1144:A:H2'    | 48:w:1145:A:C8    | 2.47                     | 0.49              |
| 58:6:77:LEU:HA     | 58:6:80:ARG:HE    | 1.77                     | 0.49              |
| 58:6:136:ARG:HA    | 58:6:141:VAL:HA   | 1.94                     | 0.49              |
| 3:D:659:G:H2'      | 3:D:660:A:C8      | 2.48                     | 0.49              |
| 3:D:660:A:N6       | 3:D:661:C:N3      | 2.60                     | 0.49              |
| 3:D:739:G:O2'      | 3:D:740:G:H8      | 1.93                     | 0.49              |
| 3:D:2667:C:O4'     | 22:W:96:MET:HG3   | 2.12                     | 0.49              |
| 3:D:5016:A:N3      | 3:D:5016:A:H2'    | 2.28                     | 0.49              |
| 11:L:220:MET:O     | 11:L:221:LYS:HG2  | 2.13                     | 0.49              |
| 30:e:89:ILE:HD13   | 30:e:121:ARG:HE   | 1.77                     | 0.49              |
| 48:w:1230:C:OP1    | 66:AE:130:ARG:NH2 | 2.46                     | 0.49              |
| 56:4:11:PRO:HG3    | 56:4:44:ASN:HD22  | 1.78                     | 0.49              |
| 67:AF:82:ARG:NH2   | 67:AF:90:SER:OG   | 2.46                     | 0.49              |
| 68:AG:111:GLU:OE1  | 68:AG:112:VAL:N   | 2.46                     | 0.49              |
| 70:AI:102:ILE:HG13 | 70:AI:113:HIS:HB3 | 1.93                     | 0.49              |
| 3:D:3599:A:H2'     | 3:D:3600:G:H8     | 1.78                     | 0.49              |
| 3:D:5021:C:H3'     | 3:D:5022:U:H5''   | 1.93                     | 0.49              |
| 6:G:116:LEU:HD23   | 6:G:164:ALA:HB2   | 1.94                     | 0.49              |
| 7:H:293:ILE:HG23   | 7:H:294:LYS:N     | 2.28                     | 0.49              |
| 12:M:156:VAL:O     | 12:M:156:VAL:HG12 | 2.12                     | 0.49              |
| 52:0:80:PRO:O      | 52:0:83:SER:OG    | 2.31                     | 0.49              |
| 54:2:43:GLU:C      | 54:2:45:TYR:H     | 2.21                     | 0.49              |
| 57:5:66:SER:HB2    | 57:5:73:THR:HG23  | 1.95                     | 0.49              |
| 61:9:4:MET:HE3     | 61:9:5:HIS:CE1    | 2.48                     | 0.49              |
| 67:AF:114:GLU:OE1  | 67:AF:114:GLU:N   | 2.46                     | 0.49              |
| 75:AN:38:PRO:O     | 75:AN:40:CYS:N    | 2.46                     | 0.49              |
| 3:D:1553:A:H62     | 3:D:1574:G:H1'    | 1.76                     | 0.49              |
| 3:D:2488:C:N4      | 5:F:126:C:OP1     | 2.46                     | 0.49              |
| 3:D:4936:G:N7      | 10:K:183:ARG:NH2  | 2.60                     | 0.49              |
| 16:Q:65:ARG:HD2    | 16:Q:66:TYR:CZ    | 2.48                     | 0.49              |
| 48:w:835:C:C5      | 72:AK:8:ARG:HD3   | 2.48                     | 0.49              |
| 50:y:146:ARG:HB2   | 50:y:149:GLN:HB2  | 1.94                     | 0.49              |
| 55:3:2:LYS:HB2     | 55:3:108:VAL:HG22 | 1.94                     | 0.49              |
| 57:5:110:ARG:HA    | 57:5:121:LEU:HD23 | 1.95                     | 0.49              |
| 63:AB:29:SER:H     | 63:AB:32:GLN:HE22 | 1.61                     | 0.49              |
| 63:AB:136:THR:HG22 | 63:AB:138:SER:H   | 1.77                     | 0.49              |
| 3:D:119:G:O6       | 12:M:113:ARG:NH2  | 2.46                     | 0.48              |
| 48:w:1452:A:C2     | 48:w:1476:A:H1'   | 2.48                     | 0.48              |
| 48:w:1636:G:H21    | 54:2:164:ARG:NH2  | 2.09                     | 0.48              |
| 68:AG:26:SER:HB2   | 68:AG:110:VAL:HA  | 1.95                     | 0.48              |
| 3:D:278:G:H5''     | 18:S:8:GLN:HE22   | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1332:C:H5''   | 35:j:29:VAL:HG23  | 1.95                     | 0.48              |
| 3:D:2705:G:H2'    | 3:D:2706:G:O4'    | 2.13                     | 0.48              |
| 28:c:67:ARG:HB2   | 28:c:67:ARG:HH11  | 1.78                     | 0.48              |
| 48:w:656:G:H5'    | 48:w:662:G:N2     | 2.27                     | 0.48              |
| 48:w:1398:G:H1'   | 79:AR:63:SER:OG   | 2.14                     | 0.48              |
| 48:w:1454:A:H5''  | 65:AD:3:ARG:HD2   | 1.94                     | 0.48              |
| 50:y:224:GLU:OE1  | 50:y:227:LYS:HG2  | 2.12                     | 0.48              |
| 53:1:185:GLY:H    | 53:1:189:LEU:HD13 | 1.78                     | 0.48              |
| 3:D:1852:U:H5''   | 31:f:22:ILE:HD11  | 1.95                     | 0.48              |
| 3:D:2529:A:O2'    | 3:D:2531:C:OP2    | 2.31                     | 0.48              |
| 3:D:3897:G:H4'    | 7:H:254:ILE:HD12  | 1.94                     | 0.48              |
| 20:U:94:MET:HG2   | 20:U:148:MET:HE3  | 1.96                     | 0.48              |
| 26:a:111:GLU:CD   | 26:a:111:GLU:H    | 2.18                     | 0.48              |
| 48:w:659:G:O2'    | 48:w:662:G:O2'    | 2.26                     | 0.48              |
| 61:9:49:GLN:O     | 61:9:53:ILE:HG22  | 2.12                     | 0.48              |
| 63:AB:85:ILE:HG12 | 63:AB:114:HIS:O   | 2.13                     | 0.48              |
| 79:AR:73:SER:H    | 79:AR:117:ASN:ND2 | 2.12                     | 0.48              |
| 3:D:1591:U:OP2    | 3:D:2856:C:O2'    | 2.23                     | 0.48              |
| 10:K:119:GLU:HG3  | 35:j:7:LEU:HD22   | 1.95                     | 0.48              |
| 30:e:9:LYS:NZ     | 30:e:83:THR:O     | 2.36                     | 0.48              |
| 48:w:641:A:H2'    | 48:w:642:U:O4'    | 2.14                     | 0.48              |
| 48:w:1432:U:H2'   | 48:w:1438:A:C8    | 2.49                     | 0.48              |
| 53:1:127:ARG:N    | 53:1:140:VAL:O    | 2.46                     | 0.48              |
| 54:2:105:GLY:O    | 54:2:106:GLU:HG3  | 2.13                     | 0.48              |
| 63:AB:49:LEU:HD12 | 63:AB:53:GLN:HB2  | 1.96                     | 0.48              |
| 64:AC:15:ARG:HA   | 64:AC:19:ALA:O    | 2.13                     | 0.48              |
| 79:AR:282:GLU:O   | 79:AR:284:PRO:HD3 | 2.13                     | 0.48              |
| 3:D:4895:C:H3'    | 3:D:4895:C:OP2    | 2.12                     | 0.48              |
| 10:K:114:ARG:HG2  | 47:v:87:ARG:HG3   | 1.95                     | 0.48              |
| 13:N:14:GLU:OE1   | 13:N:14:GLU:N     | 2.46                     | 0.48              |
| 14:O:193:ASP:OD1  | 14:O:198:LYS:HE2  | 2.14                     | 0.48              |
| 17:R:34:ASN:O     | 17:R:51:PRO:HA    | 2.13                     | 0.48              |
| 53:1:198:ARG:NE   | 53:1:200:ARG:HE   | 2.10                     | 0.48              |
| 60:8:7:GLU:OE1    | 60:8:8:ARG:N      | 2.46                     | 0.48              |
| 3:D:2758:G:O2'    | 3:D:2765:A:N3     | 2.45                     | 0.48              |
| 3:D:4924:C:N4     | 3:D:4925:U:O4     | 2.46                     | 0.48              |
| 9:J:79:TYR:O      | 9:J:82:GLU:HG2    | 2.14                     | 0.48              |
| 13:N:42:ASN:HD21  | 19:T:131:PRO:HB2  | 1.78                     | 0.48              |
| 13:N:113:GLU:OE1  | 13:N:125:ARG:NE   | 2.47                     | 0.48              |
| 17:R:32:ASP:HA    | 23:X:145:PHE:CZ   | 2.49                     | 0.48              |
| 23:X:85:ASP:OD1   | 23:X:123:SER:HB2  | 2.12                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 68:AG:88:LEU:O     | 68:AG:89:ILE:HD13 | 2.14                     | 0.48              |
| 78:AQ:102:THR:HG22 | 78:AQ:103:GLY:H   | 1.78                     | 0.48              |
| 3:D:462:G:H2'      | 3:D:463:A:C8      | 2.49                     | 0.48              |
| 3:D:1773:OMU:HM23  | 3:D:1773:OMU:H1'  | 1.64                     | 0.48              |
| 3:D:4097:G:O2'     | 3:D:4098:A:O5'    | 2.30                     | 0.48              |
| 7:H:153:MET:HB3    | 7:H:194:LEU:HD11  | 1.96                     | 0.48              |
| 10:K:112:MET:HG3   | 10:K:113:PRO:HD2  | 1.96                     | 0.48              |
| 48:w:1265:A:H2     | 48:w:1517:G:H22   | 1.61                     | 0.48              |
| 53:1:188:ASN:OD1   | 53:1:220:THR:OG1  | 2.30                     | 0.48              |
| 63:AB:29:SER:H     | 63:AB:32:GLN:NE2  | 2.11                     | 0.48              |
| 66:AE:82:TRP:CD1   | 66:AE:82:TRP:H    | 2.32                     | 0.48              |
| 5:F:96:C:OP1       | 38:m:70:ARG:NH1   | 2.46                     | 0.48              |
| 22:W:172:ARG:HH21  | 48:w:909:G:P      | 2.37                     | 0.48              |
| 28:c:127:LEU:O     | 28:c:134:LYS:HA   | 2.14                     | 0.48              |
| 33:h:21:VAL:HG11   | 33:h:96:ILE:HD12  | 1.95                     | 0.48              |
| 36:k:106:TYR:HB2   | 36:k:107:PRO:HD3  | 1.94                     | 0.48              |
| 55:3:121:ILE:N     | 55:3:125:THR:OG1  | 2.46                     | 0.48              |
| 63:AB:29:SER:OG    | 63:AB:31:GLU:OE1  | 2.32                     | 0.48              |
| 69:AH:58:ALA:O     | 69:AH:62:MET:HG3  | 2.14                     | 0.48              |
| 2:C:72:G:O2'       | 2:C:73:C:OP1      | 2.31                     | 0.48              |
| 3:D:1294:A:H1'     | 3:D:1296:G:N1     | 2.29                     | 0.48              |
| 18:S:158:HIS:HB3   | 18:S:161:MET:HG3  | 1.96                     | 0.48              |
| 29:d:53:ASP:O      | 29:d:70:VAL:HG12  | 2.14                     | 0.48              |
| 55:3:197:GLN:H     | 55:3:197:GLN:CD   | 2.21                     | 0.48              |
| 58:6:35:TYR:HA     | 58:6:123:ILE:HD13 | 1.95                     | 0.48              |
| 70:AI:86:LEU:HD21  | 70:AI:113:HIS:HB2 | 1.95                     | 0.48              |
| 79:AR:33:SER:HB3   | 79:AR:43:TRP:HE1  | 1.79                     | 0.48              |
| 79:AR:153:CYS:SG   | 79:AR:197:THR:HA  | 2.54                     | 0.48              |
| 3:D:3654:G:O2'     | 3:D:3693:U:OP1    | 2.27                     | 0.48              |
| 3:D:4733:C:H1'     | 3:D:4734:A:H2'    | 1.96                     | 0.48              |
| 4:E:117:G:OP1      | 9:J:253:TYR:OH    | 2.32                     | 0.48              |
| 7:H:56:ILE:HD12    | 7:H:365:LEU:HD22  | 1.96                     | 0.48              |
| 16:Q:178:ALA:N     | 31:f:134:GLU:OE2  | 2.44                     | 0.48              |
| 24:Y:26:PRO:O      | 24:Y:29:THR:HG22  | 2.14                     | 0.48              |
| 37:l:41:ALA:O      | 37:l:52:ARG:HD2   | 2.14                     | 0.48              |
| 48:w:475:C:H1'     | 48:w:507:G:H2'    | 1.95                     | 0.48              |
| 48:w:1535:U:O2'    | 54:2:88:MET:SD    | 2.72                     | 0.48              |
| 48:w:1743:G:N2     | 48:w:1791:A:H62   | 2.11                     | 0.48              |
| 48:w:1839:U:H1'    | 48:w:1863:A:H2    | 1.78                     | 0.48              |
| 51:z:198:ALA:HB1   | 51:z:202:THR:HG21 | 1.96                     | 0.48              |
| 53:1:250:GLU:N     | 53:1:250:GLU:OE2  | 2.47                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4:38:ALA:N      | 56:4:41:ARG:HH21   | 2.12                     | 0.48              |
| 66:AE:112:GLU:O    | 66:AE:113:ARG:NH2  | 2.46                     | 0.48              |
| 68:AG:60:THR:HG22  | 68:AG:62:ARG:HG3   | 1.95                     | 0.48              |
| 70:AI:102:ILE:HG22 | 70:AI:128:PHE:HB3  | 1.96                     | 0.48              |
| 3:D:908:G:H2'      | 3:D:909:A:H8       | 1.79                     | 0.47              |
| 3:D:2458:C:H5''    | 18:S:67:ARG:HD2    | 1.96                     | 0.47              |
| 29:d:52:ASP:OD1    | 29:d:110:LYS:HG2   | 2.12                     | 0.47              |
| 48:w:1016:U:H5'    | 61:9:15:ALA:O      | 2.14                     | 0.47              |
| 53:1:21:ASP:OD2    | 53:1:24:THR:HG23   | 2.14                     | 0.47              |
| 56:4:63:PHE:CE2    | 56:4:95:ILE:HD11   | 2.49                     | 0.47              |
| 67:AF:130:ASP:OD1  | 67:AF:130:ASP:N    | 2.39                     | 0.47              |
| 79:AR:165:ILE:HD11 | 79:AR:177:TRP:HB2  | 1.95                     | 0.47              |
| 2:C:5:C:H2'        | 2:C:6:2MG:O4'      | 2.13                     | 0.47              |
| 3:D:2579:G:N2      | 3:D:2582:A:OP2     | 2.38                     | 0.47              |
| 17:R:96:GLU:HA     | 17:R:99:GLU:HG3    | 1.96                     | 0.47              |
| 36:k:106:TYR:O     | 36:k:108:SER:N     | 2.47                     | 0.47              |
| 48:w:639:C:OP1     | 78:AQ:114:ARG:NH2  | 2.35                     | 0.47              |
| 50:y:174:ARG:HB3   | 50:y:175:GLU:OE1   | 2.13                     | 0.47              |
| 52:0:98:ALA:HB1    | 52:0:186:VAL:HG23  | 1.96                     | 0.47              |
| 56:4:66:VAL:N      | 56:4:67:PRO:HD2    | 2.29                     | 0.47              |
| 59:7:15:LEU:HG     | 59:7:71:LEU:HD11   | 1.95                     | 0.47              |
| 65:AD:71:ILE:O     | 65:AD:74:GLN:HG3   | 2.14                     | 0.47              |
| 79:AR:206:LEU:HD23 | 79:AR:218:LEU:HD23 | 1.95                     | 0.47              |
| 3:D:3641:U:OP2     | 3:D:3646:A:N6      | 2.42                     | 0.47              |
| 7:H:370:THR:O      | 7:H:370:THR:HG22   | 2.15                     | 0.47              |
| 11:L:28:LEU:HD23   | 11:L:32:ARG:NH1    | 2.28                     | 0.47              |
| 23:X:69:GLU:OE2    | 23:X:101:THR:HG22  | 2.15                     | 0.47              |
| 24:Y:159:MET:HA    | 24:Y:159:MET:HE3   | 1.96                     | 0.47              |
| 25:Z:24:ASP:HB2    | 25:Z:69:LYS:HD2    | 1.95                     | 0.47              |
| 47:v:107:ARG:O     | 47:v:111:ILE:HG12  | 2.14                     | 0.47              |
| 48:w:1523:C:OP1    | 66:AE:142:ARG:N    | 2.38                     | 0.47              |
| 49:x:63:ARG:HH12   | 69:AH:38:GLU:HA    | 1.78                     | 0.47              |
| 60:8:11:GLN:HB3    | 60:8:56:ILE:HG21   | 1.95                     | 0.47              |
| 60:8:121:GLN:OE1   | 60:8:121:GLN:N     | 2.47                     | 0.47              |
| 3:D:1570:G:N7      | 46:u:3:LYS:NZ      | 2.63                     | 0.47              |
| 10:K:165:LEU:HD11  | 10:K:176:THR:HG22  | 1.96                     | 0.47              |
| 14:O:34:PHE:HD2    | 14:O:89:VAL:HG23   | 1.78                     | 0.47              |
| 31:f:37:GLY:H      | 31:f:41:HIS:HB2    | 1.80                     | 0.47              |
| 48:w:197:U:C5      | 48:w:198:U:H1'     | 2.49                     | 0.47              |
| 48:w:606:G:H8      | 78:AQ:131:ASN:HD21 | 1.63                     | 0.47              |
| 48:w:1617:G:O6     | 63:AB:43:ARG:NH1   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:w:1636:G:H21   | 54:2:164:ARG:HH22 | 1.61                     | 0.47              |
| 48:w:1693:G:N2    | 48:w:1834:A:H8    | 2.11                     | 0.47              |
| 50:y:224:GLU:HB3  | 50:y:227:LYS:HG2  | 1.96                     | 0.47              |
| 55:3:84:TYR:CE1   | 55:3:93:LYS:HB2   | 2.49                     | 0.47              |
| 71:AJ:48:LYS:HB3  | 71:AJ:99:GLU:OE1  | 2.14                     | 0.47              |
| 79:AR:162:ASN:O   | 79:AR:164:ILE:N   | 2.47                     | 0.47              |
| 3:D:407:A:O2'     | 3:D:410:A:OP1     | 2.31                     | 0.47              |
| 3:D:739:G:O2'     | 3:D:740:G:O5'     | 2.31                     | 0.47              |
| 3:D:4741:C:H1'    | 3:D:4743:G:OP2    | 2.15                     | 0.47              |
| 10:K:153:LEU:HD11 | 10:K:195:ILE:HG13 | 1.95                     | 0.47              |
| 17:R:122:ILE:HB   | 19:T:189:ILE:HD11 | 1.97                     | 0.47              |
| 20:U:42:ARG:NH1   | 20:U:99:GLU:OE1   | 2.48                     | 0.47              |
| 21:V:76:GLU:H     | 21:V:76:GLU:CD    | 2.22                     | 0.47              |
| 25:Z:44:GLN:HA    | 25:Z:56:LEU:HD11  | 1.97                     | 0.47              |
| 45:t:71:GLU:HB3   | 45:t:80:LYS:HG2   | 1.96                     | 0.47              |
| 52:0:61:GLU:H     | 52:0:64:ARG:HG2   | 1.78                     | 0.47              |
| 53:1:209:HIS:ND1  | 53:1:219:ALA:HB2  | 2.30                     | 0.47              |
| 56:4:42:GLU:N     | 56:4:42:GLU:OE1   | 2.48                     | 0.47              |
| 64:AC:23:ALA:HA   | 64:AC:70:VAL:HG12 | 1.96                     | 0.47              |
| 71:AJ:19:ASP:OD2  | 71:AJ:20:GLN:N    | 2.48                     | 0.47              |
| 3:D:690:C:OP2     | 10:K:111:LYS:NZ   | 2.48                     | 0.47              |
| 3:D:1574:G:HO2'   | 3:D:1575:A:P      | 2.38                     | 0.47              |
| 3:D:4910:G:H22    | 19:T:107:GLY:HA3  | 1.79                     | 0.47              |
| 10:K:46:ARG:HG3   | 10:K:62:MET:HE1   | 1.97                     | 0.47              |
| 12:M:105:GLU:HB2  | 12:M:109:GLU:HB2  | 1.96                     | 0.47              |
| 16:Q:48:PRO:HB2   | 38:m:120:ALA:HB2  | 1.96                     | 0.47              |
| 17:R:128:LYS:HB2  | 17:R:128:LYS:NZ   | 2.29                     | 0.47              |
| 25:Z:49:VAL:HG12  | 25:Z:50:ASN:OD1   | 2.15                     | 0.47              |
| 52:0:164:VAL:O    | 52:0:168:VAL:HG22 | 2.15                     | 0.47              |
| 3:D:109:G:OP2     | 16:Q:74:ARG:NH1   | 2.42                     | 0.47              |
| 3:D:2560:C:H2'    | 3:D:2561:C:C6     | 2.50                     | 0.47              |
| 9:J:121:GLY:HA3   | 9:J:168:ASP:O     | 2.15                     | 0.47              |
| 10:K:50:LEU:HD12  | 10:K:51:VAL:H     | 1.78                     | 0.47              |
| 48:w:204:G:H2'    | 48:w:205:G:H8     | 1.80                     | 0.47              |
| 48:w:303:C:O4'    | 57:5:64:ASN:ND2   | 2.48                     | 0.47              |
| 48:w:955:A:N1     | 48:w:968:U:O2'    | 2.47                     | 0.47              |
| 54:2:99:ILE:HD11  | 54:2:171:GLU:HA   | 1.95                     | 0.47              |
| 55:3:223:LYS:O    | 55:3:227:GLN:N    | 2.39                     | 0.47              |
| 62:AA:34:PHE:HB3  | 62:AA:41:PHE:HB2  | 1.97                     | 0.47              |
| 64:AC:40:GLU:N    | 64:AC:40:GLU:OE2  | 2.46                     | 0.47              |
| 66:AE:63:GLU:HB3  | 66:AE:66:ARG:HH21 | 1.79                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 72:AK:15:ASN:HB3  | 72:AK:20:ARG:HB3   | 1.96                     | 0.47              |
| 79:AR:73:SER:HB2  | 79:AR:117:ASN:HD21 | 1.79                     | 0.47              |
| 3:D:1326:A2M:OP2  | 3:D:4445:U:O2'     | 2.28                     | 0.47              |
| 3:D:4345:C:O2'    | 45:t:82:MET:HE3    | 2.14                     | 0.47              |
| 18:S:189:ARG:HG2  | 18:S:193:ARG:NH1   | 2.30                     | 0.47              |
| 48:w:316:G:H5''   | 55:3:183:ARG:NH1   | 2.30                     | 0.47              |
| 48:w:346:C:OP1    | 53:1:38:LEU:N      | 2.39                     | 0.47              |
| 48:w:985:G:H4'    | 62:AA:138:ASP:OD1  | 2.14                     | 0.47              |
| 48:w:1289:U:H2'   | 48:w:1290:G:C8     | 2.50                     | 0.47              |
| 48:w:1454:A:H2    | 48:w:1476:A:H2'    | 1.80                     | 0.47              |
| 48:w:1621:U:OP1   | 63:AB:40:ARG:HG2   | 2.15                     | 0.47              |
| 50:y:71:LEU:HA    | 50:y:74:LEU:HB2    | 1.96                     | 0.47              |
| 56:4:32:MET:HE3   | 56:4:32:MET:N      | 2.29                     | 0.47              |
| 60:8:61:PRO:HA    | 60:8:66:VAL:HG23   | 1.97                     | 0.47              |
| 68:AG:68:THR:O    | 77:AP:40:ARG:NH1   | 2.48                     | 0.47              |
| 74:AM:60:ASP:N    | 74:AM:60:ASP:OD1   | 2.45                     | 0.47              |
| 79:AR:178:ASN:HB3 | 79:AR:183:LYS:N    | 2.29                     | 0.47              |
| 3:D:1699:A:H1'    | 11:L:177:ARG:HD3   | 1.96                     | 0.47              |
| 34:i:64:ILE:HG23  | 34:i:68:LEU:HD23   | 1.97                     | 0.47              |
| 40:o:33:THR:HA    | 40:o:40:PRO:HD3    | 1.97                     | 0.47              |
| 42:q:30:LYS:HB2   | 42:q:33:ASN:HB2    | 1.97                     | 0.47              |
| 48:w:360:A:N6     | 48:w:400:C:O2'     | 2.48                     | 0.47              |
| 55:3:76:LEU:HD21  | 55:3:92:ARG:HD2    | 1.96                     | 0.47              |
| 56:4:138:GLU:H    | 56:4:159:ASP:HB3   | 1.80                     | 0.47              |
| 70:AI:53:ILE:HD13 | 75:AN:24:LEU:HD22  | 1.97                     | 0.47              |
| 3:D:1769:G:H2'    | 3:D:1770:A:H8      | 1.80                     | 0.47              |
| 15:P:15:LEU:HD23  | 15:P:15:LEU:H      | 1.80                     | 0.47              |
| 16:Q:19:GLN:HA    | 16:Q:22:VAL:HG13   | 1.96                     | 0.47              |
| 16:Q:135:LYS:HD3  | 16:Q:136:LYS:HG2   | 1.96                     | 0.47              |
| 29:d:51:LYS:O     | 29:d:70:VAL:HG13   | 2.14                     | 0.47              |
| 48:w:142:C:N4     | 48:w:330:G:OP2     | 2.46                     | 0.47              |
| 48:w:639:C:H2'    | 48:w:640:A:C8      | 2.49                     | 0.47              |
| 48:w:907:G:H2'    | 48:w:908:A:C8      | 2.50                     | 0.47              |
| 48:w:1434:C:H5'   | 48:w:1437:C:H42    | 1.79                     | 0.47              |
| 54:2:35:LEU:O     | 54:2:39:ILE:HG12   | 2.14                     | 0.47              |
| 56:4:76:GLN:OE1   | 56:4:94:PHE:HB2    | 2.15                     | 0.47              |
| 65:AD:20:TYR:O    | 65:AD:24:LEU:HD13  | 2.15                     | 0.47              |
| 3:D:1780:A:N3     | 14:O:198:LYS:NZ    | 2.63                     | 0.46              |
| 3:D:3599:A:H2'    | 3:D:3600:G:C8      | 2.50                     | 0.46              |
| 3:D:4363:A:H5''   | 45:t:36:GLN:HG2    | 1.97                     | 0.46              |
| 12:M:48:LYS:HB3   | 28:c:42:THR:HG23   | 1.96                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:U:54:GLN:HA    | 20:U:83:TRP:CD1    | 2.50                     | 0.46              |
| 32:g:65:MET:HE3   | 32:g:65:MET:HB2    | 1.72                     | 0.46              |
| 48:w:1016:U:H5''  | 61:9:14:SER:HB3    | 1.96                     | 0.46              |
| 55:3:188:LYS:O    | 55:3:192:ILE:HG22  | 2.14                     | 0.46              |
| 60:8:117:PHE:C    | 60:8:119:ASP:H     | 2.23                     | 0.46              |
| 63:AB:35:GLN:H    | 63:AB:35:GLN:CD    | 2.23                     | 0.46              |
| 66:AE:38:ARG:O    | 66:AE:42:HIS:ND1   | 2.42                     | 0.46              |
| 68:AG:92:HIS:HD2  | 68:AG:93:SER:N     | 2.12                     | 0.46              |
| 3:D:1503:A:H4'    | 3:D:1504:G:H5'     | 1.96                     | 0.46              |
| 3:D:4229:U:OP1    | 45:t:63:THR:OG1    | 2.33                     | 0.46              |
| 15:P:146:ARG:HG2  | 15:P:147:ARG:HG2   | 1.95                     | 0.46              |
| 21:V:71:LYS:HD2   | 21:V:71:LYS:O      | 2.15                     | 0.46              |
| 48:w:527:C:H5'    | 58:6:125:HIS:HB2   | 1.96                     | 0.46              |
| 48:w:1130:G:H4'   | 61:9:10:GLY:HA2    | 1.98                     | 0.46              |
| 48:w:1606:G:N2    | 48:w:1632:G:H2'    | 2.30                     | 0.46              |
| 48:w:1746:U:OP1   | 55:3:31:ARG:NH1    | 2.49                     | 0.46              |
| 48:w:1747:C:H2'   | 48:w:1748:G:O4'    | 2.15                     | 0.46              |
| 55:3:42:GLY:O     | 55:3:46:LYS:NZ     | 2.48                     | 0.46              |
| 58:6:130:ILE:HG12 | 58:6:135:ILE:HD11  | 1.97                     | 0.46              |
| 66:AE:63:GLU:O    | 66:AE:67:VAL:HG23  | 2.16                     | 0.46              |
| 3:D:433:A:C2      | 3:D:3867:A:H4'     | 2.50                     | 0.46              |
| 3:D:1171:G:N1     | 3:D:1190:C:N3      | 2.56                     | 0.46              |
| 3:D:2474:G:H2'    | 3:D:2502:G:N2      | 2.31                     | 0.46              |
| 6:G:109:GLU:OE1   | 6:G:109:GLU:N      | 2.48                     | 0.46              |
| 52:0:135:GLU:HG2  | 52:0:153:VAL:HG12  | 1.96                     | 0.46              |
| 55:3:183:ARG:O    | 55:3:186:GLN:NE2   | 2.47                     | 0.46              |
| 55:3:221:LYS:HG3  | 55:3:224:ARG:NH1   | 2.30                     | 0.46              |
| 69:AH:71:ARG:HB3  | 69:AH:71:ARG:HH11  | 1.81                     | 0.46              |
| 79:AR:3:GLU:HB3   | 79:AR:267:VAL:HG13 | 1.97                     | 0.46              |
| 3:D:181:C:H2'     | 3:D:182:G:C8       | 2.51                     | 0.46              |
| 3:D:385:A:N3      | 3:D:387:G:H5''     | 2.31                     | 0.46              |
| 3:D:387:G:O2'     | 3:D:412:G:O6       | 2.21                     | 0.46              |
| 3:D:1301:C:H41    | 3:D:2316:G:H5'     | 1.79                     | 0.46              |
| 3:D:3783:A:OP2    | 3:D:3808:OMC:N4    | 2.42                     | 0.46              |
| 3:D:4859:C:H3'    | 3:D:4860:G:H8      | 1.80                     | 0.46              |
| 7:H:92:TYR:HB2    | 7:H:159:VAL:HB     | 1.97                     | 0.46              |
| 16:Q:51:ALA:HB2   | 16:Q:149:GLN:HE22  | 1.80                     | 0.46              |
| 18:S:124:ASP:OD1  | 18:S:125:SER:N     | 2.42                     | 0.46              |
| 24:Y:64:VAL:HG13  | 24:Y:72:VAL:HG13   | 1.96                     | 0.46              |
| 30:e:92:ASP:HB3   | 30:e:95:VAL:HG22   | 1.96                     | 0.46              |
| 48:w:125:C:OP1    | 48:w:127:C:N4      | 2.45                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:w:1865:C:C2     | 74:AM:5:ARG:HB2   | 2.51                     | 0.46              |
| 54:2:162:ALA:HB2   | 54:2:172:CYS:SG   | 2.56                     | 0.46              |
| 61:9:11:LEU:HD12   | 61:9:11:LEU:O     | 2.15                     | 0.46              |
| 79:AR:169:GLY:O    | 79:AR:195:LEU:HB2 | 2.15                     | 0.46              |
| 3:D:280:G:H5''     | 18:S:14:LYS:HE2   | 1.98                     | 0.46              |
| 3:D:684:G:OP2      | 3:D:685:C:N4      | 2.38                     | 0.46              |
| 6:G:205:ASN:HB2    | 6:G:206:PRO:HD2   | 1.97                     | 0.46              |
| 34:i:92:ARG:HA     | 34:i:102:LEU:HD23 | 1.96                     | 0.46              |
| 40:o:2:THR:O       | 40:o:7:SER:OG     | 2.26                     | 0.46              |
| 48:w:21:U:O2'      | 48:w:22:A:H5'     | 2.16                     | 0.46              |
| 48:w:811:A:HO2'    | 48:w:812:A:P      | 2.39                     | 0.46              |
| 54:2:124:ASP:N     | 54:2:124:ASP:OD1  | 2.48                     | 0.46              |
| 55:3:221:LYS:HG2   | 55:3:225:GLN:HE22 | 1.79                     | 0.46              |
| 3:D:2104:G:HO2'    | 3:D:2105:A:H8     | 1.60                     | 0.46              |
| 3:D:4738:C:H2'     | 3:D:4739:C:O4'    | 2.15                     | 0.46              |
| 3:D:5006:U:H4'     | 3:D:5007:A:H5'    | 1.98                     | 0.46              |
| 7:H:76:VAL:HA      | 7:H:334:LYS:O     | 2.16                     | 0.46              |
| 7:H:294:LYS:HA     | 7:H:294:LYS:HE2   | 1.97                     | 0.46              |
| 48:w:830:A:H61     | 48:w:844:U:H3     | 1.62                     | 0.46              |
| 48:w:1330:G:H4'    | 48:w:1331:C:H3'   | 1.97                     | 0.46              |
| 48:w:1482:C:OP1    | 77:AP:54:LYS:NZ   | 2.42                     | 0.46              |
| 50:y:52:THR:HA     | 50:y:57:ILE:HA    | 1.98                     | 0.46              |
| 53:1:11:ARG:NH2    | 53:1:20:LEU:HB3   | 2.30                     | 0.46              |
| 53:1:141:THR:OG1   | 53:1:143:ASP:OD1  | 2.23                     | 0.46              |
| 55:3:67:VAL:CG2    | 55:3:99:GLY:HA2   | 2.45                     | 0.46              |
| 70:AI:42:MET:HE3   | 70:AI:50:PHE:CD2  | 2.50                     | 0.46              |
| 71:AJ:68:LYS:HD2   | 71:AJ:91:LEU:HD22 | 1.98                     | 0.46              |
| 3:D:1380:G:N2      | 3:D:1381:U:O4     | 2.45                     | 0.46              |
| 3:D:4325:A:N3      | 9:J:36:LEU:HB3    | 2.30                     | 0.46              |
| 3:D:4743:G:H2'     | 3:D:4744:A:C8     | 2.51                     | 0.46              |
| 17:R:119:ARG:HG3   | 19:T:189:ILE:HG23 | 1.96                     | 0.46              |
| 18:S:9:GLU:HB3     | 39:n:44:ILE:HG13  | 1.98                     | 0.46              |
| 48:w:588:G:H5''    | 48:w:590:A2M:H4'  | 1.98                     | 0.46              |
| 74:AM:22:ARG:NH1   | 74:AM:27:ALA:O    | 2.49                     | 0.46              |
| 79:AR:143:GLN:HE21 | 79:AR:145:GLU:HG2 | 1.79                     | 0.46              |
| 3:D:759:G:OP1      | 13:N:50:LYS:HB3   | 2.15                     | 0.46              |
| 3:D:959:G:N7       | 10:K:123:ARG:HG3  | 2.31                     | 0.46              |
| 3:D:1773:OMU:H2'   | 3:D:1774:C:C6     | 2.50                     | 0.46              |
| 3:D:4635:A:H8      | 3:D:5048:A:N6     | 2.13                     | 0.46              |
| 3:D:4734:A:O2'     | 3:D:4735:G:OP2    | 2.31                     | 0.46              |
| 20:U:29:THR:HA     | 20:U:32:THR:HG22  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:W:173:ARG:HG3   | 22:W:176:ARG:HH11  | 1.80                     | 0.46              |
| 30:e:83:THR:HG22   | 30:e:85:TYR:H      | 1.81                     | 0.46              |
| 36:k:43:LEU:HA     | 36:k:43:LEU:HD12   | 1.79                     | 0.46              |
| 47:v:108:MET:O     | 47:v:112:ARG:HG2   | 2.16                     | 0.46              |
| 48:w:573:U:O2      | 48:w:576:A2M:H8    | 2.16                     | 0.46              |
| 48:w:1320:G:H2'    | 48:w:1321:G:O4'    | 2.16                     | 0.46              |
| 49:x:52:LYS:HD2    | 49:x:52:LYS:O      | 2.16                     | 0.46              |
| 55:3:230:LYS:HA    | 55:3:233:ARG:HG2   | 1.97                     | 0.46              |
| 58:6:11:LYS:HA     | 58:6:11:LYS:HD3    | 1.56                     | 0.46              |
| 65:AD:102:THR:HG23 | 65:AD:105:MET:HE2  | 1.98                     | 0.46              |
| 70:AI:114:GLU:OE1  | 70:AI:117:ARG:NH1  | 2.49                     | 0.46              |
| 2:B:30:G:P         | 63:AB:136:THR:HG23 | 2.56                     | 0.46              |
| 3:D:6:C:H5''       | 12:M:197:LYS:HG2   | 1.96                     | 0.46              |
| 3:D:124:C:OP1      | 18:S:144:ARG:HD2   | 2.16                     | 0.46              |
| 4:E:22:A:H5'       | 4:E:23:A:OP2       | 2.16                     | 0.46              |
| 12:M:50:ASP:OD2    | 12:M:51:LEU:N      | 2.48                     | 0.46              |
| 25:Z:24:ASP:OD1    | 25:Z:111:GLU:HB2   | 2.15                     | 0.46              |
| 29:d:31:SER:HA     | 29:d:48:PRO:HA     | 1.98                     | 0.46              |
| 33:h:26:LYS:HG3    | 33:h:97:ILE:HB     | 1.97                     | 0.46              |
| 41:p:33:LYS:HG2    | 41:p:46:VAL:HG22   | 1.97                     | 0.46              |
| 48:w:1114:U:O2'    | 48:w:1115:U:H2'    | 2.16                     | 0.46              |
| 52:0:39:VAL:HG13   | 52:0:48:ILE:HG22   | 1.98                     | 0.46              |
| 52:0:58:VAL:HG23   | 52:0:59:LEU:HD12   | 1.98                     | 0.46              |
| 55:3:32:MET:HA     | 55:3:52:ILE:HG23   | 1.98                     | 0.46              |
| 58:6:128:VAL:O     | 58:6:132:GLN:HG2   | 2.16                     | 0.46              |
| 3:D:711:A:HO2'     | 10:K:136:HIS:HD1   | 1.60                     | 0.46              |
| 3:D:2382:A:N1      | 3:D:2829:U:O2'     | 2.41                     | 0.46              |
| 23:X:7:LEU:O       | 23:X:103:ALA:HB1   | 2.16                     | 0.46              |
| 32:g:12:GLN:HB3    | 32:g:16:TRP:CZ3    | 2.51                     | 0.46              |
| 38:m:4:ILE:O       | 38:m:4:ILE:HG13    | 2.16                     | 0.46              |
| 43:r:79:GLU:CD     | 43:r:81:SER:HG     | 2.21                     | 0.46              |
| 48:w:465:A:H5'     | 48:w:466:G:C4      | 2.51                     | 0.46              |
| 48:w:1736:G:H2'    | 48:w:1737:G:H8     | 1.81                     | 0.46              |
| 50:y:127:VAL:HG21  | 50:y:173:THR:HA    | 1.98                     | 0.46              |
| 52:0:151:LYS:O     | 52:0:153:VAL:HG13  | 2.16                     | 0.46              |
| 54:2:191:LYS:HE3   | 54:2:191:LYS:HB2   | 1.69                     | 0.46              |
| 55:3:10:THR:HB     | 55:3:129:VAL:H     | 1.81                     | 0.46              |
| 55:3:144:LEU:HD23  | 55:3:145:PHE:CE2   | 2.51                     | 0.46              |
| 56:4:134:VAL:HG12  | 56:4:173:PHE:CE2   | 2.50                     | 0.46              |
| 61:9:83:ASP:N      | 61:9:83:ASP:OD1    | 2.46                     | 0.46              |
| 67:AF:74:SER:O     | 67:AF:78:ILE:HD12  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 68:AG:66:ARG:NH2  | 68:AG:75:LYS:HG2   | 2.30                     | 0.46              |
| 3:D:175:C:H2'     | 3:D:176:G:C8       | 2.51                     | 0.45              |
| 3:D:2464:C:HO2'   | 3:D:2465:C:H6      | 1.59                     | 0.45              |
| 3:D:4397:A:H2'    | 3:D:4452:U:O4      | 2.16                     | 0.45              |
| 4:E:23:A:N3       | 4:E:118:C:O2'      | 2.47                     | 0.45              |
| 12:M:210:GLU:OE1  | 12:M:210:GLU:N     | 2.48                     | 0.45              |
| 30:e:103:ASP:OD2  | 30:e:106:LEU:HG    | 2.16                     | 0.45              |
| 48:w:223:C:H2'    | 48:w:224:A:C8      | 2.50                     | 0.45              |
| 49:x:58:LEU:HD12  | 49:x:174:MET:HE1   | 1.98                     | 0.45              |
| 52:0:102:ALA:HB2  | 52:0:186:VAL:HG21  | 1.98                     | 0.45              |
| 53:1:100:ARG:HB2  | 53:1:114:ILE:HD13  | 1.98                     | 0.45              |
| 56:4:49:LYS:HD3   | 56:4:49:LYS:HA     | 1.76                     | 0.45              |
| 62:AA:47:LEU:HD23 | 62:AA:47:LEU:HA    | 1.79                     | 0.45              |
| 62:AA:56:VAL:HG23 | 62:AA:60:MET:SD    | 2.56                     | 0.45              |
| 68:AG:22:ILE:HA   | 68:AG:113:GLU:O    | 2.16                     | 0.45              |
| 68:AG:90:ASP:O    | 68:AG:91:LEU:HD23  | 2.15                     | 0.45              |
| 3:D:4739:C:H2'    | 3:D:4740:G:H5'     | 1.98                     | 0.45              |
| 48:w:525:A:H2'    | 48:w:526:A:C8      | 2.48                     | 0.45              |
| 48:w:529:A:H61    | 48:w:554:A:H61     | 1.64                     | 0.45              |
| 49:x:33:GLN:OE1   | 49:x:33:GLN:HA     | 2.16                     | 0.45              |
| 49:x:76:VAL:HG12  | 49:x:123:VAL:HB    | 1.97                     | 0.45              |
| 52:0:57:ASN:C     | 52:0:57:ASN:HD22   | 2.23                     | 0.45              |
| 57:5:202:ILE:HG13 | 57:5:203:LYS:N     | 2.31                     | 0.45              |
| 59:7:25:LYS:HA    | 59:7:46:MET:SD     | 2.56                     | 0.45              |
| 64:AC:128:GLU:OE2 | 64:AC:138:ARG:NH2  | 2.49                     | 0.45              |
| 66:AE:113:ARG:HD3 | 66:AE:117:ILE:HD11 | 1.98                     | 0.45              |
| 3:D:1431:C:H2'    | 3:D:1432:G:O4'     | 2.16                     | 0.45              |
| 3:D:1443:A:H2'    | 3:D:1444:G:O4'     | 2.16                     | 0.45              |
| 3:D:3792:OMG:HM23 | 3:D:3792:OMG:H1'   | 1.82                     | 0.45              |
| 14:O:179:ASP:OD2  | 14:O:180:GLU:N     | 2.49                     | 0.45              |
| 16:Q:8:MET:HE3    | 16:Q:8:MET:HB2     | 1.85                     | 0.45              |
| 17:R:63:LYS:HB3   | 17:R:63:LYS:HE3    | 1.73                     | 0.45              |
| 36:k:54:LYS:O     | 36:k:66:LYS:NZ     | 2.43                     | 0.45              |
| 49:x:11:LYS:HD3   | 49:x:11:LYS:N      | 2.31                     | 0.45              |
| 51:z:121:ARG:HH12 | 51:z:123:ARG:NH2   | 2.13                     | 0.45              |
| 58:6:40:LYS:O     | 58:6:43:VAL:HG22   | 2.17                     | 0.45              |
| 75:AN:56:CYS:SG   | 75:AN:59:CYS:HB2   | 2.56                     | 0.45              |
| 75:AN:80:ARG:HD2  | 75:AN:80:ARG:O     | 2.16                     | 0.45              |
| 3:D:651:C:N4      | 3:D:652:G:O6       | 2.49                     | 0.45              |
| 3:D:1617:G:H1'    | 3:D:2513:A:N6      | 2.32                     | 0.45              |
| 10:K:99:ASP:N     | 10:K:99:ASP:OD1    | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:w:676:C:H5''   | 61:9:5:HIS:CD2    | 2.52                     | 0.45              |
| 48:w:1256:G:H8    | 68:AG:66:ARG:HB2  | 1.81                     | 0.45              |
| 48:w:1600:G:H4'   | 73:AL:43:LYS:HE3  | 1.99                     | 0.45              |
| 49:x:184:ARG:HG2  | 49:x:191:ARG:HG2  | 1.98                     | 0.45              |
| 49:x:204:TYR:CE2  | 49:x:206:ASP:HB2  | 2.51                     | 0.45              |
| 52:0:48:ILE:HG13  | 52:0:86:LEU:HG    | 1.98                     | 0.45              |
| 53:1:11:ARG:NH1   | 53:1:24:THR:OG1   | 2.50                     | 0.45              |
| 55:3:22:ARG:HA    | 55:3:25:ARG:HG2   | 1.98                     | 0.45              |
| 62:AA:42:VAL:HG22 | 62:AA:56:VAL:O    | 2.16                     | 0.45              |
| 62:AA:82:ALA:O    | 62:AA:86:LYS:HG2  | 2.17                     | 0.45              |
| 79:AR:17:TRP:HE1  | 79:AR:36:ARG:CZ   | 2.29                     | 0.45              |
| 79:AR:38:LYS:HA   | 79:AR:66:VAL:HG23 | 1.99                     | 0.45              |
| 79:AR:40:ILE:HB   | 79:AR:59:LEU:HD12 | 1.98                     | 0.45              |
| 3:D:1716:G:H4'    | 24:Y:125:TRP:CZ3  | 2.51                     | 0.45              |
| 11:L:199:LYS:HB2  | 11:L:199:LYS:HE3  | 1.61                     | 0.45              |
| 30:e:128:LYS:O    | 30:e:132:GLN:HG2  | 2.16                     | 0.45              |
| 48:w:158:A:H2'    | 48:w:159:A2M:H8   | 1.99                     | 0.45              |
| 48:w:1436:C:O2    | 48:w:1438:A:H5'   | 2.16                     | 0.45              |
| 48:w:1495:G:H21   | 77:AP:42:CYS:HB3  | 1.82                     | 0.45              |
| 55:3:194:LEU:O    | 55:3:197:GLN:NE2  | 2.49                     | 0.45              |
| 63:AB:15:PHE:CZ   | 63:AB:22:LEU:HB2  | 2.52                     | 0.45              |
| 70:AI:77:PRO:HG2  | 70:AI:79:PHE:CE2  | 2.51                     | 0.45              |
| 79:AR:203:ASP:OD1 | 79:AR:204:GLY:N   | 2.48                     | 0.45              |
| 3:D:158:A:H5''    | 3:D:159:C:H2'     | 1.99                     | 0.45              |
| 3:D:238:C:OP2     | 29:d:45:ARG:NH2   | 2.50                     | 0.45              |
| 3:D:965:G:N2      | 3:D:2092:G:H1'    | 2.31                     | 0.45              |
| 3:D:1354:A:OP2    | 21:V:106:THR:HG21 | 2.16                     | 0.45              |
| 3:D:4996:C:OP1    | 34:i:32:ARG:NH1   | 2.39                     | 0.45              |
| 12:M:206:GLN:O    | 12:M:206:GLN:CD   | 2.60                     | 0.45              |
| 14:O:60:LEU:HD11  | 14:O:91:LEU:HD23  | 1.98                     | 0.45              |
| 16:Q:65:ARG:HD2   | 16:Q:66:TYR:CE2   | 2.52                     | 0.45              |
| 30:e:89:ILE:HG22  | 30:e:91:LEU:HG    | 1.99                     | 0.45              |
| 35:j:98:GLU:OE1   | 35:j:123:THR:OG1  | 2.30                     | 0.45              |
| 45:t:105:GLN:HG3  | 45:t:106:PHE:H    | 1.81                     | 0.45              |
| 48:w:556:U:O2'    | 48:w:558:G:OP1    | 2.31                     | 0.45              |
| 48:w:1030:A:H2'   | 48:w:1031:A2M:H8  | 1.99                     | 0.45              |
| 58:6:164:PRO:HB3  | 58:6:170:PRO:HA   | 1.99                     | 0.45              |
| 66:AE:62:ASP:OD1  | 66:AE:62:ASP:N    | 2.50                     | 0.45              |
| 3:D:3668:C:H5'    | 6:G:8:GLN:O       | 2.17                     | 0.45              |
| 11:L:31:LYS:HD3   | 11:L:31:LYS:HA    | 1.79                     | 0.45              |
| 13:N:63:ASN:O     | 13:N:67:LEU:HB2   | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:N:77:VAL:O      | 13:N:80:MET:HG2    | 2.17                     | 0.45              |
| 42:q:28:ARG:HE     | 42:q:28:ARG:HB3    | 1.65                     | 0.45              |
| 53:1:102:ILE:HG13  | 53:1:182:MET:HE1   | 1.98                     | 0.45              |
| 54:2:102:LEU:O     | 73:AL:66:LYS:NZ    | 2.44                     | 0.45              |
| 72:AK:20:ARG:HD3   | 72:AK:74:MET:SD    | 2.57                     | 0.45              |
| 8:I:235:LEU:HD23   | 8:I:240:LEU:HD11   | 1.98                     | 0.45              |
| 10:K:157:HIS:HB3   | 10:K:160:LYS:HD2   | 1.98                     | 0.45              |
| 11:L:232:ASP:OD1   | 11:L:236:ARG:NH2   | 2.50                     | 0.45              |
| 16:Q:64:VAL:HA     | 16:Q:67:HIS:HD2    | 1.81                     | 0.45              |
| 28:c:39:LYS:O      | 28:c:40:ILE:HD13   | 2.17                     | 0.45              |
| 34:i:37:GLY:O      | 34:i:41:ARG:HG3    | 2.17                     | 0.45              |
| 45:t:101:GLY:HA2   | 45:t:102:GLN:HB3   | 1.99                     | 0.45              |
| 48:w:170:A:O2'     | 55:3:136:LYS:NZ    | 2.50                     | 0.45              |
| 48:w:1232:PSU:H2'  | 48:w:1233:G:C8     | 2.51                     | 0.45              |
| 50:y:108:ASP:N     | 50:y:108:ASP:OD1   | 2.48                     | 0.45              |
| 51:z:76:LYS:HD2    | 51:z:76:LYS:HA     | 1.76                     | 0.45              |
| 65:AD:16:ILE:HD11  | 65:AD:54:VAL:HG21  | 1.98                     | 0.45              |
| 3:D:1210:C:H41     | 11:L:66:ARG:CZ     | 2.30                     | 0.45              |
| 3:D:4623:OMG:N2    | 7:H:279:GLU:OE2    | 2.45                     | 0.45              |
| 3:D:4635:A:O2'     | 3:D:4637:OMG:OP1   | 2.32                     | 0.45              |
| 48:w:1388:A:H61    | 52:0:161:GLY:HA3   | 1.82                     | 0.45              |
| 54:2:35:LEU:HD21   | 54:2:146:ARG:HD3   | 1.98                     | 0.45              |
| 62:AA:124:MET:HE2  | 62:AA:124:MET:HB2  | 1.78                     | 0.45              |
| 64:AC:118:THR:C    | 64:AC:120:LEU:N    | 2.65                     | 0.45              |
| 65:AD:58:MET:O     | 65:AD:62:GLN:HG2   | 2.17                     | 0.45              |
| 72:AK:55:ILE:O     | 72:AK:55:ILE:HD12  | 2.16                     | 0.45              |
| 79:AR:152:SER:HB2  | 79:AR:168:CYS:SG   | 2.57                     | 0.45              |
| 3:D:4620:OMU:OP2   | 3:D:4670:C:N4      | 2.40                     | 0.45              |
| 16:Q:42:LYS:O      | 16:Q:46:ILE:HG12   | 2.17                     | 0.45              |
| 23:X:15:ARG:HB3    | 23:X:27:LEU:HD23   | 1.99                     | 0.45              |
| 48:w:58:C:H5''     | 48:w:499:G:H21     | 1.81                     | 0.45              |
| 48:w:444:G:H22     | 48:w:447:A:H5'     | 1.82                     | 0.45              |
| 48:w:902:G:C6      | 48:w:903:A:H8      | 2.35                     | 0.45              |
| 48:w:923:G:OP1     | 61:9:2:GLY:HA3     | 2.17                     | 0.45              |
| 48:w:1453:C:H5'    | 65:AD:48:ASN:HB2   | 1.99                     | 0.45              |
| 48:w:1623:A:H5''   | 66:AE:133:GLY:HA3  | 1.98                     | 0.45              |
| 48:w:1639:G7M:H5'' | 73:AL:34:LYS:HE3   | 1.99                     | 0.45              |
| 55:3:231:ARG:HH11  | 55:3:234:LEU:HD13  | 1.82                     | 0.45              |
| 58:6:84:ILE:O      | 58:6:108:ARG:NE    | 2.46                     | 0.45              |
| 64:AC:89:SER:HB3   | 64:AC:112:LEU:HD13 | 1.99                     | 0.45              |
| 73:AL:101:SER:HB3  | 73:AL:108:ILE:HD11 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 75:AN:21:LYS:C    | 75:AN:23:ARG:H    | 2.25                     | 0.45              |
| 79:AR:30:MET:HE3  | 79:AR:30:MET:O    | 2.17                     | 0.45              |
| 79:AR:217:MET:HE2 | 79:AR:217:MET:HB3 | 1.80                     | 0.45              |
| 3:D:208:A:C2      | 3:D:233:U:H5''    | 2.53                     | 0.44              |
| 3:D:1179:U:H3'    | 3:D:1180:C:H5''   | 2.00                     | 0.44              |
| 3:D:2544:G:H5''   | 3:D:2545:U:H5''   | 1.98                     | 0.44              |
| 3:D:4377:G:O6     | 31:f:42:ARG:NH2   | 2.50                     | 0.44              |
| 7:H:17:LEU:O      | 7:H:19:ARG:N      | 2.50                     | 0.44              |
| 22:W:170:ARG:HH21 | 22:W:173:ARG:NE   | 2.15                     | 0.44              |
| 31:f:125:LYS:HA   | 31:f:145:VAL:O    | 2.17                     | 0.44              |
| 39:n:43:MET:HA    | 39:n:43:MET:HE2   | 2.00                     | 0.44              |
| 47:v:68:SER:OG    | 47:v:69:GLY:N     | 2.49                     | 0.44              |
| 48:w:334:C:OP2    | 55:3:190:ARG:NH2  | 2.37                     | 0.44              |
| 48:w:1217:A:H2'   | 48:w:1218:C:C6    | 2.53                     | 0.44              |
| 50:y:28:LYS:HE2   | 50:y:28:LYS:HB3   | 1.73                     | 0.44              |
| 58:6:121:LYS:HE3  | 58:6:121:LYS:HB3  | 1.72                     | 0.44              |
| 63:AB:18:ARG:HD3  | 66:AE:90:VAL:HA   | 1.99                     | 0.44              |
| 65:AD:36:GLU:HG2  | 65:AD:37:GLU:OE2  | 2.16                     | 0.44              |
| 76:AO:26:GLN:OE1  | 76:AO:26:GLN:N    | 2.49                     | 0.44              |
| 79:AR:64:HIS:HB3  | 79:AR:84:ASP:H    | 1.82                     | 0.44              |
| 3:D:983:C:H2'     | 3:D:984:C:O4'     | 2.17                     | 0.44              |
| 3:D:1083:U:H3     | 3:D:1216:C:N4     | 2.16                     | 0.44              |
| 3:D:1475:G:H2'    | 3:D:1476:C:C6     | 2.52                     | 0.44              |
| 3:D:2101:C:O2'    | 3:D:2102:G:OP1    | 2.29                     | 0.44              |
| 3:D:4731:G:H1     | 3:D:4734:A:N6     | 2.15                     | 0.44              |
| 48:w:818:A:OP1    | 58:6:80:ARG:NH2   | 2.43                     | 0.44              |
| 51:z:183:LYS:HA   | 51:z:195:LEU:O    | 2.17                     | 0.44              |
| 52:0:40:ARG:HH12  | 68:AG:108:PRO:C   | 2.26                     | 0.44              |
| 53:1:21:ASP:OD2   | 53:1:24:THR:N     | 2.51                     | 0.44              |
| 53:1:40:GLU:N     | 53:1:40:GLU:OE2   | 2.50                     | 0.44              |
| 59:7:25:LYS:HB3   | 59:7:67:PHE:CE2   | 2.52                     | 0.44              |
| 79:AR:215:GLN:HA  | 79:AR:231:ASP:HA  | 2.00                     | 0.44              |
| 3:D:1855:G:OP1    | 32:g:4:SER:HB2    | 2.16                     | 0.44              |
| 3:D:2755:A:OP2    | 30:e:51:ARG:NH1   | 2.50                     | 0.44              |
| 3:D:4742:G:H2'    | 3:D:4743:G:H8     | 1.82                     | 0.44              |
| 7:H:185:VAL:HG13  | 7:H:193:LYS:HG2   | 1.98                     | 0.44              |
| 7:H:297:LYS:HE2   | 7:H:297:LYS:HB3   | 1.70                     | 0.44              |
| 15:P:111:GLU:OE1  | 66:AE:14:ARG:NH2  | 2.50                     | 0.44              |
| 48:w:564:A:H2'    | 48:w:565:G:O4'    | 2.17                     | 0.44              |
| 48:w:607:U:O2'    | 48:w:630:U:O4'    | 2.33                     | 0.44              |
| 48:w:640:A:H2'    | 48:w:641:A:C8     | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:w:957:A:OP1    | 62:AA:57:THR:OG1  | 2.32                     | 0.44              |
| 49:x:158:ASP:OD2  | 69:AH:32:ILE:HD13 | 2.16                     | 0.44              |
| 50:y:137:LEU:HG   | 50:y:215:VAL:HG12 | 1.99                     | 0.44              |
| 51:z:78:LEU:HB3   | 51:z:97:PHE:CD2   | 2.51                     | 0.44              |
| 56:4:130:LEU:HD21 | 56:4:156:VAL:HG21 | 1.99                     | 0.44              |
| 57:5:105:ASP:HA   | 57:5:169:GLY:O    | 2.17                     | 0.44              |
| 57:5:122:GLY:O    | 57:5:167:GLN:NE2  | 2.50                     | 0.44              |
| 58:6:60:LEU:HA    | 58:6:63:LEU:HD12  | 1.99                     | 0.44              |
| 60:8:135:SER:HB3  | 60:8:138:VAL:HB   | 1.99                     | 0.44              |
| 66:AE:99:LEU:HD13 | 66:AE:99:LEU:HA   | 1.87                     | 0.44              |
| 76:AO:13:ARG:NH1  | 76:AO:55:VAL:HG22 | 2.32                     | 0.44              |
| 3:D:44:A:OP2      | 18:S:85:VAL:HG21  | 2.18                     | 0.44              |
| 3:D:389:A:H1'     | 29:d:91:ASN:HA    | 1.98                     | 0.44              |
| 3:D:1701:A:H5'    | 3:D:2096:G:H22    | 1.82                     | 0.44              |
| 3:D:3860:A:N3     | 20:U:131:ARG:NH1  | 2.65                     | 0.44              |
| 3:D:3925:OMU:HM23 | 3:D:3925:OMU:H1'  | 1.78                     | 0.44              |
| 3:D:4342:C:O3'    | 45:t:37:GLY:HA3   | 2.17                     | 0.44              |
| 3:D:4731:G:N3     | 3:D:4732:G:H1'    | 2.33                     | 0.44              |
| 5:F:85:U:H4'      | 5:F:86:U:H5'      | 1.99                     | 0.44              |
| 5:F:110:U:OP2     | 42:q:8:ARG:NH2    | 2.50                     | 0.44              |
| 13:N:36:ARG:HD3   | 13:N:38:PHE:CZ    | 2.53                     | 0.44              |
| 21:V:148:VAL:HG12 | 21:V:152:PHE:CZ   | 2.53                     | 0.44              |
| 49:x:158:ASP:OD1  | 69:AH:60:ARG:NH1  | 2.51                     | 0.44              |
| 54:2:160:GLU:OE1  | 54:2:160:GLU:HA   | 2.18                     | 0.44              |
| 55:3:160:LYS:HE3  | 55:3:162:LEU:HD11 | 2.00                     | 0.44              |
| 57:5:81:VAL:HA    | 57:5:102:VAL:HA   | 1.99                     | 0.44              |
| 58:6:142:VAL:HG12 | 58:6:144:ILE:H    | 1.83                     | 0.44              |
| 59:7:65:ARG:NH2   | 77:AP:20:SER:OG   | 2.49                     | 0.44              |
| 61:9:132:LYS:HA   | 61:9:132:LYS:HD3  | 1.64                     | 0.44              |
| 71:AJ:124:LYS:HG2 | 71:AJ:129:SER:HA  | 1.99                     | 0.44              |
| 73:AL:77:LEU:HB3  | 73:AL:79:ILE:HG12 | 1.99                     | 0.44              |
| 3:D:43:U:H5''     | 18:S:85:VAL:HG23  | 1.99                     | 0.44              |
| 3:D:494:U:H2'     | 3:D:495:C:C6      | 2.53                     | 0.44              |
| 3:D:659:G:C6      | 3:D:660:A:C6      | 3.05                     | 0.44              |
| 3:D:1442:C:O2'    | 3:D:1443:A:H5'    | 2.17                     | 0.44              |
| 3:D:1660:U:H2'    | 31:f:12:ARG:O     | 2.18                     | 0.44              |
| 3:D:3607:U:OP1    | 22:W:88:ARG:NH1   | 2.51                     | 0.44              |
| 3:D:3877:A:N3     | 3:D:4401:G:O2'    | 2.42                     | 0.44              |
| 3:D:4773:C:O2'    | 3:D:4774:C:H5'    | 2.18                     | 0.44              |
| 9:J:33:ARG:O      | 9:J:37:VAL:HG12   | 2.17                     | 0.44              |
| 20:U:111:SER:HB2  | 20:U:153:LYS:O    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:W:38:ARG:O     | 22:W:39:GLN:HB2   | 2.18                     | 0.44              |
| 38:m:3:LYS:HB3    | 38:m:4:ILE:H      | 1.59                     | 0.44              |
| 39:n:63:VAL:HG12  | 39:n:65:LYS:HG3   | 1.98                     | 0.44              |
| 48:w:186:C:H2'    | 48:w:187:G:C8     | 2.53                     | 0.44              |
| 48:w:465:A:H5'    | 48:w:466:G:C8     | 2.52                     | 0.44              |
| 48:w:570:C:O2     | 72:AK:34:THR:OG1  | 2.23                     | 0.44              |
| 48:w:1370:A:N3    | 48:w:1372:U:H5'   | 2.32                     | 0.44              |
| 49:x:34:MET:HE3   | 49:x:34:MET:HB3   | 1.76                     | 0.44              |
| 52:0:126:ILE:HG21 | 52:0:134:CYS:HB3  | 1.98                     | 0.44              |
| 53:1:160:ILE:HA   | 53:1:172:PHE:HA   | 2.00                     | 0.44              |
| 57:5:101:ILE:HD12 | 57:5:190:LEU:HD11 | 2.00                     | 0.44              |
| 59:7:41:PRO:HB2   | 59:7:43:LEU:HD23  | 1.99                     | 0.44              |
| 59:7:49:MET:HE3   | 59:7:49:MET:HB2   | 1.82                     | 0.44              |
| 61:9:29:THR:OG1   | 61:9:30:SER:N     | 2.51                     | 0.44              |
| 63:AB:93:MET:HA   | 63:AB:93:MET:HE2  | 1.99                     | 0.44              |
| 65:AD:81:ARG:HD3  | 65:AD:81:ARG:HA   | 1.72                     | 0.44              |
| 66:AE:26:ILE:HG13 | 66:AE:45:LEU:HD11 | 2.00                     | 0.44              |
| 67:AF:39:LEU:HD23 | 67:AF:39:LEU:HA   | 1.81                     | 0.44              |
| 79:AR:104:HIS:NE2 | 79:AR:122:SER:HB3 | 2.33                     | 0.44              |
| 79:AR:213:ASP:OD1 | 79:AR:213:ASP:N   | 2.50                     | 0.44              |
| 3:D:182:G:H1      | 3:D:254:G:H22     | 1.65                     | 0.44              |
| 3:D:255:C:H2'     | 3:D:256:G:C8      | 2.53                     | 0.44              |
| 3:D:3844:U:OP2    | 7:H:239:LYS:HG2   | 2.18                     | 0.44              |
| 3:D:4769:G:H5''   | 19:T:176:ARG:HD3  | 2.00                     | 0.44              |
| 14:O:55:ASP:HA    | 14:O:131:ILE:HG23 | 1.98                     | 0.44              |
| 25:Z:45:GLU:O     | 25:Z:53:ALA:HB1   | 2.17                     | 0.44              |
| 30:e:35:ASP:OD1   | 30:e:35:ASP:N     | 2.50                     | 0.44              |
| 38:m:60:VAL:O     | 38:m:64:THR:HG22  | 2.17                     | 0.44              |
| 48:w:557:U:H2'    | 48:w:558:G:C8     | 2.53                     | 0.44              |
| 48:w:1466:G:OP1   | 65:AD:5:ARG:HG2   | 2.18                     | 0.44              |
| 49:x:205:ARG:NH2  | 49:x:210:ILE:HD13 | 2.33                     | 0.44              |
| 57:5:79:ILE:HG12  | 57:5:103:LEU:O    | 2.17                     | 0.44              |
| 58:6:113:GLN:HA   | 58:6:116:LYS:HG2  | 2.00                     | 0.44              |
| 60:8:37:TYR:HE1   | 60:8:51:ILE:HG23  | 1.81                     | 0.44              |
| 65:AD:29:HIS:HA   | 65:AD:32:LYS:HE2  | 1.99                     | 0.44              |
| 66:AE:8:LYS:HD2   | 66:AE:10:GLN:H    | 1.83                     | 0.44              |
| 3:D:966:A:H5''    | 3:D:2092:G:H22    | 1.83                     | 0.44              |
| 3:D:1412:G:H2'    | 3:D:1413:C:C6     | 2.53                     | 0.44              |
| 3:D:1574:G:O2'    | 3:D:1575:A:H8     | 2.01                     | 0.44              |
| 7:H:219:VAL:HG11  | 7:H:337:VAL:HG21  | 2.00                     | 0.44              |
| 9:J:211:LEU:HB3   | 9:J:219:TYR:HB2   | 1.99                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:R:31:ILE:HD11   | 17:R:37:LEU:HB2   | 2.00                     | 0.44              |
| 24:Y:79:GLN:HE21   | 24:Y:79:GLN:C     | 2.19                     | 0.44              |
| 25:Z:18:VAL:HG22   | 25:Z:75:GLU:HG3   | 1.99                     | 0.44              |
| 48:w:867:G:H21     | 56:4:111:LYS:NZ   | 2.16                     | 0.44              |
| 49:x:33:GLN:HB3    | 49:x:154:LEU:HD12 | 1.99                     | 0.44              |
| 55:3:21:GLU:OE1    | 55:3:25:ARG:NH1   | 2.51                     | 0.44              |
| 55:3:226:GLU:O     | 55:3:230:LYS:HG3  | 2.18                     | 0.44              |
| 64:AC:97:GLN:HG3   | 64:AC:105:LYS:HD2 | 1.99                     | 0.44              |
| 67:AF:1:MET:HE3    | 67:AF:4:VAL:HG21  | 1.98                     | 0.44              |
| 77:AP:22:ARG:HD2   | 77:AP:36:LEU:O    | 2.16                     | 0.44              |
| 3:D:2487:G:O2'     | 3:D:2488:C:OP2    | 2.36                     | 0.44              |
| 3:D:2487:G:N2      | 3:D:2492:C:H1'    | 2.27                     | 0.44              |
| 13:N:8:GLN:HG2     | 13:N:74:CYS:SG    | 2.57                     | 0.44              |
| 19:T:5:GLN:HG3     | 19:T:6:VAL:N      | 2.32                     | 0.44              |
| 24:Y:107:LYS:HE3   | 24:Y:107:LYS:HB2  | 1.73                     | 0.44              |
| 28:c:72:ASP:O      | 28:c:76:ILE:HG12  | 2.18                     | 0.44              |
| 48:w:130:G:H2'     | 48:w:130:G:N3     | 2.33                     | 0.44              |
| 48:w:1442:OMU:O5'  | 48:w:1442:OMU:H6  | 2.16                     | 0.44              |
| 49:x:52:LYS:HD2    | 49:x:52:LYS:C     | 2.43                     | 0.44              |
| 49:x:144:THR:O     | 49:x:158:ASP:HB2  | 2.17                     | 0.44              |
| 64:AC:101:ASP:OD1  | 64:AC:102:GLU:N   | 2.51                     | 0.44              |
| 65:AD:92:ASP:N     | 65:AD:92:ASP:OD1  | 2.51                     | 0.44              |
| 77:AP:53:ILE:O     | 77:AP:53:ILE:HG13 | 2.17                     | 0.44              |
| 3:D:106:A:H2'      | 3:D:107:G:O4'     | 2.18                     | 0.44              |
| 3:D:981:C:H2'      | 10:K:73:TYR:HE1   | 1.82                     | 0.44              |
| 3:D:3911:C:H2'     | 3:D:3912:U:C6     | 2.53                     | 0.44              |
| 3:D:4967:A:H2'     | 3:D:4968:A:C8     | 2.52                     | 0.44              |
| 9:J:41:LYS:HB2     | 24:Y:68:THR:O     | 2.17                     | 0.44              |
| 9:J:291:GLN:HA     | 9:J:291:GLN:NE2   | 2.33                     | 0.44              |
| 18:S:45:PRO:O      | 18:S:49:ARG:HG3   | 2.17                     | 0.44              |
| 21:V:66:MET:HE2    | 21:V:66:MET:HB3   | 1.90                     | 0.44              |
| 28:c:82:THR:HA     | 28:c:87:MET:HE3   | 2.00                     | 0.44              |
| 30:e:10:VAL:O      | 30:e:83:THR:HB    | 2.18                     | 0.44              |
| 48:w:1230:C:H5'    | 48:w:1607:A:O2'   | 2.17                     | 0.44              |
| 48:w:1442:OMU:HM23 | 48:w:1442:OMU:H1' | 1.64                     | 0.44              |
| 49:x:110:ASN:C     | 49:x:111:GLN:HG3  | 2.43                     | 0.44              |
| 49:x:198:MET:SD    | 65:AD:89:SER:HB3  | 2.58                     | 0.44              |
| 50:y:222:LYS:HD2   | 50:y:223:PHE:H    | 1.82                     | 0.44              |
| 55:3:126:ASP:OD1   | 55:3:126:ASP:N    | 2.50                     | 0.44              |
| 57:5:113:TYR:O     | 57:5:117:TYR:HB2  | 2.18                     | 0.44              |
| 58:6:159:PHE:CE1   | 58:6:165:TYR:HB3  | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:9:99:ARG:O      | 61:9:103:GLU:HG3   | 2.17                     | 0.44              |
| 62:AA:28:PHE:HA    | 62:AA:92:ALA:O     | 2.18                     | 0.44              |
| 72:AK:62:THR:HB    | 72:AK:69:THR:HG22  | 1.99                     | 0.44              |
| 79:AR:191:HIS:NE2  | 79:AR:209:SER:OG   | 2.24                     | 0.44              |
| 79:AR:223:GLU:HB2  | 79:AR:225:LYS:CE   | 2.46                     | 0.44              |
| 79:AR:231:ASP:OD1  | 79:AR:232:GLY:N    | 2.50                     | 0.44              |
| 3:D:1174:G:H22     | 3:D:1186:U:H3      | 1.66                     | 0.43              |
| 3:D:1202:C:H3'     | 3:D:1203:G:C5'     | 2.48                     | 0.43              |
| 3:D:1705:G:H2'     | 3:D:1706:A:O4'     | 2.18                     | 0.43              |
| 3:D:4095:G:N2      | 3:D:4114:C:O4'     | 2.50                     | 0.43              |
| 3:D:4600:G:O2'     | 3:D:4601:U:P       | 2.76                     | 0.43              |
| 6:G:178:PRO:HG2    | 46:u:26:VAL:HG13   | 1.98                     | 0.43              |
| 9:J:256:LYS:HD2    | 9:J:256:LYS:N      | 2.32                     | 0.43              |
| 12:M:145:THR:O     | 12:M:149:ASN:ND2   | 2.51                     | 0.43              |
| 37:l:10:ARG:HA     | 37:l:10:ARG:HD3    | 1.78                     | 0.43              |
| 48:w:1639:G7M:O2'  | 48:w:1640:A:OP1    | 2.30                     | 0.43              |
| 50:y:60:ASP:OD1    | 50:y:60:ASP:N      | 2.49                     | 0.43              |
| 51:z:77:SER:C      | 51:z:79:GLU:H      | 2.26                     | 0.43              |
| 53:1:18:TRP:N      | 53:1:18:TRP:CD1    | 2.83                     | 0.43              |
| 53:1:21:ASP:OD1    | 53:1:24:THR:OG1    | 2.28                     | 0.43              |
| 71:AJ:125:VAL:O    | 71:AJ:128:VAL:HG12 | 2.18                     | 0.43              |
| 2:C:52:G:O2'       | 2:C:53:5MU:OP1     | 2.35                     | 0.43              |
| 3:D:121:A:H62      | 3:D:152:U:H3       | 1.64                     | 0.43              |
| 3:D:4637:OMG:H1'   | 3:D:4637:OMG:HM23  | 1.73                     | 0.43              |
| 48:w:22:A:H4'      | 58:6:17:ARG:HA     | 2.00                     | 0.43              |
| 48:w:107:A:H2'     | 48:w:108:G:C8      | 2.53                     | 0.43              |
| 48:w:492:C:H42     | 48:w:508:A:N6      | 2.16                     | 0.43              |
| 48:w:608:C:H5'     | 78:AQ:132:SER:HA   | 2.00                     | 0.43              |
| 48:w:1804:OMU:H1'  | 48:w:1804:OMU:HM23 | 1.59                     | 0.43              |
| 48:w:1842:4AC:O7   | 48:w:1842:4AC:H5   | 2.18                     | 0.43              |
| 49:x:50:ASN:HB3    | 49:x:53:ARG:HG2    | 1.99                     | 0.43              |
| 54:2:20:PHE:CD1    | 54:2:20:PHE:C      | 2.95                     | 0.43              |
| 54:2:144:LEU:HD23  | 76:AO:49:PRO:HG2   | 2.01                     | 0.43              |
| 55:3:14:LYS:HB2    | 55:3:124:LEU:HD21  | 2.00                     | 0.43              |
| 56:4:38:ALA:N      | 56:4:41:ARG:NH2    | 2.66                     | 0.43              |
| 57:5:129:LEU:O     | 57:5:133:GLU:HG2   | 2.18                     | 0.43              |
| 58:6:64:ASP:OD1    | 58:6:65:GLU:N      | 2.51                     | 0.43              |
| 59:7:53:LYS:HE3    | 59:7:53:LYS:HB3    | 1.83                     | 0.43              |
| 71:AJ:123:VAL:HG12 | 71:AJ:124:LYS:HG3  | 1.99                     | 0.43              |
| 79:AR:89:LEU:HD13  | 79:AR:101:PHE:HE1  | 1.83                     | 0.43              |
| 2:B:73:C:O2'       | 2:B:74:C:OP2       | 2.33                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D:4621:C:OP1     | 26:a:48:ARG:HD2    | 2.18                     | 0.43              |
| 24:Y:114:GLN:OE1   | 24:Y:115:LYS:N     | 2.51                     | 0.43              |
| 34:i:105:LEU:HG    | 34:i:107:THR:HG23  | 2.00                     | 0.43              |
| 48:w:869:A:C5      | 56:4:114:GLN:HG3   | 2.53                     | 0.43              |
| 48:w:1204:A:H2'    | 48:w:1205:C:O4'    | 2.19                     | 0.43              |
| 48:w:1678:A2M:HM'3 | 48:w:1678:A2M:H1'  | 1.73                     | 0.43              |
| 49:x:34:MET:HE2    | 49:x:149:ASN:O     | 2.18                     | 0.43              |
| 52:0:154:ASP:C     | 52:0:154:ASP:OD2   | 2.61                     | 0.43              |
| 53:1:11:ARG:HH21   | 53:1:20:LEU:HB3    | 1.83                     | 0.43              |
| 53:1:103:TYR:CE1   | 53:1:189:LEU:HD11  | 2.53                     | 0.43              |
| 54:2:124:ASP:HA    | 54:2:200:ALA:HB2   | 2.00                     | 0.43              |
| 63:AB:86:LEU:O     | 63:AB:89:MET:HG2   | 2.18                     | 0.43              |
| 70:AI:32:LYS:O     | 70:AI:36:ARG:HG2   | 2.17                     | 0.43              |
| 3:D:4260:U:H2'     | 3:D:4261:C:C6      | 2.53                     | 0.43              |
| 3:D:4685:U:H2'     | 3:D:4686:G:C8      | 2.53                     | 0.43              |
| 8:I:228:THR:HG23   | 8:I:248:ARG:HH22   | 1.83                     | 0.43              |
| 8:I:315:LYS:HD2    | 11:L:168:ALA:HB1   | 2.00                     | 0.43              |
| 11:L:29:LYS:HD2    | 11:L:32:ARG:NH1    | 2.33                     | 0.43              |
| 11:L:137:GLU:N     | 11:L:138:PRO:HD2   | 2.33                     | 0.43              |
| 13:N:12:ILE:HG22   | 13:N:81:ILE:HD11   | 2.00                     | 0.43              |
| 17:R:36:ALA:HB2    | 17:R:52:PHE:CZ     | 2.53                     | 0.43              |
| 30:e:88:ASP:O      | 30:e:121:ARG:NH2   | 2.52                     | 0.43              |
| 37:l:19:LYS:HA     | 37:l:19:LYS:HD3    | 1.75                     | 0.43              |
| 38:m:15:GLU:H      | 38:m:15:GLU:CD     | 2.26                     | 0.43              |
| 40:o:52:LYS:HG2    | 40:o:55:ARG:NH1    | 2.34                     | 0.43              |
| 45:t:33:LEU:HA     | 45:t:38:LYS:HG2    | 1.99                     | 0.43              |
| 45:t:74:GLU:OE1    | 45:t:76:ASN:HB2    | 2.18                     | 0.43              |
| 48:w:874:G:H2'     | 48:w:875:A:C8      | 2.54                     | 0.43              |
| 48:w:1237:C:H5'    | 63:AB:131:PRO:O    | 2.17                     | 0.43              |
| 51:z:172:ASN:OD1   | 51:z:172:ASN:N     | 2.50                     | 0.43              |
| 52:0:162:ASP:O     | 52:0:164:VAL:N     | 2.48                     | 0.43              |
| 62:AA:42:VAL:HG23  | 62:AA:43:HIS:N     | 2.33                     | 0.43              |
| 67:AF:37:VAL:C     | 67:AF:39:LEU:H     | 2.27                     | 0.43              |
| 71:AJ:46:HIS:CD2   | 71:AJ:103:ALA:HB2  | 2.53                     | 0.43              |
| 79:AR:17:TRP:HE3   | 79:AR:303:THR:HA   | 1.83                     | 0.43              |
| 79:AR:64:HIS:CG    | 79:AR:65:PHE:H     | 2.35                     | 0.43              |
| 79:AR:87:LEU:HD21  | 79:AR:111:VAL:HG11 | 1.99                     | 0.43              |
| 3:D:216:C:OP2      | 3:D:220:C:H5'      | 2.19                     | 0.43              |
| 3:D:2094:G:C8      | 3:D:2095:A:C6      | 3.06                     | 0.43              |
| 3:D:2266:C:O2'     | 47:v:39:ARG:NH1    | 2.52                     | 0.43              |
| 10:K:164:PHE:HA    | 10:K:175:VAL:HG23  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:N:91:LYS:HG2    | 13:N:145:ILE:HG12  | 2.00                     | 0.43              |
| 22:W:90:PRO:HB2    | 22:W:93:VAL:HG12   | 2.01                     | 0.43              |
| 34:i:50:ARG:NH1    | 34:i:62:VAL:O      | 2.51                     | 0.43              |
| 36:k:93:PRO:O      | 36:k:95:LYS:N      | 2.51                     | 0.43              |
| 48:w:1332:A:H2'    | 52:0:141:LYS:HE2   | 1.99                     | 0.43              |
| 49:x:40:LYS:HE3    | 65:AD:101:ASP:CG   | 2.44                     | 0.43              |
| 56:4:70:LYS:HA     | 56:4:73:GLN:HG3    | 2.00                     | 0.43              |
| 57:5:8:TRP:CZ3     | 57:5:20:PRO:HB3    | 2.54                     | 0.43              |
| 57:5:135:GLU:O     | 57:5:138:ASN:ND2   | 2.52                     | 0.43              |
| 64:AC:116:ASP:C    | 64:AC:116:ASP:OD1  | 2.61                     | 0.43              |
| 65:AD:119:VAL:HG12 | 65:AD:120:THR:C    | 2.43                     | 0.43              |
| 69:AH:27:LYS:HA    | 69:AH:27:LYS:HD2   | 1.93                     | 0.43              |
| 76:AO:62:GLU:N     | 76:AO:62:GLU:OE1   | 2.52                     | 0.43              |
| 3:D:1646:A:O2'     | 40:o:49:TRP:O      | 2.34                     | 0.43              |
| 5:F:16:G:O2'       | 5:F:17:A:H8        | 2.01                     | 0.43              |
| 7:H:285:TYR:CD1    | 7:H:363:ILE:HD13   | 2.53                     | 0.43              |
| 8:I:293:LEU:O      | 8:I:298:ILE:HD11   | 2.19                     | 0.43              |
| 9:J:112:ARG:C      | 9:J:114:GLY:H      | 2.25                     | 0.43              |
| 12:M:157:ILE:H     | 12:M:157:ILE:HG13  | 1.60                     | 0.43              |
| 15:P:160:GLU:OE1   | 15:P:160:GLU:N     | 2.50                     | 0.43              |
| 22:W:99:MET:HE1    | 22:W:127:VAL:O     | 2.18                     | 0.43              |
| 43:r:92:ASP:O      | 43:r:105:PRO:HG3   | 2.18                     | 0.43              |
| 50:y:78:GLU:HG2    | 50:y:79:VAL:H      | 1.83                     | 0.43              |
| 56:4:105:THR:O     | 56:4:105:THR:OG1   | 2.35                     | 0.43              |
| 69:AH:20:SER:OG    | 69:AH:22:ARG:HG2   | 2.19                     | 0.43              |
| 70:AI:69:LEU:HG    | 70:AI:70:ASN:O     | 2.18                     | 0.43              |
| 3:D:717:U:H2'      | 3:D:718:C:C6       | 2.54                     | 0.43              |
| 3:D:4755:G:N7      | 10:K:279:ASN:ND2   | 2.66                     | 0.43              |
| 26:a:13:LYS:HD2    | 26:a:128:LEU:HD11  | 2.00                     | 0.43              |
| 33:h:18:LEU:HD12   | 33:h:18:LEU:HA     | 1.86                     | 0.43              |
| 48:w:292:A:O2'     | 48:w:293:C:OP2     | 2.30                     | 0.43              |
| 48:w:563:G:H2'     | 48:w:564:A:H8      | 1.84                     | 0.43              |
| 48:w:676:C:H5''    | 61:9:5:HIS:HD2     | 1.84                     | 0.43              |
| 48:w:921:G:C2      | 75:AN:22:LYS:HG2   | 2.52                     | 0.43              |
| 48:w:1101:U:H2'    | 48:w:1102:G:C8     | 2.54                     | 0.43              |
| 48:w:1454:A:C2     | 48:w:1476:A:H2'    | 2.52                     | 0.43              |
| 49:x:41:ARG:HB2    | 49:x:47:TYR:CE2    | 2.53                     | 0.43              |
| 50:y:136:ARG:HB2   | 50:y:218:LEU:HD11  | 2.01                     | 0.43              |
| 58:6:78:LEU:HB3    | 58:6:92:MET:SD     | 2.59                     | 0.43              |
| 79:AR:212:LYS:HD2  | 79:AR:235:ILE:HD12 | 2.01                     | 0.43              |
| 2:C:4:U:H3         | 2:C:68:G:H1        | 1.66                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1601:A:O2'    | 40:o:2:THR:HG21   | 2.18                     | 0.43              |
| 10:K:209:PRO:HB2  | 10:K:211:HIS:CE1  | 2.53                     | 0.43              |
| 11:L:182:TYR:HB3  | 11:L:200:ARG:HG3  | 2.00                     | 0.43              |
| 48:w:27:A2M:H1'   | 48:w:27:A2M:HM'3  | 1.77                     | 0.43              |
| 48:w:291:G:H5''   | 53:1:203:GLY:H    | 1.83                     | 0.43              |
| 48:w:526:A:O2'    | 58:6:125:HIS:ND1  | 2.51                     | 0.43              |
| 48:w:827:A:OP1    | 58:6:10:ARG:HB3   | 2.18                     | 0.43              |
| 48:w:1387:G:H21   | 65:AD:8:THR:HG21  | 1.83                     | 0.43              |
| 48:w:1543:U:P     | 64:AC:37:ARG:HH12 | 2.41                     | 0.43              |
| 52:0:210:ILE:HD12 | 65:AD:38:ILE:O    | 2.18                     | 0.43              |
| 54:2:33:ILE:HA    | 54:2:36:GLN:HG3   | 2.01                     | 0.43              |
| 55:3:190:ARG:O    | 55:3:194:LEU:HG   | 2.19                     | 0.43              |
| 56:4:12:ASN:OD1   | 56:4:12:ASN:N     | 2.51                     | 0.43              |
| 57:5:12:ARG:HG2   | 57:5:16:GLY:O     | 2.19                     | 0.43              |
| 57:5:190:LEU:HD13 | 57:5:198:TYR:HD2  | 1.83                     | 0.43              |
| 59:7:64:TRP:CE3   | 77:AP:23:VAL:HG12 | 2.54                     | 0.43              |
| 68:AG:36:CYS:SG   | 68:AG:37:ALA:N    | 2.92                     | 0.43              |
| 70:AI:49:GLU:O    | 70:AI:64:ASN:ND2  | 2.50                     | 0.43              |
| 3:D:1332:C:H2'    | 3:D:1333:A:C8     | 2.54                     | 0.43              |
| 15:P:96:LYS:HG3   | 15:P:174:ILE:HG21 | 2.00                     | 0.43              |
| 32:g:35:VAL:HG23  | 32:g:40:LEU:HG    | 2.01                     | 0.43              |
| 33:h:51:ASN:HB2   | 33:h:77:ASN:HB2   | 2.01                     | 0.43              |
| 48:w:39:A:H62     | 48:w:515:G:N2     | 2.17                     | 0.43              |
| 58:6:21:GLU:HG3   | 58:6:24:ARG:HB3   | 2.00                     | 0.43              |
| 58:6:82:VAL:HA    | 58:6:87:LEU:O     | 2.19                     | 0.43              |
| 60:8:2:ALA:HB1    | 60:8:5:GLN:HB2    | 2.00                     | 0.43              |
| 69:AH:80:SER:O    | 69:AH:82:ASN:N    | 2.52                     | 0.43              |
| 79:AR:16:GLY:H    | 79:AR:305:ASN:CB  | 2.32                     | 0.43              |
| 79:AR:29:ASP:HB3  | 79:AR:45:LEU:HB3  | 2.00                     | 0.43              |
| 3:D:1590:C:H5''   | 3:D:1591:U:O5'    | 2.19                     | 0.43              |
| 3:D:1701:A:H8     | 3:D:2096:G:N2     | 2.16                     | 0.43              |
| 3:D:2583:C:OP2    | 37:l:76:ARG:NH1   | 2.45                     | 0.43              |
| 7:H:14:LEU:O      | 7:H:17:LEU:HB2    | 2.19                     | 0.43              |
| 11:L:164:LYS:HD3  | 11:L:164:LYS:HA   | 1.75                     | 0.43              |
| 12:M:166:LEU:HA   | 18:S:7:ILE:HD11   | 2.00                     | 0.43              |
| 31:f:92:LYS:HE2   | 31:f:92:LYS:HB2   | 1.82                     | 0.43              |
| 48:w:491:C:OP1    | 72:AK:103:SER:OG  | 2.26                     | 0.43              |
| 48:w:844:U:H2'    | 48:w:845:G:H8     | 1.84                     | 0.43              |
| 50:y:57:ILE:HG13  | 50:y:58:ALA:N     | 2.27                     | 0.43              |
| 52:0:34:TYR:CE1   | 52:0:37:VAL:HG13  | 2.54                     | 0.43              |
| 55:3:167:LYS:HB3  | 55:3:167:LYS:HE3  | 1.76                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 57:5:65:PHE:CE1   | 57:5:78:ILE:HD11  | 2.54                     | 0.43              |
| 60:8:57:ASP:HB2   | 60:8:84:ARG:NH1   | 2.34                     | 0.43              |
| 71:AJ:51:VAL:HG22 | 71:AJ:70:VAL:HG11 | 2.01                     | 0.43              |
| 3:D:278:G:H5''    | 18:S:8:GLN:NE2    | 2.34                     | 0.42              |
| 3:D:1411:C:O2'    | 3:D:1412:G:O5'    | 2.36                     | 0.42              |
| 3:D:1846:G:H2'    | 3:D:1847:C:C6     | 2.54                     | 0.42              |
| 3:D:4196:OMG:H1'  | 3:D:4196:OMG:HM23 | 1.73                     | 0.42              |
| 9:J:191:ASN:OD1   | 9:J:194:VAL:HG23  | 2.19                     | 0.42              |
| 21:V:20:SER:O     | 21:V:26:ARG:NH1   | 2.52                     | 0.42              |
| 45:t:102:GLN:OE1  | 45:t:102:GLN:HA   | 2.19                     | 0.42              |
| 48:w:416:U:O4     | 48:w:417:C:N4     | 2.51                     | 0.42              |
| 48:w:608:C:H2'    | 48:w:609:PSU:H6   | 1.84                     | 0.42              |
| 48:w:616:A:N1     | 48:w:632:C:H1'    | 2.34                     | 0.42              |
| 48:w:839:C:N4     | 72:AK:10:ARG:HA   | 2.33                     | 0.42              |
| 48:w:1112:U:H2'   | 48:w:1113:A:C8    | 2.54                     | 0.42              |
| 49:x:22:GLY:C     | 49:x:24:HIS:H     | 2.26                     | 0.42              |
| 53:1:191:ARG:NH2  | 53:1:245:ARG:HD2  | 2.34                     | 0.42              |
| 57:5:74:ARG:HD3   | 57:5:74:ARG:HA    | 1.81                     | 0.42              |
| 57:5:106:SER:OG   | 57:5:169:GLY:HA2  | 2.19                     | 0.42              |
| 57:5:150:ASP:OD1  | 57:5:150:ASP:N    | 2.51                     | 0.42              |
| 65:AD:53:TYR:CZ   | 65:AD:57:LEU:HD21 | 2.54                     | 0.42              |
| 75:AN:24:LEU:HA   | 75:AN:24:LEU:HD23 | 1.72                     | 0.42              |
| 2:C:21:A:N6       | 2:C:47:5MC:OP2    | 2.52                     | 0.42              |
| 3:D:188:G:N1      | 3:D:191:G:O6      | 2.30                     | 0.42              |
| 3:D:302:C:OP1     | 18:S:68:ARG:HB2   | 2.19                     | 0.42              |
| 3:D:494:U:H2'     | 3:D:495:C:H6      | 1.84                     | 0.42              |
| 3:D:741:C:H42     | 3:D:923:C:H42     | 1.67                     | 0.42              |
| 3:D:965:G:H2'     | 3:D:2092:G:N2     | 2.34                     | 0.42              |
| 3:D:4322:G:N2     | 3:D:4325:A:OP2    | 2.51                     | 0.42              |
| 7:H:80:GLU:OE1    | 7:H:323:TYR:OH    | 2.18                     | 0.42              |
| 7:H:240:LEU:HB3   | 7:H:244:THR:HG21  | 2.00                     | 0.42              |
| 8:I:138:MET:HE3   | 8:I:138:MET:HB3   | 1.77                     | 0.42              |
| 8:I:150:LEU:HB3   | 8:I:151:PRO:HD3   | 2.00                     | 0.42              |
| 16:Q:126:LEU:N    | 16:Q:138:ASP:OD2  | 2.44                     | 0.42              |
| 30:e:41:ALA:HB2   | 30:e:77:TYR:HE1   | 1.84                     | 0.42              |
| 47:v:97:ILE:CG2   | 47:v:107:ARG:HB3  | 2.49                     | 0.42              |
| 48:w:1446:A:O2'   | 48:w:1447:G:H5''  | 2.19                     | 0.42              |
| 50:y:190:PRO:O    | 50:y:192:SER:N    | 2.49                     | 0.42              |
| 50:y:193:ILE:H    | 50:y:193:ILE:HG12 | 1.68                     | 0.42              |
| 51:z:76:LYS:HA    | 51:z:97:PHE:HE1   | 1.84                     | 0.42              |
| 53:1:11:ARG:NH2   | 53:1:21:ASP:OD1   | 2.52                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 53:1:92:ILE:HG22   | 53:1:97:GLU:H     | 1.84                     | 0.42              |
| 55:3:79:LYS:HD3    | 55:3:86:PRO:HG3   | 2.01                     | 0.42              |
| 58:6:65:GLU:O      | 58:6:66:LYS:HG2   | 2.19                     | 0.42              |
| 58:6:176:LYS:HG3   | 58:6:179:LYS:NZ   | 2.34                     | 0.42              |
| 2:B:16:U:O2'       | 2:B:59:U:O2       | 2.25                     | 0.42              |
| 3:D:737:C:C5       | 3:D:739:G:H5''    | 2.53                     | 0.42              |
| 3:D:2561:C:H2'     | 3:D:2562:G:O4'    | 2.19                     | 0.42              |
| 3:D:3746:A:H5''    | 6:G:244:GLY:HA3   | 2.01                     | 0.42              |
| 3:D:4749:C:H2'     | 3:D:4750:G:O4'    | 2.19                     | 0.42              |
| 7:H:189:THR:O      | 7:H:193:LYS:HB2   | 2.19                     | 0.42              |
| 10:K:278:THR:OG1   | 10:K:279:ASN:N    | 2.53                     | 0.42              |
| 14:O:51:HIS:CD2    | 14:O:168:SER:HB2  | 2.55                     | 0.42              |
| 17:R:95:ILE:C      | 17:R:97:ALA:H     | 2.27                     | 0.42              |
| 17:R:133:ALA:O     | 17:R:137:LYS:NZ   | 2.51                     | 0.42              |
| 19:T:34:VAL:HG22   | 19:T:103:LYS:HB2  | 2.02                     | 0.42              |
| 20:U:154:GLU:CD    | 20:U:154:GLU:N    | 2.77                     | 0.42              |
| 29:d:89:LYS:HB3    | 29:d:89:LYS:HE3   | 1.88                     | 0.42              |
| 38:m:103:LYS:HD2   | 38:m:107:GLN:NE2  | 2.34                     | 0.42              |
| 48:w:456:C:H1'     | 48:w:1800:A:C8    | 2.55                     | 0.42              |
| 48:w:527:C:OP1     | 58:6:122:SER:OG   | 2.20                     | 0.42              |
| 51:z:253:PRO:HA    | 51:z:256:TRP:CD1  | 2.54                     | 0.42              |
| 56:4:127:ASP:O     | 56:4:131:GLU:HG2  | 2.19                     | 0.42              |
| 60:8:55:TYR:CD1    | 60:8:55:TYR:C     | 2.97                     | 0.42              |
| 62:AA:32:HIS:CE1   | 62:AA:96:LYS:HE2  | 2.55                     | 0.42              |
| 75:AN:19:HIS:HB3   | 75:AN:21:LYS:O    | 2.19                     | 0.42              |
| 3:D:75:G:O2'       | 16:Q:101:ARG:NH1  | 2.45                     | 0.42              |
| 3:D:1919:G:H1'     | 23:X:164:LYS:NZ   | 2.34                     | 0.42              |
| 3:D:4635:A:H3'     | 3:D:4636:U:H4'    | 2.01                     | 0.42              |
| 16:Q:130:LYS:HD3   | 16:Q:130:LYS:HA   | 1.91                     | 0.42              |
| 18:S:64:ILE:HD11   | 18:S:106:ALA:HB2  | 2.01                     | 0.42              |
| 18:S:75:VAL:HG21   | 18:S:80:THR:HG22  | 2.01                     | 0.42              |
| 34:i:106:VAL:O     | 34:i:106:VAL:HG12 | 2.19                     | 0.42              |
| 35:j:81:ASN:OD1    | 35:j:84:GLU:HG3   | 2.20                     | 0.42              |
| 48:w:166:A2M:HM'2  | 55:3:11:GLY:HA2   | 2.01                     | 0.42              |
| 48:w:1153:C:OP2    | 70:AI:71:LYS:NZ   | 2.53                     | 0.42              |
| 48:w:1639:G7M:HO2' | 48:w:1640:A:P     | 2.41                     | 0.42              |
| 50:y:25:PHE:CD2    | 50:y:28:LYS:HD2   | 2.54                     | 0.42              |
| 51:z:80:GLU:H      | 51:z:80:GLU:CD    | 2.24                     | 0.42              |
| 55:3:200:LYS:O     | 55:3:204:GLU:N    | 2.46                     | 0.42              |
| 58:6:58:ARG:O      | 58:6:62:THR:HG23  | 2.19                     | 0.42              |
| 60:8:151:THR:HG22  | 61:9:133:ARG:HH22 | 1.84                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:AB:37:TYR:OH   | 63:AB:45:LEU:HD11  | 2.19                     | 0.42              |
| 64:AC:96:TYR:HA   | 64:AC:100:VAL:HG22 | 2.01                     | 0.42              |
| 71:AJ:54:LYS:HD3  | 71:AJ:94:ILE:HG22  | 2.01                     | 0.42              |
| 73:AL:66:LYS:HD3  | 73:AL:111:ARG:NH1  | 2.33                     | 0.42              |
| 79:AR:119:GLN:O   | 79:AR:120:ILE:HD13 | 2.20                     | 0.42              |
| 3:D:1464:C:H5''   | 32:g:32:LEU:HD12   | 1.99                     | 0.42              |
| 3:D:2083:C:P      | 21:V:14:ARG:HH12   | 2.41                     | 0.42              |
| 3:D:4734:A:H1'    | 3:D:4735:G:C8      | 2.53                     | 0.42              |
| 3:D:4859:C:H5''   | 3:D:4860:G:C8      | 2.54                     | 0.42              |
| 15:P:151:ILE:HG13 | 15:P:152:GLY:H     | 1.84                     | 0.42              |
| 17:R:40:GLY:H     | 17:R:45:VAL:HG23   | 1.84                     | 0.42              |
| 48:w:146:G:P      | 55:3:140:ARG:HH22  | 2.43                     | 0.42              |
| 48:w:560:A:H5'    | 58:6:174:LYS:HB3   | 1.99                     | 0.42              |
| 48:w:943:U:O2'    | 62:AA:135:ILE:O    | 2.38                     | 0.42              |
| 48:w:1229:G:O2'   | 48:w:1607:A:O2'    | 2.32                     | 0.42              |
| 48:w:1621:U:H5'   | 48:w:1623:A:O2'    | 2.20                     | 0.42              |
| 48:w:1754:G:N1    | 48:w:1779:G:O6     | 2.53                     | 0.42              |
| 49:x:57:LYS:NZ    | 69:AH:66:ASP:OD1   | 2.51                     | 0.42              |
| 50:y:52:THR:HG22  | 50:y:57:ILE:HB     | 2.01                     | 0.42              |
| 50:y:217:MET:HE2  | 50:y:217:MET:HB2   | 1.76                     | 0.42              |
| 51:z:206:SER:OG   | 51:z:210:PRO:HG2   | 2.18                     | 0.42              |
| 53:1:18:TRP:HH2   | 53:1:31:PRO:HG3    | 1.84                     | 0.42              |
| 53:1:180:LEU:HD23 | 53:1:180:LEU:HA    | 1.85                     | 0.42              |
| 56:4:10:LYS:NZ    | 56:4:17:ASP:OD1    | 2.51                     | 0.42              |
| 76:AO:13:ARG:HH11 | 76:AO:55:VAL:HG22  | 1.84                     | 0.42              |
| 77:AP:38:MET:HE1  | 77:AP:50:ILE:HD11  | 2.01                     | 0.42              |
| 3:D:189:G:H2'     | 3:D:190:G:H8       | 1.84                     | 0.42              |
| 3:D:1296:G:H2'    | 3:D:1297:U:O4'     | 2.19                     | 0.42              |
| 3:D:1716:G:H4'    | 24:Y:125:TRP:CH2   | 2.55                     | 0.42              |
| 3:D:1802:A:N3     | 24:Y:130:ARG:NH1   | 2.67                     | 0.42              |
| 3:D:3928:A:H2'    | 3:D:3929:G:O4'     | 2.20                     | 0.42              |
| 3:D:4138:C:H2'    | 3:D:4139:G:C8      | 2.54                     | 0.42              |
| 16:Q:65:ARG:HG3   | 31:f:69:PHE:CD1    | 2.55                     | 0.42              |
| 31:f:137:ILE:O    | 31:f:140:VAL:HG12  | 2.19                     | 0.42              |
| 43:r:126:LYS:HD3  | 43:r:126:LYS:HA    | 1.86                     | 0.42              |
| 45:t:101:GLY:HA2  | 45:t:102:GLN:C     | 2.45                     | 0.42              |
| 48:w:303:C:H2'    | 48:w:304:C:H6      | 1.85                     | 0.42              |
| 50:y:71:LEU:H     | 50:y:71:LEU:HD23   | 1.85                     | 0.42              |
| 53:1:42:LEU:HD13  | 53:1:109:PHE:HD2   | 1.84                     | 0.42              |
| 53:1:104:ASP:N    | 53:1:108:ARG:O     | 2.48                     | 0.42              |
| 55:3:22:ARG:HA    | 55:3:25:ARG:HD3    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 58:6:75:ASN:HA    | 58:6:78:LEU:HD12   | 2.01                     | 0.42              |
| 67:AF:75:MET:SD   | 67:AF:78:ILE:HD13  | 2.60                     | 0.42              |
| 70:AI:10:ALA:HB1  | 70:AI:27:ILE:HD13  | 2.01                     | 0.42              |
| 75:AN:50:ALA:O    | 75:AN:51:GLN:HB3   | 2.20                     | 0.42              |
| 76:AO:13:ARG:NE   | 76:AO:13:ARG:HA    | 2.34                     | 0.42              |
| 3:D:1081:C:O2'    | 3:D:1082:C:H2'     | 2.19                     | 0.42              |
| 3:D:2487:G:N1     | 3:D:2492:C:O2      | 2.28                     | 0.42              |
| 3:D:4578:G:H2'    | 3:D:4579:PSU:C6    | 2.54                     | 0.42              |
| 6:G:14:SER:HA     | 6:G:17:ARG:HH21    | 1.85                     | 0.42              |
| 7:H:61:ASP:O      | 7:H:63:PRO:HD3     | 2.20                     | 0.42              |
| 7:H:359:ALA:C     | 7:H:360:LEU:HD23   | 2.44                     | 0.42              |
| 23:X:30:MET:HE2   | 23:X:30:MET:HB3    | 1.77                     | 0.42              |
| 35:j:86:GLU:OE1   | 35:j:86:GLU:N      | 2.53                     | 0.42              |
| 48:w:561:A:H5''   | 58:6:164:PRO:HG2   | 2.01                     | 0.42              |
| 48:w:562:U:H4'    | 58:6:132:GLN:HB2   | 2.00                     | 0.42              |
| 48:w:799:OMU:OP2  | 56:4:111:LYS:HG3   | 2.20                     | 0.42              |
| 48:w:951:C:H1'    | 62:AA:50:LYS:NZ    | 2.35                     | 0.42              |
| 48:w:1275:G:OP2   | 59:7:47:LYS:NZ     | 2.39                     | 0.42              |
| 48:w:1520:G:OP1   | 66:AE:136:THR:N    | 2.43                     | 0.42              |
| 49:x:61:ALA:HB2   | 49:x:159:ILE:HG21  | 2.02                     | 0.42              |
| 50:y:59:SER:HB3   | 50:y:63:LYS:NZ     | 2.35                     | 0.42              |
| 51:z:193:VAL:HG11 | 51:z:240:THR:HA    | 2.01                     | 0.42              |
| 51:z:194:ARG:O    | 51:z:224:THR:HA    | 2.20                     | 0.42              |
| 51:z:254:ASP:OD1  | 51:z:254:ASP:N     | 2.53                     | 0.42              |
| 52:0:76:ARG:HB2   | 59:7:22:VAL:HG11   | 2.02                     | 0.42              |
| 53:1:175:PHE:HE2  | 53:1:198:ARG:HD2   | 1.83                     | 0.42              |
| 53:1:180:LEU:O    | 53:1:227:VAL:HG23  | 2.19                     | 0.42              |
| 55:3:164:LYS:HE2  | 55:3:164:LYS:HB3   | 1.90                     | 0.42              |
| 66:AE:39:ARG:NH1  | 67:AF:38:LYS:HB2   | 2.34                     | 0.42              |
| 66:AE:85:ASN:OD1  | 66:AE:85:ASN:N     | 2.53                     | 0.42              |
| 75:AN:33:MET:HE2  | 75:AN:79:PHE:CD1   | 2.55                     | 0.42              |
| 79:AR:209:SER:O   | 79:AR:216:ALA:HA   | 2.20                     | 0.42              |
| 79:AR:301:GLY:HA2 | 79:AR:307:VAL:HG12 | 2.02                     | 0.42              |
| 2:B:30:G:OP1      | 48:w:1524:G:O2'    | 2.36                     | 0.42              |
| 3:D:516:C:OP2     | 3:D:516:C:H6       | 2.01                     | 0.42              |
| 3:D:1834:U:OP1    | 24:Y:116:LYS:NZ    | 2.35                     | 0.42              |
| 3:D:3669:G:H21    | 3:D:3672:G:N2      | 2.18                     | 0.42              |
| 3:D:4741:C:H4'    | 3:D:4742:G:H5'     | 2.01                     | 0.42              |
| 5:F:125:C:O3'     | 5:F:126:C:H2'      | 2.20                     | 0.42              |
| 8:I:108:TRP:CE3   | 16:Q:22:VAL:HG21   | 2.55                     | 0.42              |
| 11:L:240:ILE:HD12 | 11:L:240:ILE:HA    | 1.92                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:O:190:LEU:HD23  | 14:O:199:TYR:HA    | 2.02                     | 0.42              |
| 16:Q:164:GLU:OE2   | 16:Q:164:GLU:N     | 2.53                     | 0.42              |
| 48:w:504:G:N1      | 48:w:505:G:C6      | 2.88                     | 0.42              |
| 48:w:1864:U:H5'    | 74:AM:79:ILE:HD11  | 2.02                     | 0.42              |
| 49:x:111:GLN:HA    | 49:x:116:PHE:CG    | 2.53                     | 0.42              |
| 53:1:72:ILE:HG12   | 53:1:90:ILE:HG13   | 2.01                     | 0.42              |
| 53:1:103:TYR:CD1   | 53:1:189:LEU:HD11  | 2.55                     | 0.42              |
| 56:4:83:LEU:HD21   | 56:4:92:VAL:HG21   | 2.01                     | 0.42              |
| 57:5:37:LYS:HE3    | 57:5:95:THR:HB     | 2.02                     | 0.42              |
| 57:5:76:THR:HG21   | 57:5:104:ILE:HD12  | 2.01                     | 0.42              |
| 62:AA:76:LEU:HA    | 62:AA:79:GLN:HG2   | 2.02                     | 0.42              |
| 66:AE:23:ARG:O     | 66:AE:55:ARG:NH2   | 2.51                     | 0.42              |
| 68:AG:45:GLU:H     | 68:AG:45:GLU:CD    | 2.28                     | 0.42              |
| 68:AG:63:ILE:HD11  | 77:AP:43:PHE:CZ    | 2.55                     | 0.42              |
| 72:AK:114:MET:HA   | 72:AK:125:VAL:HG11 | 2.01                     | 0.42              |
| 79:AR:17:TRP:HE1   | 79:AR:36:ARG:NH1   | 2.18                     | 0.42              |
| 79:AR:225:LYS:H    | 79:AR:225:LYS:HD2  | 1.85                     | 0.42              |
| 3:D:4945:G:H1'     | 10:K:158:ARG:HH12  | 1.85                     | 0.42              |
| 4:E:39:C:N3        | 15:P:73:THR:HG22   | 2.35                     | 0.42              |
| 10:K:118:THR:HG21  | 35:j:92:ASN:OD1    | 2.18                     | 0.42              |
| 11:L:87:PRO:HG2    | 11:L:144:TYR:CD2   | 2.55                     | 0.42              |
| 12:M:110:LYS:HA    | 12:M:113:ARG:HG2   | 2.01                     | 0.42              |
| 48:w:343:A:H2'     | 48:w:344:U:O4'     | 2.19                     | 0.42              |
| 48:w:1383:A2M:HM'3 | 48:w:1383:A2M:H1'  | 1.81                     | 0.42              |
| 48:w:1435:C:O2'    | 48:w:1437:C:N4     | 2.51                     | 0.42              |
| 69:AH:21:ASN:O     | 69:AH:22:ARG:HD2   | 2.20                     | 0.42              |
| 3:D:908:G:H2'      | 3:D:909:A:C8       | 2.55                     | 0.42              |
| 3:D:1446:C:H2'     | 3:D:1447:C:O4'     | 2.20                     | 0.42              |
| 3:D:2527:A:P       | 22:W:38:ARG:HH22   | 2.43                     | 0.42              |
| 5:F:93:C:O2'       | 5:F:94:G:H8        | 2.03                     | 0.42              |
| 6:G:117:GLU:OE2    | 6:G:163:ARG:NH1    | 2.53                     | 0.42              |
| 9:J:125:VAL:HG23   | 9:J:126:THR:H      | 1.84                     | 0.42              |
| 15:P:109:ILE:HD13  | 15:P:109:ILE:HA    | 1.88                     | 0.42              |
| 19:T:10:ASP:OD1    | 19:T:37:ARG:HD3    | 2.20                     | 0.42              |
| 21:V:103:LEU:HD23  | 21:V:103:LEU:H     | 1.84                     | 0.42              |
| 30:e:117:LYS:HA    | 30:e:117:LYS:HD2   | 1.82                     | 0.42              |
| 39:n:16:LYS:HA     | 39:n:16:LYS:HD3    | 1.86                     | 0.42              |
| 48:w:1482:C:P      | 77:AP:54:LYS:HZ1   | 2.42                     | 0.42              |
| 48:w:1556:A:H5''   | 77:AP:13:LYS:HZ1   | 1.85                     | 0.42              |
| 48:w:1777:G:H4'    | 48:w:1778:C:OP1    | 2.20                     | 0.42              |
| 49:x:128:ARG:NH2   | 49:x:153:PRO:HD3   | 2.35                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:O:157:MET:HE1  | 52:O:187:LYS:HB3   | 2.02                     | 0.42              |
| 57:5:206:LYS:HD3  | 57:5:206:LYS:HA    | 1.85                     | 0.42              |
| 71:AJ:142:ARG:HE  | 71:AJ:142:ARG:HB2  | 1.75                     | 0.42              |
| 73:AL:41:ARG:HA   | 73:AL:41:ARG:HD2   | 1.84                     | 0.42              |
| 79:AR:302:TYR:HE2 | 79:AR:308:ARG:HD2  | 1.84                     | 0.42              |
| 3:D:1083:U:H3     | 3:D:1216:C:H41     | 1.67                     | 0.41              |
| 4:E:47:G:C2       | 4:E:48:G:H1'       | 2.55                     | 0.41              |
| 11:L:29:LYS:HD2   | 11:L:29:LYS:HA     | 1.91                     | 0.41              |
| 12:M:170:LEU:HD12 | 12:M:170:LEU:HA    | 1.91                     | 0.41              |
| 14:O:55:ASP:OD1   | 14:O:55:ASP:N      | 2.52                     | 0.41              |
| 14:O:61:SER:HA    | 14:O:126:VAL:HG12  | 2.02                     | 0.41              |
| 48:w:1636:G:OP1   | 48:w:1636:G:H3'    | 2.20                     | 0.41              |
| 49:x:42:LYS:HD3   | 65:AD:99:ASP:OD2   | 2.20                     | 0.41              |
| 53:1:18:TRP:O     | 53:1:20:LEU:N      | 2.53                     | 0.41              |
| 57:5:136:ILE:HG22 | 57:5:137:LEU:HD12  | 2.02                     | 0.41              |
| 65:AD:98:VAL:O    | 65:AD:119:VAL:HG23 | 2.20                     | 0.41              |
| 66:AE:67:VAL:O    | 66:AE:71:MET:HG3   | 2.19                     | 0.41              |
| 72:AK:57:VAL:HA   | 72:AK:73:GLY:HA2   | 2.02                     | 0.41              |
| 74:AM:45:VAL:HG23 | 74:AM:46:GLU:N     | 2.35                     | 0.41              |
| 3:D:3777:G:N2     | 3:D:3815:G:H2'     | 2.35                     | 0.41              |
| 3:D:4414:A:H5''   | 14:O:154:ARG:NH1   | 2.34                     | 0.41              |
| 3:D:4524:G:C2     | 7:H:252:ALA:HB1    | 2.55                     | 0.41              |
| 6:G:82:ILE:HD11   | 6:G:99:GLY:HA3     | 2.02                     | 0.41              |
| 6:G:117:GLU:HA    | 6:G:124:GLY:HA2    | 2.02                     | 0.41              |
| 14:O:40:LYS:HE2   | 14:O:40:LYS:HB3    | 1.86                     | 0.41              |
| 14:O:48:LEU:HD12  | 14:O:48:LEU:HA     | 1.88                     | 0.41              |
| 17:R:89:THR:O     | 17:R:93:LYS:HG2    | 2.20                     | 0.41              |
| 21:V:128:LEU:HD12 | 21:V:128:LEU:HA    | 1.89                     | 0.41              |
| 29:d:2:LYS:HB3    | 29:d:2:LYS:HE3     | 1.82                     | 0.41              |
| 34:i:117:LEU:HD23 | 34:i:117:LEU:HA    | 1.90                     | 0.41              |
| 37:l:15:THR:O     | 37:l:19:LYS:HE3    | 2.20                     | 0.41              |
| 45:t:69:ARG:NH2   | 45:t:80:LYS:HD3    | 2.35                     | 0.41              |
| 48:w:144:U:H2'    | 48:w:145:G:H8      | 1.84                     | 0.41              |
| 48:w:303:C:H2'    | 48:w:304:C:C6      | 2.55                     | 0.41              |
| 48:w:596:U:O2'    | 48:w:645:C:O2      | 2.37                     | 0.41              |
| 48:w:1535:U:O2'   | 48:w:1536:G:OP2    | 2.37                     | 0.41              |
| 49:x:121:LEU:HD21 | 49:x:145:ILE:HD13  | 2.02                     | 0.41              |
| 51:z:88:ILE:O     | 51:z:160:LEU:HD12  | 2.19                     | 0.41              |
| 51:z:135:GLY:HA2  | 51:z:167:ARG:HH22  | 1.85                     | 0.41              |
| 53:1:230:LYS:H    | 53:1:235:TRP:NE1   | 2.15                     | 0.41              |
| 57:5:110:ARG:HG3  | 57:5:121:LEU:HB3   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:7:52:LEU:HB3   | 59:7:58:VAL:HG22  | 2.02                     | 0.41              |
| 3:D:385:A:H1'     | 3:D:386:A:H5''    | 2.01                     | 0.41              |
| 3:D:1397:A:H5''   | 31:f:113:GLY:O    | 2.20                     | 0.41              |
| 3:D:4219:A:C6     | 3:D:4220:6MZ:H9   | 2.55                     | 0.41              |
| 3:D:4894:A:C3'    | 3:D:4895:C:H5'    | 2.50                     | 0.41              |
| 5:F:83:C:O2'      | 5:F:84:A:H5''     | 2.20                     | 0.41              |
| 8:I:94:ASN:OD1    | 8:I:94:ASN:N      | 2.49                     | 0.41              |
| 10:K:150:LEU:HD11 | 10:K:164:PHE:HB2  | 2.02                     | 0.41              |
| 10:K:207:LYS:HA   | 10:K:207:LYS:HD3  | 1.90                     | 0.41              |
| 11:L:29:LYS:HA    | 11:L:32:ARG:HH11  | 1.85                     | 0.41              |
| 13:N:61:TRP:CH2   | 17:R:33:GLN:HG3   | 2.55                     | 0.41              |
| 18:S:104:GLU:HA   | 18:S:160:GLU:HG3  | 2.03                     | 0.41              |
| 29:d:53:ASP:OD1   | 29:d:110:LYS:HB3  | 2.20                     | 0.41              |
| 29:d:55:VAL:HG22  | 29:d:104:VAL:HB   | 2.02                     | 0.41              |
| 41:p:34:PHE:HE1   | 41:p:47:ILE:HD11  | 1.85                     | 0.41              |
| 48:w:64:A:H2      | 48:w:83:A:H62     | 1.67                     | 0.41              |
| 48:w:179:C:H3'    | 48:w:180:G:C8     | 2.55                     | 0.41              |
| 48:w:1754:G:N2    | 48:w:1778:C:N3    | 2.60                     | 0.41              |
| 57:5:17:LYS:HE3   | 57:5:17:LYS:HB2   | 1.82                     | 0.41              |
| 66:AE:9:PHE:CG    | 66:AE:9:PHE:O     | 2.72                     | 0.41              |
| 3:D:1097:C:H2'    | 3:D:1098:G:C8     | 2.56                     | 0.41              |
| 3:D:1249:C:H2'    | 3:D:1250:C:C6     | 2.56                     | 0.41              |
| 3:D:1339:U:H2'    | 3:D:1340:OMC:C6   | 2.54                     | 0.41              |
| 3:D:2362:U:H2'    | 3:D:2363:A2M:H8   | 2.02                     | 0.41              |
| 5:F:75:OMG:HM23   | 5:F:75:OMG:H1'    | 1.80                     | 0.41              |
| 6:G:114:CYS:HB2   | 6:G:169:VAL:HG23  | 2.02                     | 0.41              |
| 21:V:122:THR:OG1  | 21:V:124:ASP:OD1  | 2.28                     | 0.41              |
| 42:q:2:SER:O      | 42:q:5:LYS:NZ     | 2.51                     | 0.41              |
| 48:w:197:U:N3     | 48:w:202:G:O6     | 2.54                     | 0.41              |
| 48:w:511:U:H2'    | 48:w:512:A2M:C8   | 2.47                     | 0.41              |
| 48:w:1455:A:N1    | 48:w:1476:A:N6    | 2.69                     | 0.41              |
| 50:y:71:LEU:CD2   | 50:y:82:ARG:HB3   | 2.50                     | 0.41              |
| 53:1:31:PRO:HG2   | 53:1:38:LEU:HG    | 2.02                     | 0.41              |
| 56:4:103:LYS:HA   | 56:4:104:PRO:HD3  | 1.93                     | 0.41              |
| 57:5:142:SER:O    | 57:5:146:GLN:HB3  | 2.20                     | 0.41              |
| 58:6:147:PHE:CD1  | 58:6:147:PHE:C    | 2.98                     | 0.41              |
| 68:AG:20:ILE:HG13 | 68:AG:91:LEU:HB2  | 2.03                     | 0.41              |
| 74:AM:44:ILE:HG12 | 74:AM:65:PRO:O    | 2.21                     | 0.41              |
| 79:AR:113:PHE:HE2 | 79:AR:117:ASN:ND2 | 2.18                     | 0.41              |
| 15:P:144:LYS:HE2  | 15:P:146:ARG:O    | 2.21                     | 0.41              |
| 23:X:155:PRO:O    | 23:X:156:HIS:C    | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:d:50:ARG:HD2   | 29:d:115:ARG:HH11 | 1.85                     | 0.41              |
| 30:e:101:PHE:C    | 30:e:102:ARG:HD3  | 2.46                     | 0.41              |
| 48:w:520:A:O5'    | 58:6:11:LYS:HD2   | 2.21                     | 0.41              |
| 48:w:1102:G:H22   | 48:w:1130:G:N2    | 2.18                     | 0.41              |
| 49:x:57:LYS:HE2   | 49:x:160:ALA:O    | 2.20                     | 0.41              |
| 49:x:84:GLN:OE1   | 49:x:101:GLY:N    | 2.53                     | 0.41              |
| 50:y:129:THR:OG1  | 50:y:131:ASP:OD1  | 2.30                     | 0.41              |
| 51:z:85:SER:O     | 51:z:85:SER:OG    | 2.34                     | 0.41              |
| 53:1:102:ILE:HG21 | 53:1:239:PRO:HG3  | 2.02                     | 0.41              |
| 53:1:138:HIS:CD2  | 53:1:148:ARG:HB3  | 2.56                     | 0.41              |
| 56:4:163:GLN:HA   | 56:4:167:GLU:OE2  | 2.21                     | 0.41              |
| 59:7:15:LEU:HD11  | 59:7:71:LEU:HG    | 2.02                     | 0.41              |
| 60:8:117:PHE:O    | 60:8:119:ASP:N    | 2.53                     | 0.41              |
| 68:AG:44:LYS:HE3  | 68:AG:44:LYS:HB3  | 1.89                     | 0.41              |
| 74:AM:10:ARG:HB2  | 74:AM:33:ASP:OD2  | 2.20                     | 0.41              |
| 3:D:189:G:H2'     | 3:D:190:G:C8      | 2.55                     | 0.41              |
| 3:D:665:C:H4'     | 3:D:666:G:O5'     | 2.20                     | 0.41              |
| 3:D:760:G:H4'     | 3:D:905:C:H1'     | 2.03                     | 0.41              |
| 3:D:987:C:H2'     | 3:D:988:C:C6      | 2.56                     | 0.41              |
| 3:D:1418:C:H2'    | 3:D:1419:G:O4'    | 2.21                     | 0.41              |
| 3:D:5060:A:O2'    | 3:D:5061:A:OP1    | 2.36                     | 0.41              |
| 11:L:87:PRO:HG2   | 11:L:144:TYR:CE2  | 2.55                     | 0.41              |
| 11:L:107:LYS:O    | 11:L:110:GLN:HG2  | 2.20                     | 0.41              |
| 13:N:115:ARG:O    | 13:N:116:ASN:C    | 2.63                     | 0.41              |
| 23:X:60:GLU:OE2   | 24:Y:139:HIS:NE2  | 2.51                     | 0.41              |
| 48:w:1035:A:H2'   | 48:w:1036:A:O4'   | 2.21                     | 0.41              |
| 50:y:144:LYS:HG3  | 50:y:208:HIS:HB3  | 2.02                     | 0.41              |
| 52:0:146:ARG:O    | 52:0:148:LYS:HD3  | 2.20                     | 0.41              |
| 54:2:88:MET:HE3   | 54:2:91:ARG:NH2   | 2.36                     | 0.41              |
| 55:3:23:LYS:HG3   | 55:3:41:LEU:HA    | 2.01                     | 0.41              |
| 59:7:4:PRO:HD2    | 59:7:7:ASN:OD1    | 2.21                     | 0.41              |
| 64:AC:39:LEU:HD11 | 64:AC:51:LEU:HB3  | 2.03                     | 0.41              |
| 79:AR:31:ILE:HG23 | 79:AR:43:TRP:HB2  | 2.02                     | 0.41              |
| 3:D:491:G:O3'     | 8:I:268:ARG:NH1   | 2.44                     | 0.41              |
| 3:D:691:C:H2'     | 3:D:692:A:C8      | 2.56                     | 0.41              |
| 3:D:981:C:H2'     | 10:K:73:TYR:CE1   | 2.55                     | 0.41              |
| 3:D:2591:A:N6     | 3:D:2754:G:O2'    | 2.53                     | 0.41              |
| 7:H:28:LYS:HE3    | 7:H:28:LYS:HB2    | 1.71                     | 0.41              |
| 8:I:64:ALA:HB3    | 8:I:92:PHE:CE2    | 2.55                     | 0.41              |
| 8:I:347:HIS:O     | 8:I:351:VAL:HG22  | 2.20                     | 0.41              |
| 14:O:32:ARG:O     | 14:O:33:ILE:C     | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:167:ARG:O    | 31:f:98:ALA:N     | 2.52                     | 0.41              |
| 25:Z:55:ASN:OD1   | 25:Z:55:ASN:C     | 2.64                     | 0.41              |
| 31:f:74:ASN:HA    | 31:f:112:LEU:O    | 2.21                     | 0.41              |
| 33:h:21:VAL:N     | 33:h:101:ASP:OD2  | 2.54                     | 0.41              |
| 48:w:70:G:H21     | 48:w:79:A:H62     | 1.67                     | 0.41              |
| 48:w:1255:G:OP1   | 48:w:1256:G:O2'   | 2.21                     | 0.41              |
| 48:w:1679:A:H2'   | 54:2:60:ARG:HD2   | 2.03                     | 0.41              |
| 55:3:197:GLN:HA   | 55:3:200:LYS:HG3  | 2.02                     | 0.41              |
| 56:4:83:LEU:HG    | 56:4:92:VAL:HG11  | 2.01                     | 0.41              |
| 58:6:35:TYR:N     | 58:6:35:TYR:CD1   | 2.88                     | 0.41              |
| 58:6:54:ARG:HG2   | 58:6:58:ARG:HH12  | 1.86                     | 0.41              |
| 59:7:57:TYR:HD2   | 59:7:75:GLY:HA2   | 1.84                     | 0.41              |
| 64:AC:42:ILE:O    | 64:AC:45:ARG:HG3  | 2.20                     | 0.41              |
| 79:AR:78:ALA:HB2  | 79:AR:92:LEU:HD11 | 2.03                     | 0.41              |
| 3:D:75:G:H3'      | 16:Q:74:ARG:HD2   | 2.03                     | 0.41              |
| 3:D:4731:G:N2     | 3:D:4732:G:N3     | 2.69                     | 0.41              |
| 6:G:140:ASN:OD1   | 6:G:142:GLU:HG2   | 2.21                     | 0.41              |
| 7:H:36:ASP:HA     | 7:H:37:PRO:HD3    | 1.89                     | 0.41              |
| 8:I:74:ALA:O      | 8:I:76:ILE:N      | 2.54                     | 0.41              |
| 10:K:176:THR:HG23 | 10:K:176:THR:O    | 2.21                     | 0.41              |
| 12:M:261:LEU:HD23 | 12:M:261:LEU:HA   | 1.88                     | 0.41              |
| 48:w:436:OMG:HM23 | 48:w:436:OMG:H1'  | 1.83                     | 0.41              |
| 48:w:583:C:OP1    | 58:6:162:ARG:NH1  | 2.54                     | 0.41              |
| 48:w:879:C:N4     | 48:w:880:G:O6     | 2.53                     | 0.41              |
| 48:w:1737:G:H2'   | 48:w:1738:C:C6    | 2.55                     | 0.41              |
| 52:0:23:GLU:HG3   | 77:AP:46:TYR:OH   | 2.21                     | 0.41              |
| 52:0:27:ARG:HG2   | 59:7:61:GLN:NE2   | 2.35                     | 0.41              |
| 52:0:162:ASP:C    | 52:0:164:VAL:H    | 2.27                     | 0.41              |
| 54:2:98:GLU:OE2   | 54:2:98:GLU:HA    | 2.20                     | 0.41              |
| 54:2:185:SER:H    | 54:2:190:ILE:HD12 | 1.86                     | 0.41              |
| 55:3:55:GLY:HA3   | 55:3:108:VAL:O    | 2.21                     | 0.41              |
| 58:6:12:THR:HA    | 58:6:48:PHE:CD2   | 2.56                     | 0.41              |
| 58:6:109:ARG:HH22 | 58:6:127:ARG:HH12 | 1.68                     | 0.41              |
| 60:8:132:ARG:O    | 60:8:134:LEU:HD23 | 2.20                     | 0.41              |
| 70:AI:82:GLN:HB2  | 70:AI:85:ASP:OD1  | 2.20                     | 0.41              |
| 71:AJ:26:GLN:OE1  | 71:AJ:26:GLN:HA   | 2.21                     | 0.41              |
| 76:AO:16:LYS:HE3  | 76:AO:16:LYS:HB2  | 1.64                     | 0.41              |
| 2:B:9:1MA:O4'     | 2:B:46:A:H1'      | 2.21                     | 0.41              |
| 2:B:14:A:H2'      | 2:B:15:G:O4'      | 2.21                     | 0.41              |
| 3:D:668:C:H4'     | 8:I:6:PRO:HB3     | 2.03                     | 0.41              |
| 3:D:683:C:H2'     | 3:D:684:G:O4'     | 2.20                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:D:1927:U:OP1     | 3:D:1949:U:O2'    | 2.32                     | 0.41              |
| 3:D:4139:G:H1      | 3:D:4145:C:H42    | 1.67                     | 0.41              |
| 3:D:4523:A2M:H5''  | 3:D:4524:G:H5'    | 2.02                     | 0.41              |
| 5:F:121:G:H2'      | 5:F:122:G:C8      | 2.55                     | 0.41              |
| 8:I:25:PRO:HG2     | 8:I:28:PHE:CE2    | 2.55                     | 0.41              |
| 9:J:125:VAL:HG23   | 9:J:126:THR:N     | 2.36                     | 0.41              |
| 10:K:251:LYS:HB2   | 10:K:251:LYS:HE2  | 1.88                     | 0.41              |
| 12:M:180:PRO:HG2   | 12:M:219:VAL:HG13 | 2.02                     | 0.41              |
| 13:N:47:LEU:HA     | 13:N:47:LEU:HD23  | 1.74                     | 0.41              |
| 15:P:151:ILE:HG13  | 15:P:152:GLY:N    | 2.36                     | 0.41              |
| 29:d:47:MET:HB3    | 29:d:47:MET:HE3   | 1.71                     | 0.41              |
| 35:j:84:GLU:CD     | 47:v:20:ARG:HH22  | 2.29                     | 0.41              |
| 48:w:174:OMC:HM23  | 48:w:174:OMC:H1'  | 1.75                     | 0.41              |
| 48:w:184:G:H2'     | 48:w:185:G:C8     | 2.56                     | 0.41              |
| 48:w:1033:G:N1     | 48:w:1080:A:O2'   | 2.41                     | 0.41              |
| 48:w:1139:C:H2'    | 48:w:1140:G:O4'   | 2.21                     | 0.41              |
| 48:w:1452:A:H4'    | 48:w:1453:C:O5'   | 2.21                     | 0.41              |
| 48:w:1606:G:HO2'   | 48:w:1607:A:P     | 2.44                     | 0.41              |
| 53:1:52:LEU:HD21   | 53:1:111:VAL:HG21 | 2.03                     | 0.41              |
| 53:1:85:GLY:N      | 53:1:88:ASP:OD2   | 2.37                     | 0.41              |
| 53:1:102:ILE:CG2   | 53:1:239:PRO:HG3  | 2.51                     | 0.41              |
| 54:2:97:PHE:HE2    | 54:2:109:LEU:HD12 | 1.86                     | 0.41              |
| 54:2:158:ALA:N     | 54:2:176:GLU:OE2  | 2.54                     | 0.41              |
| 55:3:67:VAL:HG23   | 55:3:99:GLY:HA2   | 2.03                     | 0.41              |
| 55:3:221:LYS:HG2   | 55:3:225:GLN:NE2  | 2.36                     | 0.41              |
| 55:3:221:LYS:HA    | 55:3:224:ARG:HB2  | 2.03                     | 0.41              |
| 57:5:42:ARG:HE     | 57:5:59:ARG:CZ    | 2.33                     | 0.41              |
| 58:6:70:ARG:NH2    | 58:6:94:LEU:HD21  | 2.34                     | 0.41              |
| 63:AB:81:ARG:HB3   | 63:AB:117:GLY:HA3 | 2.02                     | 0.41              |
| 66:AE:15:VAL:HG13  | 66:AE:68:ILE:HD11 | 2.03                     | 0.41              |
| 72:AK:80:ASP:OD1   | 72:AK:81:TYR:N    | 2.54                     | 0.41              |
| 72:AK:117:VAL:HG23 | 72:AK:122:LYS:HG2 | 2.03                     | 0.41              |
| 77:AP:13:LYS:HE3   | 77:AP:13:LYS:HB3  | 1.83                     | 0.41              |
| 79:AR:72:SER:HA    | 79:AR:113:PHE:CE2 | 2.56                     | 0.41              |
| 79:AR:104:HIS:CD2  | 79:AR:108:VAL:HB  | 2.55                     | 0.41              |
| 3:D:685:C:O2'      | 3:D:686:A:N7      | 2.53                     | 0.41              |
| 3:D:1742:A:OP2     | 9:J:10:LYS:HD2    | 2.21                     | 0.41              |
| 3:D:4122:G:O2'     | 30:e:136:PHE:OXT  | 2.38                     | 0.41              |
| 3:D:4625:C:O2'     | 3:D:4626:A:H5'    | 2.21                     | 0.41              |
| 14:O:31:ILE:HG12   | 14:O:32:ARG:N     | 2.36                     | 0.41              |
| 15:P:154:LYS:H     | 15:P:154:LYS:HG2  | 1.58                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:135:LYS:C    | 16:Q:136:LYS:HG2  | 2.46                     | 0.41              |
| 16:Q:145:LYS:C    | 16:Q:146:LEU:HD12 | 2.46                     | 0.41              |
| 17:R:104:MET:HE3  | 17:R:109:ARG:HG2  | 2.02                     | 0.41              |
| 30:e:58:GLY:O     | 30:e:62:ILE:HG13  | 2.21                     | 0.41              |
| 39:n:94:LEU:HD23  | 39:n:94:LEU:HA    | 1.91                     | 0.41              |
| 48:w:926:A:H61    | 48:w:1015:U:H3    | 1.67                     | 0.41              |
| 51:z:105:GLU:OE1  | 51:z:106:VAL:N    | 2.53                     | 0.41              |
| 55:3:5:ILE:HG21   | 55:3:45:TRP:HH2   | 1.86                     | 0.41              |
| 55:3:163:ASN:HB3  | 55:3:169:PRO:HB3  | 2.03                     | 0.41              |
| 56:4:116:ARG:CZ   | 56:4:121:THR:HG22 | 2.51                     | 0.41              |
| 67:AF:112:MET:C   | 67:AF:124:THR:HG1 | 2.28                     | 0.41              |
| 79:AR:94:THR:HG23 | 79:AR:96:THR:H    | 1.86                     | 0.41              |
| 79:AR:172:LYS:HG3 | 79:AR:193:GLY:N   | 2.36                     | 0.41              |
| 3:D:418:A:H62     | 5:F:16:G:H1'      | 1.83                     | 0.40              |
| 3:D:1574:G:O2'    | 3:D:1575:A:P      | 2.79                     | 0.40              |
| 3:D:1699:A:H5''   | 3:D:1700:G:H21    | 1.86                     | 0.40              |
| 3:D:2055:G:H4'    | 3:D:2056:G:OP2    | 2.21                     | 0.40              |
| 3:D:2416:G:C2     | 3:D:2425:U:H5'    | 2.56                     | 0.40              |
| 3:D:4115:G:O2'    | 3:D:4116:C:P      | 2.80                     | 0.40              |
| 7:H:238:LYS:HE2   | 7:H:238:LYS:HB2   | 1.94                     | 0.40              |
| 8:I:218:ILE:O     | 8:I:222:ARG:HB2   | 2.21                     | 0.40              |
| 11:L:44:LYS:HB2   | 11:L:44:LYS:HE2   | 1.85                     | 0.40              |
| 19:T:175:MET:HE2  | 19:T:179:LYS:HE2  | 2.03                     | 0.40              |
| 36:k:11:PHE:HB2   | 36:k:101:ILE:HD12 | 2.03                     | 0.40              |
| 44:s:20:MET:HE3   | 44:s:20:MET:HB3   | 1.77                     | 0.40              |
| 48:w:655:A:H4'    | 48:w:656:G:H3'    | 2.03                     | 0.40              |
| 48:w:927:C:H1'    | 75:AN:51:GLN:HE21 | 1.86                     | 0.40              |
| 48:w:927:C:H1'    | 75:AN:51:GLN:NE2  | 2.36                     | 0.40              |
| 48:w:1391:OMC:H4' | 77:AP:55:LEU:HD11 | 2.04                     | 0.40              |
| 48:w:1532:C:O2'   | 48:w:1635:C:O2    | 2.35                     | 0.40              |
| 48:w:1599:U:N3    | 54:2:165:ASN:O    | 2.53                     | 0.40              |
| 60:8:111:VAL:HG12 | 60:8:140:PHE:HB2  | 2.02                     | 0.40              |
| 65:AD:132:ARG:HD2 | 65:AD:132:ARG:N   | 2.36                     | 0.40              |
| 70:AI:43:LYS:HB3  | 70:AI:43:LYS:HE3  | 1.86                     | 0.40              |
| 3:D:1760:OMG:HM23 | 3:D:1760:OMG:H1'  | 1.92                     | 0.40              |
| 19:T:53:LYS:HB2   | 19:T:53:LYS:HE2   | 1.90                     | 0.40              |
| 34:i:56:GLU:OE1   | 34:i:56:GLU:HA    | 2.22                     | 0.40              |
| 47:v:32:LEU:O     | 47:v:33:LYS:HB2   | 2.21                     | 0.40              |
| 48:w:149:A:H3'    | 48:w:150:A:H8     | 1.86                     | 0.40              |
| 48:w:582:C:H2'    | 48:w:583:C:C6     | 2.56                     | 0.40              |
| 48:w:878:G:C2     | 48:w:909:G:C2     | 3.09                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:w:1622:U:O2'    | 48:w:1623:A:OP1   | 2.32                     | 0.40              |
| 49:x:11:LYS:O      | 49:x:13:GLU:N     | 2.55                     | 0.40              |
| 49:x:12:GLU:CD     | 49:x:12:GLU:H     | 2.28                     | 0.40              |
| 49:x:110:ASN:HB3   | 49:x:113:GLN:HG3  | 2.02                     | 0.40              |
| 52:0:129:SER:O     | 52:0:129:SER:OG   | 2.28                     | 0.40              |
| 57:5:23:LYS:HE2    | 57:5:23:LYS:HB3   | 1.82                     | 0.40              |
| 57:5:172:LEU:HD11  | 57:5:195:LEU:HD12 | 2.04                     | 0.40              |
| 59:7:76:ILE:HD12   | 59:7:76:ILE:N     | 2.35                     | 0.40              |
| 63:AB:136:THR:HG22 | 63:AB:138:SER:N   | 2.36                     | 0.40              |
| 70:AI:20:ARG:HA    | 70:AI:20:ARG:HD2  | 1.94                     | 0.40              |
| 72:AK:114:MET:HE3  | 72:AK:114:MET:HB2 | 1.78                     | 0.40              |
| 79:AR:104:HIS:NE2  | 79:AR:124:SER:HB3 | 2.36                     | 0.40              |
| 3:D:978:G:OP1      | 10:K:47:ASN:ND2   | 2.52                     | 0.40              |
| 3:D:2847:G:O2'     | 26:a:21:PRO:HD2   | 2.21                     | 0.40              |
| 3:D:3688:U:OP2     | 6:G:198:ARG:NH1   | 2.54                     | 0.40              |
| 3:D:4227:OMU:HM23  | 3:D:4227:OMU:H1'  | 1.65                     | 0.40              |
| 3:D:4306:OMU:HM23  | 3:D:4306:OMU:H1'  | 1.84                     | 0.40              |
| 7:H:47:LEU:HD13    | 7:H:84:MET:HE1    | 2.03                     | 0.40              |
| 10:K:66:LYS:O      | 10:K:71:ARG:NH1   | 2.52                     | 0.40              |
| 22:W:114:LYS:O     | 22:W:146:LYS:NZ   | 2.42                     | 0.40              |
| 28:c:145:ASP:OD2   | 28:c:147:LEU:N    | 2.54                     | 0.40              |
| 31:f:119:LYS:HB3   | 31:f:119:LYS:HE3  | 1.57                     | 0.40              |
| 34:i:40:LYS:HE2    | 34:i:40:LYS:HB3   | 1.66                     | 0.40              |
| 40:o:21:ARG:C      | 40:o:23:GLY:H     | 2.29                     | 0.40              |
| 48:w:155:G:OP1     | 55:3:15:LEU:HD12  | 2.21                     | 0.40              |
| 48:w:1448:A:O2'    | 48:w:1449:G:O5'   | 2.38                     | 0.40              |
| 48:w:1673:U:O2'    | 54:2:84:GLY:O     | 2.35                     | 0.40              |
| 48:w:1781:A:O2'    | 48:w:1782:G:N7    | 2.53                     | 0.40              |
| 52:0:77:PHE:HD1    | 52:0:77:PHE:HA    | 1.80                     | 0.40              |
| 53:1:122:LYS:NZ    | 53:1:143:ASP:OD2  | 2.42                     | 0.40              |
| 54:2:152:TRP:O     | 54:2:156:THR:HG22 | 2.21                     | 0.40              |
| 55:3:3:LEU:HB2     | 55:3:5:ILE:HD11   | 2.03                     | 0.40              |
| 79:AR:126:ASP:OD1  | 79:AR:126:ASP:N   | 2.53                     | 0.40              |
| 3:D:218:A:H1'      | 3:D:219:G:O4'     | 2.22                     | 0.40              |
| 6:G:206:PRO:HD3    | 6:G:213:GLY:CA    | 2.51                     | 0.40              |
| 9:J:34:LYS:O       | 9:J:38:ILE:HG12   | 2.22                     | 0.40              |
| 48:w:344:U:OP1     | 53:1:128:LYS:NZ   | 2.52                     | 0.40              |
| 48:w:924:G:N2      | 61:9:87:ASP:OD2   | 2.35                     | 0.40              |
| 49:x:94:THR:HG23   | 49:x:186:ARG:HH21 | 1.86                     | 0.40              |
| 57:5:139:LYS:HA    | 57:5:139:LYS:HD2  | 1.97                     | 0.40              |
| 57:5:149:TYR:O     | 57:5:153:LYS:HG2  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 61:9:54:LEU:O     | 61:9:60:VAL:HG22  | 2.21                     | 0.40              |
| 72:AK:25:ILE:HD11 | 72:AK:73:GLY:HA3  | 2.03                     | 0.40              |
| 76:AO:60:GLU:OE1  | 76:AO:62:GLU:N    | 2.50                     | 0.40              |
| 2:B:12:A:HO2'     | 3:D:3770:PSU:HO2' | 1.62                     | 0.40              |
| 3:D:75:G:N7       | 16:Q:102:ARG:HG2  | 2.36                     | 0.40              |
| 3:D:963:G:C8      | 3:D:964:A:N6      | 2.90                     | 0.40              |
| 3:D:1699:A:H2'    | 3:D:1704:C:N4     | 2.37                     | 0.40              |
| 3:D:2100:A:C6     | 3:D:2101:C:C4     | 3.10                     | 0.40              |
| 3:D:2487:G:OP2    | 3:D:2487:G:H2'    | 2.21                     | 0.40              |
| 3:D:4744:A:H2'    | 3:D:4745:G:O4'    | 2.21                     | 0.40              |
| 8:I:163:LYS:O     | 8:I:166:GLU:HG2   | 2.21                     | 0.40              |
| 9:J:65:ALA:HB2    | 9:J:74:ILE:HD13   | 2.04                     | 0.40              |
| 9:J:258:LYS:HE3   | 9:J:258:LYS:HB2   | 1.97                     | 0.40              |
| 10:K:69:TYR:O     | 10:K:70:LYS:HB3   | 2.22                     | 0.40              |
| 15:P:118:LYS:HG3  | 15:P:119:TYR:N    | 2.33                     | 0.40              |
| 32:g:55:LYS:O     | 32:g:58:GLN:NE2   | 2.54                     | 0.40              |
| 36:k:93:PRO:C     | 36:k:95:LYS:H     | 2.28                     | 0.40              |
| 48:w:184:G:H2'    | 48:w:185:G:H8     | 1.85                     | 0.40              |
| 48:w:528:A:H61    | 48:w:557:U:H3     | 1.70                     | 0.40              |
| 48:w:651:PSU:H2'  | 48:w:652:U:C6     | 2.56                     | 0.40              |
| 48:w:688:U:OP2    | 56:4:123:THR:OG1  | 2.32                     | 0.40              |
| 48:w:1746:U:H4'   | 55:3:65:GLN:NE2   | 2.37                     | 0.40              |
| 54:2:149:GLN:O    | 54:2:153:LEU:HB2  | 2.21                     | 0.40              |
| 55:3:118:GLU:HG3  | 55:3:119:LYS:N    | 2.36                     | 0.40              |
| 55:3:177:GLN:HG3  | 55:3:178:ARG:N    | 2.37                     | 0.40              |
| 62:AA:83:GLN:O    | 62:AA:87:GLU:HG2  | 2.21                     | 0.40              |
| 63:AB:53:GLN:CD   | 63:AB:53:GLN:H    | 2.28                     | 0.40              |
| 66:AE:76:GLN:HG2  | 66:AE:77:TYR:CD2  | 2.57                     | 0.40              |
| 67:AF:127:GLY:O   | 67:AF:131:LEU:HG  | 2.22                     | 0.40              |
| 72:AK:47:MET:O    | 72:AK:47:MET:HE2  | 2.21                     | 0.40              |
| 74:AM:51:ARG:NH2  | 76:AO:39:SER:OG   | 2.50                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6   | G     | 245/257 (95%) | 227 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 7   | H     | 396/403 (98%) | 375 (95%) | 21 (5%)  | 0        | 100         | 100 |
| 8   | I     | 361/427 (84%) | 338 (94%) | 23 (6%)  | 0        | 100         | 100 |
| 9   | J     | 291/297 (98%) | 271 (93%) | 20 (7%)  | 0        | 100         | 100 |
| 10  | K     | 211/288 (73%) | 189 (90%) | 22 (10%) | 0        | 100         | 100 |
| 11  | L     | 223/248 (90%) | 212 (95%) | 11 (5%)  | 0        | 100         | 100 |
| 12  | M     | 223/266 (84%) | 208 (93%) | 14 (6%)  | 1 (0%)   | 30          | 49  |
| 13  | N     | 188/192 (98%) | 174 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 14  | O     | 202/214 (94%) | 186 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 15  | P     | 168/178 (94%) | 158 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 16  | Q     | 206/211 (98%) | 192 (93%) | 12 (6%)  | 2 (1%)   | 12          | 24  |
| 17  | R     | 134/215 (62%) | 120 (90%) | 14 (10%) | 0        | 100         | 100 |
| 18  | S     | 201/204 (98%) | 196 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 19  | T     | 198/203 (98%) | 195 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 20  | U     | 155/184 (84%) | 144 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 21  | V     | 185/188 (98%) | 173 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 22  | W     | 178/196 (91%) | 177 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 23  | X     | 173/176 (98%) | 159 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 24  | Y     | 157/160 (98%) | 147 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 25  | Z     | 99/128 (77%)  | 93 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 26  | a     | 129/140 (92%) | 120 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 27  | b     | 61/157 (39%)  | 60 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 28  | c     | 118/156 (76%) | 111 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 29  | d     | 132/145 (91%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 30  | e     | 133/136 (98%) | 126 (95%) | 6 (4%)   | 1 (1%)   | 16          | 31  |
| 31  | f     | 145/148 (98%) | 131 (90%) | 14 (10%) | 0        | 100         | 100 |
| 32  | g     | 100/159 (63%) | 90 (90%)  | 8 (8%)   | 2 (2%)   | 6           | 10  |
| 33  | h     | 95/115 (83%)  | 91 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 34  | i     | 105/125 (84%) | 100 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 35  | j     | 126/135 (93%) | 124 (98%) | 2 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 36  | k     | 107/110 (97%) | 99 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 37  | l     | 110/117 (94%) | 106 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 38  | m     | 119/123 (97%) | 116 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 39  | n     | 100/105 (95%) | 98 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 40  | o     | 84/97 (87%)   | 79 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 41  | p     | 67/70 (96%)   | 61 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 42  | q     | 48/51 (94%)   | 46 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 43  | r     | 50/128 (39%)  | 49 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 44  | s     | 23/25 (92%)   | 23 (100%) | 0        | 0        | 100         | 100 |
| 45  | t     | 103/106 (97%) | 98 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 46  | u     | 89/92 (97%)   | 84 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 47  | v     | 123/137 (90%) | 116 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 49  | x     | 213/295 (72%) | 200 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 50  | y     | 210/264 (80%) | 193 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 51  | z     | 210/293 (72%) | 200 (95%) | 9 (4%)   | 1 (0%)   | 24          | 43  |
| 52  | 0     | 210/243 (86%) | 188 (90%) | 22 (10%) | 0        | 100         | 100 |
| 53  | 1     | 260/263 (99%) | 245 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 54  | 2     | 185/204 (91%) | 166 (90%) | 19 (10%) | 0        | 100         | 100 |
| 55  | 3     | 235/249 (94%) | 226 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 56  | 4     | 185/194 (95%) | 168 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 57  | 5     | 204/208 (98%) | 192 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 58  | 6     | 180/194 (93%) | 171 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 59  | 7     | 94/165 (57%)  | 86 (92%)  | 7 (7%)   | 1 (1%)   | 11          | 22  |
| 60  | 8     | 138/158 (87%) | 126 (91%) | 11 (8%)  | 1 (1%)   | 18          | 34  |
| 61  | 9     | 148/151 (98%) | 142 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 62  | AA    | 132/151 (87%) | 123 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 63  | AB    | 132/145 (91%) | 126 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 64  | AC    | 140/146 (96%) | 124 (89%) | 15 (11%) | 1 (1%)   | 18          | 34  |
| 65  | AD    | 129/135 (96%) | 107 (83%) | 20 (16%) | 2 (2%)   | 7           | 14  |
| 66  | AE    | 142/152 (93%) | 128 (90%) | 14 (10%) | 0        | 100         | 100 |
| 67  | AF    | 141/145 (97%) | 132 (94%) | 9 (6%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 68  | AG    | 100/119 (84%)     | 92 (92%)    | 8 (8%)   | 0        | 100         | 100 |
| 69  | AH    | 81/83 (98%)       | 72 (89%)    | 9 (11%)  | 0        | 100         | 100 |
| 70  | AI    | 127/130 (98%)     | 119 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 71  | AJ    | 139/143 (97%)     | 135 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 72  | AK    | 121/133 (91%)     | 118 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 73  | AL    | 84/125 (67%)      | 74 (88%)    | 10 (12%) | 0        | 100         | 100 |
| 74  | AM    | 97/115 (84%)      | 91 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| 75  | AN    | 81/84 (96%)       | 71 (88%)    | 9 (11%)  | 1 (1%)   | 10          | 20  |
| 76  | AO    | 59/69 (86%)       | 53 (90%)    | 6 (10%)  | 0        | 100         | 100 |
| 77  | AP    | 43/56 (77%)       | 42 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 78  | AQ    | 55/59 (93%)       | 50 (91%)    | 5 (9%)   | 0        | 100         | 100 |
| 79  | AR    | 311/317 (98%)     | 261 (84%)   | 50 (16%) | 0        | 100         | 100 |
| All | All   | 10947/12400 (88%) | 10208 (93%) | 726 (7%) | 13 (0%)  | 49          | 68  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | Q     | 48  | PRO  |
| 32  | g     | 111 | ARG  |
| 64  | AC    | 119 | LEU  |
| 51  | z     | 78  | LEU  |
| 65  | AD    | 119 | VAL  |
| 32  | g     | 110 | ALA  |
| 65  | AD    | 118 | GLN  |
| 16  | Q     | 47  | ALA  |
| 30  | e     | 33  | THR  |
| 12  | M     | 106 | THR  |
| 60  | 8     | 118 | ARG  |
| 59  | 7     | 30  | PRO  |
| 75  | AN    | 39  | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 6   | G     | 189/199 (95%) | 189 (100%) | 0        | 100         | 100 |
| 7   | H     | 346/349 (99%) | 345 (100%) | 1 (0%)   | 86          | 94  |
| 8   | I     | 301/348 (86%) | 300 (100%) | 1 (0%)   | 86          | 94  |
| 9   | J     | 245/250 (98%) | 243 (99%)  | 2 (1%)   | 73          | 88  |
| 10  | K     | 193/252 (77%) | 191 (99%)  | 2 (1%)   | 68          | 86  |
| 11  | L     | 194/215 (90%) | 194 (100%) | 0        | 100         | 100 |
| 12  | M     | 195/223 (87%) | 194 (100%) | 1 (0%)   | 81          | 92  |
| 13  | N     | 169/171 (99%) | 169 (100%) | 0        | 100         | 100 |
| 14  | O     | 174/181 (96%) | 173 (99%)  | 1 (1%)   | 78          | 91  |
| 15  | P     | 143/149 (96%) | 141 (99%)  | 2 (1%)   | 59          | 81  |
| 16  | Q     | 174/177 (98%) | 173 (99%)  | 1 (1%)   | 78          | 91  |
| 17  | R     | 116/161 (72%) | 114 (98%)  | 2 (2%)   | 53          | 78  |
| 18  | S     | 171/172 (99%) | 171 (100%) | 0        | 100         | 100 |
| 19  | T     | 172/174 (99%) | 170 (99%)  | 2 (1%)   | 63          | 83  |
| 20  | U     | 138/163 (85%) | 138 (100%) | 0        | 100         | 100 |
| 21  | V     | 164/165 (99%) | 164 (100%) | 0        | 100         | 100 |
| 22  | W     | 159/175 (91%) | 159 (100%) | 0        | 100         | 100 |
| 23  | X     | 156/157 (99%) | 155 (99%)  | 1 (1%)   | 78          | 91  |
| 24  | Y     | 139/140 (99%) | 138 (99%)  | 1 (1%)   | 76          | 89  |
| 25  | Z     | 90/115 (78%)  | 90 (100%)  | 0        | 100         | 100 |
| 26  | a     | 101/107 (94%) | 101 (100%) | 0        | 100         | 100 |
| 27  | b     | 55/126 (44%)  | 55 (100%)  | 0        | 100         | 100 |
| 28  | c     | 107/133 (80%) | 107 (100%) | 0        | 100         | 100 |
| 29  | d     | 124/135 (92%) | 122 (98%)  | 2 (2%)   | 55          | 79  |
| 30  | e     | 117/118 (99%) | 116 (99%)  | 1 (1%)   | 70          | 87  |
| 31  | f     | 120/121 (99%) | 119 (99%)  | 1 (1%)   | 73          | 88  |
| 32  | g     | 81/126 (64%)  | 81 (100%)  | 0        | 100         | 100 |
| 33  | h     | 82/97 (84%)   | 82 (100%)  | 0        | 100         | 100 |
| 34  | i     | 98/110 (89%)  | 96 (98%)   | 2 (2%)   | 48          | 75  |
| 35  | j     | 114/121 (94%) | 114 (100%) | 0        | 100         | 100 |
| 36  | k     | 88/89 (99%)   | 88 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 37  | l     | 96/100 (96%)  | 96 (100%)  | 0        | 100         | 100 |
| 38  | m     | 109/110 (99%) | 109 (100%) | 0        | 100         | 100 |
| 39  | n     | 86/89 (97%)   | 86 (100%)  | 0        | 100         | 100 |
| 40  | o     | 73/80 (91%)   | 72 (99%)   | 1 (1%)   | 59          | 81  |
| 41  | p     | 64/65 (98%)   | 63 (98%)   | 1 (2%)   | 55          | 79  |
| 42  | q     | 47/48 (98%)   | 46 (98%)   | 1 (2%)   | 47          | 74  |
| 43  | r     | 48/116 (41%)  | 48 (100%)  | 0        | 100         | 100 |
| 44  | s     | 24/24 (100%)  | 24 (100%)  | 0        | 100         | 100 |
| 45  | t     | 93/94 (99%)   | 93 (100%)  | 0        | 100         | 100 |
| 46  | u     | 74/75 (99%)   | 72 (97%)   | 2 (3%)   | 39          | 67  |
| 47  | v     | 109/121 (90%) | 107 (98%)  | 2 (2%)   | 51          | 77  |
| 49  | x     | 178/243 (73%) | 178 (100%) | 0        | 100         | 100 |
| 50  | y     | 194/231 (84%) | 192 (99%)  | 2 (1%)   | 68          | 86  |
| 51  | z     | 176/225 (78%) | 176 (100%) | 0        | 100         | 100 |
| 52  | 0     | 175/202 (87%) | 175 (100%) | 0        | 100         | 100 |
| 53  | 1     | 223/225 (99%) | 223 (100%) | 0        | 100         | 100 |
| 54  | 2     | 154/170 (91%) | 154 (100%) | 0        | 100         | 100 |
| 55  | 3     | 206/218 (94%) | 206 (100%) | 0        | 100         | 100 |
| 56  | 4     | 168/174 (97%) | 168 (100%) | 0        | 100         | 100 |
| 57  | 5     | 175/180 (97%) | 174 (99%)  | 1 (1%)   | 78          | 91  |
| 58  | 6     | 160/168 (95%) | 159 (99%)  | 1 (1%)   | 78          | 91  |
| 59  | 7     | 87/136 (64%)  | 87 (100%)  | 0        | 100         | 100 |
| 60  | 8     | 125/142 (88%) | 125 (100%) | 0        | 100         | 100 |
| 61  | 9     | 130/131 (99%) | 128 (98%)  | 2 (2%)   | 57          | 80  |
| 62  | AA    | 104/119 (87%) | 104 (100%) | 0        | 100         | 100 |
| 63  | AB    | 120/130 (92%) | 118 (98%)  | 2 (2%)   | 53          | 78  |
| 64  | AC    | 117/121 (97%) | 111 (95%)  | 6 (5%)   | 21          | 43  |
| 65  | AD    | 117/122 (96%) | 115 (98%)  | 2 (2%)   | 53          | 78  |
| 66  | AE    | 119/132 (90%) | 118 (99%)  | 1 (1%)   | 73          | 88  |
| 67  | AF    | 113/115 (98%) | 111 (98%)  | 2 (2%)   | 51          | 77  |
| 68  | AG    | 89/107 (83%)  | 89 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 69  | AH    | 67/67 (100%)     | 67 (100%)  | 0        | 100         | 100 |
| 70  | AI    | 112/113 (99%)    | 111 (99%)  | 1 (1%)   | 70          | 87  |
| 71  | AJ    | 113/115 (98%)    | 113 (100%) | 0        | 100         | 100 |
| 72  | AK    | 106/115 (92%)    | 106 (100%) | 0        | 100         | 100 |
| 73  | AL    | 73/103 (71%)     | 72 (99%)   | 1 (1%)   | 59          | 81  |
| 74  | AM    | 86/98 (88%)      | 84 (98%)   | 2 (2%)   | 44          | 72  |
| 75  | AN    | 73/76 (96%)      | 72 (99%)   | 1 (1%)   | 59          | 81  |
| 76  | AO    | 54/62 (87%)      | 53 (98%)   | 1 (2%)   | 50          | 76  |
| 77  | AP    | 39/49 (80%)      | 39 (100%)  | 0        | 100         | 100 |
| 78  | AQ    | 46/48 (96%)      | 46 (100%)  | 0        | 100         | 100 |
| 79  | AR    | 272/275 (99%)    | 272 (100%) | 0        | 100         | 100 |
| All | All   | 9509/10553 (90%) | 9454 (99%) | 55 (1%)  | 76          | 91  |

All (55) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | H     | 345 | LEU  |
| 8   | I     | 111 | TRP  |
| 9   | J     | 131 | ASN  |
| 9   | J     | 291 | GLN  |
| 10  | K     | 50  | LEU  |
| 10  | K     | 106 | VAL  |
| 12  | M     | 166 | LEU  |
| 14  | O     | 60  | LEU  |
| 15  | P     | 112 | HIS  |
| 15  | P     | 148 | THR  |
| 16  | Q     | 149 | GLN  |
| 17  | R     | 43  | THR  |
| 17  | R     | 108 | ASP  |
| 19  | T     | 106 | ASP  |
| 19  | T     | 198 | THR  |
| 23  | X     | 7   | LEU  |
| 24  | Y     | 79  | GLN  |
| 29  | d     | 111 | LEU  |
| 29  | d     | 118 | ILE  |
| 30  | e     | 35  | ASP  |
| 31  | f     | 140 | VAL  |
| 34  | i     | 22  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | i     | 46  | LEU  |
| 40  | o     | 48  | ASN  |
| 41  | p     | 28  | ASN  |
| 42  | q     | 16  | LYS  |
| 46  | u     | 5   | THR  |
| 46  | u     | 88  | GLU  |
| 47  | v     | 43  | LEU  |
| 47  | v     | 101 | LYS  |
| 50  | y     | 77  | ASP  |
| 50  | y     | 193 | ILE  |
| 57  | 5     | 186 | ASP  |
| 58  | 6     | 148 | ILE  |
| 61  | 9     | 35  | GLU  |
| 61  | 9     | 134 | VAL  |
| 63  | AB    | 37  | TYR  |
| 63  | AB    | 139 | SER  |
| 64  | AC    | 35  | ASN  |
| 64  | AC    | 46  | THR  |
| 64  | AC    | 68  | ILE  |
| 64  | AC    | 89  | SER  |
| 64  | AC    | 97  | GLN  |
| 64  | AC    | 111 | ILE  |
| 65  | AD    | 8   | THR  |
| 65  | AD    | 16  | ILE  |
| 66  | AE    | 85  | ASN  |
| 67  | AF    | 55  | THR  |
| 67  | AF    | 131 | LEU  |
| 70  | AI    | 42  | MET  |
| 73  | AL    | 90  | GLU  |
| 74  | AM    | 2   | THR  |
| 74  | AM    | 74  | CYS  |
| 75  | AN    | 8   | LEU  |
| 76  | AO    | 45  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | G     | 139 | HIS  |
| 7   | H     | 302 | ASN  |
| 8   | I     | 43  | ASN  |
| 8   | I     | 112 | HIS  |
| 8   | I     | 347 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | J     | 202 | GLN  |
| 9   | J     | 229 | ASN  |
| 9   | J     | 267 | ASN  |
| 10  | K     | 268 | GLN  |
| 11  | L     | 239 | GLN  |
| 12  | M     | 94  | GLN  |
| 12  | M     | 108 | GLN  |
| 12  | M     | 149 | ASN  |
| 12  | M     | 153 | GLN  |
| 12  | M     | 206 | GLN  |
| 13  | N     | 42  | ASN  |
| 13  | N     | 98  | HIS  |
| 13  | N     | 102 | ASN  |
| 14  | O     | 51  | HIS  |
| 14  | O     | 73  | ASN  |
| 15  | P     | 168 | GLN  |
| 16  | Q     | 205 | GLN  |
| 17  | R     | 34  | ASN  |
| 17  | R     | 66  | HIS  |
| 18  | S     | 29  | GLN  |
| 19  | T     | 26  | GLN  |
| 20  | U     | 145 | HIS  |
| 21  | V     | 7   | HIS  |
| 22  | W     | 40  | GLN  |
| 23  | X     | 173 | ASN  |
| 24  | Y     | 144 | ASN  |
| 27  | b     | 48  | GLN  |
| 29  | d     | 14  | ASN  |
| 31  | f     | 60  | HIS  |
| 32  | g     | 6   | ASN  |
| 33  | h     | 72  | HIS  |
| 34  | i     | 116 | ASN  |
| 34  | i     | 121 | ASN  |
| 35  | j     | 52  | GLN  |
| 36  | k     | 21  | GLN  |
| 36  | k     | 24  | HIS  |
| 39  | n     | 15  | HIS  |
| 40  | o     | 66  | HIS  |
| 42  | q     | 17  | GLN  |
| 47  | v     | 4   | HIS  |
| 47  | v     | 30  | ASN  |
| 49  | x     | 36  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | x     | 50  | ASN  |
| 49  | x     | 110 | ASN  |
| 49  | x     | 113 | GLN  |
| 50  | y     | 92  | GLN  |
| 50  | y     | 186 | ASN  |
| 52  | 0     | 57  | ASN  |
| 52  | 0     | 74  | GLN  |
| 53  | 1     | 50  | ASN  |
| 53  | 1     | 142 | HIS  |
| 53  | 1     | 209 | HIS  |
| 55  | 3     | 81  | HIS  |
| 55  | 3     | 110 | ASN  |
| 55  | 3     | 186 | GLN  |
| 55  | 3     | 187 | HIS  |
| 55  | 3     | 197 | GLN  |
| 55  | 3     | 225 | GLN  |
| 56  | 4     | 163 | GLN  |
| 57  | 5     | 146 | GLN  |
| 58  | 6     | 154 | GLN  |
| 61  | 9     | 5   | HIS  |
| 64  | AC    | 8   | GLN  |
| 65  | AD    | 127 | ASN  |
| 68  | AG    | 92  | HIS  |
| 69  | AH    | 35  | ASN  |
| 70  | AI    | 24  | GLN  |
| 70  | AI    | 64  | ASN  |
| 71  | AJ    | 92  | ASN  |
| 72  | AK    | 124 | ASN  |
| 75  | AN    | 83  | GLN  |
| 77  | AP    | 26  | ASN  |
| 78  | AQ    | 88  | GLN  |
| 79  | AR    | 117 | ASN  |
| 79  | AR    | 143 | GLN  |
| 79  | AR    | 188 | HIS  |
| 79  | AR    | 196 | ASN  |
| 79  | AR    | 311 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 1   | A     | 13/14 (92%) | 1 (7%)            | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2   | B     | 74/75 (98%)     | 13 (17%)          | 0               |
| 2   | C     | 74/75 (98%)     | 12 (16%)          | 2 (2%)          |
| 3   | D     | 3496/5070 (68%) | 623 (17%)         | 26 (0%)         |
| 4   | E     | 119/120 (99%)   | 15 (12%)          | 0               |
| 48  | w     | 1624/1869 (86%) | 390 (24%)         | 0               |
| 5   | F     | 155/156 (99%)   | 28 (18%)          | 3 (1%)          |
| All | All   | 5555/7379 (75%) | 1082 (19%)        | 31 (0%)         |

All (1082) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | A    |
| 2   | B     | 4   | U    |
| 2   | B     | 9   | 1MA  |
| 2   | B     | 12  | A    |
| 2   | B     | 13  | PSU  |
| 2   | B     | 17  | G    |
| 2   | B     | 21  | A    |
| 2   | B     | 46  | A    |
| 2   | B     | 47  | 5MC  |
| 2   | B     | 48  | 5MC  |
| 2   | B     | 53  | 5MU  |
| 2   | B     | 73  | C    |
| 2   | B     | 74  | C    |
| 2   | B     | 75  | A    |
| 2   | C     | 4   | U    |
| 2   | C     | 6   | 2MG  |
| 2   | C     | 9   | 1MA  |
| 2   | C     | 17  | G    |
| 2   | C     | 18  | G    |
| 2   | C     | 21  | A    |
| 2   | C     | 26  | C    |
| 2   | C     | 46  | A    |
| 2   | C     | 47  | 5MC  |
| 2   | C     | 48  | 5MC  |
| 2   | C     | 53  | 5MU  |
| 2   | C     | 73  | C    |
| 3   | D     | 2   | G    |
| 3   | D     | 39  | A    |
| 3   | D     | 42  | A    |
| 3   | D     | 48  | G    |
| 3   | D     | 56  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 59  | A    |
| 3   | D     | 64  | A    |
| 3   | D     | 65  | A    |
| 3   | D     | 69  | A    |
| 3   | D     | 91  | G    |
| 3   | D     | 98  | A    |
| 3   | D     | 108 | A    |
| 3   | D     | 109 | G    |
| 3   | D     | 110 | C    |
| 3   | D     | 116 | G    |
| 3   | D     | 117 | C    |
| 3   | D     | 119 | G    |
| 3   | D     | 120 | A    |
| 3   | D     | 143 | C    |
| 3   | D     | 144 | G    |
| 3   | D     | 152 | U    |
| 3   | D     | 159 | C    |
| 3   | D     | 170 | C    |
| 3   | D     | 171 | U    |
| 3   | D     | 172 | C    |
| 3   | D     | 180 | C    |
| 3   | D     | 181 | C    |
| 3   | D     | 183 | C    |
| 3   | D     | 185 | C    |
| 3   | D     | 186 | G    |
| 3   | D     | 188 | G    |
| 3   | D     | 189 | G    |
| 3   | D     | 200 | U    |
| 3   | D     | 209 | U    |
| 3   | D     | 210 | C    |
| 3   | D     | 218 | A    |
| 3   | D     | 220 | C    |
| 3   | D     | 234 | G    |
| 3   | D     | 256 | G    |
| 3   | D     | 257 | C    |
| 3   | D     | 259 | C    |
| 3   | D     | 261 | G    |
| 3   | D     | 265 | C    |
| 3   | D     | 266 | C    |
| 3   | D     | 267 | G    |
| 3   | D     | 269 | G    |
| 3   | D     | 275 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 276 | C    |
| 3   | D     | 280 | G    |
| 3   | D     | 296 | A    |
| 3   | D     | 306 | A    |
| 3   | D     | 315 | G    |
| 3   | D     | 316 | U    |
| 3   | D     | 340 | C    |
| 3   | D     | 344 | A    |
| 3   | D     | 345 | C    |
| 3   | D     | 350 | C    |
| 3   | D     | 387 | G    |
| 3   | D     | 407 | A    |
| 3   | D     | 410 | A    |
| 3   | D     | 412 | G    |
| 3   | D     | 413 | G    |
| 3   | D     | 449 | C    |
| 3   | D     | 450 | G    |
| 3   | D     | 452 | A    |
| 3   | D     | 453 | G    |
| 3   | D     | 454 | U    |
| 3   | D     | 467 | U    |
| 3   | D     | 468 | U    |
| 3   | D     | 484 | U    |
| 3   | D     | 485 | C    |
| 3   | D     | 486 | C    |
| 3   | D     | 487 | G    |
| 3   | D     | 491 | G    |
| 3   | D     | 494 | U    |
| 3   | D     | 495 | C    |
| 3   | D     | 496 | G    |
| 3   | D     | 498 | C    |
| 3   | D     | 499 | G    |
| 3   | D     | 500 | G    |
| 3   | D     | 507 | G    |
| 3   | D     | 509 | A    |
| 3   | D     | 510 | U    |
| 3   | D     | 513 | U    |
| 3   | D     | 514 | U    |
| 3   | D     | 515 | C    |
| 3   | D     | 516 | C    |
| 3   | D     | 517 | C    |
| 3   | D     | 645 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 657 | C    |
| 3   | D     | 659 | G    |
| 3   | D     | 661 | C    |
| 3   | D     | 665 | C    |
| 3   | D     | 667 | A    |
| 3   | D     | 668 | C    |
| 3   | D     | 670 | G    |
| 3   | D     | 673 | C    |
| 3   | D     | 686 | A    |
| 3   | D     | 688 | U    |
| 3   | D     | 703 | G    |
| 3   | D     | 704 | C    |
| 3   | D     | 731 | G    |
| 3   | D     | 738 | C    |
| 3   | D     | 739 | G    |
| 3   | D     | 740 | G    |
| 3   | D     | 746 | A    |
| 3   | D     | 754 | U    |
| 3   | D     | 760 | G    |
| 3   | D     | 904 | C    |
| 3   | D     | 905 | C    |
| 3   | D     | 913 | U    |
| 3   | D     | 914 | U    |
| 3   | D     | 915 | A    |
| 3   | D     | 917 | A    |
| 3   | D     | 918 | G    |
| 3   | D     | 923 | C    |
| 3   | D     | 924 | C    |
| 3   | D     | 926 | G    |
| 3   | D     | 932 | A    |
| 3   | D     | 933 | G    |
| 3   | D     | 935 | A    |
| 3   | D     | 936 | C    |
| 3   | D     | 937 | U    |
| 3   | D     | 943 | A    |
| 3   | D     | 944 | A    |
| 3   | D     | 945 | U    |
| 3   | D     | 959 | G    |
| 3   | D     | 960 | A    |
| 3   | D     | 961 | G    |
| 3   | D     | 962 | C    |
| 3   | D     | 965 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 966  | A    |
| 3   | D     | 970  | G    |
| 3   | D     | 971  | U    |
| 3   | D     | 972  | C    |
| 3   | D     | 977  | C    |
| 3   | D     | 982  | U    |
| 3   | D     | 984  | C    |
| 3   | D     | 988  | C    |
| 3   | D     | 989  | U    |
| 3   | D     | 1071 | C    |
| 3   | D     | 1075 | G    |
| 3   | D     | 1082 | C    |
| 3   | D     | 1083 | U    |
| 3   | D     | 1094 | G    |
| 3   | D     | 1168 | G    |
| 3   | D     | 1170 | G    |
| 3   | D     | 1171 | G    |
| 3   | D     | 1173 | G    |
| 3   | D     | 1178 | G    |
| 3   | D     | 1179 | U    |
| 3   | D     | 1180 | C    |
| 3   | D     | 1181 | C    |
| 3   | D     | 1182 | C    |
| 3   | D     | 1183 | C    |
| 3   | D     | 1184 | A    |
| 3   | D     | 1192 | C    |
| 3   | D     | 1193 | C    |
| 3   | D     | 1196 | G    |
| 3   | D     | 1202 | C    |
| 3   | D     | 1203 | G    |
| 3   | D     | 1211 | G    |
| 3   | D     | 1214 | C    |
| 3   | D     | 1215 | C    |
| 3   | D     | 1217 | G    |
| 3   | D     | 1219 | G    |
| 3   | D     | 1241 | C    |
| 3   | D     | 1262 | G    |
| 3   | D     | 1266 | G    |
| 3   | D     | 1269 | G    |
| 3   | D     | 1270 | A    |
| 3   | D     | 1271 | G    |
| 3   | D     | 1272 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1273 | G    |
| 3   | D     | 1275 | G    |
| 3   | D     | 1277 | G    |
| 3   | D     | 1280 | C    |
| 3   | D     | 1284 | G    |
| 3   | D     | 1285 | U    |
| 3   | D     | 1287 | G    |
| 3   | D     | 1294 | A    |
| 3   | D     | 1295 | C    |
| 3   | D     | 1296 | G    |
| 3   | D     | 1301 | C    |
| 3   | D     | 1302 | U    |
| 3   | D     | 1303 | A    |
| 3   | D     | 1304 | C    |
| 3   | D     | 1313 | C    |
| 3   | D     | 1326 | A2M  |
| 3   | D     | 1337 | A    |
| 3   | D     | 1354 | A    |
| 3   | D     | 1358 | G    |
| 3   | D     | 1359 | G    |
| 3   | D     | 1365 | C    |
| 3   | D     | 1366 | G    |
| 3   | D     | 1377 | G    |
| 3   | D     | 1379 | C    |
| 3   | D     | 1387 | A    |
| 3   | D     | 1393 | G    |
| 3   | D     | 1394 | G    |
| 3   | D     | 1397 | A    |
| 3   | D     | 1398 | A    |
| 3   | D     | 1403 | G    |
| 3   | D     | 1404 | G    |
| 3   | D     | 1407 | C    |
| 3   | D     | 1408 | G    |
| 3   | D     | 1409 | C    |
| 3   | D     | 1410 | U    |
| 3   | D     | 1411 | C    |
| 3   | D     | 1412 | G    |
| 3   | D     | 1415 | G    |
| 3   | D     | 1417 | C    |
| 3   | D     | 1420 | A    |
| 3   | D     | 1439 | C    |
| 3   | D     | 1442 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1443 | A    |
| 3   | D     | 1452 | A    |
| 3   | D     | 1481 | C    |
| 3   | D     | 1482 | G    |
| 3   | D     | 1483 | C    |
| 3   | D     | 1497 | A    |
| 3   | D     | 1498 | G    |
| 3   | D     | 1502 | G    |
| 3   | D     | 1514 | U    |
| 3   | D     | 1534 | A2M  |
| 3   | D     | 1535 | C    |
| 3   | D     | 1547 | A    |
| 3   | D     | 1564 | A    |
| 3   | D     | 1566 | C    |
| 3   | D     | 1575 | A    |
| 3   | D     | 1578 | U    |
| 3   | D     | 1591 | U    |
| 3   | D     | 1596 | U    |
| 3   | D     | 1624 | G    |
| 3   | D     | 1625 | OMG  |
| 3   | D     | 1631 | A    |
| 3   | D     | 1633 | G    |
| 3   | D     | 1634 | A    |
| 3   | D     | 1640 | C    |
| 3   | D     | 1641 | G    |
| 3   | D     | 1642 | A    |
| 3   | D     | 1654 | G    |
| 3   | D     | 1661 | C    |
| 3   | D     | 1676 | C    |
| 3   | D     | 1677 | PSU  |
| 3   | D     | 1678 | C    |
| 3   | D     | 1698 | C    |
| 3   | D     | 1699 | A    |
| 3   | D     | 1700 | G    |
| 3   | D     | 1701 | A    |
| 3   | D     | 1702 | C    |
| 3   | D     | 1703 | C    |
| 3   | D     | 1705 | G    |
| 3   | D     | 1715 | C    |
| 3   | D     | 1716 | G    |
| 3   | D     | 1734 | G    |
| 3   | D     | 1735 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1741 | G    |
| 3   | D     | 1742 | A    |
| 3   | D     | 1750 | G    |
| 3   | D     | 1756 | U    |
| 3   | D     | 1757 | U    |
| 3   | D     | 1758 | G    |
| 3   | D     | 1760 | OMG  |
| 3   | D     | 1763 | C    |
| 3   | D     | 1787 | A    |
| 3   | D     | 1797 | G    |
| 3   | D     | 1804 | A    |
| 3   | D     | 1810 | G    |
| 3   | D     | 1821 | G    |
| 3   | D     | 1822 | U    |
| 3   | D     | 1834 | U    |
| 3   | D     | 1836 | G    |
| 3   | D     | 1837 | A    |
| 3   | D     | 1842 | G    |
| 3   | D     | 1843 | A    |
| 3   | D     | 1855 | G    |
| 3   | D     | 1869 | G    |
| 3   | D     | 1882 | U    |
| 3   | D     | 1889 | U    |
| 3   | D     | 1897 | A    |
| 3   | D     | 1918 | U    |
| 3   | D     | 1919 | G    |
| 3   | D     | 1920 | C    |
| 3   | D     | 1921 | C    |
| 3   | D     | 1922 | G    |
| 3   | D     | 1925 | G    |
| 3   | D     | 1931 | C    |
| 3   | D     | 1932 | A    |
| 3   | D     | 1940 | G    |
| 3   | D     | 1948 | G    |
| 3   | D     | 1951 | G    |
| 3   | D     | 1959 | U    |
| 3   | D     | 1960 | A    |
| 3   | D     | 1961 | G    |
| 3   | D     | 1962 | A    |
| 3   | D     | 2024 | G    |
| 3   | D     | 2025 | A    |
| 3   | D     | 2026 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 2046 | G    |
| 3   | D     | 2048 | U    |
| 3   | D     | 2055 | G    |
| 3   | D     | 2056 | G    |
| 3   | D     | 2069 | A    |
| 3   | D     | 2084 | C    |
| 3   | D     | 2085 | G    |
| 3   | D     | 2089 | G    |
| 3   | D     | 2092 | G    |
| 3   | D     | 2093 | A    |
| 3   | D     | 2095 | A    |
| 3   | D     | 2096 | G    |
| 3   | D     | 2097 | U    |
| 3   | D     | 2098 | G    |
| 3   | D     | 2099 | G    |
| 3   | D     | 2102 | G    |
| 3   | D     | 2103 | G    |
| 3   | D     | 2104 | G    |
| 3   | D     | 2105 | A    |
| 3   | D     | 2107 | C    |
| 3   | D     | 2257 | C    |
| 3   | D     | 2258 | C    |
| 3   | D     | 2259 | G    |
| 3   | D     | 2289 | C    |
| 3   | D     | 2300 | A    |
| 3   | D     | 2301 | G    |
| 3   | D     | 2313 | A    |
| 3   | D     | 2316 | G    |
| 3   | D     | 2333 | G    |
| 3   | D     | 2348 | G    |
| 3   | D     | 2351 | OMC  |
| 3   | D     | 2395 | A    |
| 3   | D     | 2397 | G    |
| 3   | D     | 2415 | OMU  |
| 3   | D     | 2416 | G    |
| 3   | D     | 2421 | G    |
| 3   | D     | 2422 | OMC  |
| 3   | D     | 2424 | OMG  |
| 3   | D     | 2425 | U    |
| 3   | D     | 2450 | G    |
| 3   | D     | 2453 | A    |
| 3   | D     | 2465 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 2474 | G    |
| 3   | D     | 2475 | G    |
| 3   | D     | 2479 | G    |
| 3   | D     | 2483 | G    |
| 3   | D     | 2484 | A    |
| 3   | D     | 2485 | U    |
| 3   | D     | 2487 | G    |
| 3   | D     | 2488 | C    |
| 3   | D     | 2489 | C    |
| 3   | D     | 2491 | C    |
| 3   | D     | 2493 | G    |
| 3   | D     | 2494 | U    |
| 3   | D     | 2503 | G    |
| 3   | D     | 2504 | C    |
| 3   | D     | 2505 | C    |
| 3   | D     | 2506 | G    |
| 3   | D     | 2511 | A    |
| 3   | D     | 2513 | A    |
| 3   | D     | 2519 | U    |
| 3   | D     | 2520 | C    |
| 3   | D     | 2529 | A    |
| 3   | D     | 2537 | A    |
| 3   | D     | 2545 | U    |
| 3   | D     | 2546 | G    |
| 3   | D     | 2547 | G    |
| 3   | D     | 2554 | U    |
| 3   | D     | 2567 | G    |
| 3   | D     | 2583 | C    |
| 3   | D     | 2587 | A    |
| 3   | D     | 2601 | A    |
| 3   | D     | 2618 | G    |
| 3   | D     | 2627 | C    |
| 3   | D     | 2653 | C    |
| 3   | D     | 2662 | G    |
| 3   | D     | 2669 | C    |
| 3   | D     | 2676 | A    |
| 3   | D     | 2687 | U    |
| 3   | D     | 2694 | G    |
| 3   | D     | 2695 | A    |
| 3   | D     | 2696 | A    |
| 3   | D     | 2706 | G    |
| 3   | D     | 2707 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 2708 | U    |
| 3   | D     | 2711 | G    |
| 3   | D     | 2712 | G    |
| 3   | D     | 2721 | G    |
| 3   | D     | 2724 | G    |
| 3   | D     | 2726 | G    |
| 3   | D     | 2739 | C    |
| 3   | D     | 2742 | G    |
| 3   | D     | 2743 | A    |
| 3   | D     | 2746 | A    |
| 3   | D     | 2754 | G    |
| 3   | D     | 2760 | G    |
| 3   | D     | 2761 | U    |
| 3   | D     | 2763 | U    |
| 3   | D     | 2764 | A    |
| 3   | D     | 2770 | C    |
| 3   | D     | 2788 | U    |
| 3   | D     | 2790 | U    |
| 3   | D     | 2814 | C    |
| 3   | D     | 2815 | A2M  |
| 3   | D     | 2826 | U    |
| 3   | D     | 2827 | G    |
| 3   | D     | 2838 | G    |
| 3   | D     | 2855 | G    |
| 3   | D     | 2856 | C    |
| 3   | D     | 2867 | C    |
| 3   | D     | 2874 | U    |
| 3   | D     | 2877 | G    |
| 3   | D     | 2892 | C    |
| 3   | D     | 2900 | U    |
| 3   | D     | 3604 | A    |
| 3   | D     | 3605 | C    |
| 3   | D     | 3615 | G    |
| 3   | D     | 3618 | C    |
| 3   | D     | 3626 | G    |
| 3   | D     | 3635 | A    |
| 3   | D     | 3644 | U    |
| 3   | D     | 3648 | A    |
| 3   | D     | 3662 | A    |
| 3   | D     | 3664 | G    |
| 3   | D     | 3673 | C    |
| 3   | D     | 3674 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 3711 | A    |
| 3   | D     | 3712 | A    |
| 3   | D     | 3735 | G    |
| 3   | D     | 3736 | A    |
| 3   | D     | 3748 | A    |
| 3   | D     | 3750 | G    |
| 3   | D     | 3753 | G    |
| 3   | D     | 3757 | G    |
| 3   | D     | 3758 | PSU  |
| 3   | D     | 3760 | A2M  |
| 3   | D     | 3763 | A    |
| 3   | D     | 3771 | C    |
| 3   | D     | 3776 | G    |
| 3   | D     | 3777 | G    |
| 3   | D     | 3783 | A    |
| 3   | D     | 3784 | A    |
| 3   | D     | 3786 | U    |
| 3   | D     | 3802 | U    |
| 3   | D     | 3811 | G    |
| 3   | D     | 3812 | C    |
| 3   | D     | 3814 | U    |
| 3   | D     | 3817 | A    |
| 3   | D     | 3818 | UY1  |
| 3   | D     | 3819 | G    |
| 3   | D     | 3823 | G    |
| 3   | D     | 3838 | U    |
| 3   | D     | 3840 | U    |
| 3   | D     | 3867 | A    |
| 3   | D     | 3877 | A    |
| 3   | D     | 3878 | C    |
| 3   | D     | 3879 | G    |
| 3   | D     | 3885 | G    |
| 3   | D     | 3897 | G    |
| 3   | D     | 3901 | A    |
| 3   | D     | 3906 | A    |
| 3   | D     | 3907 | G    |
| 3   | D     | 3908 | A    |
| 3   | D     | 3915 | U    |
| 3   | D     | 3938 | G    |
| 3   | D     | 3939 | G    |
| 3   | D     | 3943 | A    |
| 3   | D     | 3944 | OMG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 3946 | G    |
| 3   | D     | 4076 | G    |
| 3   | D     | 4086 | G    |
| 3   | D     | 4093 | G    |
| 3   | D     | 4094 | G    |
| 3   | D     | 4097 | G    |
| 3   | D     | 4098 | A    |
| 3   | D     | 4113 | U    |
| 3   | D     | 4114 | C    |
| 3   | D     | 4115 | G    |
| 3   | D     | 4116 | C    |
| 3   | D     | 4119 | C    |
| 3   | D     | 4122 | G    |
| 3   | D     | 4127 | A    |
| 3   | D     | 4140 | C    |
| 3   | D     | 4142 | C    |
| 3   | D     | 4143 | G    |
| 3   | D     | 4144 | C    |
| 3   | D     | 4145 | C    |
| 3   | D     | 4150 | G    |
| 3   | D     | 4162 | C    |
| 3   | D     | 4163 | U    |
| 3   | D     | 4170 | A    |
| 3   | D     | 4183 | G    |
| 3   | D     | 4184 | G    |
| 3   | D     | 4191 | G    |
| 3   | D     | 4203 | A    |
| 3   | D     | 4229 | U    |
| 3   | D     | 4233 | A    |
| 3   | D     | 4251 | A    |
| 3   | D     | 4254 | G    |
| 3   | D     | 4257 | A    |
| 3   | D     | 4268 | A    |
| 3   | D     | 4273 | A    |
| 3   | D     | 4281 | A    |
| 3   | D     | 4291 | G    |
| 3   | D     | 4297 | G    |
| 3   | D     | 4304 | A    |
| 3   | D     | 4305 | G    |
| 3   | D     | 4314 | C    |
| 3   | D     | 4330 | G    |
| 3   | D     | 4332 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 4339 | A    |
| 3   | D     | 4349 | C    |
| 3   | D     | 4364 | G    |
| 3   | D     | 4373 | G    |
| 3   | D     | 4376 | A    |
| 3   | D     | 4377 | G    |
| 3   | D     | 4378 | A    |
| 3   | D     | 4380 | A    |
| 3   | D     | 4387 | C    |
| 3   | D     | 4391 | G    |
| 3   | D     | 4394 | A    |
| 3   | D     | 4405 | G    |
| 3   | D     | 4421 | C    |
| 3   | D     | 4422 | A    |
| 3   | D     | 4444 | C    |
| 3   | D     | 4448 | G    |
| 3   | D     | 4449 | A    |
| 3   | D     | 4452 | U    |
| 3   | D     | 4453 | C    |
| 3   | D     | 4464 | A    |
| 3   | D     | 4466 | C    |
| 3   | D     | 4475 | G    |
| 3   | D     | 4500 | PSU  |
| 3   | D     | 4512 | U    |
| 3   | D     | 4513 | A    |
| 3   | D     | 4519 | C    |
| 3   | D     | 4524 | G    |
| 3   | D     | 4545 | G    |
| 3   | D     | 4548 | A    |
| 3   | D     | 4554 | G    |
| 3   | D     | 4560 | C    |
| 3   | D     | 4567 | G    |
| 3   | D     | 4570 | G    |
| 3   | D     | 4573 | G    |
| 3   | D     | 4575 | G    |
| 3   | D     | 4590 | A    |
| 3   | D     | 4600 | G    |
| 3   | D     | 4601 | U    |
| 3   | D     | 4617 | G    |
| 3   | D     | 4636 | U    |
| 3   | D     | 4637 | OMG  |
| 3   | D     | 4656 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 4670 | C    |
| 3   | D     | 4672 | A    |
| 3   | D     | 4679 | G    |
| 3   | D     | 4695 | C    |
| 3   | D     | 4700 | A    |
| 3   | D     | 4708 | A    |
| 3   | D     | 4709 | U    |
| 3   | D     | 4719 | G    |
| 3   | D     | 4720 | C    |
| 3   | D     | 4730 | C    |
| 3   | D     | 4731 | G    |
| 3   | D     | 4732 | G    |
| 3   | D     | 4733 | C    |
| 3   | D     | 4734 | A    |
| 3   | D     | 4741 | C    |
| 3   | D     | 4742 | G    |
| 3   | D     | 4745 | G    |
| 3   | D     | 4754 | G    |
| 3   | D     | 4757 | C    |
| 3   | D     | 4759 | C    |
| 3   | D     | 4761 | G    |
| 3   | D     | 4765 | G    |
| 3   | D     | 4774 | C    |
| 3   | D     | 4860 | G    |
| 3   | D     | 4862 | G    |
| 3   | D     | 4870 | G    |
| 3   | D     | 4871 | C    |
| 3   | D     | 4875 | G    |
| 3   | D     | 4882 | U    |
| 3   | D     | 4883 | C    |
| 3   | D     | 4888 | U    |
| 3   | D     | 4889 | G    |
| 3   | D     | 4895 | C    |
| 3   | D     | 4896 | G    |
| 3   | D     | 4899 | G    |
| 3   | D     | 4900 | C    |
| 3   | D     | 4901 | G    |
| 3   | D     | 4902 | C    |
| 3   | D     | 4910 | G    |
| 3   | D     | 4912 | G    |
| 3   | D     | 4914 | C    |
| 3   | D     | 4927 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 4928 | C    |
| 3   | D     | 4934 | A    |
| 3   | D     | 4940 | C    |
| 3   | D     | 4941 | G    |
| 3   | D     | 4943 | A    |
| 3   | D     | 4955 | A    |
| 3   | D     | 4960 | G    |
| 3   | D     | 4963 | G    |
| 3   | D     | 4966 | A    |
| 3   | D     | 4976 | U    |
| 3   | D     | 4985 | U    |
| 3   | D     | 4989 | U    |
| 3   | D     | 4990 | C    |
| 3   | D     | 4991 | U    |
| 3   | D     | 5014 | A    |
| 3   | D     | 5016 | A    |
| 3   | D     | 5017 | G    |
| 3   | D     | 5024 | C    |
| 3   | D     | 5025 | C    |
| 3   | D     | 5026 | U    |
| 3   | D     | 5028 | G    |
| 3   | D     | 5030 | U    |
| 3   | D     | 5034 | A    |
| 3   | D     | 5041 | G    |
| 3   | D     | 5050 | C    |
| 3   | D     | 5054 | C    |
| 3   | D     | 5060 | A    |
| 3   | D     | 5061 | A    |
| 3   | D     | 5062 | G    |
| 3   | D     | 5069 | U    |
| 4   | E     | 7    | G    |
| 4   | E     | 22   | A    |
| 4   | E     | 31   | G    |
| 4   | E     | 47   | G    |
| 4   | E     | 48   | G    |
| 4   | E     | 53   | U    |
| 4   | E     | 54   | A    |
| 4   | E     | 64   | G    |
| 4   | E     | 97   | G    |
| 4   | E     | 100  | A    |
| 4   | E     | 102  | U    |
| 4   | E     | 103  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 110 | G    |
| 4   | E     | 117 | G    |
| 4   | E     | 120 | U    |
| 5   | F     | 2   | G    |
| 5   | F     | 17  | A    |
| 5   | F     | 23  | C    |
| 5   | F     | 34  | U    |
| 5   | F     | 35  | C    |
| 5   | F     | 48  | A    |
| 5   | F     | 59  | A    |
| 5   | F     | 63  | U    |
| 5   | F     | 80  | A    |
| 5   | F     | 81  | C    |
| 5   | F     | 82  | A    |
| 5   | F     | 83  | C    |
| 5   | F     | 84  | A    |
| 5   | F     | 85  | U    |
| 5   | F     | 86  | U    |
| 5   | F     | 87  | G    |
| 5   | F     | 103 | A    |
| 5   | F     | 105 | C    |
| 5   | F     | 110 | U    |
| 5   | F     | 114 | G    |
| 5   | F     | 124 | U    |
| 5   | F     | 125 | C    |
| 5   | F     | 126 | C    |
| 5   | F     | 127 | U    |
| 5   | F     | 128 | C    |
| 5   | F     | 150 | C    |
| 5   | F     | 151 | G    |
| 5   | F     | 153 | C    |
| 48  | w     | 2   | A    |
| 48  | w     | 17  | C    |
| 48  | w     | 21  | U    |
| 48  | w     | 22  | A    |
| 48  | w     | 33  | G    |
| 48  | w     | 34  | PSU  |
| 48  | w     | 35  | C    |
| 48  | w     | 41  | G    |
| 48  | w     | 43  | U    |
| 48  | w     | 44  | U    |
| 48  | w     | 45  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | w     | 46  | A    |
| 48  | w     | 49  | C    |
| 48  | w     | 59  | U    |
| 48  | w     | 60  | A    |
| 48  | w     | 61  | A    |
| 48  | w     | 62  | G    |
| 48  | w     | 66  | G    |
| 48  | w     | 67  | C    |
| 48  | w     | 68  | A    |
| 48  | w     | 69  | C    |
| 48  | w     | 78  | C    |
| 48  | w     | 79  | A    |
| 48  | w     | 80  | G    |
| 48  | w     | 81  | U    |
| 48  | w     | 83  | A    |
| 48  | w     | 89  | C    |
| 48  | w     | 97  | U    |
| 48  | w     | 103 | A    |
| 48  | w     | 112 | U    |
| 48  | w     | 113 | G    |
| 48  | w     | 115 | U    |
| 48  | w     | 116 | OMU  |
| 48  | w     | 120 | U    |
| 48  | w     | 121 | OMU  |
| 48  | w     | 126 | G    |
| 48  | w     | 129 | C    |
| 48  | w     | 130 | G    |
| 48  | w     | 143 | U    |
| 48  | w     | 149 | A    |
| 48  | w     | 150 | A    |
| 48  | w     | 154 | U    |
| 48  | w     | 155 | G    |
| 48  | w     | 159 | A2M  |
| 48  | w     | 161 | U    |
| 48  | w     | 162 | C    |
| 48  | w     | 163 | U    |
| 48  | w     | 166 | A2M  |
| 48  | w     | 173 | A    |
| 48  | w     | 182 | C    |
| 48  | w     | 190 | G    |
| 48  | w     | 191 | A    |
| 48  | w     | 194 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | w     | 195 | C    |
| 48  | w     | 196 | C    |
| 48  | w     | 197 | U    |
| 48  | w     | 198 | U    |
| 48  | w     | 199 | C    |
| 48  | w     | 200 | G    |
| 48  | w     | 214 | U    |
| 48  | w     | 215 | G    |
| 48  | w     | 226 | A    |
| 48  | w     | 291 | G    |
| 48  | w     | 292 | A    |
| 48  | w     | 293 | C    |
| 48  | w     | 294 | U    |
| 48  | w     | 295 | C    |
| 48  | w     | 311 | C    |
| 48  | w     | 312 | G    |
| 48  | w     | 313 | A    |
| 48  | w     | 318 | A    |
| 48  | w     | 319 | C    |
| 48  | w     | 332 | G    |
| 48  | w     | 345 | U    |
| 48  | w     | 346 | C    |
| 48  | w     | 347 | G    |
| 48  | w     | 362 | C    |
| 48  | w     | 364 | A    |
| 48  | w     | 370 | G    |
| 48  | w     | 380 | G    |
| 48  | w     | 381 | C    |
| 48  | w     | 385 | G    |
| 48  | w     | 386 | C    |
| 48  | w     | 398 | A    |
| 48  | w     | 400 | C    |
| 48  | w     | 407 | G    |
| 48  | w     | 408 | A    |
| 48  | w     | 409 | C    |
| 48  | w     | 413 | G    |
| 48  | w     | 418 | A    |
| 48  | w     | 421 | G    |
| 48  | w     | 428 | OMU  |
| 48  | w     | 438 | G    |
| 48  | w     | 441 | C    |
| 48  | w     | 447 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | w     | 448 | A    |
| 48  | w     | 449 | A    |
| 48  | w     | 450 | C    |
| 48  | w     | 451 | G    |
| 48  | w     | 452 | G    |
| 48  | w     | 464 | A    |
| 48  | w     | 466 | G    |
| 48  | w     | 467 | G    |
| 48  | w     | 468 | A2M  |
| 48  | w     | 471 | G    |
| 48  | w     | 472 | C    |
| 48  | w     | 473 | A    |
| 48  | w     | 474 | G    |
| 48  | w     | 482 | G    |
| 48  | w     | 485 | A    |
| 48  | w     | 487 | U    |
| 48  | w     | 488 | U    |
| 48  | w     | 489 | A    |
| 48  | w     | 491 | C    |
| 48  | w     | 493 | A    |
| 48  | w     | 496 | C    |
| 48  | w     | 497 | C    |
| 48  | w     | 498 | C    |
| 48  | w     | 500 | A    |
| 48  | w     | 506 | G    |
| 48  | w     | 507 | G    |
| 48  | w     | 512 | A2M  |
| 48  | w     | 516 | A    |
| 48  | w     | 519 | A    |
| 48  | w     | 523 | A    |
| 48  | w     | 528 | A    |
| 48  | w     | 531 | A    |
| 48  | w     | 532 | C    |
| 48  | w     | 533 | A    |
| 48  | w     | 534 | G    |
| 48  | w     | 551 | U    |
| 48  | w     | 552 | G    |
| 48  | w     | 554 | A    |
| 48  | w     | 556 | U    |
| 48  | w     | 557 | U    |
| 48  | w     | 558 | G    |
| 48  | w     | 560 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | w     | 575 | A    |
| 48  | w     | 576 | A2M  |
| 48  | w     | 583 | C    |
| 48  | w     | 587 | A    |
| 48  | w     | 588 | G    |
| 48  | w     | 589 | G    |
| 48  | w     | 590 | A2M  |
| 48  | w     | 592 | C    |
| 48  | w     | 594 | A    |
| 48  | w     | 595 | U    |
| 48  | w     | 596 | U    |
| 48  | w     | 597 | G    |
| 48  | w     | 598 | G    |
| 48  | w     | 604 | A    |
| 48  | w     | 605 | A    |
| 48  | w     | 606 | G    |
| 48  | w     | 608 | C    |
| 48  | w     | 614 | C    |
| 48  | w     | 616 | A    |
| 48  | w     | 617 | G    |
| 48  | w     | 627 | OMU  |
| 48  | w     | 628 | A    |
| 48  | w     | 632 | C    |
| 48  | w     | 643 | A    |
| 48  | w     | 655 | A    |
| 48  | w     | 659 | G    |
| 48  | w     | 660 | C    |
| 48  | w     | 664 | A    |
| 48  | w     | 668 | A2M  |
| 48  | w     | 669 | A    |
| 48  | w     | 671 | A    |
| 48  | w     | 672 | A    |
| 48  | w     | 688 | U    |
| 48  | w     | 810 | A    |
| 48  | w     | 811 | A    |
| 48  | w     | 812 | A    |
| 48  | w     | 821 | G    |
| 48  | w     | 822 | PSU  |
| 48  | w     | 830 | A    |
| 48  | w     | 834 | C    |
| 48  | w     | 835 | C    |
| 48  | w     | 836 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | w     | 837 | A    |
| 48  | w     | 838 | G    |
| 48  | w     | 839 | C    |
| 48  | w     | 840 | C    |
| 48  | w     | 841 | G    |
| 48  | w     | 842 | C    |
| 48  | w     | 847 | A    |
| 48  | w     | 853 | C    |
| 48  | w     | 869 | A    |
| 48  | w     | 870 | A    |
| 48  | w     | 872 | A    |
| 48  | w     | 874 | G    |
| 48  | w     | 878 | G    |
| 48  | w     | 880 | G    |
| 48  | w     | 881 | G    |
| 48  | w     | 882 | U    |
| 48  | w     | 883 | U    |
| 48  | w     | 884 | C    |
| 48  | w     | 888 | U    |
| 48  | w     | 889 | U    |
| 48  | w     | 890 | U    |
| 48  | w     | 891 | G    |
| 48  | w     | 893 | U    |
| 48  | w     | 895 | G    |
| 48  | w     | 896 | U    |
| 48  | w     | 897 | U    |
| 48  | w     | 898 | U    |
| 48  | w     | 899 | U    |
| 48  | w     | 900 | C    |
| 48  | w     | 901 | G    |
| 48  | w     | 904 | A    |
| 48  | w     | 909 | G    |
| 48  | w     | 912 | C    |
| 48  | w     | 913 | A    |
| 48  | w     | 917 | U    |
| 48  | w     | 920 | A    |
| 48  | w     | 930 | C    |
| 48  | w     | 933 | G    |
| 48  | w     | 934 | G    |
| 48  | w     | 943 | U    |
| 48  | w     | 958 | G    |
| 48  | w     | 963 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | w     | 970  | G    |
| 48  | w     | 990  | A    |
| 48  | w     | 992  | A    |
| 48  | w     | 999  | G    |
| 48  | w     | 1001 | A    |
| 48  | w     | 1017 | U    |
| 48  | w     | 1023 | A    |
| 48  | w     | 1027 | A    |
| 48  | w     | 1032 | C    |
| 48  | w     | 1060 | A    |
| 48  | w     | 1061 | U    |
| 48  | w     | 1062 | A    |
| 48  | w     | 1083 | A    |
| 48  | w     | 1085 | C    |
| 48  | w     | 1109 | C    |
| 48  | w     | 1114 | U    |
| 48  | w     | 1115 | U    |
| 48  | w     | 1116 | C    |
| 48  | w     | 1118 | C    |
| 48  | w     | 1119 | A    |
| 48  | w     | 1126 | G    |
| 48  | w     | 1133 | A    |
| 48  | w     | 1153 | C    |
| 48  | w     | 1154 | U    |
| 48  | w     | 1157 | G    |
| 48  | w     | 1183 | A    |
| 48  | w     | 1195 | A    |
| 48  | w     | 1207 | G    |
| 48  | w     | 1208 | A    |
| 48  | w     | 1215 | C    |
| 48  | w     | 1217 | A    |
| 48  | w     | 1221 | G    |
| 48  | w     | 1224 | G    |
| 48  | w     | 1242 | U    |
| 48  | w     | 1243 | U    |
| 48  | w     | 1251 | A    |
| 48  | w     | 1253 | A    |
| 48  | w     | 1256 | G    |
| 48  | w     | 1257 | G    |
| 48  | w     | 1259 | A    |
| 48  | w     | 1265 | A    |
| 48  | w     | 1271 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | w     | 1274 | G    |
| 48  | w     | 1275 | G    |
| 48  | w     | 1284 | A    |
| 48  | w     | 1285 | G    |
| 48  | w     | 1288 | OMU  |
| 48  | w     | 1293 | A    |
| 48  | w     | 1295 | A    |
| 48  | w     | 1298 | G    |
| 48  | w     | 1301 | A    |
| 48  | w     | 1302 | G    |
| 48  | w     | 1308 | U    |
| 48  | w     | 1309 | C    |
| 48  | w     | 1332 | A    |
| 48  | w     | 1342 | U    |
| 48  | w     | 1371 | U    |
| 48  | w     | 1372 | U    |
| 48  | w     | 1373 | C    |
| 48  | w     | 1378 | A    |
| 48  | w     | 1396 | A    |
| 48  | w     | 1397 | U    |
| 48  | w     | 1401 | A    |
| 48  | w     | 1402 | A    |
| 48  | w     | 1403 | C    |
| 48  | w     | 1404 | U    |
| 48  | w     | 1408 | U    |
| 48  | w     | 1417 | C    |
| 48  | w     | 1428 | G    |
| 48  | w     | 1429 | G    |
| 48  | w     | 1430 | C    |
| 48  | w     | 1433 | C    |
| 48  | w     | 1434 | C    |
| 48  | w     | 1435 | C    |
| 48  | w     | 1436 | C    |
| 48  | w     | 1438 | A    |
| 48  | w     | 1447 | G    |
| 48  | w     | 1449 | G    |
| 48  | w     | 1450 | G    |
| 48  | w     | 1452 | A    |
| 48  | w     | 1454 | A    |
| 48  | w     | 1462 | U    |
| 48  | w     | 1463 | U    |
| 48  | w     | 1464 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | w     | 1476 | A    |
| 48  | w     | 1477 | U    |
| 48  | w     | 1487 | A    |
| 48  | w     | 1489 | A    |
| 48  | w     | 1490 | OMG  |
| 48  | w     | 1495 | G    |
| 48  | w     | 1497 | G    |
| 48  | w     | 1498 | A    |
| 48  | w     | 1508 | A    |
| 48  | w     | 1515 | G    |
| 48  | w     | 1521 | C    |
| 48  | w     | 1522 | A    |
| 48  | w     | 1523 | C    |
| 48  | w     | 1528 | G    |
| 48  | w     | 1533 | A    |
| 48  | w     | 1536 | G    |
| 48  | w     | 1543 | U    |
| 48  | w     | 1545 | A    |
| 48  | w     | 1546 | G    |
| 48  | w     | 1548 | G    |
| 48  | w     | 1550 | G    |
| 48  | w     | 1551 | U    |
| 48  | w     | 1552 | G    |
| 48  | w     | 1553 | C    |
| 48  | w     | 1555 | U    |
| 48  | w     | 1556 | A    |
| 48  | w     | 1569 | A    |
| 48  | w     | 1570 | G    |
| 48  | w     | 1574 | C    |
| 48  | w     | 1580 | A    |
| 48  | w     | 1585 | U    |
| 48  | w     | 1586 | U    |
| 48  | w     | 1588 | A    |
| 48  | w     | 1599 | U    |
| 48  | w     | 1601 | A    |
| 48  | w     | 1602 | U    |
| 48  | w     | 1607 | A    |
| 48  | w     | 1610 | G    |
| 48  | w     | 1621 | U    |
| 48  | w     | 1623 | A    |
| 48  | w     | 1624 | U    |
| 48  | w     | 1630 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | w     | 1632 | G    |
| 48  | w     | 1633 | A    |
| 48  | w     | 1635 | C    |
| 48  | w     | 1637 | A    |
| 48  | w     | 1639 | G7M  |
| 48  | w     | 1640 | A    |
| 48  | w     | 1648 | G    |
| 48  | w     | 1654 | G    |
| 48  | w     | 1663 | A    |
| 48  | w     | 1665 | G    |
| 48  | w     | 1671 | G    |
| 48  | w     | 1680 | G    |
| 48  | w     | 1698 | C    |
| 48  | w     | 1721 | U    |
| 48  | w     | 1722 | G    |
| 48  | w     | 1742 | C    |
| 48  | w     | 1744 | G    |
| 48  | w     | 1745 | A    |
| 48  | w     | 1748 | G    |
| 48  | w     | 1751 | C    |
| 48  | w     | 1753 | C    |
| 48  | w     | 1754 | G    |
| 48  | w     | 1778 | C    |
| 48  | w     | 1779 | G    |
| 48  | w     | 1782 | G    |
| 48  | w     | 1783 | C    |
| 48  | w     | 1784 | G    |
| 48  | w     | 1786 | U    |
| 48  | w     | 1801 | A    |
| 48  | w     | 1813 | A    |
| 48  | w     | 1824 | A    |
| 48  | w     | 1829 | G    |
| 48  | w     | 1831 | A    |
| 48  | w     | 1838 | U    |
| 48  | w     | 1849 | G    |
| 48  | w     | 1850 | MA6  |
| 48  | w     | 1851 | MA6  |
| 48  | w     | 1852 | C    |
| 48  | w     | 1861 | G    |
| 48  | w     | 1862 | G    |
| 48  | w     | 1863 | A    |
| 48  | w     | 1865 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | w     | 1869 | A    |

All (31) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 5    | C    |
| 2   | C     | 72   | G    |
| 3   | D     | 1    | C    |
| 3   | D     | 406  | C    |
| 3   | D     | 515  | C    |
| 3   | D     | 914  | U    |
| 3   | D     | 922  | C    |
| 3   | D     | 987  | C    |
| 3   | D     | 1081 | C    |
| 3   | D     | 1574 | G    |
| 3   | D     | 1625 | OMG  |
| 3   | D     | 1633 | G    |
| 3   | D     | 1755 | C    |
| 3   | D     | 2101 | C    |
| 3   | D     | 2102 | G    |
| 3   | D     | 2675 | G    |
| 3   | D     | 3614 | G    |
| 3   | D     | 3673 | C    |
| 3   | D     | 4092 | G    |
| 3   | D     | 4113 | U    |
| 3   | D     | 4115 | G    |
| 3   | D     | 4348 | A    |
| 3   | D     | 4378 | A    |
| 3   | D     | 4600 | G    |
| 3   | D     | 4678 | G    |
| 3   | D     | 4699 | U    |
| 3   | D     | 4913 | G    |
| 3   | D     | 5016 | A    |
| 5   | F     | 16   | G    |
| 5   | F     | 86   | U    |
| 5   | F     | 126  | C    |

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

216 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$ |
| 3   | A2M  | D     | 3760 | 3     | 22,25,26     | 1.40 | 1 (4%)      | 31,36,39    | 1.15 | 3 (9%)      |
| 3   | PSU  | D     | 3758 | 3     | 18,21,22     | 0.97 | 1 (5%)      | 22,30,33    | 1.81 | 4 (18%)     |
| 3   | OMG  | D     | 3899 | 3     | 23,26,27     | 2.55 | 10 (43%)    | 33,38,41    | 1.95 | 10 (30%)    |
| 3   | OMG  | D     | 4499 | 3,2   | 23,26,27     | 2.57 | 9 (39%)     | 33,38,41    | 1.94 | 9 (27%)     |
| 3   | PSU  | D     | 1860 | 3     | 18,21,22     | 1.05 | 1 (5%)      | 22,30,33    | 1.86 | 4 (18%)     |
| 48  | A2M  | w     | 166  | 48    | 22,25,26     | 1.53 | 3 (13%)     | 31,36,39    | 1.04 | 3 (9%)      |
| 3   | PSU  | D     | 1792 | 3     | 18,21,22     | 0.99 | 1 (5%)      | 22,30,33    | 1.75 | 3 (13%)     |
| 2   | 1MA  | C     | 9    | 2     | 21,25,26     | 0.88 | 1 (4%)      | 31,37,40    | 0.75 | 1 (3%)      |
| 48  | OMC  | w     | 1703 | 80,48 | 19,22,23     | 2.89 | 8 (42%)     | 26,31,34    | 0.73 | 0           |
| 3   | 6MZ  | D     | 4220 | 3     | 22,25,26     | 2.82 | 4 (18%)     | 30,36,39    | 2.23 | 10 (33%)    |
| 3   | PSU  | D     | 1677 | 3     | 18,21,22     | 1.06 | 2 (11%)     | 22,30,33    | 1.75 | 4 (18%)     |
| 48  | PSU  | w     | 649  | 48    | 18,21,22     | 1.04 | 1 (5%)      | 22,30,33    | 1.85 | 5 (22%)     |
| 3   | OMU  | D     | 3925 | 3     | 19,22,23     | 2.78 | 6 (31%)     | 26,31,34    | 1.84 | 5 (19%)     |
| 48  | PSU  | w     | 651  | 48    | 18,21,22     | 1.03 | 1 (5%)      | 22,30,33    | 1.87 | 5 (22%)     |
| 3   | OMG  | D     | 4228 | 3     | 23,26,27     | 2.55 | 9 (39%)     | 33,38,41    | 2.00 | 10 (30%)    |
| 2   | PSU  | B     | 54   | 2     | 18,21,22     | 1.04 | 1 (5%)      | 22,30,33    | 1.76 | 4 (18%)     |
| 3   | PSU  | D     | 1683 | 3     | 18,21,22     | 1.07 | 2 (11%)     | 22,30,33    | 1.95 | 5 (22%)     |
| 3   | PSU  | D     | 4500 | 3,2   | 18,21,22     | 1.10 | 1 (5%)      | 22,30,33    | 1.84 | 4 (18%)     |
| 3   | A2M  | D     | 2815 | 3     | 22,25,26     | 1.43 | 1 (4%)      | 31,36,39    | 1.00 | 3 (9%)      |
| 3   | OMG  | D     | 4623 | 3     | 23,26,27     | 2.55 | 9 (39%)     | 33,38,41    | 1.94 | 10 (30%)    |
| 2   | PSU  | C     | 13   | 2     | 18,21,22     | 1.05 | 1 (5%)      | 22,30,33    | 1.78 | 4 (18%)     |
| 48  | PSU  | w     | 1238 | 48    | 18,21,22     | 1.05 | 1 (5%)      | 22,30,33    | 1.82 | 5 (22%)     |
| 48  | A2M  | w     | 1678 | 48    | 22,25,26     | 1.44 | 1 (4%)      | 31,36,39    | 0.99 | 2 (6%)      |
| 48  | 4AC  | w     | 1337 | 48    | 21,24,25     | 0.56 | 0           | 29,34,37    | 1.19 | 5 (17%)     |
| 48  | PSU  | w     | 34   | 48    | 18,21,22     | 1.05 | 1 (5%)      | 22,30,33    | 1.70 | 4 (18%)     |
| 48  | PSU  | w     | 681  | 80,48 | 18,21,22     | 1.04 | 1 (5%)      | 22,30,33    | 1.90 | 5 (22%)     |
| 48  | OMG  | w     | 1490 | 80,48 | 23,26,27     | 2.58 | 8 (34%)     | 33,38,41    | 1.92 | 9 (27%)     |
| 48  | PSU  | w     | 815  | 48    | 18,21,22     | 1.08 | 1 (5%)      | 22,30,33    | 1.86 | 5 (22%)     |
| 3   | OMU  | D     | 1773 | 3     | 19,22,23     | 2.92 | 8 (42%)     | 26,31,34    | 1.68 | 4 (15%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | D     | 3734 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 3   | PSU  | D     | 4361 | 3     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 2   | H2U  | B     | 19   | 2     | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 0.82 | 0        |
| 2   | 5MC  | B     | 48   | 2     | 18,22,23     | 3.79 | 8 (44%)  | 26,32,35    | 1.03 | 2 (7%)   |
| 48  | A2M  | w     | 1383 | 48    | 22,25,26     | 1.44 | 1 (4%)   | 31,36,39    | 1.15 | 4 (12%)  |
| 48  | A2M  | w     | 99   | 80,48 | 22,25,26     | 1.40 | 1 (4%)   | 31,36,39    | 1.05 | 3 (9%)   |
| 3   | OMU  | D     | 2837 | 3     | 19,22,23     | 2.75 | 6 (31%)  | 26,31,34    | 1.85 | 5 (19%)  |
| 3   | PSU  | D     | 4420 | 3     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.80 | 5 (22%)  |
| 3   | OMG  | D     | 3744 | 3     | 23,26,27     | 2.58 | 9 (39%)  | 33,38,41    | 1.94 | 10 (30%) |
| 48  | OMC  | w     | 462  | 48    | 19,22,23     | 3.01 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 2   | 1MA  | B     | 57   | 2     | 21,25,26     | 0.88 | 1 (4%)   | 31,37,40    | 0.75 | 1 (3%)   |
| 3   | PSU  | D     | 3639 | 3     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.76 | 4 (18%)  |
| 3   | PSU  | D     | 3920 | 3,80  | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.85 | 4 (18%)  |
| 3   | PSU  | D     | 4576 | 3     | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.84 | 4 (18%)  |
| 3   | OMU  | D     | 4227 | 3     | 19,22,23     | 2.81 | 6 (31%)  | 26,31,34    | 1.75 | 4 (15%)  |
| 48  | PSU  | w     | 866  | 48    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 48  | OMU  | w     | 1326 | 48    | 19,22,23     | 2.88 | 7 (36%)  | 26,31,34    | 1.78 | 6 (23%)  |
| 3   | 5MC  | D     | 3782 | 3,80  | 18,22,23     | 3.61 | 7 (38%)  | 26,32,35    | 1.08 | 2 (7%)   |
| 2   | 5MC  | B     | 38   | 2     | 18,22,23     | 3.71 | 8 (44%)  | 26,32,35    | 1.06 | 2 (7%)   |
| 3   | A2M  | D     | 1534 | 3,80  | 22,25,26     | 1.34 | 1 (4%)   | 31,36,39    | 1.29 | 6 (19%)  |
| 3   | PSU  | D     | 1536 | 3     | 18,21,22     | 1.05 | 2 (11%)  | 22,30,33    | 1.88 | 4 (18%)  |
| 48  | B8N  | w     | 1248 | 48    | 24,29,30     | 0.80 | 0        | 29,42,45    | 0.97 | 2 (6%)   |
| 3   | A2M  | D     | 3718 | 3     | 22,25,26     | 1.39 | 1 (4%)   | 31,36,39    | 1.00 | 2 (6%)   |
| 3   | OMG  | D     | 4370 | 3     | 23,26,27     | 2.56 | 9 (39%)  | 33,38,41    | 1.94 | 10 (30%) |
| 3   | OMG  | D     | 1625 | 3,80  | 23,26,27     | 2.60 | 8 (34%)  | 33,38,41    | 1.93 | 9 (27%)  |
| 48  | PSU  | w     | 1174 | 80,48 | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 3   | PSU  | D     | 4457 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 48  | PSU  | w     | 1347 | 48    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 3   | OMC  | D     | 3808 | 3     | 19,22,23     | 2.84 | 8 (42%)  | 26,31,34    | 0.76 | 0        |
| 3   | PSU  | D     | 4423 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 3   | OMG  | D     | 1760 | 3     | 23,26,27     | 2.61 | 8 (34%)  | 33,38,41    | 1.92 | 10 (30%) |
| 48  | A2M  | w     | 590  | 48    | 22,25,26     | 1.46 | 3 (13%)  | 31,36,39    | 1.02 | 2 (6%)   |
| 3   | PSU  | D     | 4471 | 3     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 48  | A2M  | w     | 576  | 48    | 22,25,26     | 1.43 | 2 (9%)   | 31,36,39    | 1.01 | 2 (6%)   |
| 48  | OMC  | w     | 174  | 48    | 19,22,23     | 3.02 | 8 (42%)  | 26,31,34    | 0.77 | 0        |

| Mol | Type | Chain | Res  | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | PSU  | w     | 1046 | 48     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.83 | 4 (18%)  |
| 3   | PSU  | D     | 3637 | 3,80   | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.90 | 4 (18%)  |
| 48  | G7M  | w     | 1639 | 2,48   | 23,26,27     | 2.81 | 8 (34%)  | 35,39,42    | 1.81 | 8 (22%)  |
| 2   | 5MC  | C     | 48   | 2      | 18,22,23     | 3.79 | 8 (44%)  | 26,32,35    | 1.02 | 2 (7%)   |
| 3   | OMG  | D     | 3792 | 3      | 23,26,27     | 2.55 | 9 (39%)  | 33,38,41    | 1.89 | 9 (27%)  |
| 3   | OMG  | D     | 4196 | 3,80,2 | 23,26,27     | 2.54 | 9 (39%)  | 33,38,41    | 1.89 | 9 (27%)  |
| 48  | PSU  | w     | 966  | 48     | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.82 | 5 (22%)  |
| 48  | OMU  | w     | 1804 | 48     | 19,22,23     | 2.86 | 6 (31%)  | 26,31,34    | 1.76 | 4 (15%)  |
| 3   | PSU  | D     | 4296 | 3      | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 48  | PSU  | w     | 686  | 48     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.83 | 4 (18%)  |
| 3   | PSU  | D     | 3764 | 3      | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 3   | PSU  | D     | 1744 | 3,80   | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 48  | PSU  | w     | 1643 | 80,48  | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.81 | 5 (22%)  |
| 3   | OMG  | D     | 4637 | 3      | 23,26,27     | 2.55 | 9 (39%)  | 33,38,41    | 1.95 | 9 (27%)  |
| 3   | PSU  | D     | 4293 | 3      | 18,21,22     | 1.06 | 2 (11%)  | 22,30,33    | 1.83 | 4 (18%)  |
| 3   | PSU  | D     | 3695 | 3      | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.86 | 4 (18%)  |
| 2   | 2MG  | B     | 6    | 2      | 23,26,27     | 2.63 | 7 (30%)  | 32,38,41    | 2.18 | 9 (28%)  |
| 3   | A2M  | D     | 400  | 3      | 22,25,26     | 1.43 | 1 (4%)   | 31,36,39    | 1.01 | 2 (6%)   |
| 3   | OMC  | D     | 3887 | 3      | 19,22,23     | 2.86 | 8 (42%)  | 26,31,34    | 0.76 | 0        |
| 48  | PSU  | w     | 1045 | 48     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 3   | OMU  | D     | 4498 | 3,80   | 19,22,23     | 2.79 | 6 (31%)  | 26,31,34    | 1.75 | 5 (19%)  |
| 48  | PSU  | w     | 1177 | 48     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 48  | OMC  | w     | 1391 | 48     | 19,22,23     | 2.93 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 3   | PSU  | D     | 4403 | 3,80   | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.88 | 5 (22%)  |
| 3   | 1MA  | D     | 1322 | 3      | 21,25,26     | 0.71 | 0        | 31,37,40    | 0.77 | 1 (3%)   |
| 3   | OMC  | D     | 2804 | 3      | 19,22,23     | 2.85 | 8 (42%)  | 26,31,34    | 0.69 | 0        |
| 3   | OMC  | D     | 4456 | 3      | 19,22,23     | 2.82 | 8 (42%)  | 26,31,34    | 0.69 | 0        |
| 48  | PSU  | w     | 801  | 48     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 3   | A2M  | D     | 3825 | 3      | 22,25,26     | 1.37 | 1 (4%)   | 31,36,39    | 1.02 | 2 (6%)   |
| 3   | PSU  | D     | 3853 | 3,80   | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.74 | 4 (18%)  |
| 48  | OMG  | w     | 1328 | 48     | 23,26,27     | 2.61 | 8 (34%)  | 33,38,41    | 1.94 | 10 (30%) |
| 48  | PSU  | w     | 1692 | 48     | 18,21,22     | 1.00 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 48  | PSU  | w     | 406  | 48     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 48  | PSU  | w     | 109  | 48     | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.81 | 4 (18%)  |
| 3   | OMC  | D     | 3841 | 3      | 19,22,23     | 2.81 | 8 (42%)  | 26,31,34    | 0.68 | 0        |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | D     | 4299 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.84 | 4 (18%)  |
| 48  | PSU  | w     | 1445 | 48    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.81 | 5 (22%)  |
| 2   | PSU  | B     | 13   | 2     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 48  | PSU  | w     | 822  | 48    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.75 | 5 (22%)  |
| 2   | PSU  | C     | 54   | 2     | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 3   | OMG  | D     | 2424 | 3     | 23,26,27     | 2.59 | 9 (39%)  | 33,38,41    | 1.92 | 10 (30%) |
| 3   | PSU  | D     | 3770 | 3     | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.81 | 4 (18%)  |
| 3   | PSU  | D     | 5001 | 3,80  | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.78 | 4 (18%)  |
| 3   | PSU  | D     | 3762 | 3     | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 2   | 5MU  | B     | 53   | 2     | 19,22,23     | 4.66 | 5 (26%)  | 28,32,35    | 3.64 | 8 (28%)  |
| 3   | PSU  | D     | 4972 | 3,80  | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.85 | 4 (18%)  |
| 3   | A2M  | D     | 1524 | 3     | 22,25,26     | 1.51 | 2 (9%)   | 31,36,39    | 1.08 | 3 (9%)   |
| 3   | PSU  | D     | 3768 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 3   | PSU  | D     | 4521 | 3,80  | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.88 | 5 (22%)  |
| 48  | OMC  | w     | 517  | 80,48 | 19,22,23     | 2.99 | 8 (42%)  | 26,31,34    | 0.76 | 0        |
| 48  | PSU  | w     | 105  | 48    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.81 | 5 (22%)  |
| 48  | PSU  | w     | 1232 | 48    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 3   | PSU  | D     | 4431 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.86 | 4 (18%)  |
| 3   | 5MC  | D     | 4447 | 3,80  | 18,22,23     | 3.60 | 7 (38%)  | 26,32,35    | 1.13 | 1 (3%)   |
| 48  | PSU  | w     | 93   | 48    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.78 | 3 (13%)  |
| 3   | OMG  | D     | 4494 | 3     | 23,26,27     | 2.58 | 10 (43%) | 33,38,41    | 1.95 | 9 (27%)  |
| 48  | OMU  | w     | 172  | 48    | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 48  | PSU  | w     | 863  | 48    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.82 | 5 (22%)  |
| 3   | OMG  | D     | 3944 | 3     | 23,26,27     | 2.60 | 8 (34%)  | 33,38,41    | 1.94 | 9 (27%)  |
| 3   | PSU  | D     | 3730 | 3     | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.82 | 5 (22%)  |
| 48  | OMG  | w     | 601  | 48    | 23,26,27     | 2.61 | 8 (34%)  | 33,38,41    | 1.93 | 9 (27%)  |
| 3   | PSU  | D     | 4532 | 3     | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 5   | OMG  | F     | 75   | 5     | 23,26,27     | 2.59 | 9 (39%)  | 33,38,41    | 1.93 | 9 (27%)  |
| 3   | OMC  | D     | 3701 | 3,80  | 19,22,23     | 2.85 | 8 (42%)  | 26,31,34    | 0.73 | 0        |
| 3   | PSU  | D     | 4628 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.87 | 4 (18%)  |
| 3   | PSU  | D     | 4312 | 3     | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 48  | OMU  | w     | 799  | 48    | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 1.69 | 4 (15%)  |
| 48  | PSU  | w     | 1081 | 48    | 18,21,22     | 1.01 | 1 (5%)   | 22,30,33    | 1.81 | 4 (18%)  |
| 48  | 4AC  | w     | 1842 | 48    | 21,24,25     | 0.56 | 0        | 29,34,37    | 1.16 | 4 (13%)  |
| 3   | A2M  | D     | 1871 | 3,80  | 22,25,26     | 1.42 | 1 (4%)   | 31,36,39    | 1.13 | 3 (9%)   |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | UR3  | D     | 4530 | 3     | 19,22,23     | 2.63 | 7 (36%)  | 26,32,35    | 1.30 | 2 (7%)   |
| 3   | OMG  | D     | 1522 | 3     | 23,26,27     | 2.53 | 9 (39%)  | 33,38,41    | 1.94 | 10 (30%) |
| 2   | H2U  | C     | 19   | 2     | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 0.80 | 0        |
| 3   | PSU  | D     | 4442 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.86 | 6 (27%)  |
| 48  | PSU  | w     | 1244 | 48    | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.79 | 4 (18%)  |
| 3   | OMC  | D     | 2422 | 3,80  | 19,22,23     | 2.88 | 8 (42%)  | 26,31,34    | 0.73 | 0        |
| 3   | PSU  | D     | 3715 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.85 | 5 (22%)  |
| 48  | PSU  | w     | 119  | 48    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.76 | 4 (18%)  |
| 48  | PSU  | w     | 1004 | 48    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 3   | PSU  | D     | 1862 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.89 | 5 (22%)  |
| 3   | PSU  | D     | 4579 | 3     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.83 | 4 (18%)  |
| 48  | PSU  | w     | 572  | 48    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.79 | 3 (13%)  |
| 48  | PSU  | w     | 218  | 48    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.73 | 4 (18%)  |
| 3   | PSU  | D     | 2632 | 3     | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 3   | PSU  | D     | 2508 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.82 | 4 (18%)  |
| 48  | OMG  | w     | 509  | 48    | 23,26,27     | 2.66 | 8 (34%)  | 33,38,41    | 1.92 | 9 (27%)  |
| 48  | PSU  | w     | 36   | 48    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.86 | 5 (22%)  |
| 48  | A2M  | w     | 1031 | 48    | 22,25,26     | 1.42 | 1 (4%)   | 31,36,39    | 1.01 | 2 (6%)   |
| 3   | A2M  | D     | 2401 | 3     | 22,25,26     | 1.42 | 1 (4%)   | 31,36,39    | 1.03 | 3 (9%)   |
| 3   | OMC  | D     | 2351 | 3,80  | 19,22,23     | 2.80 | 7 (36%)  | 26,31,34    | 0.77 | 0        |
| 2   | 56B  | C     | 34   | 2     | 29,35,36     | 3.00 | 11 (37%) | 36,52,55    | 2.32 | 8 (22%)  |
| 3   | A2M  | D     | 2787 | 3,80  | 22,25,26     | 1.37 | 1 (4%)   | 31,36,39    | 1.01 | 2 (6%)   |
| 48  | OMU  | w     | 116  | 48    | 19,22,23     | 2.92 | 8 (42%)  | 26,31,34    | 1.70 | 4 (15%)  |
| 2   | 5MC  | C     | 47   | 2     | 18,22,23     | 3.79 | 8 (44%)  | 26,32,35    | 1.04 | 2 (7%)   |
| 48  | OMU  | w     | 428  | 48    | 19,22,23     | 2.93 | 8 (42%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 3   | PSU  | D     | 4353 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.85 | 4 (18%)  |
| 2   | 5MC  | B     | 47   | 2     | 18,22,23     | 3.75 | 8 (44%)  | 26,32,35    | 1.05 | 2 (7%)   |
| 3   | OMU  | D     | 4620 | 3     | 19,22,23     | 2.76 | 6 (31%)  | 26,31,34    | 1.78 | 5 (19%)  |
| 48  | OMG  | w     | 644  | 48    | 23,26,27     | 2.61 | 8 (34%)  | 33,38,41    | 1.94 | 9 (27%)  |
| 3   | OMU  | D     | 2415 | 3     | 19,22,23     | 2.83 | 6 (31%)  | 26,31,34    | 1.94 | 6 (23%)  |
| 3   | OMC  | D     | 2365 | 3,80  | 19,22,23     | 2.84 | 8 (42%)  | 26,31,34    | 0.71 | 0        |
| 48  | PSU  | w     | 814  | 48    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 3   | OMG  | D     | 4618 | 3     | 23,26,27     | 2.57 | 9 (39%)  | 33,38,41    | 1.92 | 9 (27%)  |
| 48  | PSU  | w     | 609  | 48    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 48  | 6MZ  | w     | 1832 | 80,48 | 22,25,26     | 2.77 | 4 (18%)  | 30,36,39    | 2.21 | 10 (33%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | PSU  | w     | 1056 | 48    | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.81 | 4 (18%)  |
| 48  | OMG  | w     | 683  | 48    | 23,26,27     | 2.60 | 8 (34%)  | 33,38,41    | 1.96 | 9 (27%)  |
| 3   | A2M  | D     | 1326 | 3     | 22,25,26     | 1.32 | 1 (4%)   | 31,36,39    | 1.00 | 2 (6%)   |
| 3   | OMG  | D     | 4392 | 3     | 23,26,27     | 2.56 | 9 (39%)  | 33,38,41    | 1.93 | 10 (30%) |
| 2   | 2MG  | C     | 6    | 2     | 23,26,27     | 2.64 | 7 (30%)  | 32,38,41    | 2.17 | 9 (28%)  |
| 2   | 5MC  | C     | 38   | 2     | 18,22,23     | 3.76 | 8 (44%)  | 26,32,35    | 1.02 | 2 (7%)   |
| 48  | A2M  | w     | 159  | 48    | 22,25,26     | 1.54 | 2 (9%)   | 31,36,39    | 1.12 | 3 (9%)   |
| 3   | OMC  | D     | 2824 | 3     | 19,22,23     | 2.86 | 8 (42%)  | 26,31,34    | 0.72 | 0        |
| 3   | A2M  | D     | 3830 | 3     | 22,25,26     | 1.39 | 1 (4%)   | 31,36,39    | 1.06 | 1 (3%)   |
| 3   | A2M  | D     | 3724 | 3     | 22,25,26     | 1.41 | 1 (4%)   | 31,36,39    | 1.01 | 2 (6%)   |
| 3   | PSU  | D     | 5010 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.87 | 5 (22%)  |
| 3   | A2M  | D     | 4523 | 3,80  | 22,25,26     | 1.46 | 2 (9%)   | 31,36,39    | 1.12 | 4 (12%)  |
| 48  | A2M  | w     | 484  | 48    | 22,25,26     | 1.54 | 1 (4%)   | 31,36,39    | 1.00 | 2 (6%)   |
| 48  | OMU  | w     | 627  | 48    | 19,22,23     | 2.90 | 7 (36%)  | 26,31,34    | 1.72 | 5 (19%)  |
| 2   | 1MA  | C     | 57   | 2     | 21,25,26     | 0.86 | 1 (4%)   | 31,37,40    | 0.76 | 1 (3%)   |
| 3   | A2M  | D     | 398  | 3     | 22,25,26     | 1.38 | 1 (4%)   | 31,36,39    | 0.99 | 3 (9%)   |
| 3   | UY1  | D     | 3818 | 3,80  | 19,22,23     | 1.10 | 2 (10%)  | 22,31,34    | 0.92 | 1 (4%)   |
| 3   | PSU  | D     | 4689 | 3     | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.81 | 4 (18%)  |
| 3   | OMC  | D     | 4536 | 3     | 19,22,23     | 2.83 | 8 (42%)  | 26,31,34    | 0.74 | 0        |
| 2   | 1MA  | B     | 9    | 2     | 21,25,26     | 0.84 | 1 (4%)   | 31,37,40    | 0.78 | 1 (3%)   |
| 3   | OMG  | D     | 1316 | 3     | 23,26,27     | 2.57 | 10 (43%) | 33,38,41    | 1.97 | 9 (27%)  |
| 48  | MA6  | w     | 1850 | 48    | 23,26,27     | 1.39 | 4 (17%)  | 34,38,41    | 2.21 | 11 (32%) |
| 3   | PSU  | D     | 4552 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.81 | 4 (18%)  |
| 48  | PSU  | w     | 1625 | 48    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 48  | OMU  | w     | 1288 | 48    | 19,22,23     | 2.96 | 8 (42%)  | 26,31,34    | 1.67 | 4 (15%)  |
| 3   | A2M  | D     | 2363 | 3,80  | 22,25,26     | 1.35 | 2 (9%)   | 31,36,39    | 0.97 | 2 (6%)   |
| 3   | OMC  | D     | 2861 | 3     | 19,22,23     | 2.85 | 8 (42%)  | 26,31,34    | 0.67 | 0        |
| 48  | PSU  | w     | 1367 | 48    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.87 | 5 (22%)  |
| 3   | A2M  | D     | 3785 | 3,80  | 22,25,26     | 1.39 | 1 (4%)   | 31,36,39    | 1.29 | 3 (9%)   |
| 48  | A2M  | w     | 512  | 48    | 22,25,26     | 1.48 | 2 (9%)   | 31,36,39    | 1.07 | 2 (6%)   |
| 48  | A2M  | w     | 668  | 80,48 | 22,25,26     | 1.52 | 2 (9%)   | 31,36,39    | 0.98 | 2 (6%)   |
| 2   | 56B  | B     | 34   | 2     | 29,35,36     | 2.99 | 11 (37%) | 36,52,55    | 2.33 | 7 (19%)  |
| 3   | OMU  | D     | 4306 | 3     | 19,22,23     | 2.76 | 6 (31%)  | 26,31,34    | 1.78 | 5 (19%)  |
| 48  | A2M  | w     | 27   | 48    | 22,25,26     | 1.45 | 1 (4%)   | 31,36,39    | 0.99 | 1 (3%)   |
| 48  | OMG  | w     | 436  | 48    | 23,26,27     | 2.59 | 8 (34%)  | 33,38,41    | 1.99 | 9 (27%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | 5MU  | C     | 53   | 2     | 19,22,23     | 4.66 | 6 (31%)  | 28,32,35    | 3.61 | 9 (32%)  |
| 3   | OMG  | D     | 2364 | 3     | 23,26,27     | 2.52 | 9 (39%)  | 33,38,41    | 1.91 | 10 (30%) |
| 48  | MA6  | w     | 1851 | 48    | 23,26,27     | 1.32 | 5 (21%)  | 34,38,41    | 2.27 | 12 (35%) |
| 3   | PSU  | D     | 1782 | 3     | 18,21,22     | 1.00 | 1 (5%)   | 22,30,33    | 1.85 | 4 (18%)  |
| 48  | A2M  | w     | 468  | 48    | 22,25,26     | 1.57 | 2 (9%)   | 31,36,39    | 1.08 | 2 (6%)   |
| 3   | PSU  | D     | 1781 | 3     | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.80 | 4 (18%)  |
| 48  | PSU  | w     | 210  | 48    | 18,21,22     | 1.09 | 1 (5%)   | 22,30,33    | 1.80 | 5 (22%)  |
| 3   | OMG  | D     | 3627 | 3     | 23,26,27     | 2.56 | 9 (39%)  | 33,38,41    | 1.98 | 10 (30%) |
| 48  | OMU  | w     | 1442 | 80,48 | 19,22,23     | 2.87 | 6 (31%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 3   | OMC  | D     | 1340 | 3     | 19,22,23     | 2.82 | 8 (42%)  | 26,31,34    | 0.69 | 0        |
| 3   | PSU  | D     | 3851 | 3     | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.87 | 5 (22%)  |
| 48  | OMU  | w     | 121  | 48    | 19,22,23     | 2.94 | 8 (42%)  | 26,31,34    | 1.65 | 4 (15%)  |

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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 3   | A2M  | D     | 3760 | 3     | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 3758 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | D     | 3899 | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMG  | D     | 4499 | 3,2   | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 1860 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | A2M  | w     | 166  | 48    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 1792 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | 1MA  | C     | 9    | 2     | -       | 2/7/25/26 | 0/3/3/3 |
| 48  | OMC  | w     | 1703 | 80,48 | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | 6MZ  | D     | 4220 | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 1677 | 3     | -       | 5/7/25/26 | 0/2/2/2 |
| 48  | PSU  | w     | 649  | 48    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | D     | 3925 | 3     | -       | 0/9/27/28 | 0/2/2/2 |
| 48  | PSU  | w     | 651  | 48    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | D     | 4228 | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 2   | PSU  | B     | 54   | 2     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | D     | 1683 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | D     | 4500 | 3,2   | -       | 3/7/25/26 | 0/2/2/2 |
| 3   | A2M  | D     | 2815 | 3     | -       | 3/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 3   | OMG  | D     | 4623 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | C     | 13   | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 1238 | 48    | -       | 2/7/25/26  | 0/2/2/2 |
| 48  | A2M  | w     | 1678 | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | 4AC  | w     | 1337 | 48    | -       | 0/11/29/30 | 0/2/2/2 |
| 48  | PSU  | w     | 34   | 48    | -       | 3/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 681  | 80,48 | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMG  | w     | 1490 | 80,48 | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | PSU  | w     | 815  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | D     | 1773 | 3     | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 3734 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4361 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | H2U  | B     | 19   | 2     | -       | 0/7/38/39  | 0/2/2/2 |
| 2   | 5MC  | B     | 48   | 2     | -       | 2/7/25/26  | 0/2/2/2 |
| 48  | A2M  | w     | 1383 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | A2M  | w     | 99   | 80,48 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMU  | D     | 2837 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 4420 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 3744 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMC  | w     | 462  | 48    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | 1MA  | B     | 57   | 2     | -       | 0/7/25/26  | 0/3/3/3 |
| 3   | PSU  | D     | 3639 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 3920 | 3,80  | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4576 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | D     | 4227 | 3     | -       | 1/9/27/28  | 0/2/2/2 |
| 48  | PSU  | w     | 866  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMU  | w     | 1326 | 48    | -       | 5/9/27/28  | 0/2/2/2 |
| 3   | 5MC  | D     | 3782 | 3,80  | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | B     | 38   | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | D     | 1534 | 3,80  | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 1536 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | B8N  | w     | 1248 | 48    | -       | 4/16/34/35 | 0/2/2/2 |
| 3   | A2M  | D     | 3718 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | D     | 4370 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMG  | D     | 1625 | 3,80  | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | w     | 1174 | 80,48 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4457 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 1347 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | D     | 3808 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 4423 | 3     | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link   | Chirals | Torsions  | Rings   |
|-----|------|-------|------|--------|---------|-----------|---------|
| 3   | OMG  | D     | 1760 | 3      | -       | 2/9/27/28 | 0/3/3/3 |
| 48  | A2M  | w     | 590  | 48     | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 4471 | 3      | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | A2M  | w     | 576  | 48     | -       | 2/9/27/28 | 0/3/3/3 |
| 48  | OMC  | w     | 174  | 48     | -       | 1/9/27/28 | 0/2/2/2 |
| 48  | PSU  | w     | 1046 | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | D     | 3637 | 3,80   | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | G7M  | w     | 1639 | 2,48   | -       | 2/7/25/26 | 0/3/3/3 |
| 2   | 5MC  | C     | 48   | 2      | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | OMG  | D     | 3792 | 3      | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMG  | D     | 4196 | 3,80,2 | -       | 1/9/27/28 | 0/3/3/3 |
| 48  | PSU  | w     | 966  | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMU  | w     | 1804 | 48     | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | PSU  | D     | 4296 | 3      | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | PSU  | w     | 686  | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | D     | 3764 | 3      | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | D     | 1744 | 3,80   | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | PSU  | w     | 1643 | 80,48  | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | D     | 4637 | 3      | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 4293 | 3      | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | D     | 3695 | 3      | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | 2MG  | B     | 6    | 2      | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | A2M  | D     | 400  | 3      | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMC  | D     | 3887 | 3      | -       | 1/9/27/28 | 0/2/2/2 |
| 48  | PSU  | w     | 1045 | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMU  | D     | 4498 | 3,80   | -       | 0/9/27/28 | 0/2/2/2 |
| 48  | PSU  | w     | 1177 | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMC  | w     | 1391 | 48     | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | D     | 4403 | 3,80   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | 1MA  | D     | 1322 | 3      | -       | 1/7/25/26 | 0/3/3/3 |
| 3   | OMC  | D     | 2804 | 3      | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | OMC  | D     | 4456 | 3      | -       | 0/9/27/28 | 0/2/2/2 |
| 48  | PSU  | w     | 801  | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | D     | 3825 | 3      | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | D     | 3853 | 3,80   | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | OMG  | w     | 1328 | 48     | -       | 0/9/27/28 | 0/3/3/3 |
| 48  | PSU  | w     | 1692 | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | PSU  | w     | 406  | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 48  | PSU  | w     | 109  | 48     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | D     | 3841 | 3      | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | D     | 4299 | 3      | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 48  | PSU  | w     | 1445 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | PSU  | B     | 13   | 2     | -       | 2/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 822  | 48    | -       | 2/7/25/26  | 0/2/2/2 |
| 2   | PSU  | C     | 54   | 2     | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 2424 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 3770 | 3     | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 5001 | 3,80  | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 3762 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MU  | B     | 53   | 2     | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4972 | 3,80  | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | D     | 1524 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 3768 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4521 | 3,80  | -       | 2/7/25/26  | 0/2/2/2 |
| 48  | OMC  | w     | 517  | 80,48 | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | PSU  | w     | 105  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 1232 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4431 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | 5MC  | D     | 4447 | 3,80  | -       | 4/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 93   | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 4494 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | OMU  | w     | 172  | 48    | -       | 1/9/27/28  | 0/2/2/2 |
| 48  | PSU  | w     | 863  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 3944 | 3     | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 3730 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMG  | w     | 601  | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 4532 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 5   | OMG  | F     | 75   | 5     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | D     | 3701 | 3,80  | -       | 4/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 4628 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4312 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMU  | w     | 799  | 48    | -       | 3/9/27/28  | 0/2/2/2 |
| 48  | PSU  | w     | 1081 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | 4AC  | w     | 1842 | 48    | -       | 0/11/29/30 | 0/2/2/2 |
| 3   | A2M  | D     | 1871 | 3,80  | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | UR3  | D     | 4530 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 1522 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | H2U  | C     | 19   | 2     | -       | 0/7/38/39  | 0/2/2/2 |
| 3   | PSU  | D     | 4442 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 1244 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | D     | 2422 | 3,80  | -       | 1/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 3   | PSU  | D     | 3715 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 119  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 1004 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 1862 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 4579 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 572  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 218  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 2632 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | D     | 2508 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMG  | w     | 509  | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | PSU  | w     | 36   | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | A2M  | w     | 1031 | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | D     | 2401 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMC  | D     | 2351 | 3,80  | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | 56B  | C     | 34   | 2     | -       | 3/12/43/44 | 0/4/4/4 |
| 3   | A2M  | D     | 2787 | 3,80  | -       | 3/9/27/28  | 0/3/3/3 |
| 48  | OMU  | w     | 116  | 48    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | 5MC  | C     | 47   | 2     | -       | 3/7/25/26  | 0/2/2/2 |
| 48  | OMU  | w     | 428  | 48    | -       | 7/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 4353 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | B     | 47   | 2     | -       | 3/7/25/26  | 0/2/2/2 |
| 3   | OMU  | D     | 4620 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | OMG  | w     | 644  | 48    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | OMU  | D     | 2415 | 3     | -       | 3/9/27/28  | 0/2/2/2 |
| 3   | OMC  | D     | 2365 | 3,80  | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | PSU  | w     | 814  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 4618 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | PSU  | w     | 609  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | 6MZ  | w     | 1832 | 80,48 | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | PSU  | w     | 1056 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMG  | w     | 683  | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | D     | 1326 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | D     | 4392 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 2MG  | C     | 6    | 2     | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 5MC  | C     | 38   | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | A2M  | w     | 159  | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMC  | D     | 2824 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | D     | 3830 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | D     | 3724 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 5010 | 3     | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 3   | A2M  | D     | 4523 | 3,80  | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | A2M  | w     | 484  | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMU  | w     | 627  | 48    | -       | 5/9/27/28  | 0/2/2/2 |
| 2   | 1MA  | C     | 57   | 2     | -       | 0/7/25/26  | 0/3/3/3 |
| 3   | A2M  | D     | 398  | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | UY1  | D     | 3818 | 3,80  | -       | 4/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 4689 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | D     | 4536 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | 1MA  | B     | 9    | 2     | -       | 2/7/25/26  | 0/3/3/3 |
| 3   | OMG  | D     | 1316 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | MA6  | w     | 1850 | 48    | -       | 0/11/29/30 | 0/3/3/3 |
| 3   | PSU  | D     | 4552 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 1625 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | OMU  | w     | 1288 | 48    | -       | 3/9/27/28  | 0/2/2/2 |
| 3   | A2M  | D     | 2363 | 3,80  | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | D     | 2861 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | PSU  | w     | 1367 | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | D     | 3785 | 3,80  | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | A2M  | w     | 512  | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | A2M  | w     | 668  | 80,48 | -       | 3/9/27/28  | 0/3/3/3 |
| 2   | 56B  | B     | 34   | 2     | -       | 4/12/43/44 | 0/4/4/4 |
| 3   | OMU  | D     | 4306 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 48  | A2M  | w     | 27   | 48    | -       | 1/9/27/28  | 0/3/3/3 |
| 48  | OMG  | w     | 436  | 48    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 5MU  | C     | 53   | 2     | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 2364 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 48  | MA6  | w     | 1851 | 48    | -       | 2/11/29/30 | 0/3/3/3 |
| 3   | PSU  | D     | 1782 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | A2M  | w     | 468  | 48    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | D     | 1781 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 48  | PSU  | w     | 210  | 48    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | D     | 3627 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 48  | OMU  | w     | 1442 | 80,48 | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | OMC  | D     | 1340 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | D     | 3851 | 3     | -       | 1/7/25/26  | 0/2/2/2 |
| 48  | OMU  | w     | 121  | 48    | -       | 0/9/27/28  | 0/2/2/2 |

All (800) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 4220 | 6MZ  | C6-N6 | 12.08 | 1.47        | 1.34     |
| 48  | w     | 1832 | 6MZ  | C6-N6 | 11.79 | 1.47        | 1.34     |
| 2   | B     | 53   | 5MU  | C2-N1 | 10.72 | 1.55        | 1.38     |
| 2   | C     | 53   | 5MU  | C6-N1 | 10.54 | 1.56        | 1.38     |
| 2   | C     | 53   | 5MU  | C2-N1 | 10.54 | 1.55        | 1.38     |
| 2   | B     | 53   | 5MU  | C6-N1 | 10.46 | 1.55        | 1.38     |
| 2   | C     | 48   | 5MC  | C6-C5 | 9.53  | 1.50        | 1.34     |
| 2   | C     | 47   | 5MC  | C6-C5 | 9.51  | 1.50        | 1.34     |
| 2   | B     | 48   | 5MC  | C6-C5 | 9.42  | 1.50        | 1.34     |
| 2   | C     | 38   | 5MC  | C6-C5 | 9.39  | 1.50        | 1.34     |
| 2   | B     | 47   | 5MC  | C6-C5 | 9.36  | 1.50        | 1.34     |
| 2   | B     | 38   | 5MC  | C6-C5 | 9.34  | 1.49        | 1.34     |
| 3   | D     | 4447 | 5MC  | C6-C5 | 9.32  | 1.49        | 1.34     |
| 3   | D     | 3782 | 5MC  | C6-C5 | 9.18  | 1.49        | 1.34     |
| 2   | C     | 53   | 5MU  | C4-C5 | 9.15  | 1.60        | 1.44     |
| 2   | B     | 53   | 5MU  | C4-C5 | 9.13  | 1.59        | 1.44     |
| 2   | C     | 6    | 2MG  | C2-N3 | 7.69  | 1.46        | 1.31     |
| 2   | B     | 6    | 2MG  | C2-N3 | 7.68  | 1.46        | 1.31     |
| 48  | w     | 509  | OMG  | C4-N3 | 7.40  | 1.51        | 1.34     |
| 2   | B     | 48   | 5MC  | C4-N3 | 7.40  | 1.46        | 1.34     |
| 2   | C     | 53   | 5MU  | C4-N3 | -7.37 | 1.25        | 1.38     |
| 2   | B     | 53   | 5MU  | C4-N3 | -7.36 | 1.25        | 1.38     |
| 3   | D     | 1760 | OMG  | C4-N3 | 7.33  | 1.51        | 1.34     |
| 2   | C     | 47   | 5MC  | C4-N3 | 7.30  | 1.46        | 1.34     |
| 2   | B     | 47   | 5MC  | C4-N3 | 7.30  | 1.46        | 1.34     |
| 48  | w     | 436  | OMG  | C4-N3 | 7.29  | 1.51        | 1.34     |
| 3   | D     | 3944 | OMG  | C4-N3 | 7.28  | 1.51        | 1.34     |
| 48  | w     | 601  | OMG  | C4-N3 | 7.27  | 1.51        | 1.34     |
| 2   | C     | 38   | 5MC  | C4-N3 | 7.25  | 1.46        | 1.34     |
| 2   | C     | 48   | 5MC  | C4-N3 | 7.24  | 1.46        | 1.34     |
| 48  | w     | 644  | OMG  | C4-N3 | 7.24  | 1.51        | 1.34     |
| 48  | w     | 1328 | OMG  | C4-N3 | 7.23  | 1.51        | 1.34     |
| 48  | w     | 1490 | OMG  | C4-N3 | 7.22  | 1.51        | 1.34     |
| 48  | w     | 683  | OMG  | C4-N3 | 7.21  | 1.51        | 1.34     |
| 3   | D     | 1625 | OMG  | C4-N3 | 7.19  | 1.51        | 1.34     |
| 5   | F     | 75   | OMG  | C4-N3 | 7.17  | 1.51        | 1.34     |
| 48  | w     | 121  | OMU  | C2-N1 | 7.16  | 1.49        | 1.38     |
| 48  | w     | 1288 | OMU  | C2-N1 | 7.15  | 1.49        | 1.38     |
| 3   | D     | 4370 | OMG  | C4-N3 | 7.12  | 1.51        | 1.34     |
| 2   | B     | 38   | 5MC  | C4-N3 | 7.12  | 1.46        | 1.34     |
| 3   | D     | 4637 | OMG  | C4-N3 | 7.10  | 1.51        | 1.34     |
| 3   | D     | 3744 | OMG  | C4-N3 | 7.10  | 1.51        | 1.34     |
| 3   | D     | 4494 | OMG  | C4-N3 | 7.09  | 1.51        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | D     | 3792 | OMG  | C4-N3   | 7.09 | 1.51        | 1.34     |
| 48  | w     | 172  | OMU  | C2-N1   | 7.09 | 1.49        | 1.38     |
| 48  | w     | 799  | OMU  | C2-N1   | 7.08 | 1.49        | 1.38     |
| 3   | D     | 4499 | OMG  | C4-N3   | 7.07 | 1.51        | 1.34     |
| 3   | D     | 4618 | OMG  | C4-N3   | 7.07 | 1.51        | 1.34     |
| 3   | D     | 4228 | OMG  | C4-N3   | 7.07 | 1.51        | 1.34     |
| 3   | D     | 4392 | OMG  | C4-N3   | 7.07 | 1.51        | 1.34     |
| 3   | D     | 1316 | OMG  | C4-N3   | 7.06 | 1.51        | 1.34     |
| 3   | D     | 3627 | OMG  | C4-N3   | 7.06 | 1.51        | 1.34     |
| 3   | D     | 2424 | OMG  | C4-N3   | 7.05 | 1.51        | 1.34     |
| 3   | D     | 3899 | OMG  | C4-N3   | 7.05 | 1.51        | 1.34     |
| 48  | w     | 428  | OMU  | C2-N1   | 7.05 | 1.49        | 1.38     |
| 48  | w     | 116  | OMU  | C2-N1   | 7.04 | 1.49        | 1.38     |
| 3   | D     | 4196 | OMG  | C4-N3   | 7.03 | 1.51        | 1.34     |
| 3   | D     | 1773 | OMU  | C2-N1   | 7.02 | 1.49        | 1.38     |
| 48  | w     | 627  | OMU  | C2-N1   | 7.00 | 1.49        | 1.38     |
| 2   | C     | 34   | 56B  | C14-C13 | 7.00 | 1.52        | 1.32     |
| 3   | D     | 4623 | OMG  | C4-N3   | 6.99 | 1.50        | 1.34     |
| 2   | B     | 34   | 56B  | C14-C13 | 6.98 | 1.52        | 1.32     |
| 3   | D     | 1522 | OMG  | C4-N3   | 6.97 | 1.50        | 1.34     |
| 3   | D     | 2364 | OMG  | C4-N3   | 6.94 | 1.50        | 1.34     |
| 48  | w     | 1326 | OMU  | C2-N1   | 6.90 | 1.49        | 1.38     |
| 48  | w     | 1804 | OMU  | C2-N1   | 6.87 | 1.49        | 1.38     |
| 3   | D     | 3782 | 5MC  | C4-N3   | 6.84 | 1.45        | 1.34     |
| 3   | D     | 2415 | OMU  | C2-N1   | 6.84 | 1.49        | 1.38     |
| 48  | w     | 1442 | OMU  | C2-N1   | 6.83 | 1.49        | 1.38     |
| 3   | D     | 4227 | OMU  | C2-N1   | 6.78 | 1.49        | 1.38     |
| 48  | w     | 1288 | OMU  | C2-N3   | 6.66 | 1.49        | 1.38     |
| 48  | w     | 172  | OMU  | C2-N3   | 6.65 | 1.49        | 1.38     |
| 3   | D     | 3925 | OMU  | C2-N1   | 6.64 | 1.49        | 1.38     |
| 3   | D     | 4530 | UR3  | C2-N1   | 6.63 | 1.48        | 1.38     |
| 48  | w     | 799  | OMU  | C2-N3   | 6.63 | 1.49        | 1.38     |
| 48  | w     | 121  | OMU  | C2-N3   | 6.62 | 1.49        | 1.38     |
| 3   | D     | 1773 | OMU  | C2-N3   | 6.61 | 1.49        | 1.38     |
| 48  | w     | 428  | OMU  | C2-N3   | 6.58 | 1.49        | 1.38     |
| 48  | w     | 116  | OMU  | C2-N3   | 6.57 | 1.49        | 1.38     |
| 3   | D     | 4447 | 5MC  | C4-N3   | 6.56 | 1.45        | 1.34     |
| 3   | D     | 4498 | OMU  | C2-N1   | 6.56 | 1.49        | 1.38     |
| 48  | w     | 627  | OMU  | C2-N3   | 6.54 | 1.49        | 1.38     |
| 2   | C     | 53   | 5MU  | C6-C5   | 6.51 | 1.45        | 1.34     |
| 2   | C     | 6    | 2MG  | C4-N3   | 6.50 | 1.49        | 1.34     |
| 48  | w     | 1326 | OMU  | C2-N3   | 6.49 | 1.49        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 6    | 2MG  | C4-N3   | 6.48  | 1.49        | 1.34     |
| 48  | w     | 1442 | OMU  | C2-N3   | 6.48  | 1.49        | 1.38     |
| 2   | C     | 47   | 5MC  | C2-N3   | 6.48  | 1.49        | 1.36     |
| 2   | C     | 48   | 5MC  | C2-N3   | 6.45  | 1.49        | 1.36     |
| 2   | B     | 48   | 5MC  | C2-N3   | 6.44  | 1.49        | 1.36     |
| 2   | B     | 47   | 5MC  | C2-N3   | 6.43  | 1.49        | 1.36     |
| 2   | C     | 38   | 5MC  | C2-N3   | 6.42  | 1.49        | 1.36     |
| 48  | w     | 1639 | G7M  | C2-N2   | 6.42  | 1.49        | 1.34     |
| 48  | w     | 1804 | OMU  | C2-N3   | 6.42  | 1.49        | 1.38     |
| 3   | D     | 2837 | OMU  | C2-N1   | 6.42  | 1.48        | 1.38     |
| 3   | D     | 4306 | OMU  | C2-N1   | 6.41  | 1.48        | 1.38     |
| 3   | D     | 4620 | OMU  | C2-N1   | 6.41  | 1.48        | 1.38     |
| 48  | w     | 1639 | G7M  | C4-N3   | 6.40  | 1.49        | 1.34     |
| 2   | B     | 53   | 5MU  | C6-C5   | 6.38  | 1.45        | 1.34     |
| 48  | w     | 174  | OMC  | C2-N3   | 6.32  | 1.49        | 1.36     |
| 2   | B     | 38   | 5MC  | C2-N3   | 6.32  | 1.49        | 1.36     |
| 48  | w     | 462  | OMC  | C2-N3   | 6.29  | 1.49        | 1.36     |
| 48  | w     | 517  | OMC  | C2-N3   | 6.24  | 1.49        | 1.36     |
| 2   | C     | 34   | 56B  | C4-N3   | 6.22  | 1.49        | 1.34     |
| 3   | D     | 2415 | OMU  | C2-N3   | 6.22  | 1.49        | 1.38     |
| 3   | D     | 4227 | OMU  | C2-N3   | 6.22  | 1.49        | 1.38     |
| 3   | D     | 3782 | 5MC  | C2-N3   | 6.20  | 1.48        | 1.36     |
| 3   | D     | 2837 | OMU  | C2-N3   | 6.17  | 1.49        | 1.38     |
| 2   | B     | 34   | 56B  | C4-N3   | 6.17  | 1.48        | 1.34     |
| 3   | D     | 4306 | OMU  | C2-N3   | 6.17  | 1.49        | 1.38     |
| 3   | D     | 4498 | OMU  | C2-N3   | 6.17  | 1.49        | 1.38     |
| 3   | D     | 4620 | OMU  | C2-N3   | 6.17  | 1.49        | 1.38     |
| 48  | w     | 1391 | OMC  | C2-N3   | 6.13  | 1.48        | 1.36     |
| 3   | D     | 3925 | OMU  | C2-N3   | 6.09  | 1.48        | 1.38     |
| 48  | w     | 462  | OMC  | C6-C5   | 6.09  | 1.49        | 1.35     |
| 48  | w     | 174  | OMC  | C6-C5   | 6.06  | 1.49        | 1.35     |
| 48  | w     | 517  | OMC  | C6-C5   | 6.03  | 1.49        | 1.35     |
| 2   | C     | 34   | 56B  | O11-C11 | -6.03 | 1.28        | 1.43     |
| 3   | D     | 3887 | OMC  | C2-N3   | 6.03  | 1.48        | 1.36     |
| 3   | D     | 2861 | OMC  | C2-N3   | 6.01  | 1.48        | 1.36     |
| 3   | D     | 2824 | OMC  | C2-N3   | 6.00  | 1.48        | 1.36     |
| 48  | w     | 1703 | OMC  | C2-N3   | 6.00  | 1.48        | 1.36     |
| 3   | D     | 2422 | OMC  | C2-N3   | 5.99  | 1.48        | 1.36     |
| 2   | B     | 34   | 56B  | O11-C11 | -5.98 | 1.28        | 1.43     |
| 3   | D     | 4530 | UR3  | C6-C5   | 5.96  | 1.48        | 1.35     |
| 3   | D     | 1340 | OMC  | C2-N3   | 5.95  | 1.48        | 1.36     |
| 3   | D     | 2804 | OMC  | C2-N3   | 5.94  | 1.48        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | D     | 2351 | OMC  | C2-N3 | 5.93 | 1.48        | 1.36     |
| 3   | D     | 3701 | OMC  | C2-N3 | 5.93 | 1.48        | 1.36     |
| 3   | D     | 4536 | OMC  | C2-N3 | 5.92 | 1.48        | 1.36     |
| 3   | D     | 4447 | 5MC  | C2-N3 | 5.92 | 1.48        | 1.36     |
| 3   | D     | 2365 | OMC  | C2-N3 | 5.91 | 1.48        | 1.36     |
| 48  | w     | 428  | OMU  | C6-C5 | 5.91 | 1.48        | 1.35     |
| 48  | w     | 1703 | OMC  | C6-C5 | 5.90 | 1.48        | 1.35     |
| 48  | w     | 1391 | OMC  | C6-C5 | 5.90 | 1.48        | 1.35     |
| 3   | D     | 3808 | OMC  | C2-N3 | 5.90 | 1.48        | 1.36     |
| 3   | D     | 3701 | OMC  | C6-C5 | 5.89 | 1.48        | 1.35     |
| 3   | D     | 2422 | OMC  | C6-C5 | 5.86 | 1.48        | 1.35     |
| 48  | w     | 1288 | OMU  | C6-C5 | 5.86 | 1.48        | 1.35     |
| 48  | w     | 799  | OMU  | C6-C5 | 5.85 | 1.48        | 1.35     |
| 3   | D     | 1773 | OMU  | C6-C5 | 5.84 | 1.48        | 1.35     |
| 48  | w     | 121  | OMU  | C6-C5 | 5.84 | 1.48        | 1.35     |
| 48  | w     | 172  | OMU  | C6-C5 | 5.82 | 1.48        | 1.35     |
| 3   | D     | 2861 | OMC  | C6-C5 | 5.82 | 1.48        | 1.35     |
| 48  | w     | 627  | OMU  | C6-C5 | 5.82 | 1.48        | 1.35     |
| 3   | D     | 4456 | OMC  | C2-N3 | 5.81 | 1.48        | 1.36     |
| 3   | D     | 3841 | OMC  | C6-C5 | 5.79 | 1.48        | 1.35     |
| 3   | D     | 3841 | OMC  | C2-N3 | 5.79 | 1.48        | 1.36     |
| 48  | w     | 1639 | G7M  | C2-N3 | 5.78 | 1.47        | 1.33     |
| 3   | D     | 2824 | OMC  | C6-C5 | 5.78 | 1.48        | 1.35     |
| 3   | D     | 3887 | OMC  | C6-C5 | 5.78 | 1.48        | 1.35     |
| 48  | w     | 116  | OMU  | C6-C5 | 5.75 | 1.48        | 1.35     |
| 3   | D     | 2804 | OMC  | C6-C5 | 5.74 | 1.48        | 1.35     |
| 48  | w     | 1442 | OMU  | C6-C5 | 5.74 | 1.48        | 1.35     |
| 3   | D     | 4456 | OMC  | C6-C5 | 5.74 | 1.48        | 1.35     |
| 3   | D     | 3808 | OMC  | C6-C5 | 5.73 | 1.48        | 1.35     |
| 3   | D     | 2365 | OMC  | C6-C5 | 5.72 | 1.48        | 1.35     |
| 3   | D     | 4536 | OMC  | C6-C5 | 5.71 | 1.48        | 1.35     |
| 48  | w     | 1326 | OMU  | C6-C5 | 5.71 | 1.48        | 1.35     |
| 3   | D     | 1340 | OMC  | C6-C5 | 5.69 | 1.48        | 1.35     |
| 48  | w     | 509  | OMG  | C2-N3 | 5.68 | 1.46        | 1.33     |
| 48  | w     | 1804 | OMU  | C6-C5 | 5.66 | 1.48        | 1.35     |
| 3   | D     | 2415 | OMU  | C6-C5 | 5.65 | 1.48        | 1.35     |
| 3   | D     | 2351 | OMC  | C6-C5 | 5.65 | 1.48        | 1.35     |
| 3   | D     | 4498 | OMU  | C6-C5 | 5.64 | 1.48        | 1.35     |
| 3   | D     | 4227 | OMU  | C6-C5 | 5.59 | 1.48        | 1.35     |
| 3   | D     | 3925 | OMU  | C6-C5 | 5.58 | 1.48        | 1.35     |
| 2   | C     | 34   | 56B  | C2-N3 | 5.58 | 1.46        | 1.33     |
| 3   | D     | 4620 | OMU  | C6-C5 | 5.57 | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 4306 | OMU  | C6-C5   | 5.56  | 1.48        | 1.35     |
| 48  | w     | 644  | OMG  | C2-N3   | 5.55  | 1.46        | 1.33     |
| 2   | B     | 34   | 56B  | C2-N3   | 5.54  | 1.46        | 1.33     |
| 3   | D     | 2837 | OMU  | C6-C5   | 5.54  | 1.47        | 1.35     |
| 48  | w     | 1328 | OMG  | C2-N3   | 5.49  | 1.46        | 1.33     |
| 3   | D     | 1760 | OMG  | C2-N3   | 5.45  | 1.46        | 1.33     |
| 48  | w     | 601  | OMG  | C2-N3   | 5.44  | 1.46        | 1.33     |
| 3   | D     | 1625 | OMG  | C2-N3   | 5.42  | 1.46        | 1.33     |
| 48  | w     | 1490 | OMG  | C2-N3   | 5.39  | 1.46        | 1.33     |
| 48  | w     | 436  | OMG  | C2-N3   | 5.37  | 1.46        | 1.33     |
| 3   | D     | 3944 | OMG  | C2-N3   | 5.37  | 1.46        | 1.33     |
| 48  | w     | 683  | OMG  | C2-N3   | 5.37  | 1.46        | 1.33     |
| 3   | D     | 2424 | OMG  | C2-N3   | 5.35  | 1.46        | 1.33     |
| 5   | F     | 75   | OMG  | C2-N3   | 5.33  | 1.46        | 1.33     |
| 2   | B     | 34   | 56B  | C11-C10 | 5.33  | 1.62        | 1.54     |
| 3   | D     | 4494 | OMG  | C2-N3   | 5.31  | 1.46        | 1.33     |
| 3   | D     | 1524 | A2M  | O5'-C5' | -5.29 | 1.31        | 1.44     |
| 3   | D     | 4370 | OMG  | C2-N3   | 5.26  | 1.45        | 1.33     |
| 3   | D     | 3744 | OMG  | C2-N3   | 5.26  | 1.45        | 1.33     |
| 48  | w     | 509  | OMG  | C2-N2   | 5.24  | 1.46        | 1.34     |
| 2   | C     | 34   | 56B  | C11-C10 | 5.23  | 1.62        | 1.54     |
| 3   | D     | 4637 | OMG  | C2-N3   | 5.23  | 1.45        | 1.33     |
| 3   | D     | 3627 | OMG  | C2-N3   | 5.22  | 1.45        | 1.33     |
| 3   | D     | 4499 | OMG  | C2-N3   | 5.22  | 1.45        | 1.33     |
| 3   | D     | 4618 | OMG  | C2-N3   | 5.22  | 1.45        | 1.33     |
| 3   | D     | 1316 | OMG  | C2-N3   | 5.21  | 1.45        | 1.33     |
| 48  | w     | 668  | A2M  | O5'-C5' | -5.20 | 1.32        | 1.44     |
| 3   | D     | 4196 | OMG  | C2-N3   | 5.20  | 1.45        | 1.33     |
| 3   | D     | 4228 | OMG  | C2-N3   | 5.19  | 1.45        | 1.33     |
| 2   | C     | 48   | 5MC  | C6-N1   | 5.18  | 1.46        | 1.38     |
| 2   | C     | 47   | 5MC  | C6-N1   | 5.17  | 1.46        | 1.38     |
| 3   | D     | 3792 | OMG  | C2-N3   | 5.17  | 1.45        | 1.33     |
| 2   | B     | 48   | 5MC  | C6-N1   | 5.16  | 1.46        | 1.38     |
| 3   | D     | 1760 | OMG  | C2-N2   | 5.16  | 1.46        | 1.34     |
| 48  | w     | 601  | OMG  | C2-N2   | 5.16  | 1.46        | 1.34     |
| 3   | D     | 4392 | OMG  | C2-N3   | 5.15  | 1.45        | 1.33     |
| 48  | w     | 644  | OMG  | C2-N2   | 5.15  | 1.46        | 1.34     |
| 3   | D     | 3785 | A2M  | O5'-C5' | -5.13 | 1.32        | 1.44     |
| 3   | D     | 3944 | OMG  | C2-N2   | 5.13  | 1.46        | 1.34     |
| 3   | D     | 4623 | OMG  | C2-N3   | 5.13  | 1.45        | 1.33     |
| 3   | D     | 2424 | OMG  | C2-N2   | 5.12  | 1.46        | 1.34     |
| 48  | w     | 174  | OMC  | C4-N3   | 5.10  | 1.44        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 3899 | OMG  | C2-N3   | 5.10  | 1.45        | 1.33     |
| 3   | D     | 2401 | A2M  | O5'-C5' | -5.10 | 1.32        | 1.44     |
| 3   | D     | 1522 | OMG  | C2-N3   | 5.09  | 1.45        | 1.33     |
| 48  | w     | 1328 | OMG  | C2-N2   | 5.09  | 1.46        | 1.34     |
| 48  | w     | 683  | OMG  | C2-N2   | 5.08  | 1.46        | 1.34     |
| 2   | C     | 38   | 5MC  | C6-N1   | 5.08  | 1.46        | 1.38     |
| 48  | w     | 436  | OMG  | C2-N2   | 5.08  | 1.46        | 1.34     |
| 3   | D     | 2815 | A2M  | O5'-C5' | -5.08 | 1.32        | 1.44     |
| 48  | w     | 462  | OMC  | C4-N3   | 5.07  | 1.44        | 1.34     |
| 3   | D     | 2364 | OMG  | C2-N3   | 5.05  | 1.45        | 1.33     |
| 2   | C     | 6    | 2MG  | C2-N1   | 5.04  | 1.44        | 1.36     |
| 5   | F     | 75   | OMG  | C2-N2   | 5.04  | 1.46        | 1.34     |
| 3   | D     | 400  | A2M  | O5'-C5' | -5.04 | 1.32        | 1.44     |
| 3   | D     | 4618 | OMG  | C2-N2   | 5.04  | 1.46        | 1.34     |
| 2   | B     | 47   | 5MC  | C6-N1   | 5.03  | 1.46        | 1.38     |
| 48  | w     | 484  | A2M  | O5'-C5' | -5.03 | 1.32        | 1.44     |
| 3   | D     | 1625 | OMG  | C2-N2   | 5.02  | 1.46        | 1.34     |
| 48  | w     | 517  | OMC  | C4-N3   | 5.02  | 1.44        | 1.34     |
| 48  | w     | 468  | A2M  | O5'-C5' | -5.02 | 1.32        | 1.44     |
| 3   | D     | 4523 | A2M  | O5'-C5' | -5.02 | 1.32        | 1.44     |
| 48  | w     | 1490 | OMG  | C2-N2   | 5.02  | 1.46        | 1.34     |
| 3   | D     | 1871 | A2M  | O5'-C5' | -5.01 | 1.32        | 1.44     |
| 3   | D     | 3825 | A2M  | O5'-C5' | -5.01 | 1.32        | 1.44     |
| 3   | D     | 3830 | A2M  | O5'-C5' | -5.00 | 1.32        | 1.44     |
| 2   | B     | 6    | 2MG  | C2-N1   | 4.99  | 1.44        | 1.36     |
| 3   | D     | 3744 | OMG  | C2-N2   | 4.99  | 1.46        | 1.34     |
| 2   | B     | 38   | 5MC  | C6-N1   | 4.98  | 1.46        | 1.38     |
| 3   | D     | 4499 | OMG  | C2-N2   | 4.98  | 1.46        | 1.34     |
| 3   | D     | 2787 | A2M  | O5'-C5' | -4.97 | 1.32        | 1.44     |
| 48  | w     | 1391 | OMC  | C4-N3   | 4.96  | 1.44        | 1.34     |
| 3   | D     | 4494 | OMG  | C2-N2   | 4.96  | 1.46        | 1.34     |
| 48  | w     | 1031 | A2M  | O5'-C5' | -4.95 | 1.32        | 1.44     |
| 3   | D     | 4623 | OMG  | C2-N2   | 4.95  | 1.46        | 1.34     |
| 3   | D     | 3760 | A2M  | O5'-C5' | -4.93 | 1.32        | 1.44     |
| 48  | w     | 174  | OMC  | C4-N4   | 4.93  | 1.45        | 1.33     |
| 3   | D     | 3627 | OMG  | C2-N2   | 4.93  | 1.45        | 1.34     |
| 48  | w     | 27   | A2M  | O5'-C5' | -4.93 | 1.32        | 1.44     |
| 48  | w     | 1383 | A2M  | O5'-C5' | -4.92 | 1.32        | 1.44     |
| 3   | D     | 1316 | OMG  | C2-N2   | 4.91  | 1.45        | 1.34     |
| 3   | D     | 4228 | OMG  | C2-N2   | 4.91  | 1.45        | 1.34     |
| 3   | D     | 4370 | OMG  | C2-N2   | 4.90  | 1.45        | 1.34     |
| 48  | w     | 462  | OMC  | C4-N4   | 4.88  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 4637 | OMG  | C2-N2   | 4.87  | 1.45        | 1.34     |
| 48  | w     | 159  | A2M  | O5'-C5' | -4.87 | 1.32        | 1.44     |
| 48  | w     | 517  | OMC  | C4-N4   | 4.86  | 1.45        | 1.33     |
| 3   | D     | 1326 | A2M  | O5'-C5' | -4.86 | 1.32        | 1.44     |
| 3   | D     | 4196 | OMG  | C2-N2   | 4.84  | 1.45        | 1.34     |
| 3   | D     | 3792 | OMG  | C2-N2   | 4.84  | 1.45        | 1.34     |
| 3   | D     | 4447 | 5MC  | C6-N1   | 4.84  | 1.46        | 1.38     |
| 3   | D     | 2364 | OMG  | C2-N2   | 4.84  | 1.45        | 1.34     |
| 48  | w     | 1703 | OMC  | C4-N3   | 4.84  | 1.44        | 1.34     |
| 3   | D     | 4392 | OMG  | C2-N2   | 4.84  | 1.45        | 1.34     |
| 3   | D     | 3899 | OMG  | C2-N2   | 4.83  | 1.45        | 1.34     |
| 3   | D     | 1522 | OMG  | C2-N2   | 4.83  | 1.45        | 1.34     |
| 3   | D     | 3782 | 5MC  | C6-N1   | 4.83  | 1.46        | 1.38     |
| 48  | w     | 166  | A2M  | O5'-C5' | -4.82 | 1.33        | 1.44     |
| 48  | w     | 1391 | OMC  | C4-N4   | 4.82  | 1.45        | 1.33     |
| 3   | D     | 3887 | OMC  | C4-N3   | 4.81  | 1.44        | 1.34     |
| 3   | D     | 2804 | OMC  | C4-N3   | 4.81  | 1.44        | 1.34     |
| 48  | w     | 1639 | G7M  | C5-N7   | -4.78 | 1.33        | 1.39     |
| 48  | w     | 99   | A2M  | O5'-C5' | -4.78 | 1.33        | 1.44     |
| 3   | D     | 3718 | A2M  | O5'-C5' | -4.78 | 1.33        | 1.44     |
| 48  | w     | 512  | A2M  | O5'-C5' | -4.77 | 1.33        | 1.44     |
| 3   | D     | 2824 | OMC  | C4-N3   | 4.77  | 1.44        | 1.34     |
| 48  | w     | 1703 | OMC  | C4-N4   | 4.76  | 1.45        | 1.33     |
| 3   | D     | 398  | A2M  | O5'-C5' | -4.76 | 1.33        | 1.44     |
| 3   | D     | 2422 | OMC  | C4-N3   | 4.75  | 1.44        | 1.34     |
| 3   | D     | 2365 | OMC  | C4-N3   | 4.72  | 1.44        | 1.34     |
| 2   | C     | 34   | 56B  | C2-N2   | 4.72  | 1.45        | 1.34     |
| 3   | D     | 2422 | OMC  | C4-N4   | 4.71  | 1.45        | 1.33     |
| 3   | D     | 3808 | OMC  | C4-N4   | 4.71  | 1.45        | 1.33     |
| 3   | D     | 4456 | OMC  | C4-N3   | 4.70  | 1.44        | 1.34     |
| 3   | D     | 4536 | OMC  | C4-N3   | 4.69  | 1.44        | 1.34     |
| 3   | D     | 2804 | OMC  | C4-N4   | 4.69  | 1.45        | 1.33     |
| 3   | D     | 4530 | UR3  | C2-N3   | 4.69  | 1.48        | 1.39     |
| 3   | D     | 3724 | A2M  | O5'-C5' | -4.69 | 1.33        | 1.44     |
| 3   | D     | 3701 | OMC  | C4-N3   | 4.69  | 1.44        | 1.34     |
| 3   | D     | 2861 | OMC  | C4-N4   | 4.68  | 1.44        | 1.33     |
| 3   | D     | 3887 | OMC  | C4-N4   | 4.68  | 1.44        | 1.33     |
| 3   | D     | 2363 | A2M  | O5'-C5' | -4.68 | 1.33        | 1.44     |
| 3   | D     | 4536 | OMC  | C4-N4   | 4.67  | 1.44        | 1.33     |
| 3   | D     | 3701 | OMC  | C4-N4   | 4.66  | 1.44        | 1.33     |
| 2   | B     | 34   | 56B  | C2-N2   | 4.66  | 1.45        | 1.34     |
| 3   | D     | 2365 | OMC  | C4-N4   | 4.66  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 1340 | OMC  | C4-N4   | 4.65  | 1.44        | 1.33     |
| 3   | D     | 4456 | OMC  | C4-N4   | 4.65  | 1.44        | 1.33     |
| 3   | D     | 1340 | OMC  | C4-N3   | 4.64  | 1.43        | 1.34     |
| 3   | D     | 2861 | OMC  | C4-N3   | 4.64  | 1.43        | 1.34     |
| 3   | D     | 3808 | OMC  | C4-N3   | 4.63  | 1.43        | 1.34     |
| 48  | w     | 1678 | A2M  | O5'-C5' | -4.63 | 1.33        | 1.44     |
| 3   | D     | 2824 | OMC  | C4-N4   | 4.63  | 1.44        | 1.33     |
| 3   | D     | 3841 | OMC  | C4-N4   | 4.62  | 1.44        | 1.33     |
| 3   | D     | 3841 | OMC  | C4-N3   | 4.61  | 1.43        | 1.34     |
| 3   | D     | 2351 | OMC  | C4-N3   | 4.61  | 1.43        | 1.34     |
| 48  | w     | 576  | A2M  | O5'-C5' | -4.59 | 1.33        | 1.44     |
| 48  | w     | 590  | A2M  | O5'-C5' | -4.55 | 1.33        | 1.44     |
| 48  | w     | 174  | OMC  | C2-N1   | 4.55  | 1.49        | 1.40     |
| 3   | D     | 1534 | A2M  | O5'-C5' | -4.54 | 1.33        | 1.44     |
| 3   | D     | 2351 | OMC  | C4-N4   | 4.53  | 1.44        | 1.33     |
| 48  | w     | 517  | OMC  | C2-N1   | 4.52  | 1.49        | 1.40     |
| 48  | w     | 462  | OMC  | C2-N1   | 4.44  | 1.49        | 1.40     |
| 2   | C     | 48   | 5MC  | C2-N1   | 4.30  | 1.49        | 1.40     |
| 48  | w     | 1391 | OMC  | C2-N1   | 4.28  | 1.49        | 1.40     |
| 3   | D     | 2824 | OMC  | C2-N1   | 4.21  | 1.49        | 1.40     |
| 2   | B     | 48   | 5MC  | C2-N1   | 4.20  | 1.49        | 1.40     |
| 2   | C     | 34   | 56B  | C5-C6   | 4.20  | 1.53        | 1.44     |
| 2   | C     | 47   | 5MC  | C2-N1   | 4.20  | 1.49        | 1.40     |
| 3   | D     | 3808 | OMC  | C2-N1   | 4.18  | 1.49        | 1.40     |
| 2   | C     | 38   | 5MC  | C2-N1   | 4.18  | 1.49        | 1.40     |
| 3   | D     | 2422 | OMC  | C2-N1   | 4.17  | 1.49        | 1.40     |
| 48  | w     | 1703 | OMC  | C2-N1   | 4.16  | 1.49        | 1.40     |
| 2   | B     | 38   | 5MC  | C2-N1   | 4.15  | 1.49        | 1.40     |
| 2   | B     | 47   | 5MC  | C2-N1   | 4.14  | 1.49        | 1.40     |
| 2   | C     | 48   | 5MC  | C4-N4   | 4.14  | 1.44        | 1.34     |
| 3   | D     | 2804 | OMC  | C2-N1   | 4.13  | 1.48        | 1.40     |
| 2   | C     | 47   | 5MC  | C4-N4   | 4.13  | 1.44        | 1.34     |
| 2   | B     | 48   | 5MC  | C4-N4   | 4.12  | 1.44        | 1.34     |
| 2   | B     | 47   | 5MC  | C4-N4   | 4.09  | 1.44        | 1.34     |
| 3   | D     | 3701 | OMC  | C2-N1   | 4.08  | 1.48        | 1.40     |
| 3   | D     | 2365 | OMC  | C2-N1   | 4.07  | 1.48        | 1.40     |
| 2   | C     | 38   | 5MC  | C4-N4   | 4.07  | 1.44        | 1.34     |
| 3   | D     | 2861 | OMC  | C2-N1   | 4.04  | 1.48        | 1.40     |
| 3   | D     | 2351 | OMC  | C2-N1   | 4.04  | 1.48        | 1.40     |
| 3   | D     | 4536 | OMC  | C2-N1   | 4.03  | 1.48        | 1.40     |
| 2   | B     | 38   | 5MC  | C4-N4   | 4.02  | 1.44        | 1.34     |
| 3   | D     | 3887 | OMC  | C2-N1   | 4.02  | 1.48        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | D     | 3841 | OMC  | C2-N1 | 3.97 | 1.48        | 1.40     |
| 3   | D     | 1340 | OMC  | C2-N1 | 3.97 | 1.48        | 1.40     |
| 2   | B     | 34   | 56B  | C5-C6 | 3.97 | 1.53        | 1.44     |
| 3   | D     | 3782 | 5MC  | C2-N1 | 3.93 | 1.48        | 1.40     |
| 3   | D     | 4456 | OMC  | C2-N1 | 3.93 | 1.48        | 1.40     |
| 3   | D     | 4447 | 5MC  | C2-N1 | 3.92 | 1.48        | 1.40     |
| 3   | D     | 3782 | 5MC  | C4-N4 | 3.90 | 1.44        | 1.34     |
| 3   | D     | 4447 | 5MC  | C4-N4 | 3.87 | 1.44        | 1.34     |
| 48  | w     | 1639 | G7M  | C5-C6 | 3.76 | 1.53        | 1.43     |
| 48  | w     | 210  | PSU  | C6-C5 | 3.54 | 1.39        | 1.35     |
| 48  | w     | 1288 | OMU  | C4-N3 | 3.53 | 1.44        | 1.38     |
| 48  | w     | 172  | OMU  | C4-N3 | 3.51 | 1.44        | 1.38     |
| 48  | w     | 822  | PSU  | C6-C5 | 3.48 | 1.39        | 1.35     |
| 48  | w     | 116  | OMU  | C4-N3 | 3.48 | 1.44        | 1.38     |
| 48  | w     | 815  | PSU  | C6-C5 | 3.47 | 1.39        | 1.35     |
| 2   | C     | 54   | PSU  | C6-C5 | 3.45 | 1.39        | 1.35     |
| 48  | w     | 572  | PSU  | C6-C5 | 3.43 | 1.39        | 1.35     |
| 48  | w     | 799  | OMU  | C4-N3 | 3.43 | 1.44        | 1.38     |
| 3   | D     | 1773 | OMU  | C4-N3 | 3.41 | 1.44        | 1.38     |
| 48  | w     | 428  | OMU  | C4-N3 | 3.41 | 1.44        | 1.38     |
| 48  | w     | 866  | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 48  | w     | 627  | OMU  | C4-N3 | 3.40 | 1.44        | 1.38     |
| 48  | w     | 218  | PSU  | C6-C5 | 3.40 | 1.39        | 1.35     |
| 48  | w     | 119  | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 48  | w     | 609  | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 48  | w     | 34   | PSU  | C6-C5 | 3.38 | 1.39        | 1.35     |
| 48  | w     | 863  | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 48  | w     | 109  | PSU  | C6-C5 | 3.37 | 1.39        | 1.35     |
| 48  | w     | 36   | PSU  | C6-C5 | 3.35 | 1.39        | 1.35     |
| 48  | w     | 121  | OMU  | C4-N3 | 3.35 | 1.44        | 1.38     |
| 2   | C     | 13   | PSU  | C6-C5 | 3.32 | 1.39        | 1.35     |
| 48  | w     | 93   | PSU  | C6-C5 | 3.32 | 1.39        | 1.35     |
| 48  | w     | 462  | OMC  | C6-N1 | 3.31 | 1.46        | 1.38     |
| 48  | w     | 1004 | PSU  | C6-C5 | 3.31 | 1.39        | 1.35     |
| 48  | w     | 1442 | OMU  | C4-N3 | 3.31 | 1.44        | 1.38     |
| 48  | w     | 1326 | OMU  | C4-N3 | 3.30 | 1.44        | 1.38     |
| 2   | B     | 54   | PSU  | C6-C5 | 3.29 | 1.39        | 1.35     |
| 48  | w     | 686  | PSU  | C6-C5 | 3.28 | 1.39        | 1.35     |
| 48  | w     | 1804 | OMU  | C4-N3 | 3.28 | 1.44        | 1.38     |
| 48  | w     | 801  | PSU  | C6-C5 | 3.27 | 1.39        | 1.35     |
| 3   | D     | 3762 | PSU  | C6-C5 | 3.27 | 1.39        | 1.35     |
| 48  | w     | 1625 | PSU  | C6-C5 | 3.27 | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 13   | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 3   | D     | 4392 | OMG  | C5-N7   | -3.26 | 1.32        | 1.39     |
| 48  | w     | 105  | PSU  | C6-C5   | 3.26  | 1.39        | 1.35     |
| 48  | w     | 174  | OMC  | C6-N1   | 3.25  | 1.45        | 1.38     |
| 3   | D     | 4500 | PSU  | C6-C5   | 3.24  | 1.39        | 1.35     |
| 3   | D     | 3792 | OMG  | C5-N7   | -3.24 | 1.32        | 1.39     |
| 48  | w     | 649  | PSU  | C6-C5   | 3.24  | 1.39        | 1.35     |
| 48  | w     | 814  | PSU  | C6-C5   | 3.24  | 1.39        | 1.35     |
| 48  | w     | 1232 | PSU  | C6-C5   | 3.24  | 1.39        | 1.35     |
| 3   | D     | 1316 | OMG  | C5-N7   | -3.23 | 1.32        | 1.39     |
| 48  | w     | 517  | OMC  | C6-N1   | 3.21  | 1.45        | 1.38     |
| 48  | w     | 1850 | MA6  | C8-N9   | -3.20 | 1.31        | 1.37     |
| 3   | D     | 1625 | OMG  | C5-N7   | -3.19 | 1.32        | 1.39     |
| 3   | D     | 4196 | OMG  | C5-N7   | -3.19 | 1.32        | 1.39     |
| 3   | D     | 4494 | OMG  | C5-N7   | -3.18 | 1.32        | 1.39     |
| 3   | D     | 4532 | PSU  | C6-C5   | 3.18  | 1.39        | 1.35     |
| 3   | D     | 3734 | PSU  | C6-C5   | 3.17  | 1.39        | 1.35     |
| 3   | D     | 3768 | PSU  | C6-C5   | 3.17  | 1.39        | 1.35     |
| 3   | D     | 1522 | OMG  | C5-N7   | -3.17 | 1.32        | 1.39     |
| 3   | D     | 3715 | PSU  | C6-C5   | 3.16  | 1.39        | 1.35     |
| 48  | w     | 1244 | PSU  | C6-C5   | 3.15  | 1.39        | 1.35     |
| 3   | D     | 4420 | PSU  | C6-C5   | 3.15  | 1.39        | 1.35     |
| 48  | w     | 1045 | PSU  | C6-C5   | 3.14  | 1.39        | 1.35     |
| 3   | D     | 4370 | OMG  | C5-N7   | -3.14 | 1.33        | 1.39     |
| 3   | D     | 3818 | UY1  | C2-N1   | 3.13  | 1.41        | 1.36     |
| 3   | D     | 4392 | OMG  | O6-C6   | -3.13 | 1.17        | 1.23     |
| 48  | w     | 1445 | PSU  | C6-C5   | 3.13  | 1.39        | 1.35     |
| 3   | D     | 4296 | PSU  | C6-C5   | 3.12  | 1.39        | 1.35     |
| 48  | w     | 1174 | PSU  | C6-C5   | 3.12  | 1.39        | 1.35     |
| 48  | w     | 1367 | PSU  | C6-C5   | 3.11  | 1.38        | 1.35     |
| 3   | D     | 3770 | PSU  | C6-C5   | 3.11  | 1.38        | 1.35     |
| 3   | D     | 2415 | OMU  | C4-N3   | 3.11  | 1.44        | 1.38     |
| 2   | B     | 34   | 56B  | C11-C12 | 3.11  | 1.58        | 1.53     |
| 3   | D     | 4456 | OMC  | O2-C2   | -3.10 | 1.18        | 1.23     |
| 48  | w     | 1851 | MA6  | C5-C4   | -3.10 | 1.33        | 1.39     |
| 3   | D     | 3627 | OMG  | C5-N7   | -3.10 | 1.33        | 1.39     |
| 48  | w     | 1238 | PSU  | C6-C5   | 3.10  | 1.38        | 1.35     |
| 3   | D     | 2424 | OMG  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 48  | w     | 1347 | PSU  | C6-C5   | 3.09  | 1.38        | 1.35     |
| 3   | D     | 1522 | OMG  | O6-C6   | -3.09 | 1.17        | 1.23     |
| 3   | D     | 3899 | OMG  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 48  | w     | 1490 | OMG  | C5-N7   | -3.08 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 2364 | OMG  | C5-N7 | -3.08 | 1.33        | 1.39     |
| 3   | D     | 1781 | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 3   | D     | 4637 | OMG  | C5-N7 | -3.08 | 1.33        | 1.39     |
| 48  | w     | 966  | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 3   | D     | 1860 | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 3   | D     | 4499 | OMG  | C5-N7 | -3.07 | 1.33        | 1.39     |
| 3   | D     | 4618 | OMG  | C5-N7 | -3.07 | 1.33        | 1.39     |
| 48  | w     | 1177 | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 5   | F     | 75   | OMG  | C5-N7 | -3.06 | 1.33        | 1.39     |
| 3   | D     | 3764 | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 3   | D     | 4623 | OMG  | C5-N7 | -3.06 | 1.33        | 1.39     |
| 48  | w     | 406  | PSU  | C6-C5 | 3.05  | 1.38        | 1.35     |
| 3   | D     | 3841 | OMC  | O2-C2 | -3.05 | 1.18        | 1.23     |
| 48  | w     | 651  | PSU  | C6-C5 | 3.04  | 1.38        | 1.35     |
| 3   | D     | 2632 | PSU  | C6-C5 | 3.04  | 1.38        | 1.35     |
| 3   | D     | 1316 | OMG  | O6-C6 | -3.04 | 1.17        | 1.23     |
| 3   | D     | 3899 | OMG  | O6-C6 | -3.04 | 1.17        | 1.23     |
| 48  | w     | 1046 | PSU  | C6-C5 | 3.04  | 1.38        | 1.35     |
| 3   | D     | 4498 | OMU  | C4-N3 | 3.04  | 1.44        | 1.38     |
| 3   | D     | 5010 | PSU  | C6-C5 | 3.04  | 1.38        | 1.35     |
| 3   | D     | 2351 | OMC  | O2-C2 | -3.04 | 1.18        | 1.23     |
| 3   | D     | 3744 | OMG  | C5-N7 | -3.03 | 1.33        | 1.39     |
| 3   | D     | 3730 | PSU  | C6-C5 | 3.02  | 1.38        | 1.35     |
| 48  | w     | 1391 | OMC  | C6-N1 | 3.02  | 1.45        | 1.38     |
| 3   | D     | 4228 | OMG  | O6-C6 | -3.02 | 1.17        | 1.23     |
| 3   | D     | 4370 | OMG  | O6-C6 | -3.02 | 1.17        | 1.23     |
| 3   | D     | 4536 | OMC  | O2-C2 | -3.02 | 1.18        | 1.23     |
| 3   | D     | 4306 | OMU  | O4-C4 | -3.02 | 1.18        | 1.24     |
| 3   | D     | 4227 | OMU  | C4-N3 | 3.02  | 1.44        | 1.38     |
| 3   | D     | 4423 | PSU  | C6-C5 | 3.02  | 1.38        | 1.35     |
| 3   | D     | 4228 | OMG  | C5-N7 | -3.01 | 1.33        | 1.39     |
| 3   | D     | 4494 | OMG  | O6-C6 | -3.01 | 1.17        | 1.23     |
| 3   | D     | 2861 | OMC  | O2-C2 | -3.00 | 1.18        | 1.23     |
| 48  | w     | 1703 | OMC  | C6-N1 | 3.00  | 1.45        | 1.38     |
| 3   | D     | 2861 | OMC  | C6-N1 | 3.00  | 1.45        | 1.38     |
| 3   | D     | 3925 | OMU  | O4-C4 | -2.99 | 1.18        | 1.24     |
| 3   | D     | 2365 | OMC  | O2-C2 | -2.99 | 1.18        | 1.23     |
| 3   | D     | 3627 | OMG  | O6-C6 | -2.99 | 1.17        | 1.23     |
| 3   | D     | 3701 | OMC  | C6-N1 | 2.98  | 1.45        | 1.38     |
| 3   | D     | 2837 | OMU  | O4-C4 | -2.98 | 1.18        | 1.24     |
| 3   | D     | 4552 | PSU  | C6-C5 | 2.98  | 1.38        | 1.35     |
| 3   | D     | 1744 | PSU  | C6-C5 | 2.98  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 3925 | OMU  | O2-C2   | -2.97 | 1.17        | 1.23     |
| 2   | C     | 34   | 56B  | C11-C12 | 2.97  | 1.58        | 1.53     |
| 3   | D     | 4306 | OMU  | O2-C2   | -2.97 | 1.17        | 1.23     |
| 3   | D     | 3887 | OMC  | C6-N1   | 2.97  | 1.45        | 1.38     |
| 3   | D     | 1340 | OMC  | O2-C2   | -2.97 | 1.18        | 1.23     |
| 48  | w     | 681  | PSU  | C6-C5   | 2.97  | 1.38        | 1.35     |
| 3   | D     | 2422 | OMC  | C6-N1   | 2.97  | 1.45        | 1.38     |
| 3   | D     | 2824 | OMC  | C6-N1   | 2.97  | 1.45        | 1.38     |
| 3   | D     | 3887 | OMC  | O2-C2   | -2.97 | 1.18        | 1.23     |
| 3   | D     | 4972 | PSU  | C6-C5   | 2.97  | 1.38        | 1.35     |
| 3   | D     | 2824 | OMC  | O2-C2   | -2.97 | 1.18        | 1.23     |
| 3   | D     | 4689 | PSU  | C6-C5   | 2.97  | 1.38        | 1.35     |
| 48  | w     | 1703 | OMC  | O2-C2   | -2.96 | 1.18        | 1.23     |
| 3   | D     | 3744 | OMG  | O6-C6   | -2.96 | 1.18        | 1.23     |
| 3   | D     | 4456 | OMC  | C6-N1   | 2.96  | 1.45        | 1.38     |
| 3   | D     | 2804 | OMC  | C6-N1   | 2.95  | 1.45        | 1.38     |
| 3   | D     | 5001 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 3   | D     | 3853 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 3   | D     | 3695 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 3   | D     | 4623 | OMG  | O6-C6   | -2.95 | 1.18        | 1.23     |
| 3   | D     | 3808 | OMC  | O2-C2   | -2.95 | 1.18        | 1.23     |
| 3   | D     | 1340 | OMC  | C6-N1   | 2.95  | 1.45        | 1.38     |
| 48  | w     | 1643 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 3   | D     | 4628 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 48  | w     | 1056 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 3   | D     | 4620 | OMU  | C4-N3   | 2.94  | 1.43        | 1.38     |
| 3   | D     | 4620 | OMU  | O2-C2   | -2.94 | 1.17        | 1.23     |
| 3   | D     | 4471 | PSU  | C6-C5   | 2.94  | 1.38        | 1.35     |
| 3   | D     | 4293 | PSU  | C6-C5   | 2.94  | 1.38        | 1.35     |
| 3   | D     | 4620 | OMU  | O4-C4   | -2.94 | 1.18        | 1.24     |
| 3   | D     | 4499 | OMG  | O6-C6   | -2.94 | 1.18        | 1.23     |
| 3   | D     | 2422 | OMC  | O2-C2   | -2.94 | 1.18        | 1.23     |
| 3   | D     | 4312 | PSU  | C6-C5   | 2.94  | 1.38        | 1.35     |
| 3   | D     | 4306 | OMU  | C4-N3   | 2.93  | 1.43        | 1.38     |
| 48  | w     | 683  | OMG  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 3   | D     | 2365 | OMC  | C6-N1   | 2.93  | 1.45        | 1.38     |
| 48  | w     | 1328 | OMG  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 3   | D     | 2508 | PSU  | C6-C5   | 2.93  | 1.38        | 1.35     |
| 3   | D     | 4498 | OMU  | O4-C4   | -2.93 | 1.18        | 1.24     |
| 48  | w     | 601  | OMG  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 3   | D     | 1792 | PSU  | C6-C5   | 2.93  | 1.38        | 1.35     |
| 3   | D     | 4196 | OMG  | O6-C6   | -2.93 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 48  | w     | 509  | OMG  | C5-N7 | -2.92 | 1.33        | 1.39     |
| 3   | D     | 4618 | OMG  | O6-C6 | -2.92 | 1.18        | 1.23     |
| 3   | D     | 4227 | OMU  | O4-C4 | -2.92 | 1.18        | 1.24     |
| 3   | D     | 1862 | PSU  | C6-C5 | 2.91  | 1.38        | 1.35     |
| 3   | D     | 4403 | PSU  | C6-C5 | 2.91  | 1.38        | 1.35     |
| 2   | C     | 6    | 2MG  | C5-N7 | -2.91 | 1.33        | 1.39     |
| 3   | D     | 4431 | PSU  | C6-C5 | 2.91  | 1.38        | 1.35     |
| 3   | D     | 4576 | PSU  | C6-C5 | 2.91  | 1.38        | 1.35     |
| 3   | D     | 2837 | OMU  | C4-N3 | 2.91  | 1.43        | 1.38     |
| 48  | w     | 1850 | MA6  | C5-C4 | -2.91 | 1.33        | 1.39     |
| 3   | D     | 3792 | OMG  | O6-C6 | -2.91 | 1.18        | 1.23     |
| 48  | w     | 644  | OMG  | C5-C6 | 2.91  | 1.55        | 1.44     |
| 3   | D     | 4637 | OMG  | O6-C6 | -2.90 | 1.18        | 1.23     |
| 3   | D     | 3944 | OMG  | C5-N7 | -2.90 | 1.33        | 1.39     |
| 3   | D     | 3841 | OMC  | C6-N1 | 2.90  | 1.45        | 1.38     |
| 3   | D     | 4498 | OMU  | O2-C2 | -2.90 | 1.17        | 1.23     |
| 3   | D     | 4536 | OMC  | C6-N1 | 2.90  | 1.45        | 1.38     |
| 3   | D     | 2364 | OMG  | O6-C6 | -2.90 | 1.18        | 1.23     |
| 3   | D     | 4442 | PSU  | C6-C5 | 2.90  | 1.38        | 1.35     |
| 3   | D     | 1760 | OMG  | C5-C6 | 2.90  | 1.55        | 1.44     |
| 3   | D     | 4353 | PSU  | C6-C5 | 2.90  | 1.38        | 1.35     |
| 3   | D     | 2804 | OMC  | O2-C2 | -2.90 | 1.18        | 1.23     |
| 2   | B     | 6    | 2MG  | C5-N7 | -2.89 | 1.33        | 1.39     |
| 3   | D     | 4361 | PSU  | C6-C5 | 2.88  | 1.38        | 1.35     |
| 48  | w     | 1850 | MA6  | C6-N6 | 2.88  | 1.45        | 1.36     |
| 3   | D     | 3925 | OMU  | C4-N3 | 2.88  | 1.43        | 1.38     |
| 3   | D     | 4579 | PSU  | C6-C5 | 2.88  | 1.38        | 1.35     |
| 3   | D     | 2351 | OMC  | C6-N1 | 2.88  | 1.44        | 1.38     |
| 3   | D     | 4227 | OMU  | O2-C2 | -2.87 | 1.17        | 1.23     |
| 48  | w     | 436  | OMG  | C5-C6 | 2.87  | 1.55        | 1.44     |
| 3   | D     | 4457 | PSU  | C6-C5 | 2.87  | 1.38        | 1.35     |
| 3   | D     | 4521 | PSU  | C6-C5 | 2.87  | 1.38        | 1.35     |
| 3   | D     | 2837 | OMU  | O2-C2 | -2.87 | 1.17        | 1.23     |
| 3   | D     | 2415 | OMU  | O4-C4 | -2.87 | 1.18        | 1.24     |
| 3   | D     | 1782 | PSU  | C6-C5 | 2.86  | 1.38        | 1.35     |
| 48  | w     | 1328 | OMG  | C5-C6 | 2.86  | 1.55        | 1.44     |
| 3   | D     | 3944 | OMG  | C5-C6 | 2.86  | 1.55        | 1.44     |
| 3   | D     | 1625 | OMG  | O6-C6 | -2.86 | 1.18        | 1.23     |
| 48  | w     | 509  | OMG  | C5-C6 | 2.85  | 1.55        | 1.44     |
| 48  | w     | 644  | OMG  | C5-N7 | -2.85 | 1.33        | 1.39     |
| 48  | w     | 1490 | OMG  | O6-C6 | -2.84 | 1.18        | 1.23     |
| 3   | D     | 3808 | OMC  | C6-N1 | 2.84  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 2424 | OMG  | O6-C6 | -2.84 | 1.18        | 1.23     |
| 48  | w     | 683  | OMG  | C5-C6 | 2.84  | 1.54        | 1.44     |
| 3   | D     | 4299 | PSU  | C6-C5 | 2.82  | 1.38        | 1.35     |
| 48  | w     | 1692 | PSU  | C6-C5 | 2.82  | 1.38        | 1.35     |
| 48  | w     | 1639 | G7M  | C2-N1 | 2.82  | 1.44        | 1.37     |
| 48  | w     | 683  | OMG  | O6-C6 | -2.82 | 1.18        | 1.23     |
| 3   | D     | 3637 | PSU  | C6-C5 | 2.82  | 1.38        | 1.35     |
| 48  | w     | 436  | OMG  | C5-N7 | -2.82 | 1.33        | 1.39     |
| 48  | w     | 1081 | PSU  | C6-C5 | 2.82  | 1.38        | 1.35     |
| 3   | D     | 3639 | PSU  | C6-C5 | 2.81  | 1.38        | 1.35     |
| 3   | D     | 1683 | PSU  | C6-C5 | 2.81  | 1.38        | 1.35     |
| 48  | w     | 601  | OMG  | C5-C6 | 2.80  | 1.54        | 1.44     |
| 48  | w     | 601  | OMG  | O6-C6 | -2.80 | 1.18        | 1.23     |
| 48  | w     | 1850 | MA6  | C5-N7 | -2.80 | 1.33        | 1.39     |
| 3   | D     | 3701 | OMC  | O2-C2 | -2.80 | 1.18        | 1.23     |
| 3   | D     | 2415 | OMU  | O2-C2 | -2.79 | 1.17        | 1.23     |
| 48  | w     | 1326 | OMU  | O2-C2 | -2.79 | 1.17        | 1.23     |
| 3   | D     | 3920 | PSU  | C6-C5 | 2.79  | 1.38        | 1.35     |
| 3   | D     | 4530 | UR3  | C6-N1 | 2.79  | 1.44        | 1.38     |
| 2   | B     | 57   | 1MA  | C2-N1 | 2.79  | 1.41        | 1.35     |
| 2   | C     | 57   | 1MA  | C2-N1 | 2.79  | 1.41        | 1.35     |
| 2   | C     | 9    | 1MA  | C2-N1 | 2.78  | 1.41        | 1.35     |
| 48  | w     | 1851 | MA6  | C6-N6 | 2.78  | 1.45        | 1.36     |
| 5   | F     | 75   | OMG  | O6-C6 | -2.78 | 1.18        | 1.23     |
| 3   | D     | 4618 | OMG  | C5-C6 | 2.78  | 1.54        | 1.44     |
| 5   | F     | 75   | OMG  | C5-C6 | 2.77  | 1.54        | 1.44     |
| 48  | w     | 1490 | OMG  | C5-C6 | 2.77  | 1.54        | 1.44     |
| 48  | w     | 1391 | OMC  | O2-C2 | -2.77 | 1.18        | 1.23     |
| 3   | D     | 3744 | OMG  | C5-C6 | 2.76  | 1.54        | 1.44     |
| 48  | w     | 1326 | OMU  | O4-C4 | -2.76 | 1.19        | 1.24     |
| 3   | D     | 3758 | PSU  | C6-C5 | 2.75  | 1.38        | 1.35     |
| 3   | D     | 4447 | 5MC  | O2-C2 | -2.75 | 1.18        | 1.23     |
| 48  | w     | 436  | OMG  | O6-C6 | -2.75 | 1.18        | 1.23     |
| 48  | w     | 1639 | G7M  | C6-N1 | 2.74  | 1.43        | 1.38     |
| 3   | D     | 3851 | PSU  | C6-C5 | 2.74  | 1.38        | 1.35     |
| 3   | D     | 1760 | OMG  | C5-N7 | -2.74 | 1.33        | 1.39     |
| 48  | w     | 1804 | OMU  | O4-C4 | -2.74 | 1.19        | 1.24     |
| 48  | w     | 1442 | OMU  | O4-C4 | -2.74 | 1.19        | 1.24     |
| 3   | D     | 4494 | OMG  | C5-C6 | 2.73  | 1.54        | 1.44     |
| 48  | w     | 116  | OMU  | O4-C4 | -2.73 | 1.19        | 1.24     |
| 3   | D     | 1536 | PSU  | C6-C5 | 2.73  | 1.38        | 1.35     |
| 48  | w     | 509  | OMG  | C6-N1 | 2.72  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 3899 | OMG  | C5-C6 | 2.72  | 1.54        | 1.44     |
| 48  | w     | 517  | OMC  | O2-C2 | -2.72 | 1.18        | 1.23     |
| 3   | D     | 4499 | OMG  | C5-C6 | 2.71  | 1.54        | 1.44     |
| 2   | C     | 34   | 56B  | C2-N1 | 2.71  | 1.44        | 1.37     |
| 2   | B     | 19   | H2U  | C2-N3 | -2.71 | 1.33        | 1.38     |
| 3   | D     | 2424 | OMG  | C5-C6 | 2.71  | 1.54        | 1.44     |
| 2   | B     | 34   | 56B  | O6-C6 | -2.71 | 1.18        | 1.23     |
| 3   | D     | 4228 | OMG  | C5-C6 | 2.71  | 1.54        | 1.44     |
| 48  | w     | 1832 | 6MZ  | C5-C4 | -2.70 | 1.34        | 1.39     |
| 48  | w     | 1328 | OMG  | O6-C6 | -2.70 | 1.18        | 1.23     |
| 3   | D     | 4196 | OMG  | C5-C6 | 2.70  | 1.54        | 1.44     |
| 3   | D     | 3792 | OMG  | C5-C6 | 2.70  | 1.54        | 1.44     |
| 3   | D     | 1625 | OMG  | C5-C6 | 2.70  | 1.54        | 1.44     |
| 48  | w     | 121  | OMU  | O4-C4 | -2.70 | 1.19        | 1.24     |
| 3   | D     | 3944 | OMG  | O6-C6 | -2.70 | 1.18        | 1.23     |
| 3   | D     | 1760 | OMG  | C6-N1 | 2.69  | 1.43        | 1.38     |
| 48  | w     | 462  | OMC  | O2-C2 | -2.69 | 1.18        | 1.23     |
| 48  | w     | 1442 | OMU  | O2-C2 | -2.69 | 1.18        | 1.23     |
| 3   | D     | 4623 | OMG  | C5-C6 | 2.69  | 1.54        | 1.44     |
| 3   | D     | 2364 | OMG  | C5-C6 | 2.69  | 1.54        | 1.44     |
| 2   | C     | 19   | H2U  | C2-N3 | -2.68 | 1.33        | 1.38     |
| 3   | D     | 4637 | OMG  | C5-C6 | 2.68  | 1.54        | 1.44     |
| 3   | D     | 4370 | OMG  | C5-C6 | 2.68  | 1.54        | 1.44     |
| 48  | w     | 644  | OMG  | O6-C6 | -2.68 | 1.18        | 1.23     |
| 48  | w     | 509  | OMG  | C2-N1 | 2.67  | 1.44        | 1.37     |
| 3   | D     | 3627 | OMG  | C5-C6 | 2.67  | 1.54        | 1.44     |
| 48  | w     | 428  | OMU  | O4-C4 | -2.66 | 1.19        | 1.24     |
| 3   | D     | 4392 | OMG  | C5-C6 | 2.66  | 1.54        | 1.44     |
| 3   | D     | 4220 | 6MZ  | C5-C4 | -2.66 | 1.34        | 1.39     |
| 48  | w     | 644  | OMG  | C6-N1 | 2.66  | 1.43        | 1.38     |
| 48  | w     | 799  | OMU  | O4-C4 | -2.66 | 1.19        | 1.24     |
| 48  | w     | 627  | OMU  | O4-C4 | -2.65 | 1.19        | 1.24     |
| 3   | D     | 1316 | OMG  | C5-C6 | 2.65  | 1.54        | 1.44     |
| 48  | w     | 172  | OMU  | O4-C4 | -2.65 | 1.19        | 1.24     |
| 48  | w     | 1804 | OMU  | O2-C2 | -2.65 | 1.18        | 1.23     |
| 3   | D     | 3944 | OMG  | C6-N1 | 2.64  | 1.43        | 1.38     |
| 48  | w     | 436  | OMG  | C6-N1 | 2.64  | 1.43        | 1.38     |
| 48  | w     | 509  | OMG  | O6-C6 | -2.64 | 1.18        | 1.23     |
| 48  | w     | 428  | OMU  | O2-C2 | -2.64 | 1.18        | 1.23     |
| 3   | D     | 1760 | OMG  | O6-C6 | -2.63 | 1.18        | 1.23     |
| 3   | D     | 1773 | OMU  | O2-C2 | -2.63 | 1.18        | 1.23     |
| 3   | D     | 1522 | OMG  | C5-C6 | 2.63  | 1.54        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 9    | 1MA  | C2-N1   | 2.63  | 1.40        | 1.35     |
| 48  | w     | 1328 | OMG  | C6-N1   | 2.62  | 1.43        | 1.38     |
| 2   | C     | 6    | 2MG  | C5-C6   | 2.62  | 1.54        | 1.44     |
| 3   | D     | 1773 | OMU  | O4-C4   | -2.61 | 1.19        | 1.24     |
| 48  | w     | 121  | OMU  | O2-C2   | -2.61 | 1.18        | 1.23     |
| 3   | D     | 1677 | PSU  | C6-C5   | 2.60  | 1.38        | 1.35     |
| 48  | w     | 1288 | OMU  | O4-C4   | -2.60 | 1.19        | 1.24     |
| 48  | w     | 601  | OMG  | C6-N1   | 2.60  | 1.43        | 1.38     |
| 48  | w     | 116  | OMU  | O2-C2   | -2.60 | 1.18        | 1.23     |
| 2   | B     | 34   | 56B  | C2-N1   | 2.59  | 1.44        | 1.37     |
| 48  | w     | 1288 | OMU  | O2-C2   | -2.59 | 1.18        | 1.23     |
| 2   | C     | 34   | 56B  | O6-C6   | -2.58 | 1.18        | 1.23     |
| 2   | B     | 6    | 2MG  | C5-C6   | 2.58  | 1.54        | 1.44     |
| 48  | w     | 174  | OMC  | O2-C2   | -2.58 | 1.18        | 1.23     |
| 2   | B     | 19   | H2U  | C4-N3   | -2.57 | 1.33        | 1.37     |
| 48  | w     | 1639 | G7M  | O6-C6   | -2.56 | 1.18        | 1.23     |
| 48  | w     | 683  | OMG  | C6-N1   | 2.56  | 1.43        | 1.38     |
| 48  | w     | 627  | OMU  | O2-C2   | -2.56 | 1.18        | 1.23     |
| 48  | w     | 1851 | MA6  | C5-N7   | -2.55 | 1.34        | 1.39     |
| 48  | w     | 799  | OMU  | O2-C2   | -2.55 | 1.18        | 1.23     |
| 3   | D     | 1760 | OMG  | C2-N1   | 2.54  | 1.44        | 1.37     |
| 48  | w     | 668  | A2M  | O4'-C4' | -2.54 | 1.39        | 1.45     |
| 48  | w     | 644  | OMG  | C2-N1   | 2.53  | 1.43        | 1.37     |
| 48  | w     | 172  | OMU  | O2-C2   | -2.52 | 1.18        | 1.23     |
| 2   | C     | 19   | H2U  | C4-N3   | -2.51 | 1.33        | 1.37     |
| 3   | D     | 3744 | OMG  | C6-N1   | 2.51  | 1.43        | 1.38     |
| 48  | w     | 462  | OMC  | C5-C4   | 2.51  | 1.48        | 1.42     |
| 48  | w     | 517  | OMC  | C5-C4   | 2.51  | 1.48        | 1.42     |
| 48  | w     | 174  | OMC  | C5-C4   | 2.50  | 1.48        | 1.42     |
| 48  | w     | 1328 | OMG  | C2-N1   | 2.49  | 1.43        | 1.37     |
| 5   | F     | 75   | OMG  | C6-N1   | 2.49  | 1.43        | 1.38     |
| 48  | w     | 601  | OMG  | C2-N1   | 2.49  | 1.43        | 1.37     |
| 3   | D     | 3944 | OMG  | C2-N1   | 2.49  | 1.43        | 1.37     |
| 3   | D     | 2424 | OMG  | C6-N1   | 2.48  | 1.43        | 1.38     |
| 48  | w     | 436  | OMG  | C2-N1   | 2.47  | 1.43        | 1.37     |
| 48  | w     | 1851 | MA6  | C8-N9   | -2.47 | 1.33        | 1.37     |
| 3   | D     | 4530 | UR3  | O4-C4   | -2.45 | 1.18        | 1.23     |
| 3   | D     | 1625 | OMG  | C6-N1   | 2.45  | 1.43        | 1.38     |
| 48  | w     | 683  | OMG  | C2-N1   | 2.44  | 1.43        | 1.37     |
| 3   | D     | 4499 | OMG  | C6-N1   | 2.43  | 1.43        | 1.38     |
| 3   | D     | 4618 | OMG  | C6-N1   | 2.42  | 1.43        | 1.38     |
| 48  | w     | 1490 | OMG  | C6-N1   | 2.41  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 1524 | A2M  | O4'-C4' | -2.41 | 1.39        | 1.45     |
| 3   | D     | 4530 | UR3  | O2-C2   | -2.40 | 1.18        | 1.22     |
| 2   | C     | 6    | 2MG  | C6-N1   | 2.40  | 1.43        | 1.38     |
| 3   | D     | 4637 | OMG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 3   | D     | 3782 | 5MC  | O2-C2   | -2.39 | 1.19        | 1.23     |
| 2   | B     | 38   | 5MC  | O2-C2   | -2.38 | 1.19        | 1.23     |
| 3   | D     | 4494 | OMG  | C6-N1   | 2.38  | 1.43        | 1.38     |
| 3   | D     | 2424 | OMG  | C2-N1   | 2.38  | 1.43        | 1.37     |
| 3   | D     | 3744 | OMG  | C2-N1   | 2.37  | 1.43        | 1.37     |
| 3   | D     | 4618 | OMG  | C2-N1   | 2.37  | 1.43        | 1.37     |
| 2   | B     | 6    | 2MG  | C6-N1   | 2.37  | 1.43        | 1.38     |
| 3   | D     | 2364 | OMG  | C6-N1   | 2.37  | 1.43        | 1.38     |
| 3   | D     | 4623 | OMG  | C6-N1   | 2.36  | 1.43        | 1.38     |
| 3   | D     | 4499 | OMG  | C2-N1   | 2.36  | 1.43        | 1.37     |
| 3   | D     | 4228 | OMG  | C6-N1   | 2.35  | 1.43        | 1.38     |
| 3   | D     | 3627 | OMG  | C6-N1   | 2.35  | 1.43        | 1.38     |
| 5   | F     | 75   | OMG  | C2-N1   | 2.35  | 1.43        | 1.37     |
| 3   | D     | 4220 | 6MZ  | C8-N9   | -2.35 | 1.33        | 1.37     |
| 3   | D     | 3701 | OMC  | C5-C4   | 2.33  | 1.48        | 1.42     |
| 2   | B     | 48   | 5MC  | O2-C2   | -2.33 | 1.19        | 1.23     |
| 2   | C     | 34   | 56B  | C6-N1   | 2.33  | 1.43        | 1.38     |
| 48  | w     | 1832 | 6MZ  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 48  | w     | 1391 | OMC  | C5-C4   | 2.33  | 1.48        | 1.42     |
| 3   | D     | 1522 | OMG  | C4-N9   | -2.32 | 1.32        | 1.38     |
| 3   | D     | 4623 | OMG  | C2-N1   | 2.32  | 1.43        | 1.37     |
| 3   | D     | 3899 | OMG  | C6-N1   | 2.32  | 1.43        | 1.38     |
| 2   | C     | 38   | 5MC  | O2-C2   | -2.32 | 1.19        | 1.23     |
| 3   | D     | 4370 | OMG  | C6-N1   | 2.32  | 1.43        | 1.38     |
| 48  | w     | 1832 | 6MZ  | C8-N9   | -2.30 | 1.33        | 1.37     |
| 3   | D     | 4392 | OMG  | C6-N1   | 2.30  | 1.43        | 1.38     |
| 3   | D     | 1625 | OMG  | C2-N1   | 2.30  | 1.43        | 1.37     |
| 3   | D     | 3899 | OMG  | C4-N9   | -2.29 | 1.32        | 1.38     |
| 3   | D     | 3792 | OMG  | C6-N1   | 2.29  | 1.43        | 1.38     |
| 2   | B     | 47   | 5MC  | O2-C2   | -2.28 | 1.19        | 1.23     |
| 3   | D     | 4494 | OMG  | C2-N1   | 2.28  | 1.43        | 1.37     |
| 48  | w     | 1490 | OMG  | C2-N1   | 2.27  | 1.43        | 1.37     |
| 2   | B     | 6    | 2MG  | O6-C6   | -2.27 | 1.19        | 1.23     |
| 2   | C     | 47   | 5MC  | O2-C2   | -2.27 | 1.19        | 1.23     |
| 3   | D     | 4196 | OMG  | C6-N1   | 2.26  | 1.43        | 1.38     |
| 3   | D     | 3899 | OMG  | C2-N1   | 2.25  | 1.43        | 1.37     |
| 48  | w     | 1703 | OMC  | C5-C4   | 2.25  | 1.48        | 1.42     |
| 3   | D     | 2364 | OMG  | C4-N9   | -2.25 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 3792 | OMG  | C2-N1   | 2.24  | 1.43        | 1.37     |
| 3   | D     | 4623 | OMG  | C4-N9   | -2.24 | 1.32        | 1.38     |
| 3   | D     | 2364 | OMG  | C2-N1   | 2.24  | 1.43        | 1.37     |
| 3   | D     | 3627 | OMG  | C2-N1   | 2.23  | 1.43        | 1.37     |
| 3   | D     | 3808 | OMC  | C5-C4   | 2.23  | 1.48        | 1.42     |
| 3   | D     | 2422 | OMC  | C5-C4   | 2.23  | 1.48        | 1.42     |
| 2   | C     | 48   | 5MC  | O2-C2   | -2.23 | 1.19        | 1.23     |
| 48  | w     | 166  | A2M  | C5-C4   | 2.22  | 1.43        | 1.39     |
| 2   | C     | 48   | 5MC  | CM5-C5  | 2.22  | 1.56        | 1.50     |
| 3   | D     | 1316 | OMG  | C4-N9   | -2.22 | 1.32        | 1.38     |
| 3   | D     | 3887 | OMC  | C5-C4   | 2.22  | 1.48        | 1.42     |
| 3   | D     | 4228 | OMG  | C2-N1   | 2.22  | 1.43        | 1.37     |
| 2   | B     | 48   | 5MC  | CM5-C5  | 2.21  | 1.56        | 1.50     |
| 2   | B     | 47   | 5MC  | CM5-C5  | 2.21  | 1.56        | 1.50     |
| 2   | C     | 6    | 2MG  | O6-C6   | -2.20 | 1.19        | 1.23     |
| 2   | C     | 38   | 5MC  | CM5-C5  | 2.20  | 1.56        | 1.50     |
| 3   | D     | 4637 | OMG  | C2-N1   | 2.20  | 1.43        | 1.37     |
| 3   | D     | 2824 | OMC  | C5-C4   | 2.20  | 1.48        | 1.42     |
| 3   | D     | 4196 | OMG  | C2-N1   | 2.20  | 1.43        | 1.37     |
| 3   | D     | 4228 | OMG  | C4-N9   | -2.19 | 1.32        | 1.38     |
| 2   | C     | 47   | 5MC  | CM5-C5  | 2.19  | 1.56        | 1.50     |
| 3   | D     | 4370 | OMG  | C2-N1   | 2.19  | 1.43        | 1.37     |
| 3   | D     | 4392 | OMG  | C4-N9   | -2.19 | 1.32        | 1.38     |
| 2   | B     | 38   | 5MC  | CM5-C5  | 2.19  | 1.56        | 1.50     |
| 3   | D     | 1522 | OMG  | C2-N1   | 2.18  | 1.43        | 1.37     |
| 3   | D     | 1522 | OMG  | C6-N1   | 2.18  | 1.42        | 1.38     |
| 3   | D     | 2424 | OMG  | C4-N9   | -2.18 | 1.32        | 1.38     |
| 48  | w     | 166  | A2M  | C8-N9   | 2.18  | 1.41        | 1.37     |
| 3   | D     | 4456 | OMC  | C5-C4   | 2.18  | 1.47        | 1.42     |
| 3   | D     | 4499 | OMG  | C4-N9   | -2.17 | 1.32        | 1.38     |
| 3   | D     | 1316 | OMG  | C6-N1   | 2.17  | 1.42        | 1.38     |
| 3   | D     | 2365 | OMC  | C5-C4   | 2.17  | 1.47        | 1.42     |
| 3   | D     | 3627 | OMG  | C4-N9   | -2.17 | 1.32        | 1.38     |
| 3   | D     | 4220 | 6MZ  | C5-N7   | -2.17 | 1.34        | 1.39     |
| 3   | D     | 2804 | OMC  | C5-C4   | 2.16  | 1.47        | 1.42     |
| 3   | D     | 2861 | OMC  | C5-C4   | 2.16  | 1.47        | 1.42     |
| 2   | B     | 34   | 56B  | C6-N1   | 2.16  | 1.42        | 1.38     |
| 48  | w     | 1288 | OMU  | C5-C4   | 2.15  | 1.48        | 1.43     |
| 48  | w     | 428  | OMU  | C5-C4   | 2.15  | 1.48        | 1.43     |
| 3   | D     | 3841 | OMC  | C5-C4   | 2.15  | 1.47        | 1.42     |
| 3   | D     | 3818 | UY1  | O4'-C1' | -2.15 | 1.40        | 1.43     |
| 3   | D     | 4370 | OMG  | C4-N9   | -2.15 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 4536 | OMC  | C5-C4   | 2.15  | 1.47        | 1.42     |
| 3   | D     | 4637 | OMG  | C4-N9   | -2.15 | 1.32        | 1.38     |
| 3   | D     | 4392 | OMG  | C2-N1   | 2.15  | 1.43        | 1.37     |
| 3   | D     | 1316 | OMG  | C8-N9   | -2.15 | 1.32        | 1.37     |
| 3   | D     | 1316 | OMG  | C2-N1   | 2.14  | 1.43        | 1.37     |
| 48  | w     | 576  | A2M  | C5-C4   | 2.14  | 1.43        | 1.39     |
| 3   | D     | 3744 | OMG  | C4-N9   | -2.12 | 1.32        | 1.38     |
| 48  | w     | 1288 | OMU  | C6-N1   | 2.12  | 1.43        | 1.38     |
| 48  | w     | 121  | OMU  | C6-N1   | 2.11  | 1.43        | 1.38     |
| 3   | D     | 4523 | A2M  | O4'-C4' | -2.11 | 1.40        | 1.45     |
| 3   | D     | 4494 | OMG  | C4-N9   | -2.11 | 1.32        | 1.38     |
| 48  | w     | 1326 | OMU  | C6-N1   | 2.10  | 1.43        | 1.38     |
| 3   | D     | 2363 | A2M  | O4'-C4' | -2.10 | 1.40        | 1.45     |
| 2   | C     | 53   | 5MU  | O2-C2   | -2.10 | 1.19        | 1.23     |
| 48  | w     | 590  | A2M  | C8-N9   | 2.09  | 1.41        | 1.37     |
| 3   | D     | 4196 | OMG  | C4-N9   | -2.09 | 1.32        | 1.38     |
| 3   | D     | 1773 | OMU  | C5-C4   | 2.09  | 1.48        | 1.43     |
| 48  | w     | 512  | A2M  | C5-C4   | 2.08  | 1.42        | 1.39     |
| 48  | w     | 172  | OMU  | C6-N1   | 2.08  | 1.43        | 1.38     |
| 48  | w     | 590  | A2M  | C5-C4   | 2.08  | 1.42        | 1.39     |
| 3   | D     | 3792 | OMG  | C4-N9   | -2.08 | 1.32        | 1.38     |
| 48  | w     | 627  | OMU  | C5-C4   | 2.08  | 1.48        | 1.43     |
| 3   | D     | 1683 | PSU  | C4-C5   | -2.08 | 1.38        | 1.44     |
| 48  | w     | 799  | OMU  | C5-C4   | 2.07  | 1.48        | 1.43     |
| 3   | D     | 4618 | OMG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 3   | D     | 1340 | OMC  | C5-C4   | 2.07  | 1.47        | 1.42     |
| 48  | w     | 172  | OMU  | C5-C4   | 2.07  | 1.48        | 1.43     |
| 48  | w     | 799  | OMU  | C6-N1   | 2.07  | 1.43        | 1.38     |
| 48  | w     | 468  | A2M  | C5-C4   | 2.07  | 1.42        | 1.39     |
| 48  | w     | 428  | OMU  | C6-N1   | 2.06  | 1.43        | 1.38     |
| 3   | D     | 1677 | PSU  | O4'-C1' | -2.06 | 1.41        | 1.43     |
| 3   | D     | 1773 | OMU  | C6-N1   | 2.06  | 1.43        | 1.38     |
| 5   | F     | 75   | OMG  | C4-N9   | -2.06 | 1.32        | 1.38     |
| 3   | D     | 4293 | PSU  | C4-C5   | -2.03 | 1.38        | 1.44     |
| 3   | D     | 3899 | OMG  | C8-N9   | -2.03 | 1.33        | 1.37     |
| 3   | D     | 1536 | PSU  | C4-C5   | -2.03 | 1.38        | 1.44     |
| 48  | w     | 159  | A2M  | C5-C4   | 2.02  | 1.42        | 1.39     |
| 48  | w     | 116  | OMU  | C5-C4   | 2.02  | 1.48        | 1.43     |
| 48  | w     | 121  | OMU  | C5-C4   | 2.01  | 1.48        | 1.43     |
| 48  | w     | 1851 | MA6  | C4-N9   | -2.01 | 1.33        | 1.37     |
| 48  | w     | 116  | OMU  | C6-N1   | 2.01  | 1.42        | 1.38     |
| 3   | D     | 4530 | UR3  | C5-C4   | 2.01  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 4494 | OMG  | C8-N9 | -2.01 | 1.33        | 1.37     |

All (950) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | B     | 53   | 5MU  | C5-C4-N3  | 12.26 | 125.77      | 115.31   |
| 2   | C     | 53   | 5MU  | C5-C4-N3  | 12.00 | 125.55      | 115.31   |
| 2   | C     | 53   | 5MU  | C5-C6-N1  | -9.91 | 113.14      | 123.34   |
| 2   | B     | 53   | 5MU  | C5-C6-N1  | -9.76 | 113.29      | 123.34   |
| 2   | C     | 34   | 56B  | C1'-N9-C4 | -7.37 | 104.61      | 126.50   |
| 2   | B     | 34   | 56B  | C1'-N9-C4 | -7.21 | 105.08      | 126.50   |
| 2   | B     | 34   | 56B  | C5-C4-N3  | -6.69 | 119.69      | 127.52   |
| 2   | C     | 34   | 56B  | C5-C4-N3  | -6.57 | 119.83      | 127.52   |
| 2   | C     | 6    | 2MG  | C2-N3-C4  | 6.47  | 120.06      | 112.04   |
| 2   | B     | 6    | 2MG  | C2-N3-C4  | 6.42  | 120.00      | 112.04   |
| 48  | w     | 1851 | MA6  | N1-C2-N3  | -5.85 | 119.46      | 128.60   |
| 3   | D     | 2415 | OMU  | C4-N3-C2  | -5.82 | 118.90      | 126.58   |
| 3   | D     | 4220 | 6MZ  | N1-C2-N3  | -5.72 | 119.66      | 128.60   |
| 3   | D     | 3925 | OMU  | C4-N3-C2  | -5.66 | 119.12      | 126.58   |
| 3   | D     | 2837 | OMU  | C4-N3-C2  | -5.63 | 119.15      | 126.58   |
| 48  | w     | 1832 | 6MZ  | N1-C2-N3  | -5.52 | 119.97      | 128.60   |
| 48  | w     | 1850 | MA6  | N1-C2-N3  | -5.51 | 119.98      | 128.60   |
| 3   | D     | 4498 | OMU  | C4-N3-C2  | -5.50 | 119.33      | 126.58   |
| 3   | D     | 4306 | OMU  | C4-N3-C2  | -5.47 | 119.36      | 126.58   |
| 48  | w     | 1490 | OMG  | C5-C4-N3  | -5.43 | 119.64      | 128.46   |
| 3   | D     | 4227 | OMU  | C4-N3-C2  | -5.43 | 119.42      | 126.58   |
| 48  | w     | 1804 | OMU  | C4-N3-C2  | -5.38 | 119.49      | 126.58   |
| 3   | D     | 1625 | OMG  | C5-C4-N3  | -5.37 | 119.74      | 128.46   |
| 3   | D     | 4620 | OMU  | C4-N3-C2  | -5.34 | 119.54      | 126.58   |
| 48  | w     | 627  | OMU  | C4-N3-C2  | -5.32 | 119.57      | 126.58   |
| 48  | w     | 436  | OMG  | C5-C4-N3  | -5.29 | 119.89      | 128.46   |
| 48  | w     | 428  | OMU  | C4-N3-C2  | -5.28 | 119.62      | 126.58   |
| 3   | D     | 3792 | OMG  | C5-C4-N3  | -5.27 | 119.92      | 128.46   |
| 48  | w     | 172  | OMU  | C4-N3-C2  | -5.26 | 119.64      | 126.58   |
| 3   | D     | 4196 | OMG  | C5-C4-N3  | -5.26 | 119.93      | 128.46   |
| 48  | w     | 683  | OMG  | C5-C4-N3  | -5.26 | 119.94      | 128.46   |
| 48  | w     | 1442 | OMU  | C4-N3-C2  | -5.25 | 119.65      | 126.58   |
| 2   | C     | 6    | 2MG  | C5-C4-N3  | -5.24 | 119.97      | 128.46   |
| 48  | w     | 799  | OMU  | C4-N3-C2  | -5.23 | 119.69      | 126.58   |
| 3   | D     | 3944 | OMG  | C5-C4-N3  | -5.23 | 119.98      | 128.46   |
| 48  | w     | 1832 | 6MZ  | C5-C4-N3  | -5.21 | 119.95      | 126.75   |
| 3   | D     | 4494 | OMG  | C5-C4-N3  | -5.18 | 120.05      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 48  | w     | 509  | OMG  | C5-C4-N3 | -5.17 | 120.07      | 128.46   |
| 48  | w     | 116  | OMU  | C4-N3-C2 | -5.17 | 119.76      | 126.58   |
| 3   | D     | 1773 | OMU  | C4-N3-C2 | -5.15 | 119.79      | 126.58   |
| 2   | B     | 6    | 2MG  | C5-C4-N3 | -5.14 | 120.12      | 128.46   |
| 48  | w     | 1288 | OMU  | C4-N3-C2 | -5.14 | 119.80      | 126.58   |
| 3   | D     | 1316 | OMG  | C5-C4-N3 | -5.13 | 120.14      | 128.46   |
| 3   | D     | 1683 | PSU  | N1-C2-N3 | 5.12  | 120.93      | 115.13   |
| 5   | F     | 75   | OMG  | C5-C4-N3 | -5.11 | 120.17      | 128.46   |
| 3   | D     | 4637 | OMG  | C5-C4-N3 | -5.09 | 120.21      | 128.46   |
| 3   | D     | 4618 | OMG  | C5-C4-N3 | -5.08 | 120.21      | 128.46   |
| 2   | B     | 53   | 5MU  | O4-C4-C5 | -5.08 | 119.02      | 124.90   |
| 3   | D     | 4392 | OMG  | C5-C4-N3 | -5.07 | 120.23      | 128.46   |
| 48  | w     | 1328 | OMG  | C5-C4-N3 | -5.07 | 120.24      | 128.46   |
| 48  | w     | 601  | OMG  | C5-C4-N3 | -5.06 | 120.26      | 128.46   |
| 3   | D     | 4499 | OMG  | C5-C4-N3 | -5.04 | 120.28      | 128.46   |
| 3   | D     | 3627 | OMG  | C5-C4-N3 | -5.04 | 120.29      | 128.46   |
| 48  | w     | 644  | OMG  | C5-C4-N3 | -5.03 | 120.30      | 128.46   |
| 3   | D     | 4370 | OMG  | C5-C4-N3 | -5.03 | 120.31      | 128.46   |
| 3   | D     | 3637 | PSU  | N1-C2-N3 | 5.00  | 120.79      | 115.13   |
| 3   | D     | 3744 | OMG  | C5-C4-N3 | -5.00 | 120.35      | 128.46   |
| 48  | w     | 1326 | OMU  | C4-N3-C2 | -4.99 | 120.00      | 126.58   |
| 2   | C     | 53   | 5MU  | O4-C4-C5 | -4.97 | 119.14      | 124.90   |
| 48  | w     | 121  | OMU  | C4-N3-C2 | -4.96 | 120.04      | 126.58   |
| 3   | D     | 4228 | OMG  | C5-C4-N3 | -4.96 | 120.42      | 128.46   |
| 3   | D     | 2424 | OMG  | C5-C4-N3 | -4.95 | 120.42      | 128.46   |
| 3   | D     | 2364 | OMG  | C5-C4-N3 | -4.92 | 120.49      | 128.46   |
| 3   | D     | 3637 | PSU  | C4-N3-C2 | -4.91 | 119.26      | 126.34   |
| 3   | D     | 4521 | PSU  | C4-N3-C2 | -4.91 | 119.27      | 126.34   |
| 3   | D     | 1536 | PSU  | C4-N3-C2 | -4.90 | 119.28      | 126.34   |
| 2   | B     | 13   | PSU  | N1-C2-N3 | 4.89  | 120.67      | 115.13   |
| 48  | w     | 681  | PSU  | C4-N3-C2 | -4.89 | 119.30      | 126.34   |
| 3   | D     | 4628 | PSU  | N1-C2-N3 | 4.88  | 120.66      | 115.13   |
| 3   | D     | 1862 | PSU  | N1-C2-N3 | 4.87  | 120.65      | 115.13   |
| 3   | D     | 4403 | PSU  | N1-C2-N3 | 4.86  | 120.64      | 115.13   |
| 48  | w     | 681  | PSU  | N1-C2-N3 | 4.85  | 120.63      | 115.13   |
| 3   | D     | 4220 | 6MZ  | C5-C4-N3 | -4.85 | 120.42      | 126.75   |
| 48  | w     | 651  | PSU  | C4-N3-C2 | -4.84 | 119.37      | 126.34   |
| 3   | D     | 3899 | OMG  | C5-C4-N3 | -4.84 | 120.61      | 128.46   |
| 3   | D     | 3851 | PSU  | N1-C2-N3 | 4.83  | 120.61      | 115.13   |
| 3   | D     | 1683 | PSU  | C4-N3-C2 | -4.83 | 119.37      | 126.34   |
| 48  | w     | 1850 | MA6  | C5-C4-N3 | -4.83 | 120.44      | 126.75   |
| 3   | D     | 1782 | PSU  | C4-N3-C2 | -4.83 | 119.38      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 4530 | UR3  | C4-N3-C2 | -4.83 | 120.02      | 124.56   |
| 48  | w     | 815  | PSU  | C4-N3-C2 | -4.82 | 119.39      | 126.34   |
| 3   | D     | 1760 | OMG  | C5-C4-N3 | -4.82 | 120.64      | 128.46   |
| 3   | D     | 1860 | PSU  | N1-C2-N3 | 4.81  | 120.58      | 115.13   |
| 3   | D     | 4431 | PSU  | N1-C2-N3 | 4.81  | 120.58      | 115.13   |
| 3   | D     | 3851 | PSU  | C4-N3-C2 | -4.81 | 119.41      | 126.34   |
| 3   | D     | 5010 | PSU  | C4-N3-C2 | -4.81 | 119.41      | 126.34   |
| 3   | D     | 3695 | PSU  | C4-N3-C2 | -4.80 | 119.42      | 126.34   |
| 3   | D     | 1862 | PSU  | C4-N3-C2 | -4.80 | 119.42      | 126.34   |
| 48  | w     | 1367 | PSU  | C4-N3-C2 | -4.80 | 119.42      | 126.34   |
| 3   | D     | 4521 | PSU  | N1-C2-N3 | 4.80  | 120.57      | 115.13   |
| 3   | D     | 1536 | PSU  | N1-C2-N3 | 4.79  | 120.56      | 115.13   |
| 3   | D     | 5010 | PSU  | N1-C2-N3 | 4.79  | 120.56      | 115.13   |
| 3   | D     | 3920 | PSU  | C4-N3-C2 | -4.79 | 119.44      | 126.34   |
| 48  | w     | 1045 | PSU  | C4-N3-C2 | -4.78 | 119.45      | 126.34   |
| 3   | D     | 4431 | PSU  | C4-N3-C2 | -4.78 | 119.45      | 126.34   |
| 3   | D     | 1677 | PSU  | C4-N3-C2 | -4.78 | 119.45      | 126.34   |
| 3   | D     | 3695 | PSU  | N1-C2-N3 | 4.78  | 120.54      | 115.13   |
| 3   | D     | 4353 | PSU  | C4-N3-C2 | -4.77 | 119.47      | 126.34   |
| 3   | D     | 3770 | PSU  | N1-C2-N3 | 4.77  | 120.53      | 115.13   |
| 3   | D     | 4623 | OMG  | C5-C4-N3 | -4.77 | 120.73      | 128.46   |
| 3   | D     | 4299 | PSU  | N1-C2-N3 | 4.77  | 120.53      | 115.13   |
| 48  | w     | 406  | PSU  | C4-N3-C2 | -4.77 | 119.47      | 126.34   |
| 48  | w     | 1692 | PSU  | C4-N3-C2 | -4.77 | 119.47      | 126.34   |
| 3   | D     | 3920 | PSU  | N1-C2-N3 | 4.76  | 120.53      | 115.13   |
| 3   | D     | 2508 | PSU  | C4-N3-C2 | -4.76 | 119.48      | 126.34   |
| 3   | D     | 4628 | PSU  | C4-N3-C2 | -4.76 | 119.48      | 126.34   |
| 3   | D     | 4403 | PSU  | C4-N3-C2 | -4.76 | 119.48      | 126.34   |
| 3   | D     | 4576 | PSU  | C4-N3-C2 | -4.76 | 119.48      | 126.34   |
| 3   | D     | 4457 | PSU  | C4-N3-C2 | -4.76 | 119.48      | 126.34   |
| 3   | D     | 1522 | OMG  | C5-C4-N3 | -4.75 | 120.75      | 128.46   |
| 3   | D     | 4972 | PSU  | N1-C2-N3 | 4.74  | 120.50      | 115.13   |
| 48  | w     | 814  | PSU  | C4-N3-C2 | -4.74 | 119.51      | 126.34   |
| 2   | C     | 53   | 5MU  | C4-N3-C2 | -4.74 | 121.21      | 127.35   |
| 3   | D     | 4442 | PSU  | N1-C2-N3 | 4.74  | 120.50      | 115.13   |
| 3   | D     | 4353 | PSU  | N1-C2-N3 | 4.74  | 120.50      | 115.13   |
| 48  | w     | 1367 | PSU  | N1-C2-N3 | 4.74  | 120.50      | 115.13   |
| 3   | D     | 3715 | PSU  | C4-N3-C2 | -4.74 | 119.52      | 126.34   |
| 48  | w     | 1347 | PSU  | C4-N3-C2 | -4.73 | 119.52      | 126.34   |
| 3   | D     | 4552 | PSU  | N1-C2-N3 | 4.73  | 120.49      | 115.13   |
| 48  | w     | 572  | PSU  | C4-N3-C2 | -4.73 | 119.52      | 126.34   |
| 3   | D     | 3758 | PSU  | C4-N3-C2 | -4.73 | 119.52      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 4689 | PSU  | N1-C2-N3 | 4.73  | 120.49      | 115.13   |
| 3   | D     | 1782 | PSU  | N1-C2-N3 | 4.73  | 120.49      | 115.13   |
| 48  | w     | 1081 | PSU  | C4-N3-C2 | -4.73 | 119.53      | 126.34   |
| 3   | D     | 1744 | PSU  | C4-N3-C2 | -4.73 | 119.53      | 126.34   |
| 48  | w     | 93   | PSU  | C4-N3-C2 | -4.72 | 119.53      | 126.34   |
| 3   | D     | 4972 | PSU  | C4-N3-C2 | -4.72 | 119.54      | 126.34   |
| 3   | D     | 4442 | PSU  | C4-N3-C2 | -4.72 | 119.54      | 126.34   |
| 48  | w     | 1056 | PSU  | C4-N3-C2 | -4.72 | 119.54      | 126.34   |
| 3   | D     | 1792 | PSU  | C4-N3-C2 | -4.72 | 119.54      | 126.34   |
| 48  | w     | 1177 | PSU  | C4-N3-C2 | -4.72 | 119.54      | 126.34   |
| 48  | w     | 649  | PSU  | N1-C2-N3 | 4.71  | 120.47      | 115.13   |
| 3   | D     | 3730 | PSU  | C4-N3-C2 | -4.70 | 119.56      | 126.34   |
| 48  | w     | 1004 | PSU  | N1-C2-N3 | 4.70  | 120.46      | 115.13   |
| 48  | w     | 651  | PSU  | N1-C2-N3 | 4.70  | 120.46      | 115.13   |
| 3   | D     | 4312 | PSU  | C4-N3-C2 | -4.70 | 119.57      | 126.34   |
| 48  | w     | 686  | PSU  | N1-C2-N3 | 4.70  | 120.45      | 115.13   |
| 48  | w     | 1046 | PSU  | N1-C2-N3 | 4.70  | 120.45      | 115.13   |
| 3   | D     | 1860 | PSU  | C4-N3-C2 | -4.70 | 119.57      | 126.34   |
| 3   | D     | 4293 | PSU  | C4-N3-C2 | -4.70 | 119.57      | 126.34   |
| 48  | w     | 649  | PSU  | C4-N3-C2 | -4.70 | 119.57      | 126.34   |
| 3   | D     | 4312 | PSU  | N1-C2-N3 | 4.69  | 120.45      | 115.13   |
| 3   | D     | 3715 | PSU  | N1-C2-N3 | 4.69  | 120.45      | 115.13   |
| 3   | D     | 4579 | PSU  | N1-C2-N3 | 4.69  | 120.45      | 115.13   |
| 3   | D     | 4293 | PSU  | N1-C2-N3 | 4.69  | 120.44      | 115.13   |
| 3   | D     | 1781 | PSU  | C4-N3-C2 | -4.69 | 119.58      | 126.34   |
| 3   | D     | 5001 | PSU  | C4-N3-C2 | -4.69 | 119.59      | 126.34   |
| 3   | D     | 4361 | PSU  | C4-N3-C2 | -4.68 | 119.59      | 126.34   |
| 48  | w     | 863  | PSU  | N1-C2-N3 | 4.68  | 120.44      | 115.13   |
| 2   | C     | 54   | PSU  | C4-N3-C2 | -4.68 | 119.59      | 126.34   |
| 2   | B     | 53   | 5MU  | C4-N3-C2 | -4.68 | 121.29      | 127.35   |
| 3   | D     | 4532 | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 3   | D     | 4500 | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 3   | D     | 4576 | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 3   | D     | 3734 | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 48  | w     | 1692 | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 48  | w     | 866  | PSU  | C4-N3-C2 | -4.68 | 119.60      | 126.34   |
| 48  | w     | 36   | PSU  | N1-C2-N3 | 4.68  | 120.43      | 115.13   |
| 48  | w     | 1045 | PSU  | N1-C2-N3 | 4.67  | 120.42      | 115.13   |
| 48  | w     | 815  | PSU  | N1-C2-N3 | 4.67  | 120.42      | 115.13   |
| 3   | D     | 3764 | PSU  | N1-C2-N3 | 4.67  | 120.42      | 115.13   |
| 48  | w     | 1174 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 3   | D     | 4299 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 48  | w     | 1046 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 48  | w     | 1244 | PSU  | C4-N3-C2 | -4.67 | 119.61      | 126.34   |
| 3   | D     | 4361 | PSU  | N1-C2-N3 | 4.67  | 120.42      | 115.13   |
| 3   | D     | 3734 | PSU  | C4-N3-C2 | -4.67 | 119.62      | 126.34   |
| 3   | D     | 1744 | PSU  | N1-C2-N3 | 4.66  | 120.41      | 115.13   |
| 48  | w     | 406  | PSU  | N1-C2-N3 | 4.66  | 120.41      | 115.13   |
| 3   | D     | 4296 | PSU  | N1-C2-N3 | 4.65  | 120.40      | 115.13   |
| 3   | D     | 4423 | PSU  | N1-C2-N3 | 4.65  | 120.40      | 115.13   |
| 3   | D     | 2508 | PSU  | N1-C2-N3 | 4.65  | 120.40      | 115.13   |
| 3   | D     | 4423 | PSU  | C4-N3-C2 | -4.65 | 119.64      | 126.34   |
| 48  | w     | 1445 | PSU  | C4-N3-C2 | -4.65 | 119.64      | 126.34   |
| 48  | w     | 1238 | PSU  | C4-N3-C2 | -4.65 | 119.65      | 126.34   |
| 48  | w     | 1232 | PSU  | N1-C2-N3 | 4.64  | 120.39      | 115.13   |
| 3   | D     | 3764 | PSU  | C4-N3-C2 | -4.64 | 119.66      | 126.34   |
| 48  | w     | 863  | PSU  | C4-N3-C2 | -4.64 | 119.66      | 126.34   |
| 3   | D     | 4457 | PSU  | N1-C2-N3 | 4.64  | 120.38      | 115.13   |
| 3   | D     | 3762 | PSU  | N1-C2-N3 | 4.64  | 120.38      | 115.13   |
| 3   | D     | 4579 | PSU  | C4-N3-C2 | -4.64 | 119.66      | 126.34   |
| 48  | w     | 105  | PSU  | N1-C2-N3 | 4.63  | 120.38      | 115.13   |
| 2   | B     | 13   | PSU  | C4-N3-C2 | -4.63 | 119.66      | 126.34   |
| 3   | D     | 2632 | PSU  | C4-N3-C2 | -4.63 | 119.66      | 126.34   |
| 48  | w     | 1238 | PSU  | N1-C2-N3 | 4.63  | 120.38      | 115.13   |
| 48  | w     | 686  | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 48  | w     | 1056 | PSU  | N1-C2-N3 | 4.63  | 120.38      | 115.13   |
| 3   | D     | 4420 | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 48  | w     | 966  | PSU  | N1-C2-N3 | 4.63  | 120.37      | 115.13   |
| 3   | D     | 4471 | PSU  | N1-C2-N3 | 4.63  | 120.37      | 115.13   |
| 48  | w     | 210  | PSU  | C4-N3-C2 | -4.63 | 119.67      | 126.34   |
| 3   | D     | 4689 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 3   | D     | 4471 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 3   | D     | 4500 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 48  | w     | 109  | PSU  | N1-C2-N3 | 4.62  | 120.37      | 115.13   |
| 48  | w     | 1625 | PSU  | C4-N3-C2 | -4.62 | 119.68      | 126.34   |
| 48  | w     | 1177 | PSU  | N1-C2-N3 | 4.62  | 120.36      | 115.13   |
| 3   | D     | 2632 | PSU  | N1-C2-N3 | 4.61  | 120.36      | 115.13   |
| 48  | w     | 1232 | PSU  | C4-N3-C2 | -4.61 | 119.69      | 126.34   |
| 48  | w     | 1643 | PSU  | N1-C2-N3 | 4.61  | 120.36      | 115.13   |
| 48  | w     | 966  | PSU  | C4-N3-C2 | -4.61 | 119.69      | 126.34   |
| 3   | D     | 1781 | PSU  | N1-C2-N3 | 4.61  | 120.35      | 115.13   |
| 3   | D     | 4552 | PSU  | C4-N3-C2 | -4.60 | 119.70      | 126.34   |
| 3   | D     | 3768 | PSU  | C4-N3-C2 | -4.60 | 119.71      | 126.34   |
| 48  | w     | 1004 | PSU  | C4-N3-C2 | -4.60 | 119.71      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 4220 | 6MZ  | N9-C8-N7 | -4.60 | 107.62      | 113.91   |
| 3   | D     | 3768 | PSU  | N1-C2-N3 | 4.60  | 120.34      | 115.13   |
| 3   | D     | 4532 | PSU  | C4-N3-C2 | -4.60 | 119.71      | 126.34   |
| 3   | D     | 3770 | PSU  | C4-N3-C2 | -4.59 | 119.72      | 126.34   |
| 2   | C     | 54   | PSU  | N1-C2-N3 | 4.59  | 120.33      | 115.13   |
| 48  | w     | 1347 | PSU  | N1-C2-N3 | 4.59  | 120.33      | 115.13   |
| 48  | w     | 105  | PSU  | C4-N3-C2 | -4.58 | 119.74      | 126.34   |
| 48  | w     | 1625 | PSU  | N1-C2-N3 | 4.58  | 120.32      | 115.13   |
| 48  | w     | 1850 | MA6  | C4-C5-C6 | 4.58  | 121.01      | 115.88   |
| 3   | D     | 5001 | PSU  | N1-C2-N3 | 4.58  | 120.32      | 115.13   |
| 48  | w     | 609  | PSU  | N1-C2-N3 | 4.58  | 120.32      | 115.13   |
| 2   | C     | 13   | PSU  | C4-N3-C2 | -4.58 | 119.74      | 126.34   |
| 2   | B     | 54   | PSU  | C4-N3-C2 | -4.57 | 119.75      | 126.34   |
| 48  | w     | 801  | PSU  | N1-C2-N3 | 4.57  | 120.31      | 115.13   |
| 3   | D     | 3639 | PSU  | C4-N3-C2 | -4.57 | 119.75      | 126.34   |
| 3   | D     | 3730 | PSU  | N1-C2-N3 | 4.57  | 120.30      | 115.13   |
| 3   | D     | 1677 | PSU  | N1-C2-N3 | 4.56  | 120.30      | 115.13   |
| 3   | D     | 3762 | PSU  | C4-N3-C2 | -4.56 | 119.77      | 126.34   |
| 48  | w     | 866  | PSU  | N1-C2-N3 | 4.56  | 120.30      | 115.13   |
| 48  | w     | 1643 | PSU  | C4-N3-C2 | -4.56 | 119.77      | 126.34   |
| 48  | w     | 801  | PSU  | C4-N3-C2 | -4.56 | 119.77      | 126.34   |
| 3   | D     | 3853 | PSU  | N1-C2-N3 | 4.55  | 120.28      | 115.13   |
| 48  | w     | 1081 | PSU  | N1-C2-N3 | 4.55  | 120.28      | 115.13   |
| 3   | D     | 3639 | PSU  | N1-C2-N3 | 4.55  | 120.28      | 115.13   |
| 48  | w     | 1445 | PSU  | N1-C2-N3 | 4.55  | 120.28      | 115.13   |
| 3   | D     | 4296 | PSU  | C4-N3-C2 | -4.54 | 119.79      | 126.34   |
| 3   | D     | 3853 | PSU  | C4-N3-C2 | -4.54 | 119.80      | 126.34   |
| 48  | w     | 109  | PSU  | C4-N3-C2 | -4.53 | 119.81      | 126.34   |
| 3   | D     | 3758 | PSU  | N1-C2-N3 | 4.53  | 120.26      | 115.13   |
| 48  | w     | 218  | PSU  | C4-N3-C2 | -4.53 | 119.82      | 126.34   |
| 48  | w     | 1244 | PSU  | N1-C2-N3 | 4.52  | 120.26      | 115.13   |
| 2   | C     | 34   | 56B  | C2-N3-C4 | 4.52  | 120.36      | 112.30   |
| 48  | w     | 1851 | MA6  | C5-C4-N3 | -4.52 | 120.85      | 126.75   |
| 48  | w     | 683  | OMG  | C2-N3-C4 | 4.52  | 120.35      | 112.30   |
| 2   | B     | 34   | 56B  | C2-N3-C4 | 4.51  | 120.33      | 112.30   |
| 2   | C     | 13   | PSU  | N1-C2-N3 | 4.50  | 120.23      | 115.13   |
| 48  | w     | 1174 | PSU  | N1-C2-N3 | 4.50  | 120.23      | 115.13   |
| 48  | w     | 436  | OMG  | C2-N3-C4 | 4.49  | 120.31      | 112.30   |
| 48  | w     | 36   | PSU  | C4-N3-C2 | -4.49 | 119.87      | 126.34   |
| 3   | D     | 4420 | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 48  | w     | 814  | PSU  | N1-C2-N3 | 4.49  | 120.22      | 115.13   |
| 48  | w     | 119  | PSU  | C4-N3-C2 | -4.48 | 119.88      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 48  | w     | 34   | PSU  | N1-C2-N3  | 4.48  | 120.21      | 115.13   |
| 48  | w     | 572  | PSU  | N1-C2-N3  | 4.48  | 120.20      | 115.13   |
| 48  | w     | 119  | PSU  | N1-C2-N3  | 4.47  | 120.20      | 115.13   |
| 48  | w     | 210  | PSU  | N1-C2-N3  | 4.47  | 120.19      | 115.13   |
| 48  | w     | 1851 | MA6  | C2-N1-C6  | 4.47  | 122.31      | 111.75   |
| 48  | w     | 1490 | OMG  | C2-N3-C4  | 4.44  | 120.22      | 112.30   |
| 2   | B     | 6    | 2MG  | C2-N1-C6  | -4.44 | 119.37      | 124.48   |
| 2   | C     | 6    | 2MG  | C2-N1-C6  | -4.44 | 119.37      | 124.48   |
| 2   | C     | 53   | 5MU  | N3-C2-N1  | 4.44  | 120.78      | 114.89   |
| 48  | w     | 1850 | MA6  | C2-N1-C6  | 4.43  | 122.22      | 111.75   |
| 48  | w     | 93   | PSU  | N1-C2-N3  | 4.43  | 120.15      | 115.13   |
| 3   | D     | 1792 | PSU  | N1-C2-N3  | 4.41  | 120.13      | 115.13   |
| 3   | D     | 3944 | OMG  | C2-N3-C4  | 4.40  | 120.15      | 112.30   |
| 48  | w     | 609  | PSU  | C4-N3-C2  | -4.40 | 120.00      | 126.34   |
| 2   | B     | 54   | PSU  | N1-C2-N3  | 4.40  | 120.11      | 115.13   |
| 48  | w     | 1851 | MA6  | N9-C8-N7  | -4.39 | 107.90      | 113.91   |
| 3   | D     | 1625 | OMG  | C2-N3-C4  | 4.38  | 120.11      | 112.30   |
| 48  | w     | 218  | PSU  | N1-C2-N3  | 4.37  | 120.08      | 115.13   |
| 48  | w     | 822  | PSU  | N1-C2-N3  | 4.37  | 120.08      | 115.13   |
| 48  | w     | 822  | PSU  | C4-N3-C2  | -4.37 | 120.04      | 126.34   |
| 3   | D     | 4494 | OMG  | C2-N3-C4  | 4.36  | 120.07      | 112.30   |
| 48  | w     | 1832 | 6MZ  | N9-C8-N7  | -4.36 | 107.95      | 113.91   |
| 48  | w     | 1639 | G7M  | C2-N3-C4  | 4.35  | 120.05      | 112.30   |
| 2   | B     | 53   | 5MU  | C5M-C5-C4 | 4.35  | 123.56      | 118.77   |
| 3   | D     | 4618 | OMG  | C2-N3-C4  | 4.35  | 120.04      | 112.30   |
| 48  | w     | 601  | OMG  | C2-N3-C4  | 4.34  | 120.04      | 112.30   |
| 5   | F     | 75   | OMG  | C2-N3-C4  | 4.34  | 120.03      | 112.30   |
| 3   | D     | 4228 | OMG  | C2-N3-C4  | 4.34  | 120.03      | 112.30   |
| 3   | D     | 3627 | OMG  | C2-N3-C4  | 4.34  | 120.03      | 112.30   |
| 3   | D     | 4392 | OMG  | C2-N3-C4  | 4.34  | 120.03      | 112.30   |
| 3   | D     | 4370 | OMG  | C2-N3-C4  | 4.32  | 120.00      | 112.30   |
| 3   | D     | 3792 | OMG  | C2-N3-C4  | 4.32  | 120.00      | 112.30   |
| 3   | D     | 4499 | OMG  | C2-N3-C4  | 4.30  | 119.97      | 112.30   |
| 3   | D     | 3744 | OMG  | C2-N3-C4  | 4.29  | 119.95      | 112.30   |
| 3   | D     | 4196 | OMG  | C2-N3-C4  | 4.29  | 119.94      | 112.30   |
| 3   | D     | 2364 | OMG  | C2-N3-C4  | 4.29  | 119.94      | 112.30   |
| 3   | D     | 4637 | OMG  | C2-N3-C4  | 4.27  | 119.92      | 112.30   |
| 3   | D     | 1316 | OMG  | C2-N3-C4  | 4.27  | 119.90      | 112.30   |
| 3   | D     | 3899 | OMG  | C2-N3-C4  | 4.25  | 119.87      | 112.30   |
| 3   | D     | 2424 | OMG  | C2-N3-C4  | 4.22  | 119.81      | 112.30   |
| 48  | w     | 34   | PSU  | C4-N3-C2  | -4.21 | 120.27      | 126.34   |
| 48  | w     | 1328 | OMG  | C2-N3-C4  | 4.21  | 119.80      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | D     | 1760 | OMG  | C2-N3-C4  | 4.20  | 119.78      | 112.30   |
| 48  | w     | 509  | OMG  | C2-N3-C4  | 4.20  | 119.78      | 112.30   |
| 48  | w     | 1639 | G7M  | C5-C4-N3  | -4.18 | 120.14      | 128.15   |
| 48  | w     | 644  | OMG  | C2-N3-C4  | 4.17  | 119.72      | 112.30   |
| 2   | B     | 53   | 5MU  | C5M-C5-C6 | -4.16 | 117.29      | 122.85   |
| 3   | D     | 3925 | OMU  | N3-C2-N1  | 4.16  | 120.41      | 114.89   |
| 3   | D     | 4623 | OMG  | C2-N3-C4  | 4.16  | 119.70      | 112.30   |
| 2   | B     | 53   | 5MU  | N3-C2-N1  | 4.15  | 120.40      | 114.89   |
| 3   | D     | 2415 | OMU  | N3-C2-N1  | 4.12  | 120.35      | 114.89   |
| 3   | D     | 1522 | OMG  | C2-N3-C4  | 4.11  | 119.62      | 112.30   |
| 2   | C     | 34   | 56B  | C7-C5-C4  | -4.05 | 107.97      | 112.66   |
| 2   | C     | 53   | 5MU  | C5M-C5-C6 | -4.04 | 117.45      | 122.85   |
| 3   | D     | 4306 | OMU  | N3-C2-N1  | 4.00  | 120.20      | 114.89   |
| 2   | C     | 53   | 5MU  | C5M-C5-C4 | 3.99  | 123.16      | 118.77   |
| 48  | w     | 1639 | G7M  | C5-C6-N1  | 3.97  | 120.09      | 111.79   |
| 48  | w     | 428  | OMU  | N3-C2-N1  | 3.97  | 120.16      | 114.89   |
| 3   | D     | 4620 | OMU  | N3-C2-N1  | 3.97  | 120.16      | 114.89   |
| 3   | D     | 2837 | OMU  | N3-C2-N1  | 3.97  | 120.16      | 114.89   |
| 3   | D     | 4498 | OMU  | N3-C2-N1  | 3.93  | 120.11      | 114.89   |
| 3   | D     | 4227 | OMU  | N3-C2-N1  | 3.91  | 120.08      | 114.89   |
| 3   | D     | 4447 | 5MC  | C5-C6-N1  | -3.87 | 119.36      | 123.34   |
| 2   | B     | 34   | 56B  | C7-C5-C4  | -3.85 | 108.20      | 112.66   |
| 3   | D     | 1773 | OMU  | N3-C2-N1  | 3.85  | 120.00      | 114.89   |
| 48  | w     | 1326 | OMU  | N3-C2-N1  | 3.82  | 119.97      | 114.89   |
| 3   | D     | 1625 | OMG  | N9-C4-N3  | 3.81  | 133.59      | 125.94   |
| 48  | w     | 1442 | OMU  | N3-C2-N1  | 3.80  | 119.94      | 114.89   |
| 48  | w     | 627  | OMU  | N3-C2-N1  | 3.80  | 119.94      | 114.89   |
| 48  | w     | 1851 | MA6  | C4-C5-C6  | 3.80  | 120.13      | 115.88   |
| 48  | w     | 799  | OMU  | N3-C2-N1  | 3.78  | 119.91      | 114.89   |
| 48  | w     | 1804 | OMU  | N3-C2-N1  | 3.78  | 119.90      | 114.89   |
| 48  | w     | 1832 | 6MZ  | C4-C5-C6  | 3.75  | 119.72      | 116.81   |
| 48  | w     | 1850 | MA6  | N9-C8-N7  | -3.74 | 108.80      | 113.91   |
| 48  | w     | 1490 | OMG  | N9-C4-N3  | 3.73  | 133.42      | 125.94   |
| 48  | w     | 1288 | OMU  | N3-C2-N1  | 3.71  | 119.82      | 114.89   |
| 3   | D     | 3792 | OMG  | N9-C4-N3  | 3.71  | 133.38      | 125.94   |
| 48  | w     | 172  | OMU  | N3-C2-N1  | 3.70  | 119.80      | 114.89   |
| 48  | w     | 121  | OMU  | N3-C2-N1  | 3.70  | 119.80      | 114.89   |
| 2   | B     | 34   | 56B  | N9-C4-N3  | 3.69  | 133.36      | 125.94   |
| 3   | D     | 2415 | OMU  | C5-C4-N3  | 3.69  | 120.36      | 114.84   |
| 3   | D     | 4220 | 6MZ  | C5-N7-C8  | 3.69  | 108.75      | 103.51   |
| 2   | C     | 34   | 56B  | C7-C8-N9  | -3.68 | 107.44      | 111.06   |
| 48  | w     | 509  | OMG  | N9-C4-N3  | 3.65  | 133.26      | 125.94   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 48  | w     | 1832 | 6MZ  | C2-N3-C4 | 3.61  | 120.27      | 111.75   |
| 2   | B     | 34   | 56B  | C7-C8-N9 | -3.61 | 107.52      | 111.06   |
| 3   | D     | 2837 | OMU  | C5-C4-N3 | 3.61  | 120.23      | 114.84   |
| 3   | D     | 4220 | 6MZ  | C2-N3-C4 | 3.60  | 120.26      | 111.75   |
| 3   | D     | 4196 | OMG  | N9-C4-N3 | 3.60  | 133.17      | 125.94   |
| 48  | w     | 683  | OMG  | N9-C4-N3 | 3.60  | 133.16      | 125.94   |
| 48  | w     | 1337 | 4AC  | O7-C7-N4 | 3.60  | 127.64      | 121.82   |
| 3   | D     | 3944 | OMG  | N9-C4-N3 | 3.59  | 133.15      | 125.94   |
| 48  | w     | 436  | OMG  | N9-C4-N3 | 3.58  | 133.13      | 125.94   |
| 3   | D     | 4498 | OMU  | C5-C4-N3 | 3.57  | 120.19      | 114.84   |
| 2   | C     | 34   | 56B  | N9-C4-N3 | 3.56  | 133.08      | 125.94   |
| 3   | D     | 1316 | OMG  | N9-C4-N3 | 3.54  | 133.05      | 125.94   |
| 3   | D     | 4228 | OMG  | N9-C8-N7 | -3.53 | 106.75      | 113.39   |
| 3   | D     | 4637 | OMG  | N9-C4-N3 | 3.52  | 133.00      | 125.94   |
| 3   | D     | 4494 | OMG  | N9-C4-N3 | 3.52  | 133.00      | 125.94   |
| 3   | D     | 3925 | OMU  | C5-C4-N3 | 3.51  | 120.09      | 114.84   |
| 48  | w     | 644  | OMG  | N9-C8-N7 | -3.50 | 106.80      | 113.39   |
| 5   | F     | 75   | OMG  | N9-C4-N3 | 3.50  | 132.96      | 125.94   |
| 3   | D     | 4227 | OMU  | C5-C4-N3 | 3.49  | 120.06      | 114.84   |
| 3   | D     | 1522 | OMG  | N9-C8-N7 | -3.49 | 106.82      | 113.39   |
| 3   | D     | 4623 | OMG  | N9-C8-N7 | -3.48 | 106.83      | 113.39   |
| 48  | w     | 116  | OMU  | C5-C4-N3 | 3.48  | 120.04      | 114.84   |
| 48  | w     | 1804 | OMU  | C5-C4-N3 | 3.47  | 120.04      | 114.84   |
| 3   | D     | 3782 | 5MC  | C5-C6-N1 | -3.47 | 119.77      | 123.34   |
| 3   | D     | 1760 | OMG  | N9-C8-N7 | -3.46 | 106.86      | 113.39   |
| 3   | D     | 4637 | OMG  | N9-C8-N7 | -3.46 | 106.86      | 113.39   |
| 2   | C     | 47   | 5MC  | C5-C6-N1 | -3.46 | 119.78      | 123.34   |
| 3   | D     | 3627 | OMG  | N9-C8-N7 | -3.46 | 106.88      | 113.39   |
| 48  | w     | 116  | OMU  | N3-C2-N1 | 3.46  | 119.48      | 114.89   |
| 2   | C     | 6    | 2MG  | N9-C4-N3 | 3.45  | 132.86      | 125.94   |
| 48  | w     | 1328 | OMG  | N9-C8-N7 | -3.45 | 106.90      | 113.39   |
| 3   | D     | 1316 | OMG  | N9-C8-N7 | -3.44 | 106.91      | 113.39   |
| 2   | B     | 47   | 5MC  | C5-C6-N1 | -3.44 | 119.80      | 123.34   |
| 3   | D     | 4370 | OMG  | N9-C4-N3 | 3.44  | 132.84      | 125.94   |
| 3   | D     | 4499 | OMG  | N9-C8-N7 | -3.44 | 106.92      | 113.39   |
| 3   | D     | 4306 | OMU  | C5-C4-N3 | 3.43  | 119.98      | 114.84   |
| 3   | D     | 4620 | OMU  | C5-C4-N3 | 3.43  | 119.97      | 114.84   |
| 3   | D     | 3899 | OMG  | N9-C8-N7 | -3.43 | 106.93      | 113.39   |
| 48  | w     | 601  | OMG  | N9-C4-N3 | 3.42  | 132.81      | 125.94   |
| 3   | D     | 4370 | OMG  | N9-C8-N7 | -3.42 | 106.96      | 113.39   |
| 48  | w     | 1842 | 4AC  | O7-C7-N4 | 3.41  | 127.33      | 121.82   |
| 48  | w     | 1851 | MA6  | C5-N7-C8 | 3.41  | 108.35      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | D     | 4499 | OMG  | N9-C4-N3  | 3.41  | 132.78      | 125.94   |
| 48  | w     | 436  | OMG  | N9-C8-N7  | -3.40 | 106.98      | 113.39   |
| 48  | w     | 644  | OMG  | N9-C4-N3  | 3.40  | 132.77      | 125.94   |
| 5   | F     | 75   | OMG  | N9-C8-N7  | -3.40 | 106.98      | 113.39   |
| 48  | w     | 683  | OMG  | N9-C8-N7  | -3.40 | 106.99      | 113.39   |
| 48  | w     | 601  | OMG  | N9-C8-N7  | -3.40 | 106.99      | 113.39   |
| 48  | w     | 1328 | OMG  | N9-C4-N3  | 3.39  | 132.75      | 125.94   |
| 2   | B     | 38   | 5MC  | C5-C6-N1  | -3.39 | 119.85      | 123.34   |
| 3   | D     | 3744 | OMG  | N9-C8-N7  | -3.38 | 107.02      | 113.39   |
| 3   | D     | 3627 | OMG  | N9-C4-N3  | 3.38  | 132.73      | 125.94   |
| 48  | w     | 1639 | G7M  | O6-C6-C5  | -3.37 | 120.45      | 128.06   |
| 3   | D     | 2424 | OMG  | N9-C8-N7  | -3.37 | 107.05      | 113.39   |
| 2   | B     | 6    | 2MG  | N9-C8-N7  | -3.37 | 107.05      | 113.39   |
| 2   | B     | 6    | 2MG  | N9-C4-N3  | 3.36  | 132.69      | 125.94   |
| 3   | D     | 4618 | OMG  | N9-C4-N3  | 3.36  | 132.68      | 125.94   |
| 48  | w     | 172  | OMU  | C5-C4-N3  | 3.35  | 119.85      | 114.84   |
| 3   | D     | 2364 | OMG  | N9-C8-N7  | -3.35 | 107.09      | 113.39   |
| 3   | D     | 3744 | OMG  | N9-C4-N3  | 3.34  | 132.65      | 125.94   |
| 48  | w     | 1442 | OMU  | C5-C4-N3  | 3.34  | 119.83      | 114.84   |
| 48  | w     | 1832 | 6MZ  | C5-N7-C8  | 3.33  | 108.25      | 103.51   |
| 2   | B     | 48   | 5MC  | C5-C6-N1  | -3.33 | 119.91      | 123.34   |
| 3   | D     | 2424 | OMG  | N9-C4-N3  | 3.32  | 132.61      | 125.94   |
| 3   | D     | 4392 | OMG  | N9-C4-N3  | 3.32  | 132.61      | 125.94   |
| 48  | w     | 1851 | MA6  | C2-N3-C4  | 3.32  | 119.59      | 111.75   |
| 48  | w     | 627  | OMU  | C5-C4-N3  | 3.32  | 119.81      | 114.84   |
| 3   | D     | 3944 | OMG  | N9-C8-N7  | -3.31 | 107.15      | 113.39   |
| 3   | D     | 4494 | OMG  | N9-C8-N7  | -3.31 | 107.16      | 113.39   |
| 3   | D     | 4228 | OMG  | C1'-N9-C4 | -3.31 | 116.68      | 126.50   |
| 48  | w     | 509  | OMG  | N9-C8-N7  | -3.31 | 107.17      | 113.39   |
| 3   | D     | 4618 | OMG  | N9-C8-N7  | -3.30 | 107.18      | 113.39   |
| 48  | w     | 799  | OMU  | C5-C4-N3  | 3.30  | 119.78      | 114.84   |
| 3   | D     | 4392 | OMG  | N9-C8-N7  | -3.29 | 107.19      | 113.39   |
| 2   | C     | 38   | 5MC  | C5-C6-N1  | -3.29 | 119.95      | 123.34   |
| 3   | D     | 1625 | OMG  | N9-C8-N7  | -3.28 | 107.21      | 113.39   |
| 48  | w     | 1288 | OMU  | C5-C4-N3  | 3.28  | 119.75      | 114.84   |
| 3   | D     | 1760 | OMG  | N9-C4-N3  | 3.27  | 132.51      | 125.94   |
| 48  | w     | 1326 | OMU  | C5-C4-N3  | 3.26  | 119.72      | 114.84   |
| 48  | w     | 121  | OMU  | C5-C4-N3  | 3.25  | 119.70      | 114.84   |
| 2   | C     | 6    | 2MG  | N9-C8-N7  | -3.24 | 107.28      | 113.39   |
| 3   | D     | 4228 | OMG  | N9-C4-N3  | 3.23  | 132.42      | 125.94   |
| 3   | D     | 1773 | OMU  | C5-C4-N3  | 3.21  | 119.65      | 114.84   |
| 3   | D     | 3792 | OMG  | N9-C8-N7  | -3.21 | 107.34      | 113.39   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 1522 | OMG  | C1'-N9-C4  | -3.20 | 117.00      | 126.50   |
| 48  | w     | 428  | OMU  | C5-C4-N3   | 3.20  | 119.62      | 114.84   |
| 3   | D     | 4196 | OMG  | N9-C8-N7   | -3.18 | 107.40      | 113.39   |
| 3   | D     | 4220 | 6MZ  | C4-C5-N7   | -3.18 | 106.75      | 110.62   |
| 48  | w     | 1639 | G7M  | N9-C4-N3   | 3.18  | 132.32      | 125.94   |
| 48  | w     | 1850 | MA6  | C5-N7-C8   | 3.17  | 108.01      | 103.51   |
| 2   | C     | 48   | 5MC  | C5-C6-N1   | -3.17 | 120.08      | 123.34   |
| 3   | D     | 2364 | OMG  | N9-C4-N3   | 3.16  | 132.29      | 125.94   |
| 3   | D     | 4220 | 6MZ  | C4-C5-C6   | 3.16  | 119.26      | 116.81   |
| 48  | w     | 436  | OMG  | C2-N1-C6   | -3.16 | 119.34      | 125.10   |
| 48  | w     | 1850 | MA6  | C2-N3-C4   | 3.15  | 119.20      | 111.75   |
| 48  | w     | 683  | OMG  | C2-N1-C6   | -3.15 | 119.36      | 125.10   |
| 3   | D     | 1625 | OMG  | C2-N1-C6   | -3.15 | 119.36      | 125.10   |
| 3   | D     | 4392 | OMG  | C2-N1-C6   | -3.15 | 119.36      | 125.10   |
| 3   | D     | 3899 | OMG  | C1'-N9-C4  | -3.15 | 117.16      | 126.50   |
| 3   | D     | 3899 | OMG  | N9-C4-N3   | 3.14  | 132.25      | 125.94   |
| 3   | D     | 4623 | OMG  | C1'-N9-C4  | -3.14 | 117.18      | 126.50   |
| 48  | w     | 1639 | G7M  | C2-N1-C6   | -3.14 | 119.38      | 125.10   |
| 2   | B     | 34   | 56B  | C2-N1-C6   | -3.13 | 119.40      | 125.10   |
| 3   | D     | 3785 | A2M  | C2'-C1'-N9 | -3.12 | 108.28      | 113.53   |
| 3   | D     | 2424 | OMG  | C2-N1-C6   | -3.12 | 119.42      | 125.10   |
| 3   | D     | 4196 | OMG  | C2-N1-C6   | -3.11 | 119.42      | 125.10   |
| 3   | D     | 4623 | OMG  | N9-C4-N3   | 3.11  | 132.19      | 125.94   |
| 48  | w     | 1490 | OMG  | N9-C8-N7   | -3.11 | 107.53      | 113.39   |
| 3   | D     | 1522 | OMG  | N9-C4-N3   | 3.11  | 132.18      | 125.94   |
| 48  | w     | 644  | OMG  | C2-N1-C6   | -3.10 | 119.45      | 125.10   |
| 3   | D     | 3744 | OMG  | C2-N1-C6   | -3.09 | 119.46      | 125.10   |
| 3   | D     | 3792 | OMG  | C2-N1-C6   | -3.08 | 119.48      | 125.10   |
| 3   | D     | 2364 | OMG  | C2-N1-C6   | -3.08 | 119.48      | 125.10   |
| 3   | D     | 4499 | OMG  | C2-N1-C6   | -3.08 | 119.49      | 125.10   |
| 3   | D     | 4637 | OMG  | C2-N1-C6   | -3.07 | 119.50      | 125.10   |
| 48  | w     | 1328 | OMG  | C2-N1-C6   | -3.07 | 119.51      | 125.10   |
| 2   | C     | 34   | 56B  | C2-N1-C6   | -3.06 | 119.51      | 125.10   |
| 3   | D     | 3627 | OMG  | C2-N1-C6   | -3.06 | 119.52      | 125.10   |
| 3   | D     | 1316 | OMG  | C2-N1-C6   | -3.06 | 119.52      | 125.10   |
| 3   | D     | 4228 | OMG  | C2-N1-C6   | -3.04 | 119.55      | 125.10   |
| 3   | D     | 4494 | OMG  | C2-N1-C6   | -3.03 | 119.58      | 125.10   |
| 3   | D     | 3944 | OMG  | C2-N1-C6   | -3.02 | 119.59      | 125.10   |
| 48  | w     | 116  | OMU  | O4-C4-C5   | -3.02 | 119.85      | 125.16   |
| 5   | F     | 75   | OMG  | C2-N1-C6   | -3.02 | 119.60      | 125.10   |
| 3   | D     | 1760 | OMG  | C1'-N9-C4  | -3.01 | 117.55      | 126.50   |
| 48  | w     | 1490 | OMG  | C2-N1-C6   | -3.00 | 119.62      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 48  | w     | 509  | OMG  | C2-N1-C6  | -2.99 | 119.66      | 125.10   |
| 48  | w     | 601  | OMG  | C2-N1-C6  | -2.98 | 119.66      | 125.10   |
| 3   | D     | 3627 | OMG  | C1'-N9-C4 | -2.98 | 117.66      | 126.50   |
| 3   | D     | 4370 | OMG  | C2-N1-C6  | -2.97 | 119.68      | 125.10   |
| 3   | D     | 1522 | OMG  | C2-N1-C6  | -2.97 | 119.68      | 125.10   |
| 48  | w     | 1804 | OMU  | O4-C4-C5  | -2.95 | 119.97      | 125.16   |
| 3   | D     | 4618 | OMG  | C2-N1-C6  | -2.95 | 119.73      | 125.10   |
| 3   | D     | 4576 | PSU  | O2-C2-N1  | -2.94 | 119.56      | 122.79   |
| 3   | D     | 4500 | PSU  | O2-C2-N1  | -2.93 | 119.57      | 122.79   |
| 3   | D     | 2837 | OMU  | O4-C4-C5  | -2.92 | 120.02      | 125.16   |
| 3   | D     | 1683 | PSU  | O2-C2-N1  | -2.92 | 119.58      | 122.79   |
| 48  | w     | 1851 | MA6  | C4-C5-N7  | -2.91 | 107.07      | 110.62   |
| 3   | D     | 3920 | PSU  | O2-C2-N1  | -2.91 | 119.59      | 122.79   |
| 3   | D     | 3899 | OMG  | C2-N1-C6  | -2.91 | 119.80      | 125.10   |
| 3   | D     | 2415 | OMU  | O4-C4-C5  | -2.89 | 120.08      | 125.16   |
| 3   | D     | 4623 | OMG  | C2-N1-C6  | -2.89 | 119.83      | 125.10   |
| 3   | D     | 3744 | OMG  | C1'-N9-C4 | -2.88 | 117.94      | 126.50   |
| 3   | D     | 4392 | OMG  | C5-C6-N1  | 2.87  | 120.49      | 113.19   |
| 3   | D     | 3695 | PSU  | O2-C2-N1  | -2.87 | 119.63      | 122.79   |
| 3   | D     | 2424 | OMG  | C1'-N9-C4 | -2.87 | 117.98      | 126.50   |
| 48  | w     | 1328 | OMG  | C1'-N9-C4 | -2.87 | 117.99      | 126.50   |
| 3   | D     | 4370 | OMG  | C1'-N9-C4 | -2.87 | 117.99      | 126.50   |
| 3   | D     | 4392 | OMG  | C1'-N9-C4 | -2.87 | 117.99      | 126.50   |
| 48  | w     | 172  | OMU  | O4-C4-C5  | -2.86 | 120.12      | 125.16   |
| 48  | w     | 1851 | MA6  | N1-C6-N6  | -2.86 | 113.96      | 117.08   |
| 3   | D     | 4306 | OMU  | O4-C4-C5  | -2.86 | 120.14      | 125.16   |
| 48  | w     | 1442 | OMU  | O4-C4-C5  | -2.86 | 120.14      | 125.16   |
| 3   | D     | 3925 | OMU  | O4-C4-C5  | -2.85 | 120.14      | 125.16   |
| 48  | w     | 644  | OMG  | C1'-N9-C4 | -2.85 | 118.03      | 126.50   |
| 48  | w     | 1004 | PSU  | O2-C2-N1  | -2.85 | 119.65      | 122.79   |
| 3   | D     | 4637 | OMG  | C1'-N9-C4 | -2.85 | 118.05      | 126.50   |
| 3   | D     | 2364 | OMG  | C1'-N9-C4 | -2.84 | 118.06      | 126.50   |
| 48  | w     | 109  | PSU  | O2-C2-N1  | -2.84 | 119.66      | 122.79   |
| 48  | w     | 683  | OMG  | C5-C6-N1  | 2.84  | 120.39      | 113.19   |
| 48  | w     | 1850 | MA6  | C4-C5-N7  | -2.83 | 107.17      | 110.62   |
| 3   | D     | 4228 | OMG  | C5-C6-N1  | 2.83  | 120.37      | 113.19   |
| 48  | w     | 627  | OMU  | O4-C4-C5  | -2.83 | 120.19      | 125.16   |
| 48  | w     | 36   | PSU  | O2-C2-N1  | -2.83 | 119.68      | 122.79   |
| 3   | D     | 4499 | OMG  | C1'-N9-C4 | -2.83 | 118.11      | 126.50   |
| 48  | w     | 1832 | 6MZ  | N3-C4-N9  | 2.83  | 131.74      | 127.08   |
| 3   | D     | 4227 | OMU  | O4-C4-C5  | -2.83 | 120.19      | 125.16   |
| 48  | w     | 1046 | PSU  | O2-C2-N1  | -2.82 | 119.68      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | w     | 119  | PSU  | O2-C2-N1    | -2.82 | 119.69      | 122.79   |
| 3   | D     | 4498 | OMU  | O4-C4-C5    | -2.82 | 120.20      | 125.16   |
| 48  | w     | 436  | OMG  | C5-C6-N1    | 2.82  | 120.34      | 113.19   |
| 48  | w     | 1326 | OMU  | O4-C4-C5    | -2.81 | 120.22      | 125.16   |
| 3   | D     | 1860 | PSU  | O2-C2-N1    | -2.81 | 119.70      | 122.79   |
| 48  | w     | 1288 | OMU  | O4-C4-C5    | -2.81 | 120.22      | 125.16   |
| 3   | D     | 4370 | OMG  | C5-C6-N1    | 2.81  | 120.32      | 113.19   |
| 3   | D     | 3627 | OMG  | C5-C6-N1    | 2.80  | 120.31      | 113.19   |
| 3   | D     | 1683 | PSU  | C6-N1-C2    | -2.80 | 119.82      | 122.68   |
| 3   | D     | 4620 | OMU  | O4-C4-C5    | -2.79 | 120.25      | 125.16   |
| 3   | D     | 3768 | PSU  | O2-C2-N1    | -2.79 | 119.72      | 122.79   |
| 3   | D     | 3762 | PSU  | O2-C2-N1    | -2.78 | 119.72      | 122.79   |
| 3   | D     | 1534 | A2M  | O2'-C2'-C1' | 2.78  | 114.51      | 109.08   |
| 3   | D     | 1625 | OMG  | C5-C6-N1    | 2.78  | 120.24      | 113.19   |
| 3   | D     | 2424 | OMG  | C5-C6-N1    | 2.78  | 120.24      | 113.19   |
| 3   | D     | 1534 | A2M  | C3'-C2'-C1' | -2.77 | 97.68       | 102.89   |
| 3   | D     | 1760 | OMG  | C2-N1-C6    | -2.77 | 120.05      | 125.10   |
| 3   | D     | 4431 | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 48  | w     | 822  | PSU  | O2-C2-N1    | -2.77 | 119.74      | 122.79   |
| 48  | w     | 601  | OMG  | C5-C6-N1    | 2.77  | 120.22      | 113.19   |
| 3   | D     | 1316 | OMG  | C5-C6-N1    | 2.76  | 120.21      | 113.19   |
| 3   | D     | 3744 | OMG  | C5-C6-N1    | 2.76  | 120.20      | 113.19   |
| 3   | D     | 5010 | PSU  | O2-C2-N1    | -2.76 | 119.75      | 122.79   |
| 3   | D     | 1522 | OMG  | C5-C6-N1    | 2.76  | 120.20      | 113.19   |
| 48  | w     | 799  | OMU  | O4-C4-C5    | -2.76 | 120.30      | 125.16   |
| 3   | D     | 2364 | OMG  | C5-C6-N1    | 2.76  | 120.20      | 113.19   |
| 3   | D     | 4637 | OMG  | C5-C6-N1    | 2.75  | 120.19      | 113.19   |
| 2   | B     | 6    | 2MG  | C5-C6-N1    | 2.75  | 120.17      | 113.19   |
| 3   | D     | 1536 | PSU  | O2-C2-N1    | -2.75 | 119.77      | 122.79   |
| 3   | D     | 4499 | OMG  | C5-C6-N1    | 2.74  | 120.16      | 113.19   |
| 3   | D     | 4579 | PSU  | O2-C2-N1    | -2.74 | 119.78      | 122.79   |
| 3   | D     | 4494 | OMG  | C5-C6-N1    | 2.74  | 120.14      | 113.19   |
| 3   | D     | 1773 | OMU  | O4-C4-C5    | -2.74 | 120.35      | 125.16   |
| 2   | B     | 13   | PSU  | O2-C2-N1    | -2.73 | 119.78      | 122.79   |
| 48  | w     | 609  | PSU  | O2-C2-N1    | -2.73 | 119.78      | 122.79   |
| 3   | D     | 4618 | OMG  | C1'-N9-C4   | -2.73 | 118.38      | 126.50   |
| 5   | F     | 75   | OMG  | C5-C6-N1    | 2.73  | 120.13      | 113.19   |
| 48  | w     | 1177 | PSU  | O2-C2-N1    | -2.73 | 119.79      | 122.79   |
| 48  | w     | 801  | PSU  | O2-C2-N1    | -2.72 | 119.79      | 122.79   |
| 3   | D     | 3899 | OMG  | C5-C6-N1    | 2.72  | 120.10      | 113.19   |
| 3   | D     | 4196 | OMG  | C5-C6-N1    | 2.72  | 120.09      | 113.19   |
| 48  | w     | 601  | OMG  | C1'-N9-C4   | -2.71 | 118.44      | 126.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | w     | 121  | OMU  | O4-C4-C5    | -2.71 | 120.39      | 125.16   |
| 48  | w     | 1490 | OMG  | C5-C6-N1    | 2.71  | 120.08      | 113.19   |
| 3   | D     | 3792 | OMG  | C5-C6-N1    | 2.71  | 120.07      | 113.19   |
| 2   | C     | 6    | 2MG  | C5-C6-N1    | 2.71  | 120.07      | 113.19   |
| 48  | w     | 1639 | G7M  | CN7-N7-C5   | 2.71  | 130.13      | 126.77   |
| 48  | w     | 966  | PSU  | O2-C2-N1    | -2.71 | 119.81      | 122.79   |
| 3   | D     | 3944 | OMG  | C5-C6-N1    | 2.71  | 120.06      | 113.19   |
| 48  | w     | 644  | OMG  | C5-C6-N1    | 2.70  | 120.06      | 113.19   |
| 3   | D     | 3734 | PSU  | O2-C2-N1    | -2.70 | 119.82      | 122.79   |
| 3   | D     | 4442 | PSU  | O2-C2-N1    | -2.70 | 119.82      | 122.79   |
| 48  | w     | 1328 | OMG  | C5-C6-N1    | 2.69  | 120.03      | 113.19   |
| 3   | D     | 1744 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 48  | w     | 1238 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 48  | w     | 686  | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 3   | D     | 2632 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 48  | w     | 866  | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 3   | D     | 4403 | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 48  | w     | 649  | PSU  | O2-C2-N1    | -2.68 | 119.84      | 122.79   |
| 48  | w     | 428  | OMU  | O4-C4-C5    | -2.67 | 120.46      | 125.16   |
| 5   | F     | 75   | OMG  | C1'-N9-C4   | -2.67 | 118.56      | 126.50   |
| 3   | D     | 4312 | PSU  | O2-C2-N1    | -2.67 | 119.85      | 122.79   |
| 3   | D     | 4392 | OMG  | O6-C6-C5    | -2.67 | 119.51      | 126.60   |
| 48  | w     | 1367 | PSU  | O2-C2-N1    | -2.67 | 119.86      | 122.79   |
| 3   | D     | 4623 | OMG  | C5-C6-N1    | 2.66  | 119.95      | 113.19   |
| 3   | D     | 4618 | OMG  | C5-C6-N1    | 2.66  | 119.95      | 113.19   |
| 3   | D     | 4220 | 6MZ  | C5-C4-N9    | 2.66  | 108.88      | 105.78   |
| 3   | D     | 1316 | OMG  | C1'-N9-C4   | -2.66 | 118.60      | 126.50   |
| 48  | w     | 436  | OMG  | C1'-N9-C4   | -2.66 | 118.60      | 126.50   |
| 3   | D     | 3715 | PSU  | O2-C2-N1    | -2.66 | 119.87      | 122.79   |
| 48  | w     | 509  | OMG  | C5-C6-N1    | 2.65  | 119.93      | 113.19   |
| 48  | w     | 651  | PSU  | O2-C2-N1    | -2.65 | 119.87      | 122.79   |
| 3   | D     | 4457 | PSU  | O2-C2-N1    | -2.65 | 119.87      | 122.79   |
| 3   | D     | 2424 | OMG  | O6-C6-C5    | -2.65 | 119.58      | 126.60   |
| 48  | w     | 406  | PSU  | O2-C2-N1    | -2.64 | 119.89      | 122.79   |
| 48  | w     | 1326 | OMU  | C1'-N1-C2   | 2.64  | 122.35      | 117.57   |
| 3   | D     | 4494 | OMG  | C1'-N9-C4   | -2.64 | 118.67      | 126.50   |
| 3   | D     | 1760 | OMG  | C5-C6-N1    | 2.64  | 119.89      | 113.19   |
| 3   | D     | 3760 | A2M  | C3'-C2'-C1' | -2.64 | 97.93       | 102.89   |
| 3   | D     | 1862 | PSU  | O2-C2-N1    | -2.63 | 119.90      | 122.79   |
| 48  | w     | 210  | PSU  | O2-C2-N1    | -2.62 | 119.91      | 122.79   |
| 3   | D     | 4353 | PSU  | O2-C2-N1    | -2.62 | 119.91      | 122.79   |
| 48  | w     | 1692 | PSU  | O2-C2-N1    | -2.61 | 119.91      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 4423 | PSU  | O2-C2-N1    | -2.61 | 119.91      | 122.79   |
| 48  | w     | 1643 | PSU  | O2-C2-N1    | -2.61 | 119.91      | 122.79   |
| 3   | D     | 1625 | OMG  | O6-C6-C5    | -2.61 | 119.67      | 126.60   |
| 3   | D     | 4228 | OMG  | O6-C6-C5    | -2.61 | 119.67      | 126.60   |
| 48  | w     | 36   | PSU  | C6-C5-C4    | 2.61  | 120.02      | 118.20   |
| 3   | D     | 3764 | PSU  | O2-C2-N1    | -2.61 | 119.92      | 122.79   |
| 3   | D     | 1782 | PSU  | O2-C2-N1    | -2.60 | 119.92      | 122.79   |
| 2   | C     | 54   | PSU  | O2-C2-N1    | -2.60 | 119.92      | 122.79   |
| 3   | D     | 3744 | OMG  | O6-C6-C5    | -2.60 | 119.70      | 126.60   |
| 3   | D     | 2364 | OMG  | O6-C6-C5    | -2.60 | 119.71      | 126.60   |
| 3   | D     | 4972 | PSU  | O2-C2-N1    | -2.59 | 119.94      | 122.79   |
| 48  | w     | 1625 | PSU  | O2-C2-N1    | -2.59 | 119.94      | 122.79   |
| 3   | D     | 3627 | OMG  | O6-C6-C5    | -2.59 | 119.74      | 126.60   |
| 48  | w     | 159  | A2M  | C2'-C1'-N9  | -2.58 | 109.18      | 113.53   |
| 3   | D     | 3792 | OMG  | O6-C6-C5    | -2.58 | 119.75      | 126.60   |
| 48  | w     | 1347 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 3   | D     | 3851 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 3   | D     | 4299 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 3   | D     | 4361 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 3   | D     | 4500 | PSU  | C6-N1-C2    | -2.58 | 120.05      | 122.68   |
| 48  | w     | 1232 | PSU  | O2-C2-N1    | -2.58 | 119.95      | 122.79   |
| 48  | w     | 436  | OMG  | O6-C6-C5    | -2.57 | 119.77      | 126.60   |
| 48  | w     | 1445 | PSU  | O2-C2-N1    | -2.57 | 119.96      | 122.79   |
| 3   | D     | 1316 | OMG  | O6-C6-C5    | -2.57 | 119.79      | 126.60   |
| 3   | D     | 4499 | OMG  | O6-C6-C5    | -2.57 | 119.79      | 126.60   |
| 48  | w     | 1045 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 3   | D     | 4293 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 48  | w     | 1383 | A2M  | C3'-C2'-C1' | -2.56 | 98.08       | 102.89   |
| 48  | w     | 1244 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 2   | B     | 53   | 5MU  | O4-C4-N3    | -2.56 | 115.21      | 120.12   |
| 48  | w     | 1851 | MA6  | C5-C4-N9    | 2.56  | 108.76      | 105.78   |
| 3   | D     | 3770 | PSU  | O2-C2-N1    | -2.56 | 119.98      | 122.79   |
| 48  | w     | 36   | PSU  | C6-N1-C2    | -2.56 | 120.07      | 122.68   |
| 3   | D     | 4689 | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 48  | w     | 509  | OMG  | O6-C6-C5    | -2.55 | 119.83      | 126.60   |
| 48  | w     | 863  | PSU  | O2-C2-N1    | -2.55 | 119.98      | 122.79   |
| 3   | D     | 1860 | PSU  | C6-N1-C2    | -2.55 | 120.08      | 122.68   |
| 3   | D     | 1781 | PSU  | O2-C2-N1    | -2.55 | 119.99      | 122.79   |
| 48  | w     | 681  | PSU  | O2-C2-N1    | -2.55 | 119.99      | 122.79   |
| 48  | w     | 1832 | 6MZ  | C4-C5-N7    | -2.54 | 107.53      | 110.62   |
| 48  | w     | 601  | OMG  | O6-C6-C5    | -2.53 | 119.88      | 126.60   |
| 3   | D     | 4532 | PSU  | O2-C2-N1    | -2.53 | 120.00      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | C     | 13   | PSU  | O2-C2-N1  | -2.53 | 120.00      | 122.79   |
| 3   | D     | 3730 | PSU  | O2-C2-N1  | -2.53 | 120.01      | 122.79   |
| 3   | D     | 1677 | PSU  | O2-C2-N1  | -2.52 | 120.01      | 122.79   |
| 3   | D     | 4637 | OMG  | O6-C6-C5  | -2.52 | 119.91      | 126.60   |
| 5   | F     | 75   | OMG  | O6-C6-C5  | -2.52 | 119.91      | 126.60   |
| 3   | D     | 4196 | OMG  | O6-C6-C5  | -2.52 | 119.92      | 126.60   |
| 48  | w     | 683  | OMG  | O6-C6-C5  | -2.51 | 119.93      | 126.60   |
| 2   | B     | 6    | 2MG  | O6-C6-C5  | -2.51 | 119.93      | 126.60   |
| 48  | w     | 105  | PSU  | O2-C2-N1  | -2.51 | 120.03      | 122.79   |
| 3   | D     | 4521 | PSU  | O2-C2-N1  | -2.51 | 120.03      | 122.79   |
| 2   | C     | 53   | 5MU  | O4-C4-N3  | -2.51 | 115.31      | 120.12   |
| 48  | w     | 815  | PSU  | O2-C2-N1  | -2.50 | 120.03      | 122.79   |
| 3   | D     | 4494 | OMG  | O6-C6-C5  | -2.50 | 119.96      | 126.60   |
| 2   | C     | 6    | 2MG  | O6-C6-C5  | -2.50 | 119.97      | 126.60   |
| 3   | D     | 4628 | PSU  | O2-C2-N1  | -2.50 | 120.04      | 122.79   |
| 48  | w     | 609  | PSU  | C6-N1-C2  | -2.50 | 120.13      | 122.68   |
| 48  | w     | 1081 | PSU  | O2-C2-N1  | -2.50 | 120.04      | 122.79   |
| 48  | w     | 1490 | OMG  | O6-C6-C5  | -2.49 | 119.98      | 126.60   |
| 48  | w     | 1850 | MA6  | N3-C4-N9  | 2.49  | 131.19      | 127.08   |
| 3   | D     | 4579 | PSU  | C6-N1-C2  | -2.49 | 120.14      | 122.68   |
| 3   | D     | 3944 | OMG  | O6-C6-C5  | -2.48 | 120.01      | 126.60   |
| 48  | w     | 509  | OMG  | C1'-N9-C4 | -2.48 | 119.13      | 126.50   |
| 3   | D     | 4296 | PSU  | O2-C2-N1  | -2.48 | 120.06      | 122.79   |
| 3   | D     | 4370 | OMG  | O6-C6-C5  | -2.48 | 120.03      | 126.60   |
| 3   | D     | 2837 | OMU  | O2-C2-N1  | -2.48 | 119.50      | 122.79   |
| 48  | w     | 683  | OMG  | C1'-N9-C4 | -2.47 | 119.15      | 126.50   |
| 3   | D     | 4552 | PSU  | O2-C2-N1  | -2.47 | 120.07      | 122.79   |
| 48  | w     | 1337 | 4AC  | CM7-C7-N4 | -2.47 | 111.02      | 115.29   |
| 3   | D     | 4420 | PSU  | O2-C2-N1  | -2.47 | 120.07      | 122.79   |
| 2   | B     | 54   | PSU  | O2-C2-N1  | -2.47 | 120.08      | 122.79   |
| 48  | w     | 218  | PSU  | O2-C2-N1  | -2.46 | 120.08      | 122.79   |
| 3   | D     | 3944 | OMG  | C1'-N9-C4 | -2.46 | 119.20      | 126.50   |
| 48  | w     | 1328 | OMG  | O6-C6-C5  | -2.46 | 120.08      | 126.60   |
| 2   | B     | 13   | PSU  | C6-N1-C2  | -2.46 | 120.17      | 122.68   |
| 3   | D     | 4228 | OMG  | C1'-N9-C8 | 2.46  | 133.69      | 126.70   |
| 48  | w     | 1004 | PSU  | C6-N1-C2  | -2.45 | 120.18      | 122.68   |
| 3   | D     | 3770 | PSU  | C6-N1-C2  | -2.45 | 120.18      | 122.68   |
| 48  | w     | 1643 | PSU  | C6-N1-C2  | -2.44 | 120.18      | 122.68   |
| 48  | w     | 109  | PSU  | C6-N1-C2  | -2.44 | 120.19      | 122.68   |
| 3   | D     | 4623 | OMG  | O6-C6-C5  | -2.44 | 120.13      | 126.60   |
| 3   | D     | 4628 | PSU  | C6-N1-C2  | -2.43 | 120.19      | 122.68   |
| 48  | w     | 34   | PSU  | O2-C2-N1  | -2.43 | 120.11      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | w     | 644  | OMG  | O6-C6-C5    | -2.43 | 120.16      | 126.60   |
| 3   | D     | 4299 | PSU  | C6-N1-C2    | -2.43 | 120.20      | 122.68   |
| 3   | D     | 3639 | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 48  | w     | 572  | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 3   | D     | 3899 | OMG  | O6-C6-C5    | -2.42 | 120.17      | 126.60   |
| 3   | D     | 4423 | PSU  | C6-N1-C2    | -2.42 | 120.21      | 122.68   |
| 3   | D     | 4689 | PSU  | C6-N1-C2    | -2.42 | 120.21      | 122.68   |
| 3   | D     | 3762 | PSU  | C6-N1-C2    | -2.41 | 120.22      | 122.68   |
| 3   | D     | 4552 | PSU  | C6-N1-C2    | -2.41 | 120.22      | 122.68   |
| 3   | D     | 1522 | OMG  | O6-C6-C5    | -2.41 | 120.21      | 126.60   |
| 2   | C     | 53   | 5MU  | O2-C2-N1    | -2.41 | 119.59      | 122.79   |
| 48  | w     | 34   | PSU  | C6-N1-C2    | -2.40 | 120.23      | 122.68   |
| 3   | D     | 4403 | PSU  | C6-N1-C2    | -2.40 | 120.23      | 122.68   |
| 3   | D     | 4618 | OMG  | O6-C6-C5    | -2.39 | 120.25      | 126.60   |
| 3   | D     | 2508 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 3   | D     | 1760 | OMG  | O6-C6-C5    | -2.39 | 120.25      | 126.60   |
| 3   | D     | 3758 | PSU  | O2-C2-N1    | -2.38 | 120.17      | 122.79   |
| 3   | D     | 4293 | PSU  | C6-N1-C2    | -2.38 | 120.25      | 122.68   |
| 48  | w     | 1046 | PSU  | C6-N1-C2    | -2.38 | 120.25      | 122.68   |
| 3   | D     | 2415 | OMU  | O3'-C3'-C2' | 2.38  | 117.92      | 111.17   |
| 3   | D     | 4620 | OMU  | O2-C2-N1    | -2.38 | 119.63      | 122.79   |
| 48  | w     | 93   | PSU  | O2-C2-N1    | -2.37 | 120.18      | 122.79   |
| 3   | D     | 4532 | PSU  | C6-N1-C2    | -2.37 | 120.26      | 122.68   |
| 2   | B     | 6    | 2MG  | N1-C2-N3    | -2.37 | 120.28      | 123.95   |
| 48  | w     | 1842 | 4AC  | C5-C4-N4    | -2.37 | 118.81      | 122.92   |
| 48  | w     | 686  | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 48  | w     | 1232 | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 3   | D     | 3764 | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 3   | D     | 4296 | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 3   | D     | 4361 | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 3   | D     | 4196 | OMG  | C1'-N9-C4   | -2.35 | 119.51      | 126.50   |
| 48  | w     | 651  | PSU  | C6-C5-C4    | 2.35  | 119.84      | 118.20   |
| 3   | D     | 4972 | PSU  | C6-N1-C2    | -2.35 | 120.28      | 122.68   |
| 3   | D     | 3768 | PSU  | C6-N1-C2    | -2.35 | 120.28      | 122.68   |
| 48  | w     | 822  | PSU  | O4'-C1'-C2' | 2.35  | 108.45      | 105.14   |
| 3   | D     | 3734 | PSU  | C6-C5-C4    | 2.35  | 119.84      | 118.20   |
| 3   | D     | 4431 | PSU  | C6-N1-C2    | -2.35 | 120.28      | 122.68   |
| 3   | D     | 1744 | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 48  | w     | 863  | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 2   | C     | 6    | 2MG  | N1-C2-N3    | -2.34 | 120.33      | 123.95   |
| 48  | w     | 468  | A2M  | C2'-C1'-N9  | -2.34 | 109.59      | 113.53   |
| 48  | w     | 1174 | PSU  | O2-C2-N1    | -2.34 | 120.21      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 3734 | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 48  | w     | 1056 | PSU  | O2-C2-N1    | -2.34 | 120.22      | 122.79   |
| 3   | D     | 2815 | A2M  | N3-C4-N9    | 2.34  | 130.93      | 127.08   |
| 3   | D     | 3851 | PSU  | C6-N1-C2    | -2.33 | 120.30      | 122.68   |
| 48  | w     | 644  | OMG  | C8-N7-C5    | 2.33  | 108.47      | 104.24   |
| 3   | D     | 1522 | OMG  | C1'-N9-C8   | 2.33  | 133.34      | 126.70   |
| 3   | D     | 4442 | PSU  | C6-N1-C2    | -2.33 | 120.30      | 122.68   |
| 3   | D     | 1871 | A2M  | C3'-C2'-C1' | -2.33 | 98.52       | 102.89   |
| 3   | D     | 4471 | PSU  | O2-C2-N1    | -2.32 | 120.23      | 122.79   |
| 2   | B     | 6    | 2MG  | C8-N7-C5    | 2.32  | 108.44      | 104.24   |
| 48  | w     | 1842 | 4AC  | C4-N3-C2    | -2.32 | 116.97      | 120.12   |
| 3   | D     | 1524 | A2M  | N3-C4-N9    | 2.32  | 130.90      | 127.08   |
| 3   | D     | 3639 | PSU  | C6-N1-C2    | -2.31 | 120.32      | 122.68   |
| 3   | D     | 5001 | PSU  | O2-C2-N1    | -2.31 | 120.25      | 122.79   |
| 48  | w     | 814  | PSU  | O2-C2-N1    | -2.31 | 120.25      | 122.79   |
| 3   | D     | 5010 | PSU  | C6-N1-C2    | -2.31 | 120.32      | 122.68   |
| 48  | w     | 105  | PSU  | C6-N1-C2    | -2.31 | 120.32      | 122.68   |
| 3   | D     | 3695 | PSU  | C6-N1-C2    | -2.31 | 120.33      | 122.68   |
| 48  | w     | 1238 | PSU  | C6-N1-C2    | -2.31 | 120.33      | 122.68   |
| 3   | D     | 3853 | PSU  | O2-C2-N1    | -2.31 | 120.25      | 122.79   |
| 3   | D     | 3853 | PSU  | C6-N1-C2    | -2.30 | 120.33      | 122.68   |
| 3   | D     | 1871 | A2M  | C2'-C1'-N9  | -2.30 | 109.66      | 113.53   |
| 48  | w     | 649  | PSU  | C6-N1-C2    | -2.30 | 120.33      | 122.68   |
| 3   | D     | 4306 | OMU  | O2-C2-N1    | -2.30 | 119.73      | 122.79   |
| 3   | D     | 3899 | OMG  | C1'-N9-C8   | 2.29  | 133.22      | 126.70   |
| 48  | w     | 1850 | MA6  | N1-C6-N6    | -2.29 | 114.58      | 117.08   |
| 48  | w     | 119  | PSU  | C6-N1-C2    | -2.29 | 120.34      | 122.68   |
| 48  | w     | 436  | OMG  | C8-N7-C5    | 2.29  | 108.39      | 104.24   |
| 3   | D     | 1862 | PSU  | C6-N1-C2    | -2.29 | 120.34      | 122.68   |
| 3   | D     | 1792 | PSU  | O2-C2-N1    | -2.29 | 120.27      | 122.79   |
| 48  | w     | 406  | PSU  | C6-C5-C4    | 2.29  | 119.80      | 118.20   |
| 3   | D     | 3637 | PSU  | O2-C2-N1    | -2.29 | 120.27      | 122.79   |
| 48  | w     | 512  | A2M  | N3-C4-N9    | 2.29  | 130.85      | 127.08   |
| 3   | D     | 1536 | PSU  | C6-N1-C2    | -2.28 | 120.35      | 122.68   |
| 48  | w     | 166  | A2M  | N3-C4-N9    | 2.28  | 130.84      | 127.08   |
| 48  | w     | 1625 | PSU  | C6-N1-C2    | -2.28 | 120.35      | 122.68   |
| 48  | w     | 1367 | PSU  | C6-C5-C4    | 2.28  | 119.79      | 118.20   |
| 3   | D     | 3715 | PSU  | C6-N1-C2    | -2.28 | 120.35      | 122.68   |
| 48  | w     | 1328 | OMG  | C8-N7-C5    | 2.28  | 108.37      | 104.24   |
| 48  | w     | 815  | PSU  | C6-C5-C4    | 2.28  | 119.79      | 118.20   |
| 3   | D     | 2401 | A2M  | N3-C4-N9    | 2.28  | 130.84      | 127.08   |
| 3   | D     | 4623 | OMG  | C1'-N9-C8   | 2.28  | 133.18      | 126.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 3785 | A2M  | N3-C4-N9   | 2.28  | 130.83      | 127.08   |
| 48  | w     | 1031 | A2M  | N3-C4-N9   | 2.27  | 130.83      | 127.08   |
| 2   | C     | 6    | 2MG  | C8-N7-C5   | 2.27  | 108.35      | 104.24   |
| 3   | D     | 4353 | PSU  | C6-N1-C2   | -2.26 | 120.37      | 122.68   |
| 48  | w     | 966  | PSU  | C6-N1-C2   | -2.26 | 120.37      | 122.68   |
| 3   | D     | 4457 | PSU  | C6-N1-C2   | -2.26 | 120.38      | 122.68   |
| 3   | D     | 1781 | PSU  | C6-N1-C2   | -2.26 | 120.38      | 122.68   |
| 48  | w     | 99   | A2M  | C2'-C1'-N9 | -2.25 | 109.73      | 113.53   |
| 48  | w     | 822  | PSU  | C6-N1-C2   | -2.25 | 120.38      | 122.68   |
| 3   | D     | 2632 | PSU  | C6-N1-C2   | -2.25 | 120.38      | 122.68   |
| 3   | D     | 4228 | OMG  | C8-N7-C5   | 2.24  | 108.30      | 104.24   |
| 3   | D     | 398  | A2M  | N3-C4-N9   | 2.24  | 130.77      | 127.08   |
| 48  | w     | 484  | A2M  | N3-C4-N9   | 2.24  | 130.77      | 127.08   |
| 3   | D     | 1326 | A2M  | N3-C4-N9   | 2.24  | 130.77      | 127.08   |
| 3   | D     | 3758 | PSU  | C6-N1-C2   | -2.23 | 120.40      | 122.68   |
| 48  | w     | 681  | PSU  | C6-N1-C2   | -2.23 | 120.40      | 122.68   |
| 48  | w     | 649  | PSU  | C6-C5-C4   | 2.23  | 119.76      | 118.20   |
| 48  | w     | 1045 | PSU  | C6-C5-C4   | 2.23  | 119.76      | 118.20   |
| 3   | D     | 4623 | OMG  | C8-N7-C5   | 2.23  | 108.27      | 104.24   |
| 48  | w     | 681  | PSU  | C6-C5-C4   | 2.23  | 119.75      | 118.20   |
| 3   | D     | 3785 | A2M  | C2-N1-C6   | -2.23 | 114.94      | 118.77   |
| 3   | D     | 1534 | A2M  | O4'-C1'-N9 | -2.23 | 103.67      | 108.06   |
| 48  | w     | 801  | PSU  | C6-N1-C2   | -2.22 | 120.41      | 122.68   |
| 3   | D     | 3637 | PSU  | C6-N1-C2   | -2.22 | 120.41      | 122.68   |
| 48  | w     | 1850 | MA6  | C5-C4-N9   | 2.22  | 108.36      | 105.78   |
| 48  | w     | 683  | OMG  | C8-N7-C5   | 2.22  | 108.25      | 104.24   |
| 3   | D     | 2508 | PSU  | C6-N1-C2   | -2.22 | 120.42      | 122.68   |
| 3   | D     | 4312 | PSU  | C6-N1-C2   | -2.22 | 120.42      | 122.68   |
| 3   | D     | 3830 | A2M  | N3-C4-N9   | 2.21  | 130.73      | 127.08   |
| 3   | D     | 1760 | OMG  | C8-N7-C5   | 2.21  | 108.24      | 104.24   |
| 3   | D     | 1534 | A2M  | C2-N1-C6   | -2.21 | 114.97      | 118.77   |
| 48  | w     | 601  | OMG  | C8-N7-C5   | 2.21  | 108.24      | 104.24   |
| 3   | D     | 4576 | PSU  | C6-N1-C2   | -2.21 | 120.43      | 122.68   |
| 3   | D     | 4471 | PSU  | C6-N1-C2   | -2.20 | 120.43      | 122.68   |
| 48  | w     | 1490 | OMG  | C1'-N9-C4  | -2.20 | 119.95      | 126.50   |
| 2   | B     | 13   | PSU  | C6-C5-C4   | 2.20  | 119.74      | 118.20   |
| 3   | D     | 3920 | PSU  | C6-N1-C2   | -2.20 | 120.43      | 122.68   |
| 48  | w     | 1337 | 4AC  | C5-C4-N4   | -2.20 | 119.10      | 122.92   |
| 3   | D     | 3792 | OMG  | C1'-N9-C4  | -2.20 | 119.97      | 126.50   |
| 3   | D     | 4521 | PSU  | C6-N1-C2   | -2.20 | 120.43      | 122.68   |
| 48  | w     | 1174 | PSU  | C6-N1-C2   | -2.20 | 120.43      | 122.68   |
| 5   | F     | 75   | OMG  | C8-N7-C5   | 2.20  | 108.22      | 104.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 54   | PSU  | C6-N1-C2    | -2.20 | 120.44      | 122.68   |
| 3   | D     | 4420 | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 3   | D     | 4220 | 6MZ  | N3-C4-N9    | 2.19  | 130.70      | 127.08   |
| 3   | D     | 4499 | OMG  | C8-N7-C5    | 2.19  | 108.21      | 104.24   |
| 48  | w     | 1081 | PSU  | O4'-C1'-C2' | 2.19  | 108.24      | 105.14   |
| 48  | w     | 1445 | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 3   | D     | 1316 | OMG  | C8-N7-C5    | 2.19  | 108.21      | 104.24   |
| 48  | w     | 1056 | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 48  | w     | 1692 | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 2   | C     | 13   | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 3   | D     | 1782 | PSU  | C6-N1-C2    | -2.19 | 120.44      | 122.68   |
| 3   | D     | 3944 | OMG  | C8-N7-C5    | 2.19  | 108.20      | 104.24   |
| 48  | w     | 1248 | B8N  | C32-C33-C34 | -2.19 | 105.10      | 110.30   |
| 48  | w     | 468  | A2M  | N3-C4-N9    | 2.18  | 130.68      | 127.08   |
| 3   | D     | 4494 | OMG  | C8-N7-C5    | 2.18  | 108.19      | 104.24   |
| 48  | w     | 27   | A2M  | N3-C4-N9    | 2.18  | 130.67      | 127.08   |
| 3   | D     | 3627 | OMG  | C8-N7-C5    | 2.18  | 108.18      | 104.24   |
| 3   | D     | 4637 | OMG  | C8-N7-C5    | 2.17  | 108.18      | 104.24   |
| 3   | D     | 3782 | 5MC  | CM5-C5-C6   | -2.17 | 119.94      | 122.85   |
| 48  | w     | 1347 | PSU  | C6-N1-C2    | -2.17 | 120.46      | 122.68   |
| 3   | D     | 4370 | OMG  | C8-N7-C5    | 2.17  | 108.17      | 104.24   |
| 3   | D     | 3925 | OMU  | O2-C2-N1    | -2.17 | 119.90      | 122.79   |
| 3   | D     | 4618 | OMG  | C8-N7-C5    | 2.17  | 108.17      | 104.24   |
| 48  | w     | 1045 | PSU  | C6-N1-C2    | -2.17 | 120.47      | 122.68   |
| 48  | w     | 1832 | 6MZ  | C5-C4-N9    | 2.17  | 108.31      | 105.78   |
| 3   | D     | 1534 | A2M  | N3-C4-N9    | 2.17  | 130.66      | 127.08   |
| 3   | D     | 1522 | OMG  | C8-N7-C5    | 2.17  | 108.17      | 104.24   |
| 3   | D     | 4420 | PSU  | O4'-C1'-C2' | 2.17  | 108.20      | 105.14   |
| 48  | w     | 509  | OMG  | C8-N7-C5    | 2.17  | 108.16      | 104.24   |
| 3   | D     | 3899 | OMG  | C8-N7-C5    | 2.17  | 108.16      | 104.24   |
| 3   | D     | 4523 | A2M  | C2-N1-C6    | -2.17 | 115.05      | 118.77   |
| 3   | D     | 1625 | OMG  | C8-N7-C5    | 2.16  | 108.16      | 104.24   |
| 3   | D     | 3818 | UY1  | O4-C4-N3    | -2.16 | 115.97      | 120.12   |
| 48  | w     | 1177 | PSU  | C6-N1-C2    | -2.16 | 120.47      | 122.68   |
| 3   | D     | 2815 | A2M  | C2-N1-C6    | -2.16 | 115.06      | 118.77   |
| 3   | D     | 1862 | PSU  | C6-C5-C4    | 2.16  | 119.71      | 118.20   |
| 3   | D     | 4498 | OMU  | O2-C2-N1    | -2.16 | 119.92      | 122.79   |
| 48  | w     | 1367 | PSU  | C6-N1-C2    | -2.16 | 120.48      | 122.68   |
| 3   | D     | 4523 | A2M  | C3'-C2'-C1' | -2.16 | 98.84       | 102.89   |
| 3   | D     | 3744 | OMG  | C8-N7-C5    | 2.16  | 108.14      | 104.24   |
| 48  | w     | 1678 | A2M  | N3-C4-N9    | 2.15  | 130.63      | 127.08   |
| 48  | w     | 406  | PSU  | C6-N1-C2    | -2.15 | 120.48      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | w     | 1639 | G7M  | O3'-C3'-C2' | 2.15  | 118.76      | 111.82   |
| 3   | D     | 4523 | A2M  | N3-C4-N9    | 2.14  | 130.62      | 127.08   |
| 3   | D     | 4392 | OMG  | C8-N7-C5    | 2.14  | 108.12      | 104.24   |
| 3   | D     | 1871 | A2M  | N3-C4-N9    | 2.14  | 130.61      | 127.08   |
| 3   | D     | 2815 | A2M  | C5-C4-N3    | -2.14 | 123.96      | 126.75   |
| 3   | D     | 400  | A2M  | N3-C4-N9    | 2.14  | 130.61      | 127.08   |
| 3   | D     | 4392 | OMG  | C1'-N9-C8   | 2.14  | 132.78      | 126.70   |
| 3   | D     | 2415 | OMU  | O2-C2-N1    | -2.14 | 119.94      | 122.79   |
| 3   | D     | 4523 | A2M  | C2'-C1'-N9  | -2.14 | 109.93      | 113.53   |
| 48  | w     | 1842 | 4AC  | CM7-C7-N4   | -2.14 | 111.60      | 115.29   |
| 3   | D     | 3730 | PSU  | C6-N1-C2    | -2.14 | 120.50      | 122.68   |
| 48  | w     | 159  | A2M  | N3-C4-N9    | 2.13  | 130.60      | 127.08   |
| 48  | w     | 1678 | A2M  | C2-N1-C6    | -2.13 | 115.11      | 118.77   |
| 3   | D     | 2787 | A2M  | C2-N1-C6    | -2.13 | 115.11      | 118.77   |
| 48  | w     | 218  | PSU  | C6-N1-C2    | -2.13 | 120.50      | 122.68   |
| 3   | D     | 2363 | A2M  | N3-C4-N9    | 2.13  | 130.60      | 127.08   |
| 48  | w     | 576  | A2M  | N3-C4-N9    | 2.13  | 130.59      | 127.08   |
| 48  | w     | 99   | A2M  | N3-C4-N9    | 2.13  | 130.59      | 127.08   |
| 3   | D     | 3825 | A2M  | N3-C4-N9    | 2.13  | 130.59      | 127.08   |
| 48  | w     | 159  | A2M  | C2-N1-C6    | -2.12 | 115.12      | 118.77   |
| 48  | w     | 1248 | B8N  | O4'-C1'-C2' | 2.12  | 108.14      | 105.14   |
| 48  | w     | 210  | PSU  | C6-N1-C2    | -2.12 | 120.51      | 122.68   |
| 3   | D     | 3724 | A2M  | N3-C4-N9    | 2.12  | 130.58      | 127.08   |
| 48  | w     | 651  | PSU  | C6-N1-C2    | -2.12 | 120.52      | 122.68   |
| 2   | B     | 48   | 5MC  | CM5-C5-C6   | -2.12 | 120.02      | 122.85   |
| 3   | D     | 2363 | A2M  | C2-N1-C6    | -2.12 | 115.13      | 118.77   |
| 48  | w     | 668  | A2M  | N3-C4-N9    | 2.12  | 130.57      | 127.08   |
| 3   | D     | 2401 | A2M  | C2-N1-C6    | -2.12 | 115.13      | 118.77   |
| 48  | w     | 1442 | OMU  | O2-C2-N1    | -2.12 | 119.97      | 122.79   |
| 3   | D     | 3760 | A2M  | N3-C4-N9    | 2.12  | 130.57      | 127.08   |
| 48  | w     | 1238 | PSU  | C6-C5-C4    | 2.11  | 119.67      | 118.20   |
| 3   | D     | 3715 | PSU  | C6-C5-C4    | 2.11  | 119.67      | 118.20   |
| 3   | D     | 3627 | OMG  | C1'-N9-C8   | 2.11  | 132.70      | 126.70   |
| 3   | D     | 1625 | OMG  | C1'-N9-C4   | -2.11 | 120.24      | 126.50   |
| 2   | C     | 57   | 1MA  | C6-C5-N7    | -2.11 | 128.36      | 132.20   |
| 3   | D     | 5001 | PSU  | C6-N1-C2    | -2.11 | 120.53      | 122.68   |
| 3   | D     | 1524 | A2M  | C2-N1-C6    | -2.11 | 115.15      | 118.77   |
| 48  | w     | 512  | A2M  | C3'-C2'-C1' | -2.11 | 98.93       | 102.89   |
| 3   | D     | 4220 | 6MZ  | C4-N9-C8    | 2.11  | 108.01      | 105.73   |
| 48  | w     | 99   | A2M  | C2-N1-C6    | -2.11 | 115.15      | 118.77   |
| 3   | D     | 1760 | OMG  | C1'-N9-C8   | 2.11  | 132.69      | 126.70   |
| 48  | w     | 866  | PSU  | C6-N1-C2    | -2.11 | 120.53      | 122.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 2364 | OMG  | C8-N7-C5    | 2.10  | 108.05      | 104.24   |
| 2   | B     | 54   | PSU  | C6-N1-C2    | -2.10 | 120.53      | 122.68   |
| 3   | D     | 2424 | OMG  | C8-N7-C5    | 2.10  | 108.05      | 104.24   |
| 3   | D     | 1534 | A2M  | C5-C4-N3    | -2.10 | 124.01      | 126.75   |
| 2   | B     | 9    | 1MA  | C6-C5-N7    | -2.10 | 128.38      | 132.20   |
| 3   | D     | 3724 | A2M  | C2-N1-C6    | -2.10 | 115.17      | 118.77   |
| 48  | w     | 966  | PSU  | C6-C5-C4    | 2.10  | 119.66      | 118.20   |
| 3   | D     | 3718 | A2M  | C2-N1-C6    | -2.10 | 115.17      | 118.77   |
| 3   | D     | 3825 | A2M  | C2-N1-C6    | -2.09 | 115.17      | 118.77   |
| 48  | w     | 1383 | A2M  | C2-N1-C6    | -2.09 | 115.18      | 118.77   |
| 48  | w     | 484  | A2M  | C2-N1-C6    | -2.09 | 115.19      | 118.77   |
| 3   | D     | 3851 | PSU  | C6-C5-C4    | 2.08  | 119.65      | 118.20   |
| 3   | D     | 4442 | PSU  | C6-C5-C4    | 2.08  | 119.65      | 118.20   |
| 48  | w     | 590  | A2M  | N3-C4-N9    | 2.08  | 130.51      | 127.08   |
| 48  | w     | 1490 | OMG  | C8-N7-C5    | 2.08  | 108.00      | 104.24   |
| 3   | D     | 400  | A2M  | C2-N1-C6    | -2.08 | 115.20      | 118.77   |
| 48  | w     | 1337 | 4AC  | C4-N3-C2    | -2.08 | 117.29      | 120.12   |
| 3   | D     | 1326 | A2M  | C2-N1-C6    | -2.08 | 115.20      | 118.77   |
| 48  | w     | 166  | A2M  | C5-C4-N3    | -2.07 | 124.05      | 126.75   |
| 48  | w     | 428  | OMU  | O2-C2-N1    | -2.07 | 120.03      | 122.79   |
| 3   | D     | 398  | A2M  | C2-N1-C6    | -2.07 | 115.21      | 118.77   |
| 48  | w     | 590  | A2M  | C2-N1-C6    | -2.07 | 115.22      | 118.77   |
| 3   | D     | 2787 | A2M  | N3-C4-N9    | 2.07  | 130.49      | 127.08   |
| 48  | w     | 1832 | 6MZ  | C4-N9-C8    | 2.07  | 107.97      | 105.73   |
| 3   | D     | 2401 | A2M  | C5-C4-N3    | -2.07 | 124.06      | 126.75   |
| 3   | D     | 4442 | PSU  | O4'-C1'-C2' | 2.07  | 108.06      | 105.14   |
| 48  | w     | 1383 | A2M  | C2'-C1'-N9  | -2.06 | 110.06      | 113.53   |
| 48  | w     | 815  | PSU  | C6-N1-C2    | -2.06 | 120.57      | 122.68   |
| 48  | w     | 1244 | PSU  | C6-N1-C2    | -2.06 | 120.57      | 122.68   |
| 48  | w     | 1643 | PSU  | C6-C5-C4    | 2.06  | 119.64      | 118.20   |
| 2   | B     | 47   | 5MC  | CM5-C5-C6   | -2.06 | 120.09      | 122.85   |
| 3   | D     | 3792 | OMG  | C8-N7-C5    | 2.06  | 107.97      | 104.24   |
| 3   | D     | 2364 | OMG  | C1'-N9-C8   | 2.06  | 132.56      | 126.70   |
| 2   | C     | 34   | 56B  | C8-C7-C5    | 2.05  | 108.25      | 106.08   |
| 2   | B     | 57   | 1MA  | C6-C5-N7    | -2.05 | 128.46      | 132.20   |
| 48  | w     | 210  | PSU  | C6-C5-C4    | 2.05  | 119.63      | 118.20   |
| 3   | D     | 3718 | A2M  | N3-C4-N9    | 2.05  | 130.47      | 127.08   |
| 2   | C     | 9    | 1MA  | C6-C5-N7    | -2.05 | 128.46      | 132.20   |
| 2   | B     | 38   | 5MC  | CM5-C5-C6   | -2.05 | 120.11      | 122.85   |
| 3   | D     | 3744 | OMG  | C1'-N9-C8   | 2.05  | 132.53      | 126.70   |
| 3   | D     | 4530 | UR3  | C6-N1-C2    | -2.05 | 119.95      | 121.79   |
| 2   | C     | 38   | 5MC  | CM5-C5-C6   | -2.04 | 120.12      | 122.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | w     | 166  | A2M  | C2-N1-C6    | -2.04 | 115.26      | 118.77   |
| 3   | D     | 3760 | A2M  | C2-N1-C6    | -2.04 | 115.26      | 118.77   |
| 48  | w     | 1337 | 4AC  | C5-C4-N3    | 2.04  | 125.88      | 122.59   |
| 3   | D     | 2424 | OMG  | C1'-N9-C8   | 2.04  | 132.51      | 126.70   |
| 48  | w     | 1383 | A2M  | N3-C4-N9    | 2.04  | 130.45      | 127.08   |
| 48  | w     | 627  | OMU  | O2-C2-N1    | -2.04 | 120.08      | 122.79   |
| 48  | w     | 668  | A2M  | C2-N1-C6    | -2.04 | 115.27      | 118.77   |
| 3   | D     | 1677 | PSU  | C6-N1-C2    | -2.04 | 120.60      | 122.68   |
| 2   | C     | 47   | 5MC  | CM5-C5-C6   | -2.03 | 120.13      | 122.85   |
| 48  | w     | 1326 | OMU  | O2'-C2'-C1' | 2.03  | 113.04      | 109.08   |
| 48  | w     | 1031 | A2M  | C5-C4-N3    | -2.03 | 124.10      | 126.75   |
| 3   | D     | 4521 | PSU  | O4'-C1'-C2' | 2.03  | 108.01      | 105.14   |
| 48  | w     | 576  | A2M  | C2-N1-C6    | -2.02 | 115.29      | 118.77   |
| 48  | w     | 863  | PSU  | C6-C5-C4    | 2.02  | 119.61      | 118.20   |
| 2   | C     | 48   | 5MC  | CM5-C5-C6   | -2.02 | 120.15      | 122.85   |
| 3   | D     | 398  | A2M  | C5-C4-N3    | -2.02 | 124.11      | 126.75   |
| 3   | D     | 4196 | OMG  | C8-N7-C5    | 2.02  | 107.90      | 104.24   |
| 48  | w     | 105  | PSU  | C6-C5-C4    | 2.02  | 119.61      | 118.20   |
| 48  | w     | 1328 | OMG  | C1'-N9-C8   | 2.02  | 132.43      | 126.70   |
| 48  | w     | 1851 | MA6  | C4-N9-C8    | 2.01  | 107.91      | 105.73   |
| 3   | D     | 3730 | PSU  | C6-C5-C4    | 2.01  | 119.60      | 118.20   |
| 3   | D     | 4403 | PSU  | C6-C5-C4    | 2.01  | 119.60      | 118.20   |
| 3   | D     | 4370 | OMG  | C1'-N9-C8   | 2.01  | 132.41      | 126.70   |
| 48  | w     | 814  | PSU  | C6-N1-C2    | -2.01 | 120.63      | 122.68   |
| 48  | w     | 172  | OMU  | O2-C2-N1    | -2.01 | 120.12      | 122.79   |
| 3   | D     | 1524 | A2M  | C5-C4-N3    | -2.00 | 124.14      | 126.75   |
| 48  | w     | 1851 | MA6  | N3-C4-N9    | 2.00  | 130.39      | 127.08   |
| 3   | D     | 1683 | PSU  | C6-C5-C4    | 2.00  | 119.60      | 118.20   |
| 3   | D     | 5010 | PSU  | C6-C5-C4    | 2.00  | 119.60      | 118.20   |
| 48  | w     | 1445 | PSU  | C6-C5-C4    | 2.00  | 119.60      | 118.20   |
| 3   | D     | 1322 | 1MA  | C6-C5-N7    | -2.00 | 128.55      | 132.20   |

There are no chirality outliers.

All (173) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 34  | 56B  | C14-C10-N10-C9  |
| 2   | B     | 34  | 56B  | C5-C7-C9-N10    |
| 2   | C     | 34  | 56B  | C11-C10-N10-C9  |
| 2   | C     | 34  | 56B  | C14-C10-N10-C9  |
| 2   | B     | 47  | 5MC  | O4'-C4'-C5'-O5' |
| 2   | B     | 47  | 5MC  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 48   | 5MC  | O4'-C4'-C5'-O5' |
| 2   | C     | 48   | 5MC  | O4'-C4'-C5'-O5' |
| 2   | B     | 53   | 5MU  | O4'-C4'-C5'-O5' |
| 3   | D     | 398  | A2M  | C1'-C2'-O2'-CM' |
| 3   | D     | 1534 | A2M  | C1'-C2'-O2'-CM' |
| 3   | D     | 1677 | PSU  | C2'-C1'-C5-C6   |
| 3   | D     | 1760 | OMG  | C3'-C4'-C5'-O5' |
| 3   | D     | 1773 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | D     | 2415 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | D     | 2415 | OMU  | C3'-C4'-C5'-O5' |
| 3   | D     | 2415 | OMU  | O4'-C4'-C5'-O5' |
| 3   | D     | 2424 | OMG  | O4'-C4'-C5'-O5' |
| 3   | D     | 2424 | OMG  | C3'-C4'-C5'-O5' |
| 3   | D     | 2815 | A2M  | O4'-C4'-C5'-O5' |
| 3   | D     | 2815 | A2M  | C3'-C4'-C5'-O5' |
| 3   | D     | 3785 | A2M  | O4'-C4'-C5'-O5' |
| 3   | D     | 3944 | OMG  | O4'-C4'-C5'-O5' |
| 3   | D     | 3944 | OMG  | C3'-C4'-C5'-O5' |
| 3   | D     | 4196 | OMG  | C1'-C2'-O2'-CM2 |
| 3   | D     | 4227 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | D     | 4500 | PSU  | C3'-C4'-C5'-O5' |
| 3   | D     | 4500 | PSU  | O4'-C4'-C5'-O5' |
| 3   | D     | 4637 | OMG  | C1'-C2'-O2'-CM2 |
| 48  | w     | 34   | PSU  | C3'-C4'-C5'-O5' |
| 48  | w     | 116  | OMU  | O4'-C4'-C5'-O5' |
| 48  | w     | 159  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 159  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 166  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 166  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 174  | OMC  | C1'-C2'-O2'-CM2 |
| 48  | w     | 428  | OMU  | C2'-C1'-N1-C2   |
| 48  | w     | 428  | OMU  | C2'-C1'-N1-C6   |
| 48  | w     | 428  | OMU  | C1'-C2'-O2'-CM2 |
| 48  | w     | 468  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 468  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 512  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 576  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 627  | OMU  | C1'-C2'-O2'-CM2 |
| 48  | w     | 644  | OMG  | C3'-C4'-C5'-O5' |
| 48  | w     | 668  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 668  | A2M  | C1'-C2'-O2'-CM' |
| 48  | w     | 799  | OMU  | C1'-C2'-O2'-CM2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 48  | w     | 1248 | B8N  | C31-C32-C33-N34 |
| 48  | w     | 1326 | OMU  | C1'-C2'-O2'-CM2 |
| 48  | w     | 1442 | OMU  | C1'-C2'-O2'-CM2 |
| 48  | w     | 1639 | G7M  | O4'-C4'-C5'-O5' |
| 48  | w     | 1678 | A2M  | C1'-C2'-O2'-CM' |
| 48  | w     | 1804 | OMU  | C1'-C2'-O2'-CM2 |
| 48  | w     | 1832 | 6MZ  | C5-C6-N6-C9     |
| 48  | w     | 1832 | 6MZ  | N1-C6-N6-C9     |
| 48  | w     | 1851 | MA6  | O4'-C4'-C5'-O5' |
| 3   | D     | 3701 | OMC  | C2'-C1'-N1-C6   |
| 2   | C     | 47   | 5MC  | C3'-C4'-C5'-O5' |
| 2   | B     | 48   | 5MC  | C3'-C4'-C5'-O5' |
| 2   | C     | 48   | 5MC  | C3'-C4'-C5'-O5' |
| 2   | B     | 53   | 5MU  | C3'-C4'-C5'-O5' |
| 3   | D     | 1534 | A2M  | O4'-C4'-C5'-O5' |
| 3   | D     | 3785 | A2M  | C3'-C4'-C5'-O5' |
| 3   | D     | 3818 | UY1  | C3'-C4'-C5'-O5' |
| 3   | D     | 3818 | UY1  | O4'-C4'-C5'-O5' |
| 48  | w     | 116  | OMU  | C3'-C4'-C5'-O5' |
| 48  | w     | 428  | OMU  | C3'-C4'-C5'-O5' |
| 48  | w     | 512  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 627  | OMU  | C3'-C4'-C5'-O5' |
| 48  | w     | 627  | OMU  | O4'-C4'-C5'-O5' |
| 48  | w     | 822  | PSU  | C3'-C4'-C5'-O5' |
| 48  | w     | 1238 | PSU  | C3'-C4'-C5'-O5' |
| 48  | w     | 1288 | OMU  | C3'-C4'-C5'-O5' |
| 48  | w     | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 2   | B     | 34   | 56B  | C7-C9-N10-C10   |
| 3   | D     | 1760 | OMG  | O4'-C4'-C5'-O5' |
| 3   | D     | 2364 | OMG  | O4'-C4'-C5'-O5' |
| 48  | w     | 428  | OMU  | O4'-C4'-C5'-O5' |
| 48  | w     | 576  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 668  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 799  | OMU  | C3'-C4'-C5'-O5' |
| 48  | w     | 822  | PSU  | O4'-C4'-C5'-O5' |
| 48  | w     | 1238 | PSU  | O4'-C4'-C5'-O5' |
| 48  | w     | 1639 | G7M  | C3'-C4'-C5'-O5' |
| 48  | w     | 1703 | OMC  | O4'-C4'-C5'-O5' |
| 3   | D     | 4447 | 5MC  | C2'-C1'-N1-C6   |
| 3   | D     | 3701 | OMC  | C2'-C1'-N1-C2   |
| 48  | w     | 34   | PSU  | O4'-C4'-C5'-O5' |
| 48  | w     | 799  | OMU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | D     | 4447 | 5MC  | C2'-C1'-N1-C2   |
| 2   | B     | 13   | PSU  | C3'-C4'-C5'-O5' |
| 3   | D     | 2364 | OMG  | C3'-C4'-C5'-O5' |
| 48  | w     | 1490 | OMG  | C3'-C4'-C5'-O5' |
| 2   | C     | 53   | 5MU  | O4'-C4'-C5'-O5' |
| 3   | D     | 1677 | PSU  | O4'-C4'-C5'-O5' |
| 48  | w     | 99   | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 590  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 590  | A2M  | C3'-C4'-C5'-O5' |
| 48  | w     | 644  | OMG  | O4'-C4'-C5'-O5' |
| 48  | w     | 1288 | OMU  | O4'-C4'-C5'-O5' |
| 48  | w     | 1490 | OMG  | O4'-C4'-C5'-O5' |
| 3   | D     | 1677 | PSU  | C3'-C4'-C5'-O5' |
| 48  | w     | 1490 | OMG  | C4'-C5'-O5'-P   |
| 2   | C     | 47   | 5MC  | O4'-C4'-C5'-O5' |
| 3   | D     | 3760 | A2M  | C3'-C4'-C5'-O5' |
| 3   | D     | 4447 | 5MC  | O4'-C1'-N1-C6   |
| 3   | D     | 2787 | A2M  | C2'-C1'-N9-C8   |
| 2   | C     | 34   | 56B  | C7-C9-N10-C10   |
| 3   | D     | 3701 | OMC  | O4'-C1'-N1-C6   |
| 48  | w     | 644  | OMG  | C4'-C5'-O5'-P   |
| 2   | B     | 6    | 2MG  | O4'-C4'-C5'-O5' |
| 2   | B     | 13   | PSU  | O4'-C4'-C5'-O5' |
| 48  | w     | 1248 | B8N  | C31-C32-C33-C34 |
| 3   | D     | 2401 | A2M  | C3'-C2'-O2'-CM' |
| 3   | D     | 4370 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | D     | 4499 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | w     | 172  | OMU  | C3'-C2'-O2'-CM2 |
| 2   | C     | 47   | 5MC  | C4'-C5'-O5'-P   |
| 3   | D     | 3944 | OMG  | C4'-C5'-O5'-P   |
| 3   | D     | 4500 | PSU  | C4'-C5'-O5'-P   |
| 48  | w     | 34   | PSU  | C4'-C5'-O5'-P   |
| 2   | C     | 9    | 1MA  | C3'-C4'-C5'-O5' |
| 48  | w     | 1703 | OMC  | C3'-C4'-C5'-O5' |
| 3   | D     | 4447 | 5MC  | O4'-C1'-N1-C2   |
| 3   | D     | 3701 | OMC  | O4'-C1'-N1-C2   |
| 3   | D     | 3760 | A2M  | O4'-C4'-C5'-O5' |
| 3   | D     | 3770 | PSU  | C3'-C4'-C5'-O5' |
| 48  | w     | 428  | OMU  | O4'-C1'-N1-C6   |
| 3   | D     | 1534 | A2M  | C4'-C5'-O5'-P   |
| 48  | w     | 1248 | B8N  | C32-C33-C34-O35 |
| 48  | w     | 1288 | OMU  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | D     | 2787 | A2M  | C2'-C1'-N9-C4   |
| 48  | w     | 1326 | OMU  | O4'-C1'-N1-C6   |
| 48  | w     | 1248 | B8N  | C32-C33-C34-O36 |
| 2   | B     | 47   | 5MC  | C4'-C5'-O5'-P   |
| 48  | w     | 428  | OMU  | O4'-C1'-N1-C2   |
| 48  | w     | 1326 | OMU  | C2'-C1'-N1-C6   |
| 2   | C     | 54   | PSU  | O4'-C1'-C5-C4   |
| 3   | D     | 1677 | PSU  | O4'-C1'-C5-C4   |
| 3   | D     | 3818 | UY1  | O4'-C1'-C5-C4   |
| 3   | D     | 4521 | PSU  | O4'-C1'-C5-C4   |
| 3   | D     | 1625 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | D     | 4494 | OMG  | C3'-C2'-O2'-CM2 |
| 48  | w     | 627  | OMU  | C2'-C1'-N1-C6   |
| 48  | w     | 509  | OMG  | O4'-C4'-C5'-O5' |
| 2   | B     | 9    | 1MA  | C3'-C4'-C5'-O5' |
| 2   | C     | 9    | 1MA  | O4'-C4'-C5'-O5' |
| 2   | C     | 53   | 5MU  | C3'-C4'-C5'-O5' |
| 48  | w     | 627  | OMU  | O4'-C1'-N1-C6   |
| 2   | B     | 9    | 1MA  | O4'-C4'-C5'-O5' |
| 3   | D     | 398  | A2M  | O4'-C4'-C5'-O5' |
| 48  | w     | 27   | A2M  | C1'-C2'-O2'-CM' |
| 48  | w     | 462  | OMC  | C1'-C2'-O2'-CM2 |
| 3   | D     | 1322 | 1MA  | C2'-C1'-N9-C8   |
| 3   | D     | 2787 | A2M  | O4'-C1'-N9-C8   |
| 48  | w     | 1326 | OMU  | O4'-C1'-N1-C2   |
| 3   | D     | 2422 | OMC  | O4'-C4'-C5'-O5' |
| 48  | w     | 99   | A2M  | C3'-C4'-C5'-O5' |
| 2   | C     | 54   | PSU  | O4'-C1'-C5-C6   |
| 3   | D     | 1677 | PSU  | O4'-C1'-C5-C6   |
| 3   | D     | 3818 | UY1  | O4'-C1'-C5-C6   |
| 3   | D     | 4521 | PSU  | O4'-C1'-C5-C6   |
| 48  | w     | 1326 | OMU  | C2'-C1'-N1-C2   |
| 3   | D     | 3887 | OMC  | C4'-C5'-O5'-P   |
| 3   | D     | 1524 | A2M  | O4'-C1'-N9-C8   |
| 3   | D     | 2351 | OMC  | O4'-C4'-C5'-O5' |
| 48  | w     | 1804 | OMU  | C3'-C4'-C5'-O5' |
| 3   | D     | 3944 | OMG  | C3'-C2'-O2'-CM2 |
| 2   | B     | 6    | 2MG  | C3'-C4'-C5'-O5' |
| 2   | B     | 34   | 56B  | O4'-C4'-C5'-O5' |
| 3   | D     | 2815 | A2M  | C4'-C5'-O5'-P   |
| 3   | D     | 3851 | PSU  | C3'-C4'-C5'-O5' |

There are no ring outliers.

60 monomers are involved in 79 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 48  | w     | 166  | A2M  | 2       | 0            |
| 3   | D     | 4220 | 6MZ  | 1       | 0            |
| 3   | D     | 3925 | OMU  | 1       | 0            |
| 48  | w     | 651  | PSU  | 1       | 0            |
| 3   | D     | 2815 | A2M  | 1       | 0            |
| 3   | D     | 4623 | OMG  | 2       | 0            |
| 48  | w     | 1678 | A2M  | 1       | 0            |
| 48  | w     | 681  | PSU  | 1       | 0            |
| 48  | w     | 1490 | OMG  | 1       | 0            |
| 3   | D     | 1773 | OMU  | 4       | 0            |
| 48  | w     | 1383 | A2M  | 1       | 0            |
| 3   | D     | 4227 | OMU  | 1       | 0            |
| 3   | D     | 3808 | OMC  | 1       | 0            |
| 3   | D     | 1760 | OMG  | 1       | 0            |
| 48  | w     | 590  | A2M  | 2       | 0            |
| 48  | w     | 576  | A2M  | 1       | 0            |
| 48  | w     | 174  | OMC  | 1       | 0            |
| 48  | w     | 1639 | G7M  | 3       | 0            |
| 3   | D     | 3792 | OMG  | 1       | 0            |
| 3   | D     | 4196 | OMG  | 1       | 0            |
| 48  | w     | 1804 | OMU  | 1       | 0            |
| 3   | D     | 4637 | OMG  | 2       | 0            |
| 48  | w     | 1391 | OMC  | 1       | 0            |
| 3   | D     | 3770 | PSU  | 1       | 0            |
| 2   | B     | 53   | 5MU  | 3       | 0            |
| 48  | w     | 1232 | PSU  | 2       | 0            |
| 3   | D     | 4447 | 5MC  | 1       | 0            |
| 3   | D     | 4494 | OMG  | 1       | 0            |
| 48  | w     | 172  | OMU  | 1       | 0            |
| 5   | F     | 75   | OMG  | 2       | 0            |
| 48  | w     | 799  | OMU  | 2       | 0            |
| 48  | w     | 1842 | 4AC  | 1       | 0            |
| 3   | D     | 4579 | PSU  | 1       | 0            |
| 48  | w     | 509  | OMG  | 2       | 0            |
| 48  | w     | 36   | PSU  | 1       | 0            |
| 48  | w     | 1031 | A2M  | 1       | 0            |
| 3   | D     | 2351 | OMC  | 1       | 0            |
| 2   | C     | 47   | 5MC  | 1       | 0            |
| 48  | w     | 428  | OMU  | 1       | 0            |
| 3   | D     | 4620 | OMU  | 1       | 0            |
| 3   | D     | 2415 | OMU  | 1       | 0            |
| 48  | w     | 609  | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | D     | 1326 | A2M  | 1       | 0            |
| 3   | D     | 4392 | OMG  | 1       | 0            |
| 2   | C     | 6    | 2MG  | 1       | 0            |
| 48  | w     | 159  | A2M  | 1       | 0            |
| 3   | D     | 4523 | A2M  | 1       | 0            |
| 3   | D     | 3818 | UY1  | 1       | 0            |
| 2   | B     | 9    | 1MA  | 1       | 0            |
| 48  | w     | 1850 | MA6  | 1       | 0            |
| 48  | w     | 1288 | OMU  | 1       | 0            |
| 3   | D     | 2363 | A2M  | 1       | 0            |
| 48  | w     | 512  | A2M  | 2       | 0            |
| 3   | D     | 4306 | OMU  | 1       | 0            |
| 48  | w     | 27   | A2M  | 2       | 0            |
| 48  | w     | 436  | OMG  | 2       | 0            |
| 2   | C     | 53   | 5MU  | 2       | 0            |
| 48  | w     | 1442 | OMU  | 2       | 0            |
| 3   | D     | 1340 | OMC  | 1       | 0            |
| 48  | w     | 121  | OMU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 545 ligands modelled in this entry, 545 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

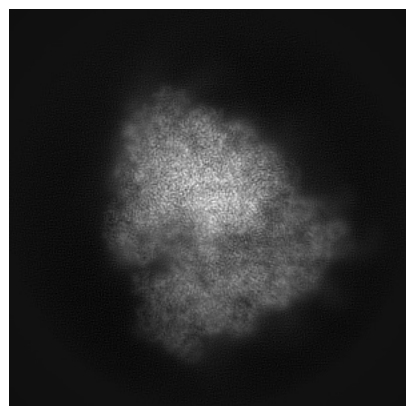
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36178. These allow visual inspection of the internal detail of the map and identification of artifacts.

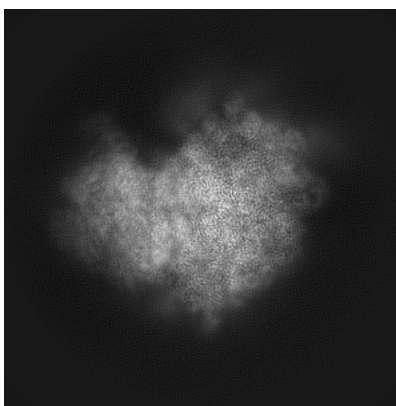
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

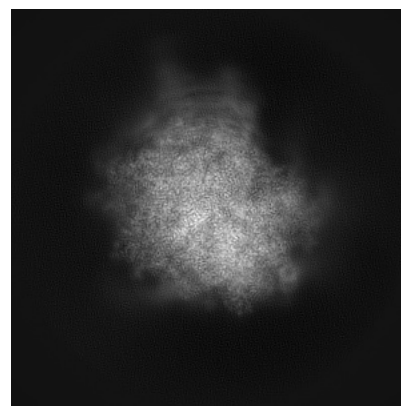
#### 6.1.1 Primary map



X

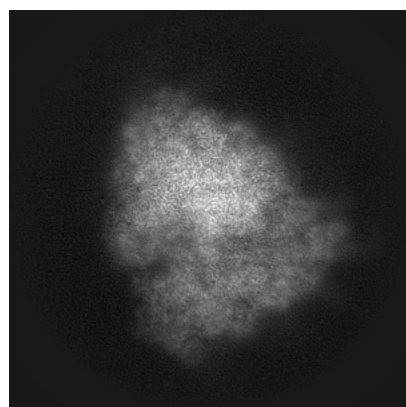


Y

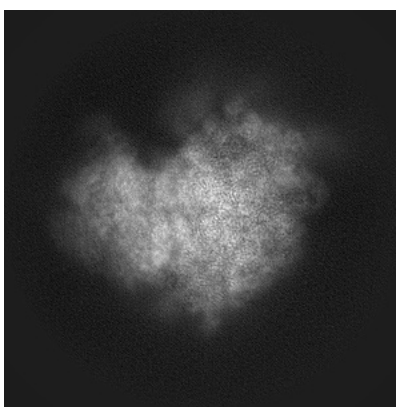


Z

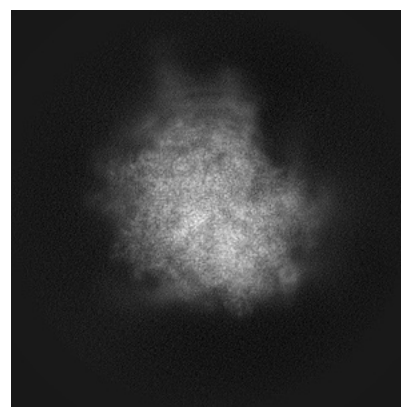
#### 6.1.2 Raw map



X



Y

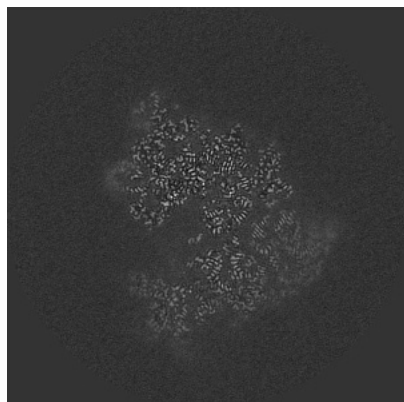


Z

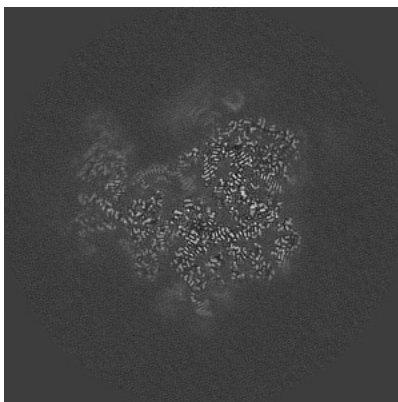
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

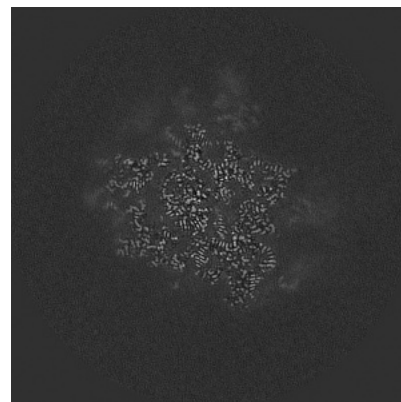
### 6.2.1 Primary map



X Index: 265

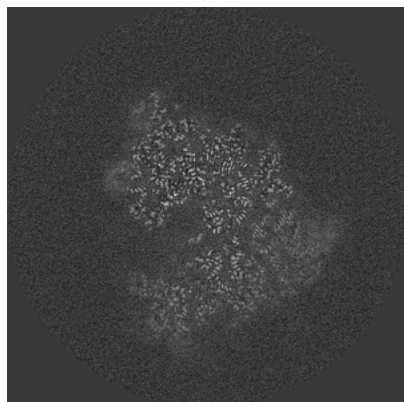


Y Index: 265

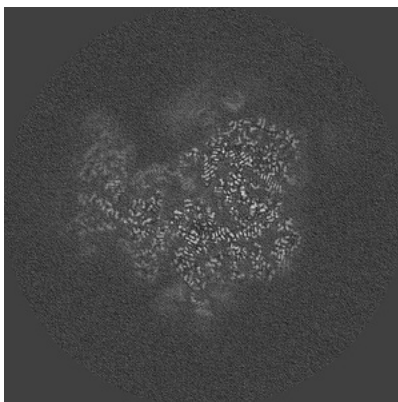


Z Index: 265

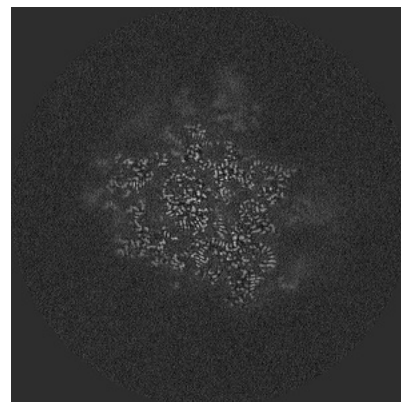
### 6.2.2 Raw map



X Index: 265



Y Index: 265

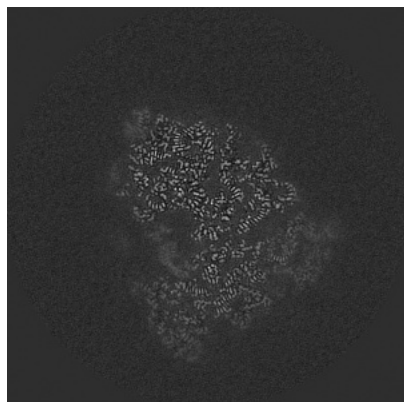


Z Index: 265

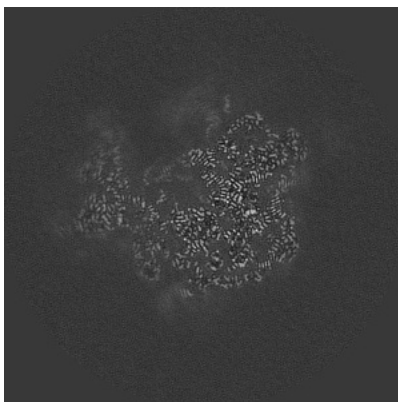
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

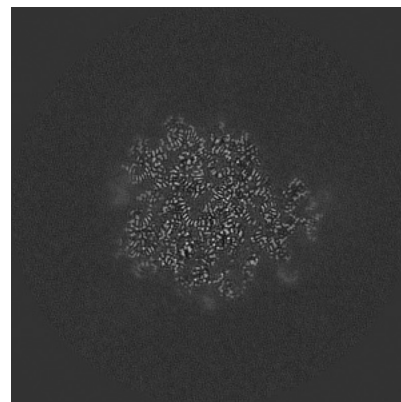
### 6.3.1 Primary map



X Index: 253

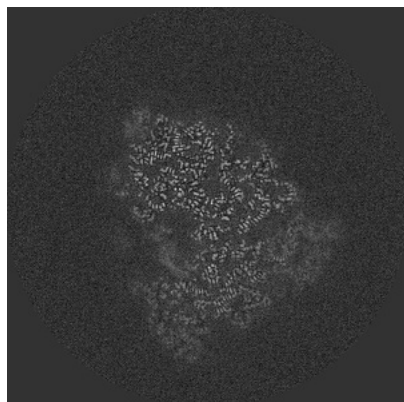


Y Index: 258

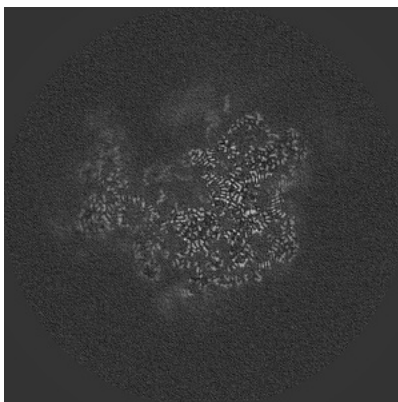


Z Index: 300

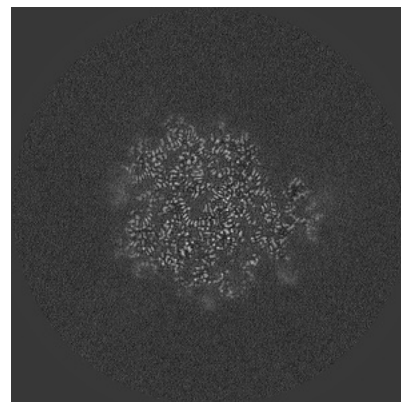
### 6.3.2 Raw map



X Index: 253



Y Index: 258

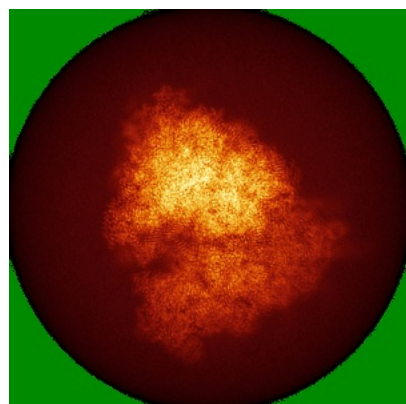


Z Index: 300

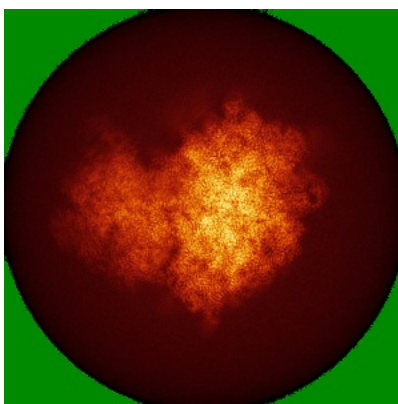
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

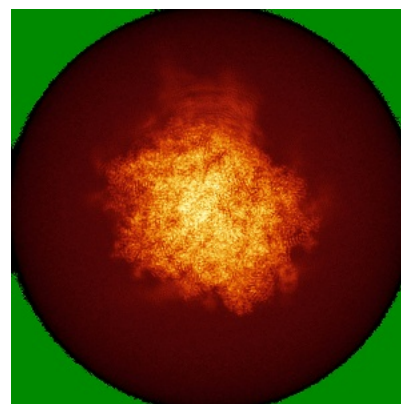
### 6.4.1 Primary map



X

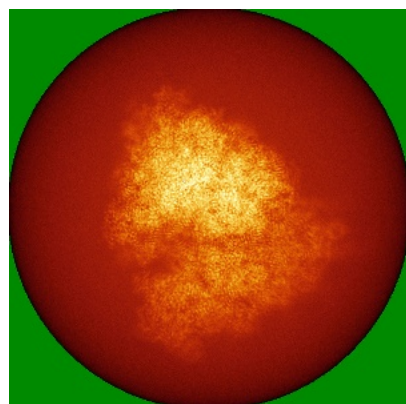


Y

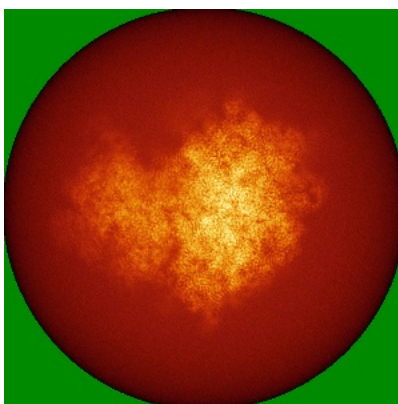


Z

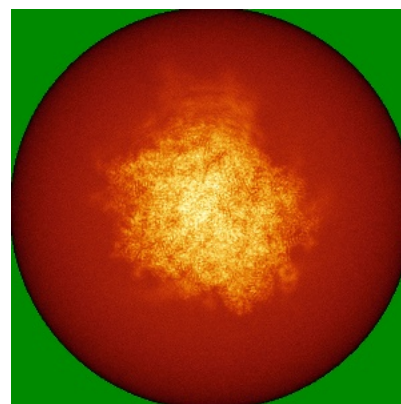
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

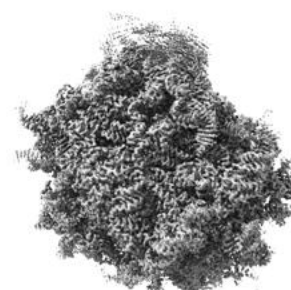
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

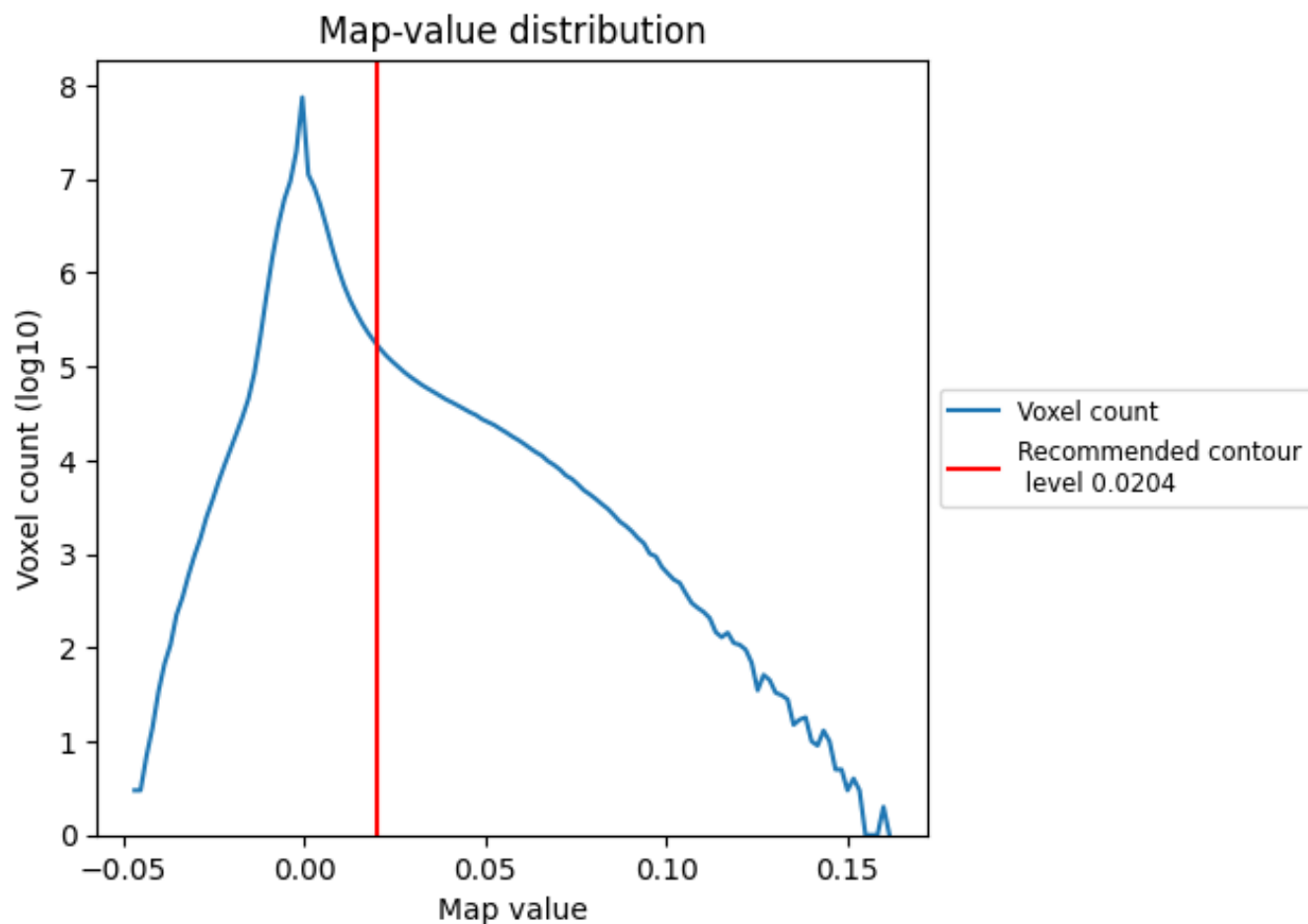
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

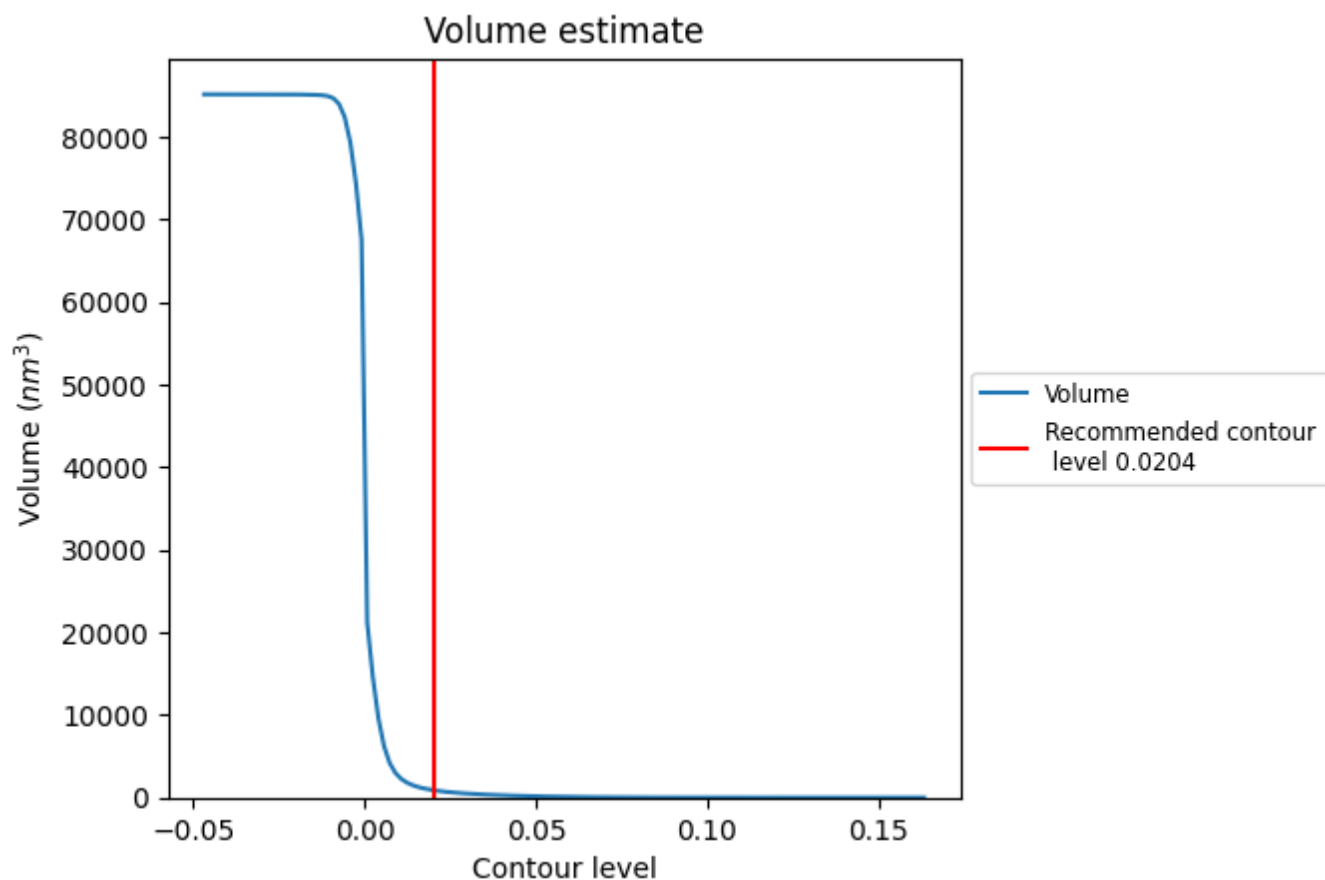
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

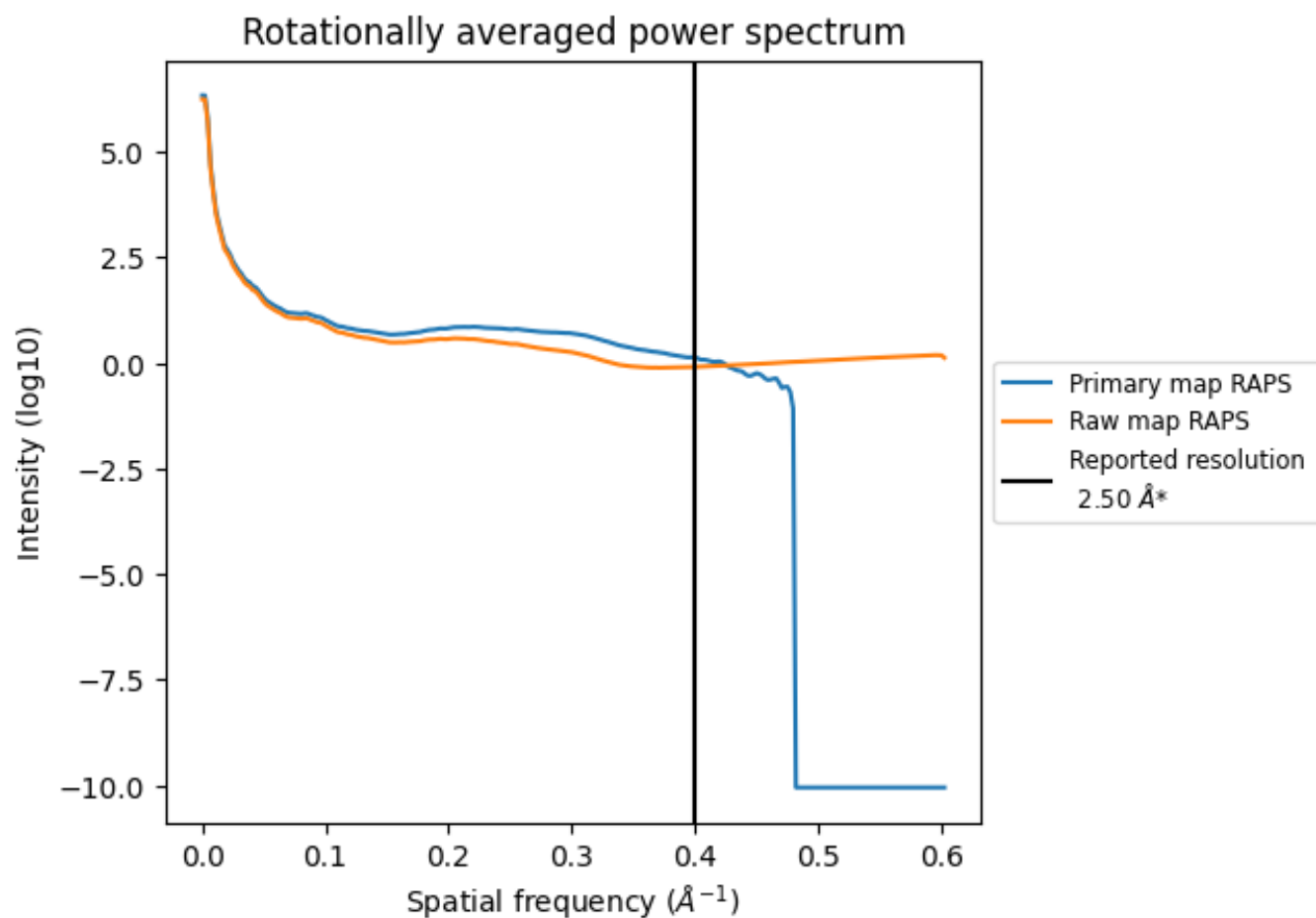
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 872  $\text{nm}^3$ ; this corresponds to an approximate mass of 788 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

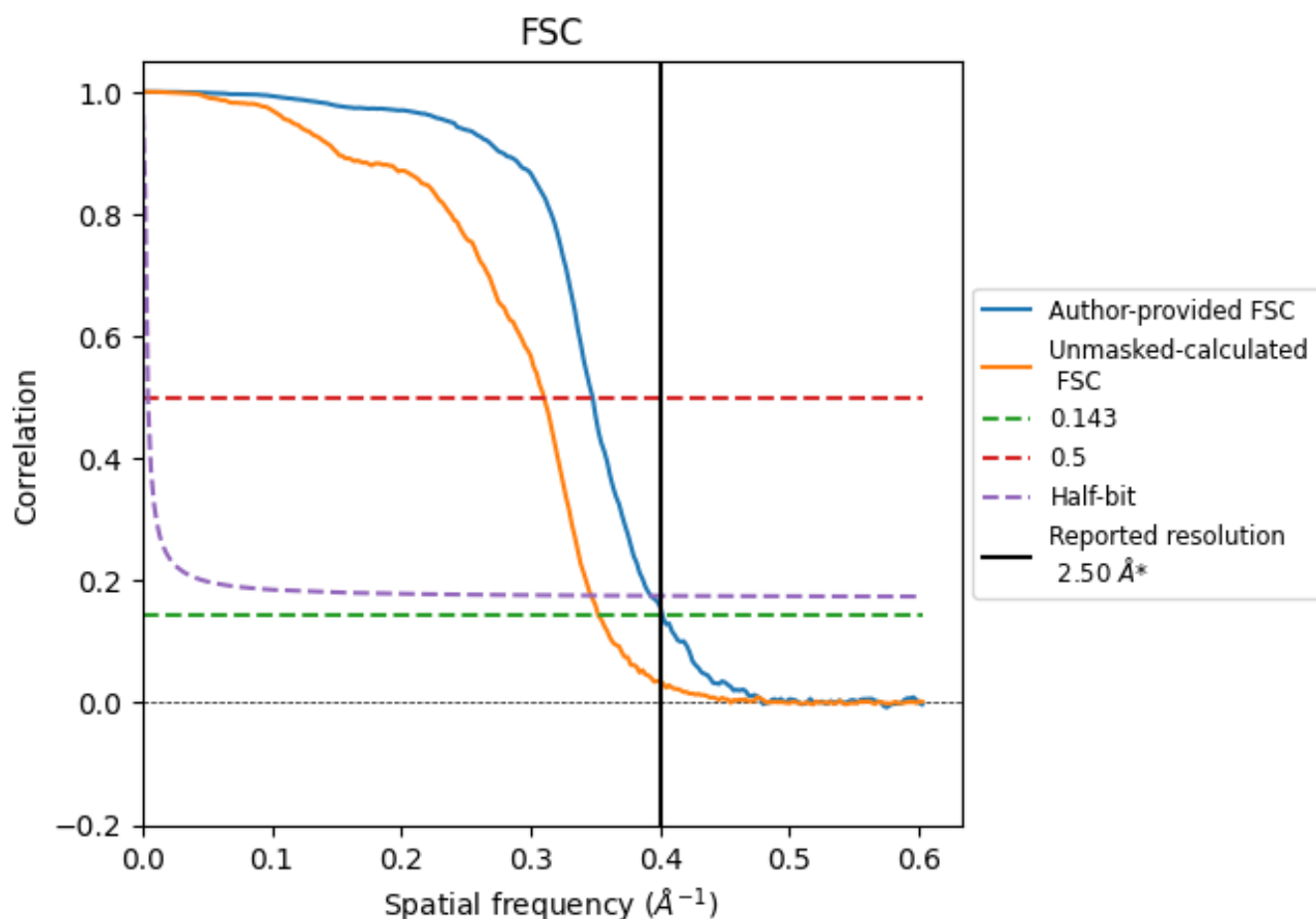


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.400 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

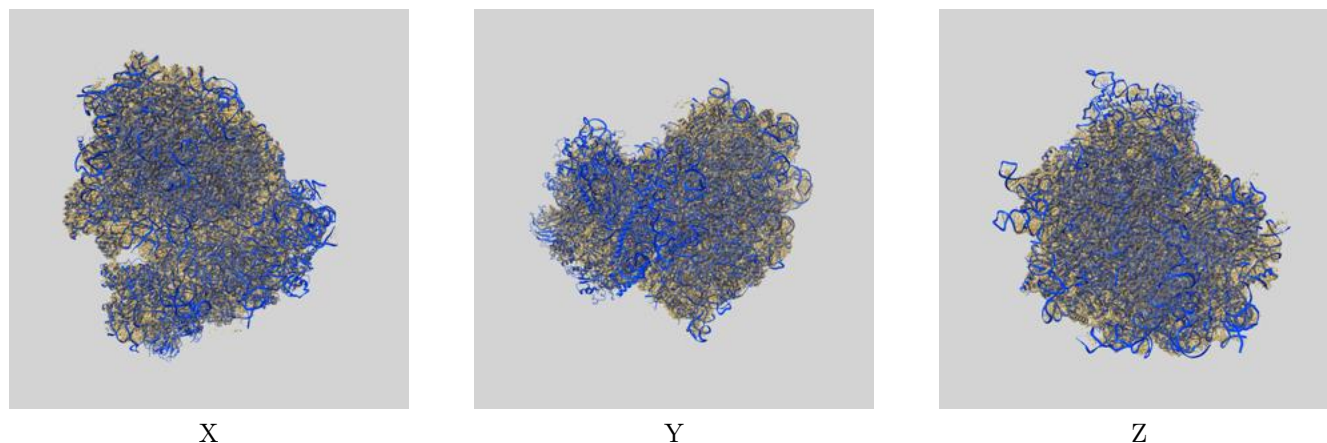
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.50                               | -    | -        |
| Author-provided FSC curve | 2.49                               | 2.87 | 2.55     |
| Unmasked-calculated*      | 2.84                               | 3.22 | 2.88     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.5 by more than 10 %

## 9 Map-model fit [i](#)

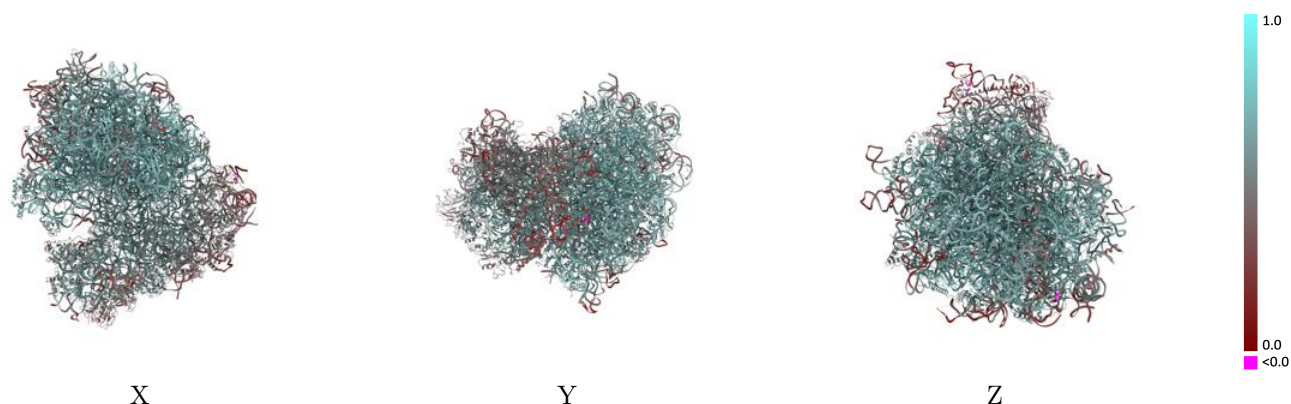
This section contains information regarding the fit between EMDB map EMD-36178 and PDB model 8JDJ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

### 9.1 Map-model overlay [i](#)



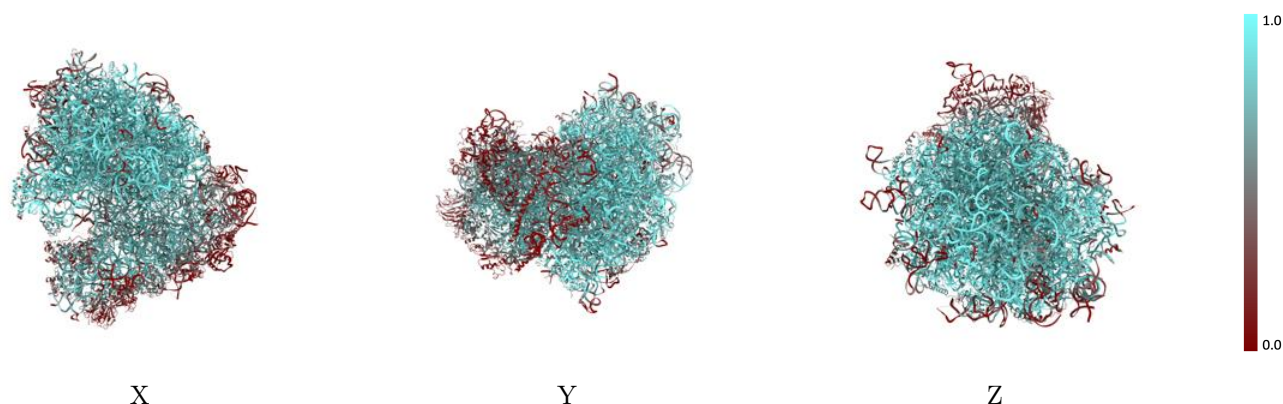
The images above show the 3D surface view of the map at the recommended contour level 0.0204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



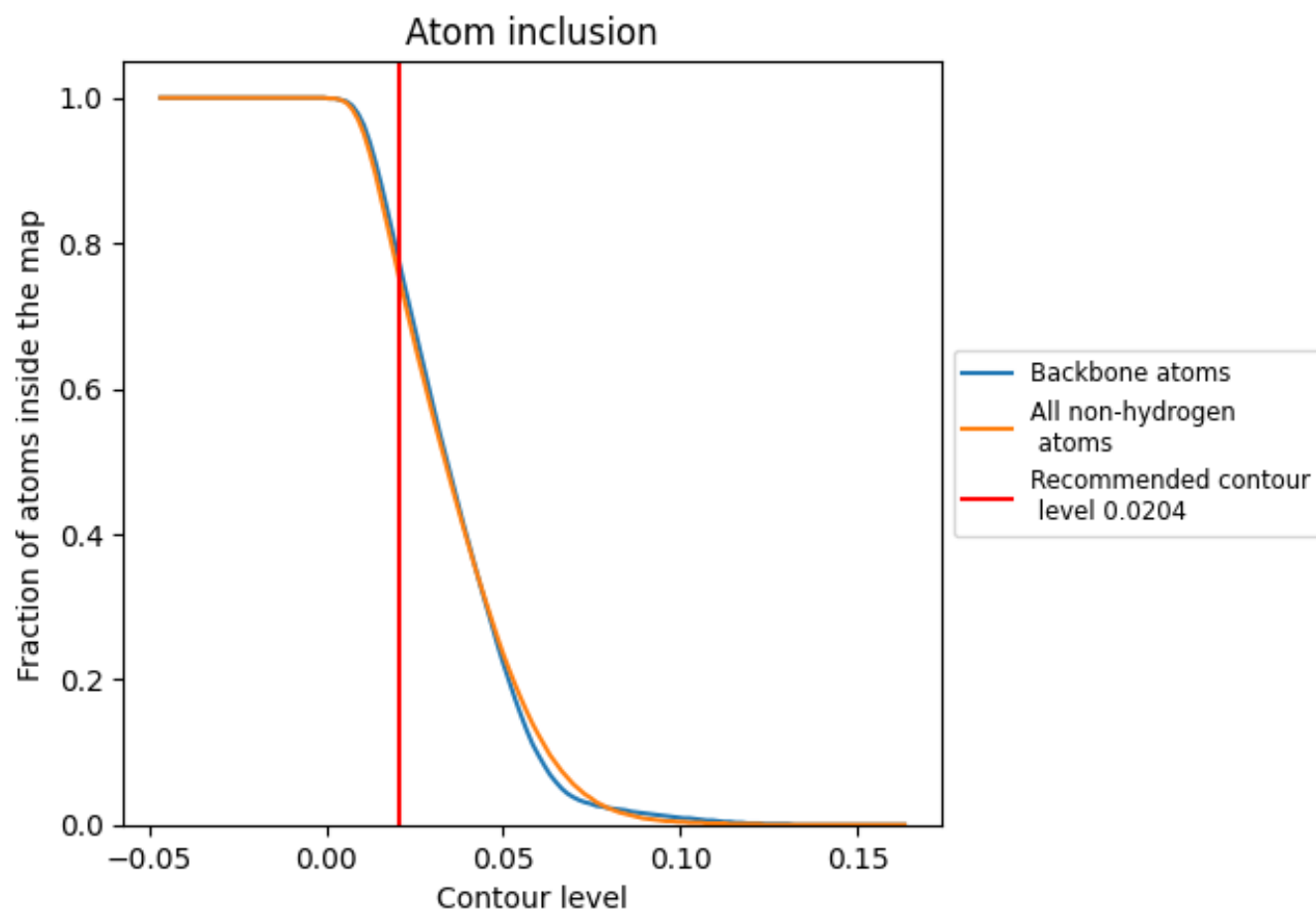
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0204).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0204) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7560   |  0.5940   |
| 0     |  0.4300   |  0.5030   |
| 1     |  0.1920   |  0.4160   |
| 2     |  0.5890   |  0.5570   |
| 3     |  0.1380   |  0.3760   |
| 4     |  0.2120   |  0.4330   |
| 5     |  0.4180   |  0.4690   |
| 6     |  0.2690   |  0.4200   |
| 7     |  0.1920   |  0.4090   |
| 8     |  0.5540   |  0.5380   |
| 9     |  0.6460   |  0.5830   |
| A     |  0.7530   |  0.5730   |
| AA    |  0.7120   |  0.5910   |
| AB    |  0.3450   |  0.5030   |
| AC    |  0.5690  |  0.5560  |
| AD    |  0.3730 |  0.4790 |
| AE    |  0.4660 |  0.5170 |
| AF    |  0.5290 |  0.5460 |
| AG    |  0.3960 |  0.4720 |
| AH    |  0.5030 |  0.5610 |
| AI    |  0.7210 |  0.6100 |
| AJ    |  0.6570 |  0.5690 |
| AK    |  0.0850 |  0.3780 |
| AL    |  0.2980 |  0.4910 |
| AM    |  0.7380 |  0.6020 |
| AN    |  0.4170 |  0.5080 |
| AO    |  0.4970 |  0.5270 |
| AP    |  0.7720 |  0.6050 |
| AQ    |  0.2430 |  0.4390 |
| AR    |  0.1450 |  0.4090 |
| B     |  0.7340 |  0.5560 |
| C     |  0.5610 |  0.5650 |
| D     |  0.8550 |  0.6220 |
| E     |  0.9800 |  0.6730 |
| F     |  0.9010 |  0.6360 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| G     |  0.9550   |  0.6850   |
| H     |  0.8850   |  0.6650   |
| I     |  0.8960   |  0.6530   |
| J     |  0.7930   |  0.6250   |
| K     |  0.7470   |  0.6060   |
| L     |  0.8990   |  0.6680   |
| M     |  0.7090   |  0.5960   |
| N     |  0.8330   |  0.6410   |
| O     |  0.8630   |  0.6450   |
| P     |  0.7060   |  0.5940   |
| Q     |  0.8040   |  0.6270   |
| R     |  0.8490   |  0.6380   |
| S     |  0.9710   |  0.6860   |
| T     |  0.9130   |  0.6740   |
| U     |  0.8890   |  0.6690   |
| V     |  0.9320   |  0.6750   |
| W     |  0.7920   |  0.6230   |
| X     |  0.9190   |  0.6720   |
| Y     |  0.8500   |  0.6450   |
| Z     |  0.5790  |  0.5520  |
| a     |  0.8970 |  0.6740 |
| b     |  0.8780 |  0.6650 |
| c     |  0.8270 |  0.6340 |
| d     |  0.8200 |  0.6300 |
| e     |  0.8170 |  0.6290 |
| f     |  0.9170 |  0.6710 |
| g     |  0.7080 |  0.5860 |
| h     |  0.8250 |  0.6290 |
| i     |  0.8220 |  0.6470 |
| j     |  0.9330 |  0.6880 |
| k     |  0.9370 |  0.6720 |
| l     |  0.8510 |  0.6420 |
| m     |  0.8160 |  0.6370 |
| n     |  0.7680 |  0.6360 |
| o     |  0.9550 |  0.6800 |
| p     |  0.6550 |  0.5890 |
| q     |  0.8960 |  0.6520 |
| r     |  0.8750 |  0.6570 |
| s     |  0.9130 |  0.6680 |
| t     |  0.8330 |  0.6340 |
| u     |  0.8800 |  0.6660 |
| v     |  0.8920 |  0.6410 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| w     |  0.7260 |  0.5470 |
| x     |  0.5390 |  0.5670 |
| y     |  0.6030 |  0.5830 |
| z     |  0.6630 |  0.5930 |