



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 02:12 AM EDT

PDB ID : 7LS2 / pdb\_00007ls2  
EMDB ID : EMD-23501  
Title : 80S ribosome from mouse bound to eEF2 (Class I)  
Authors : Loerch, S.; Smith, P.R.; Kunder, N.; Stanowick, A.D.; Lou, T.-F.; Campbell, Z.T.  
Deposited on : 2021-02-17  
Resolution : 3.10 Å(reported)

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:

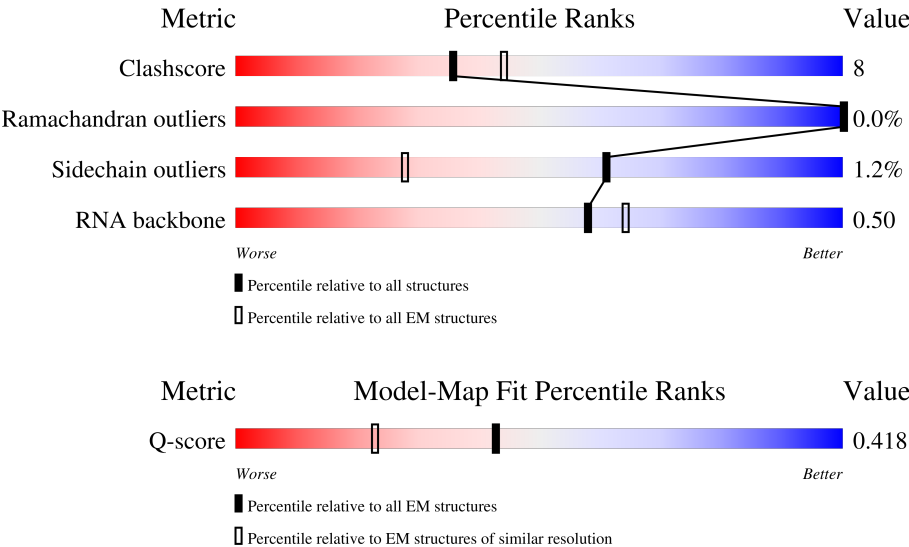
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



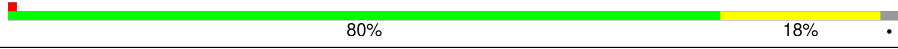
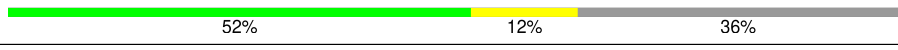
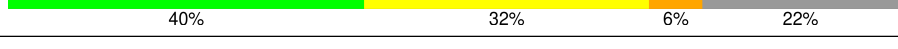
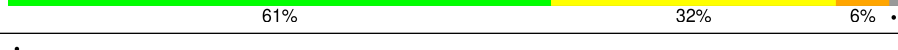
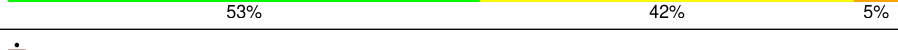
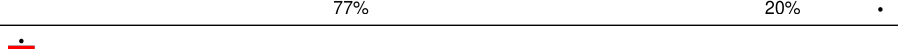
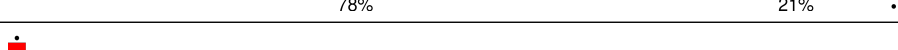
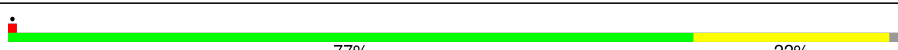
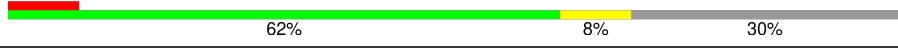
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14724 ( 2.60 - 3.60 )                                    |

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   | A1    | 270    | <div> <div>66%</div> <div>16%</div> <div>18%</div> </div> |
| 2   | B1    | 266    | <div> <div>74%</div> <div>12%</div> <div>14%</div> </div> |
| 3   | C1    | 192    | <div> <div>79%</div> <div>20%</div> </div>                |

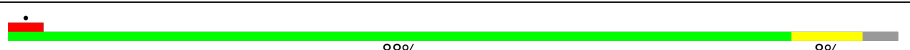
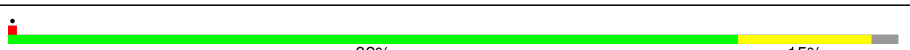
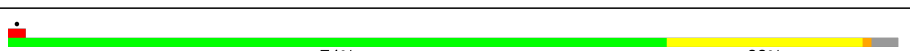
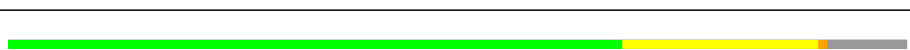
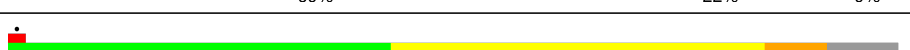
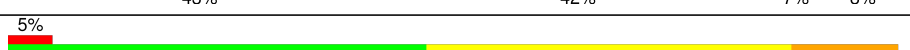
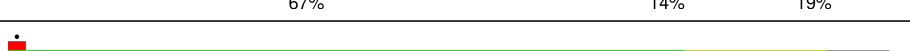
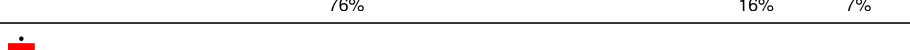
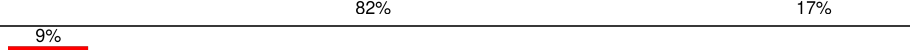
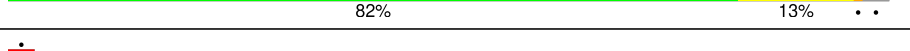
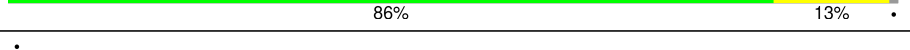
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D1    | 214    |    |
| 5   | E1    | 178    |    |
| 6   | F1    | 211    |    |
| 7   | G1    | 217    |    |
| 8   | H1    | 204    |    |
| 9   | A2    | 4731   |    |
| 10  | B2    | 121    |    |
| 11  | C2    | 156    |    |
| 12  | D2    | 257    |    |
| 13  | E2    | 403    |    |
| 14  | F2    | 419    |    |
| 15  | G2    | 297    |  |
| 16  | H2    | 296    |  |
| 17  | I2    | 203    |  |
| 18  | J2    | 184    |  |
| 19  | K2    | 188    |  |
| 20  | L2    | 196    |  |
| 21  | M2    | 176    |  |
| 22  | N2    | 160    |  |
| 23  | O2    | 128    |  |
| 24  | P2    | 140    |  |
| 25  | Q2    | 157    |  |
| 26  | R2    | 156    |  |
| 27  | S2    | 145    |  |
| 28  | T2    | 136    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | U2    | 148    |    |
| 30  | V2    | 160    |    |
| 31  | W2    | 115    |    |
| 32  | X2    | 125    |    |
| 33  | Y2    | 135    |    |
| 34  | Z2    | 110    |    |
| 35  | a2    | 117    |    |
| 36  | b2    | 123    |    |
| 37  | c2    | 105    |    |
| 38  | d2    | 97     |    |
| 39  | e2    | 70     |    |
| 40  | f2    | 51     |   |
| 41  | g2    | 128    |  |
| 42  | h2    | 25     |  |
| 43  | i2    | 106    |  |
| 44  | j2    | 92     |  |
| 45  | k2    | 137    |  |
| 46  | m2    | 1871   |  |
| 47  | n2    | 75     |  |
| 48  | p2    | 264    |  |
| 49  | q2    | 243    |  |
| 50  | r2    | 263    |  |
| 51  | w2    | 158    |  |
| 52  | z2    | 135    |  |
| 53  | o2    | 295    |  |

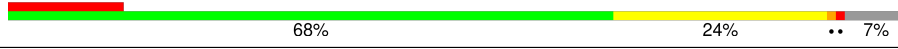
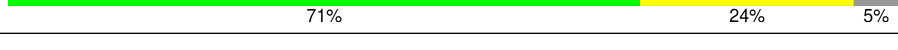
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | s2    | 204    |                  |
| 55  | v2    | 165    |                  |
| 56  | x2    | 145    |                  |
| 57  | y2    | 146    |                  |
| 58  | A3    | 152    |                  |
| 59  | B3    | 145    |                  |
| 60  | C3    | 119    |                  |
| 61  | D3    | 83     |                  |
| 62  | E3    | 143    |                  |
| 63  | F3    | 115    |                  |
| 64  | G3    | 69     |                  |
| 65  | H3    | 56     |                  |
| 66  | I3    | 317    |                  |
| 67  | J3    | 293    |                  |
| 68  | K3    | 249    |                  |
| 69  | L3    | 194    |                  |
| 70  | M3    | 132    |                  |
| 71  | N3    | 151    |                  |
| 72  | O3    | 151    |                  |
| 73  | P3    | 130    |                  |
| 74  | Q3    | 133    |                  |
| 75  | R3    | 125    |                  |
| 76  | S3    | 84     |                  |
| 77  | T3    | 133    |                  |
| 78  | U3    | 156    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 79  | m     | 858    |  |
| 80  | j     | 317    |  |
| 81  | k     | 165    |  |
| 82  | A     | 386    |  |
| 83  | t     | 194    |  |
| 84  | u     | 208    |  |
| 85  | L1    | 217    |  |

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 227130 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 protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A1    | 222      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1851  | 1190 | 356 | 297 | 8 |         |       |

- Molecule 2 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B1    | 230      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1863  | 1188 | 359 | 312 | 4 |         |       |

- Molecule 3 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C1    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1519  | 956 | 284 | 273 | 6 |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L10-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D1    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1690  | 1073 | 327 | 278 | 12 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | E1    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1397  | 880 | 260 | 251 | 6 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | F1    | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1676  | 1048 | 344 | 280 | 4 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G1    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 732 | 221 | 183 | 7 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | H1    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 9 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 9   | A2    | 3706     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 79519 | 35463 | 14497 | 25854 | 3705 |         |       |

- Molecule 10 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 10  | B2    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 11 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 11  | C2    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3315  | 1481 | 585 | 1094 | 155 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | D2    | 251      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1921  | 1204 | 393 | 318 | 6 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | E2    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3238  | 2060 | 609 | 555 | 14 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L4.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | F2    | 367      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2928  | 1842 | 583 | 488 | 15 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | G2    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2385  | 1506 | 440 | 425 | 14 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | H2    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1789  | 1145 | 342 | 298 | 4 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | I2    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1640  | 1055 | 320 | 259 | 6 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | J2    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 777 | 241 | 215 | 9 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | K2    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1511  | 946 | 313 | 248 | 4 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | L2    | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1542  | 955 | 332 | 246 | 9 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | M2    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1450  | 924 | 283 | 233 | 10 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | N2    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 253 | 216 | 6 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | O2    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 529 | 144 | 150 | 2 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | P2    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 613 | 182 | 169 | 5 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Q2    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 895   | 563 | 180 | 148 | 4 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | R2    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 618 | 181 | 167 | 1 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | S2    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | T2    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | U2    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1164  | 736 | 239 | 185 | 4 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | V2    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 596 | 198 | 146 | 5 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | W2    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 732   | 465 | 130 | 131 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | X2    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Y2    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Z2    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 143 | 4 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | a2    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 565 | 187 | 148 | 6 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | b2    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1001  | 634 | 201 | 165 | 1 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | c2    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 516 | 173 | 133 | 5 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | d2    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 39  | e2    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 568   | 365 | 103 | 99 | 1 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | f2    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | g2    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 430   | 267 | 90 | 67 | 6 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | h2    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | i2    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 528 | 172 | 136 | 6 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | j2    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 436 | 133 | 118 | 7 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | k2    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1001  | 621 | 207 | 168 | 5 |         |       |

- Molecule 46 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 46  | m2    | 1724     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36817 | 16440 | 6606 | 12048 | 1723 |         |       |

- Molecule 47 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 47  | n2    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 48 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | p2    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |

- Molecule 49 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | q2    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1756  | 1119 | 316 | 314 | 7 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | r2    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | w2    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 793 | 234 | 214 | 6 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | z2    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 678 | 201 | 197 | 4 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | o2    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1694  | 1077 | 297 | 312 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | s2    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1496  | 934 | 285 | 270 | 7 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | v2    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 534 | 147 | 133 | 5 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | x2    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1073  | 681 | 205 | 180 | 7 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | y2    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 726 | 216 | 198 | 3 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | A3    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1190  | 746 | 241 | 202 | 1 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | B3    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 691 | 215 | 196 | 2 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | C3    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 807   | 507 | 153 | 143 | 4 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | D3    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 392 | 119 | 122 | 5 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | E3    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | F3    | 100      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 811   | 506 | 169 | 131 | 5 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 64  | G3    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 65  | H3    | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 284 | 93 | 73 | 5 |         |       |

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 66  | I3    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 67  | J3    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1725  | 1116 | 298 | 302 | 9 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 68  | K3    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1840  | 1149 | 367 | 317 | 7 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | L3    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S12.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | M3    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 593 | 164 | 177 | 8 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | N3    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | O3    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 612 | 197 | 187 | 6 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | P3    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Q3    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 662 | 206 | 176 | 5 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | R3    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S27-like.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | S3    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 652   | 409 | 121 | 115 | 7 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 77  | T3    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 271 | 95 | 71 | 1 |         |       |

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78  | U3    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 505   | 317 | 96 | 85 | 7 |         |       |

- Molecule 79 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 79  | m     | 851      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6649  | 4217 | 1146 | 1242 | 44 |         |       |

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | j     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1507  | 959 | 263 | 276 | 9 |         |       |

- Molecule 81 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | k     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1159  | 721 | 218 | 217 | 3 |         |       |

- Molecule 82 is a protein called Isoform 3 of Plasminogen activator inhibitor 1 RNA-binding protein.

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 82  | A     | 61       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 486   | 289 | 94 | 103 |         |       |

- Molecule 83 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | t     | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 944 | 270 | 262 | 1 |         |       |

- Molecule 84 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 84  | u     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

- Molecule 85 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 85  | L1    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1660  | 1061 | 300 | 291 | 8 |         |       |

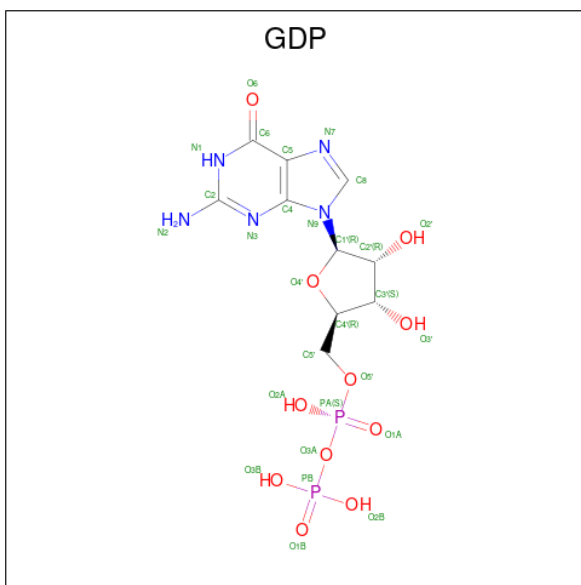
- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 86  | d2    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | g2    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | i2    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | j2    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | F3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | H3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | U3    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 87  | H3    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 88  | m     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

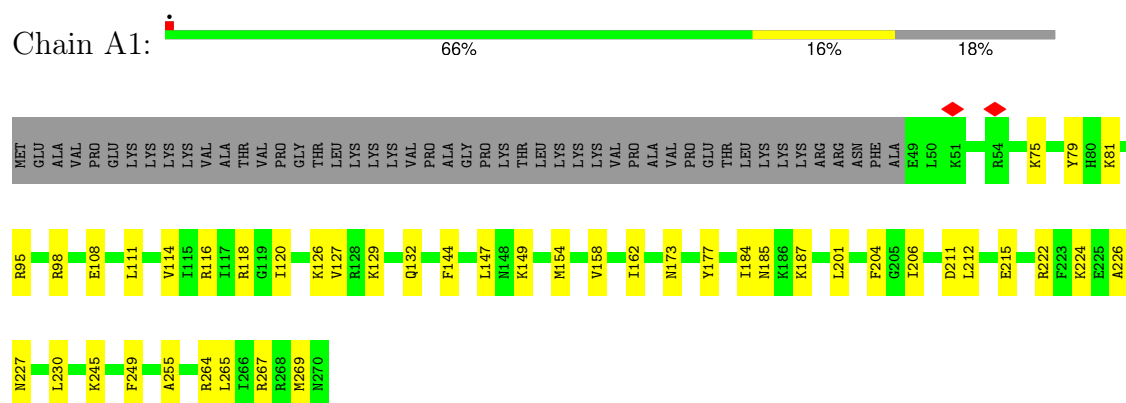
- Molecule 89 is water.

| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 89  | B1    | 1        | Total O<br>1 1 | 0       |
| 89  | A2    | 1        | Total O<br>1 1 | 0       |
| 89  | m2    | 2        | Total O<br>2 2 | 0       |

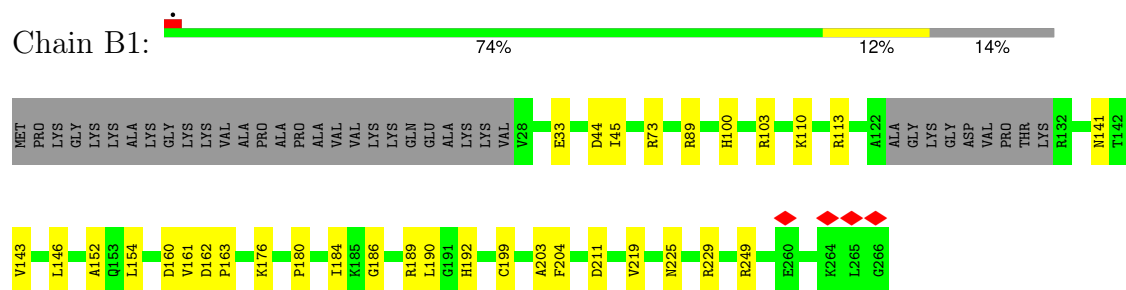
### 3 Residue-property plots

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.

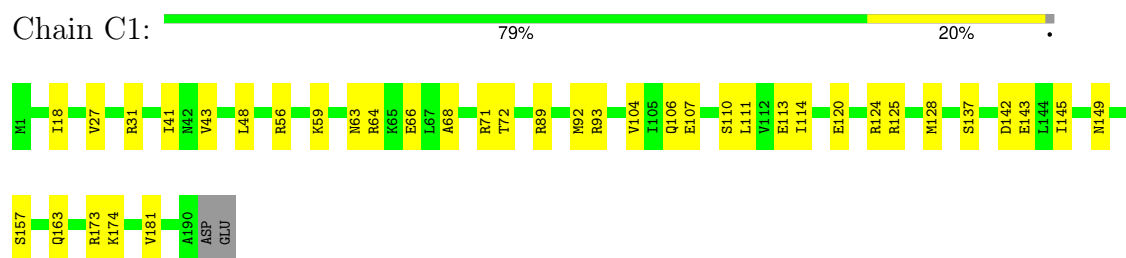
- Molecule 1: 60S ribosomal protein L7



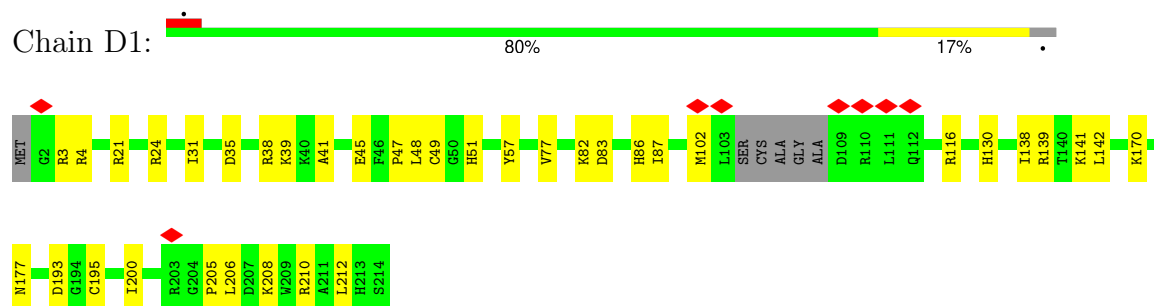
- Molecule 2: 60S ribosomal protein L7a



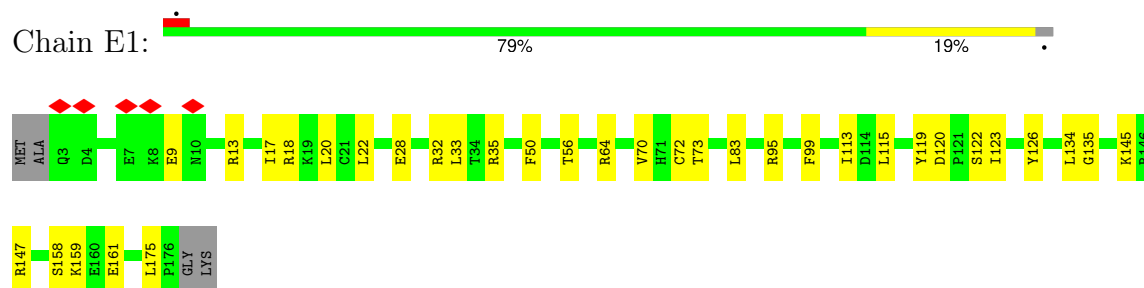
- Molecule 3: 60S ribosomal protein L9



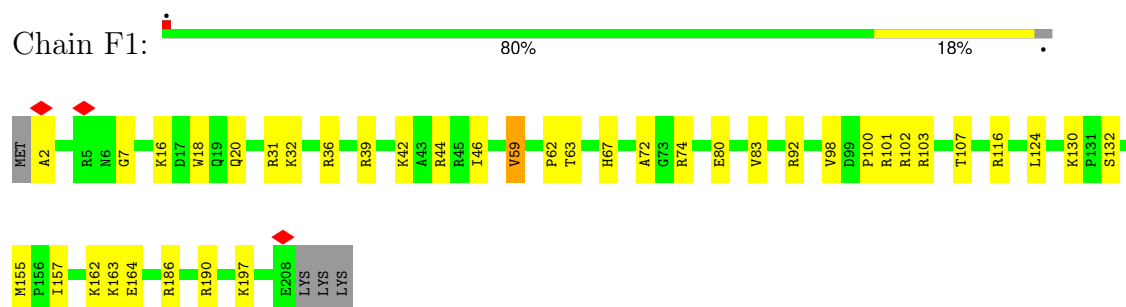
- Molecule 4: 60S ribosomal protein L10-like



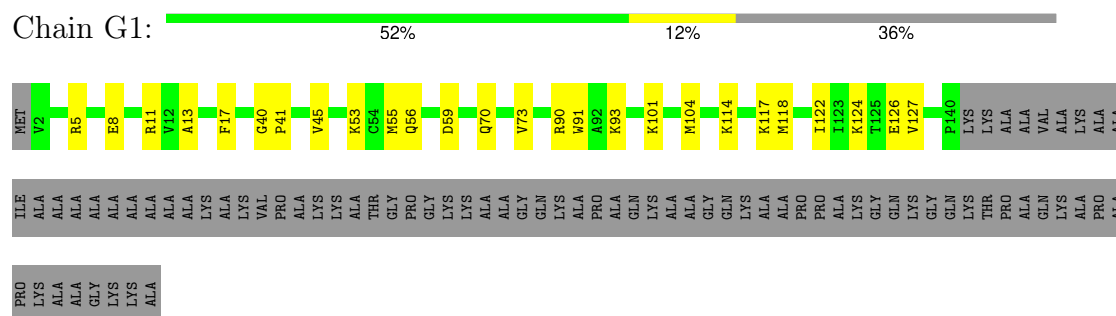
- Molecule 5: 60S ribosomal protein L11



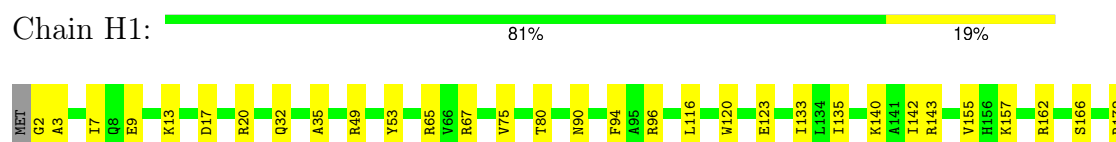
- Molecule 6: 60S ribosomal protein L13



- Molecule 7: 60S ribosomal protein L14

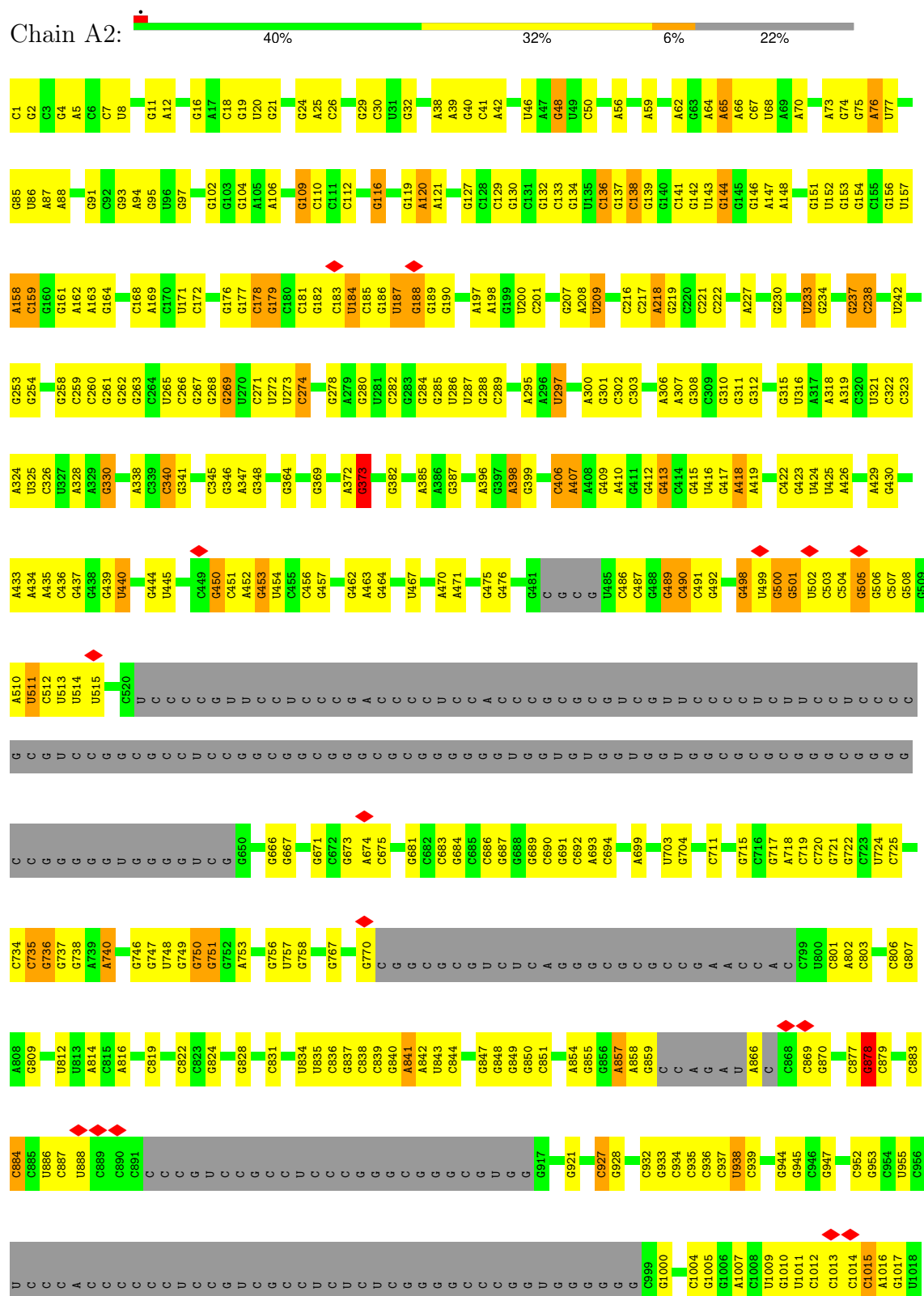


- Molecule 8: 60S ribosomal protein L15





• Molecule 9: 28S rRNA

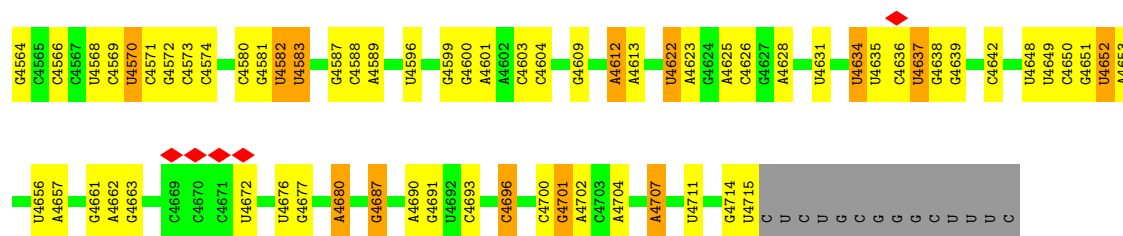


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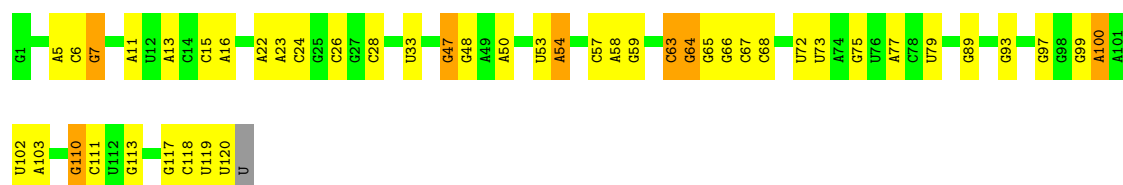




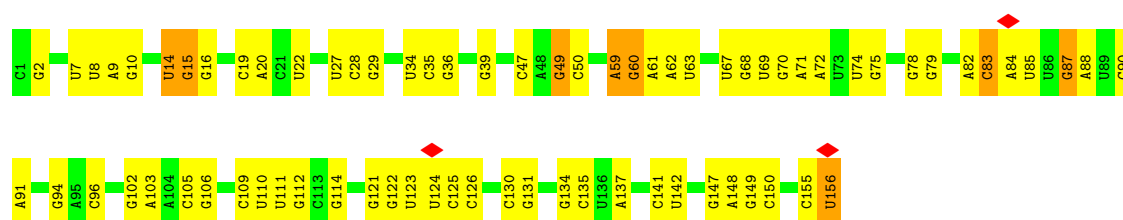
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| U | G     | U4281 | U4355 | U4188 | U4006 | U3922 | G3841 | U | C     | C3583 | C3583 |
| U | G     | U4282 | U4356 | U4189 | U4007 | U3923 | G3842 | U | C     | C3584 | C3584 |
| U | G     | U4283 | U4357 | U4190 | U4008 | U3924 | G3843 | U | C     | C3585 | C3585 |
| U | G     | U4284 | U4358 | U4191 | U4009 | U3925 | G3844 | U | C     | C3586 | C3586 |
| U | G     | U4285 | U4359 | U4192 | U4010 | U3926 | G3845 | U | C     | C3587 | C3587 |
| U | G     | U4286 | U4360 | U4193 | U4011 | U3927 | G3846 | U | C     | C3588 | C3588 |
| U | G     | U4287 | U4361 | U4194 | U4012 | U3928 | G3847 | U | C     | C3589 | C3589 |
| U | G     | U4288 | U4362 | U4195 | U4013 | U3929 | G3848 | U | C     | C3590 | C3590 |
| U | G     | U4289 | U4363 | U4196 | U4014 | U3930 | G3849 | U | C     | C3591 | C3591 |
| U | G     | U4290 | U4364 | U4197 | U4015 | U3931 | G3850 | U | C     | C3592 | C3592 |
| U | G     | U4291 | U4365 | U4198 | U4016 | U3932 | G3851 | U | C     | C3593 | C3593 |
| U | G     | U4292 | U4366 | U4199 | U4017 | U3933 | G3852 | U | C     | C3594 | C3594 |
| U | G     | U4293 | U4367 | U4200 | U4018 | U3934 | G3853 | U | C     | C3595 | C3595 |
| U | G     | U4294 | U4368 | U4201 | U4019 | U3935 | G3854 | U | C     | C3596 | C3596 |
| U | G     | U4295 | U4369 | U4202 | U4020 | U3936 | G3855 | U | C     | C3597 | C3597 |
| U | G     | U4296 | U4370 | U4203 | U4021 | U3937 | G3856 | U | C     | C3598 | C3598 |
| U | G     | U4297 | U4371 | U4204 | U4022 | U3938 | G3857 | U | C     | C3599 | C3599 |
| U | G     | U4298 | U4372 | U4205 | U4023 | U3939 | G3858 | U | C     | C3600 | C3600 |
| U | G     | U4299 | U4373 | U4206 | U4024 | U3940 | G3859 | U | C     | C3601 | C3601 |
| U | G     | U4300 | U4374 | U4207 | U4025 | U3941 | G3860 | U | C     | C3602 | C3602 |
| U | G     | U4301 | U4375 | U4208 | U4026 | U3942 | G3861 | U | C     | C3603 | C3603 |
| U | G     | U4302 | U4376 | U4209 | U4027 | U3943 | G3862 | U | C     | C3604 | C3604 |
| U | G     | U4303 | U4377 | U4210 | U4028 | U3944 | G3863 | U | C     | C3605 | C3605 |
| U | G     | U4304 | U4378 | U4211 | U4029 | U3945 | G3864 | U | C     | C3606 | C3606 |
| U | G     |       |       |       |       |       |       |   |       |       |       |



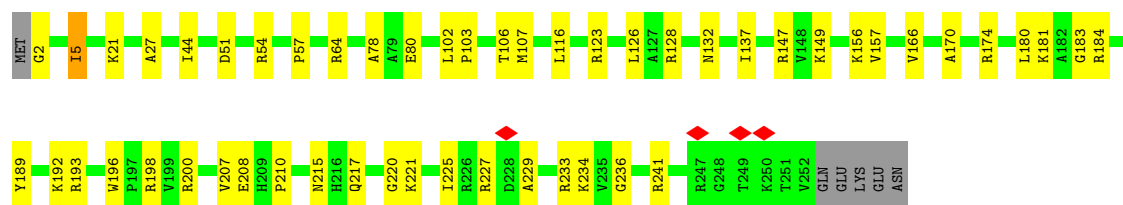
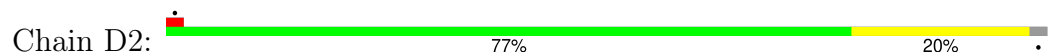
• Molecule 10: 5S rRNA



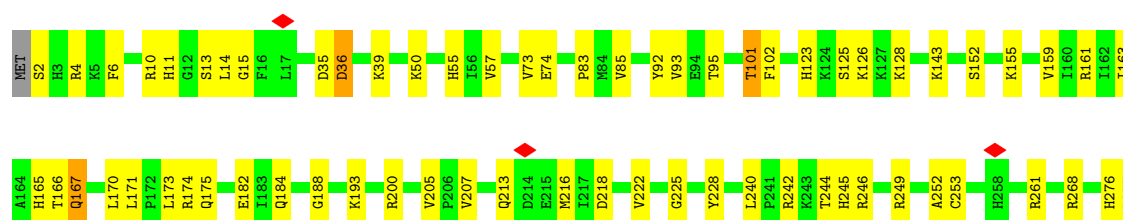
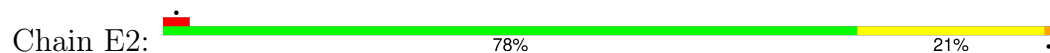
• Molecule 11: 5.8S rRNA



• Molecule 12: 60S ribosomal protein L8

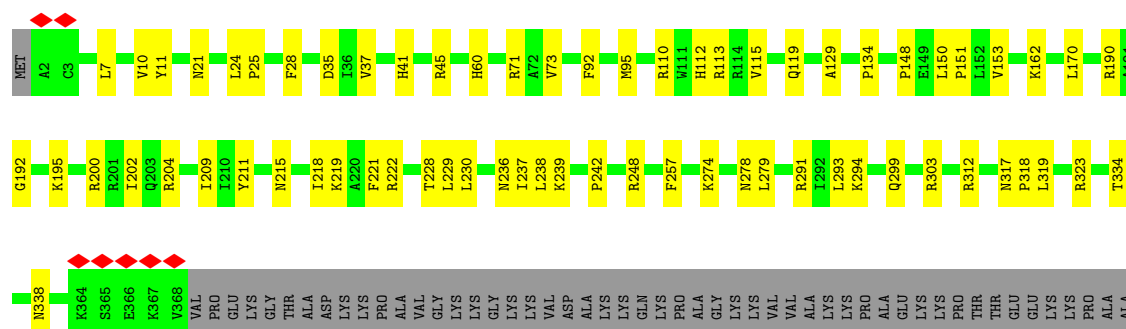


• Molecule 13: 60S ribosomal protein L3

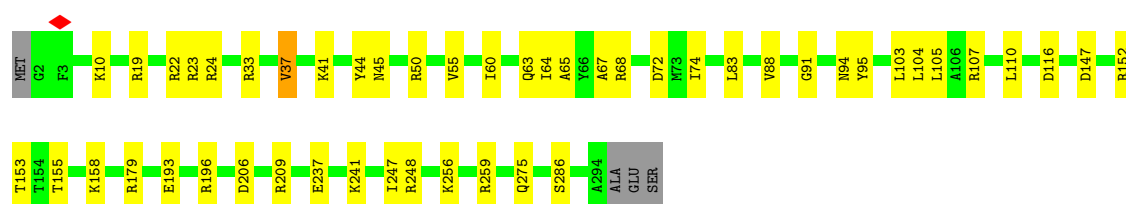
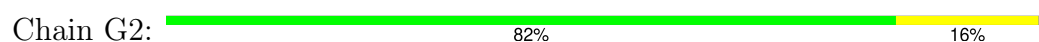




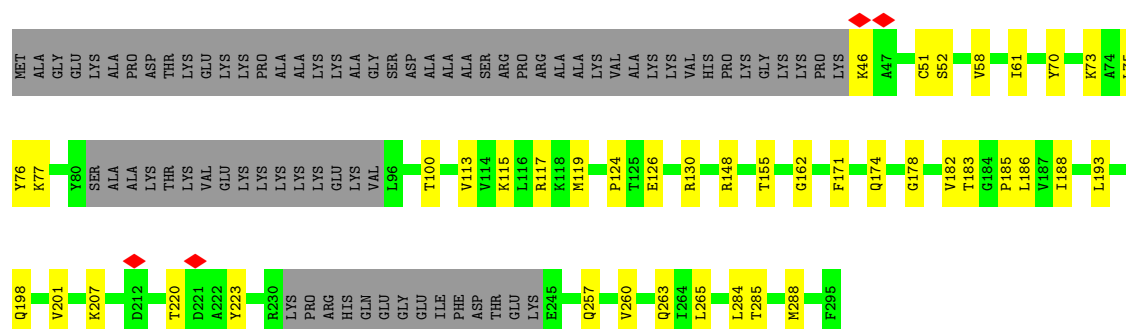
- Molecule 14: 60S ribosomal protein L4



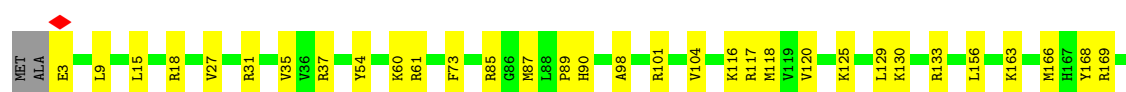
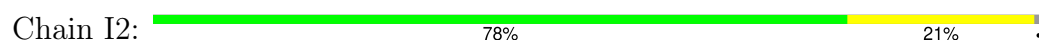
- Molecule 15: 60S ribosomal protein L5



- Molecule 16: 60S ribosomal protein L6



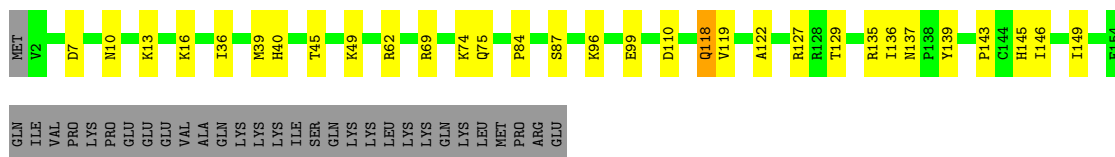
- Molecule 17: 60S ribosomal protein L13a





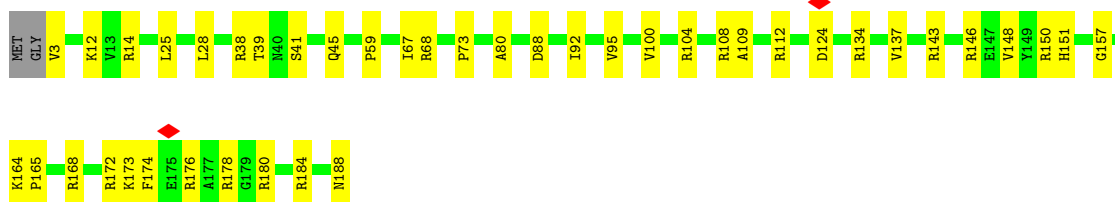
- Molecule 18: 60S ribosomal protein L17

Chain J2: 66% 16% 17%



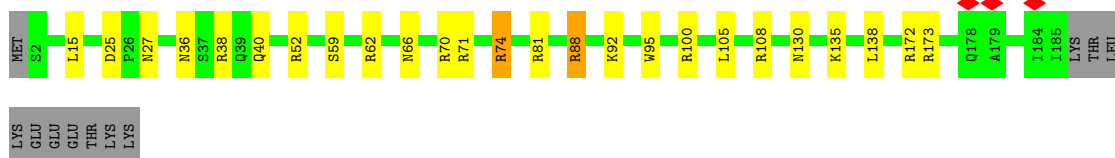
- Molecule 19: 60S ribosomal protein L18

Chain K2: 77% 22%



- Molecule 20: 60S ribosomal protein L19

Chain L2: 81% 12% 6%



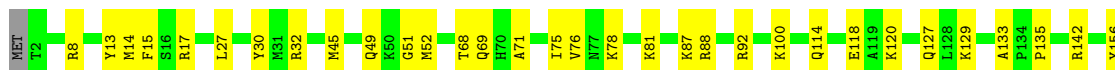
- Molecule 21: 60S ribosomal protein L18a

Chain M2: 88% 11%



- Molecule 22: 60S ribosomal protein L21

Chain N2: 79% 20%

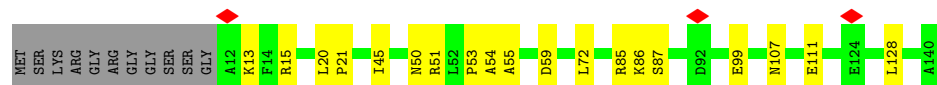
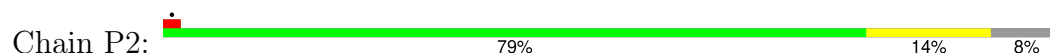




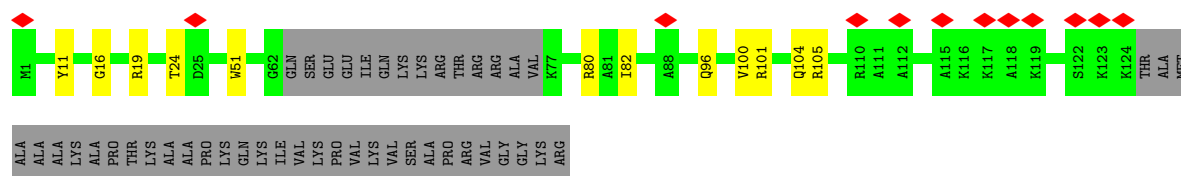
- Molecule 23: 60S ribosomal protein L22



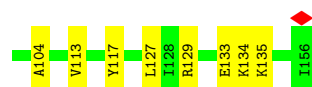
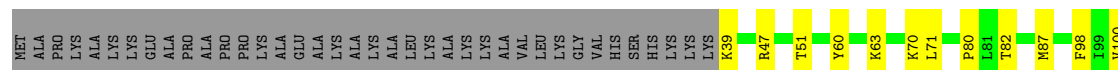
- Molecule 24: 60S ribosomal protein L23



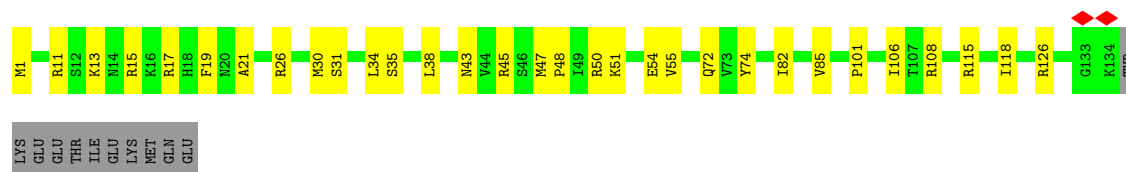
- Molecule 25: 60S ribosomal protein L24



- Molecule 26: 60S ribosomal protein L23a



- Molecule 27: 60S ribosomal protein L26



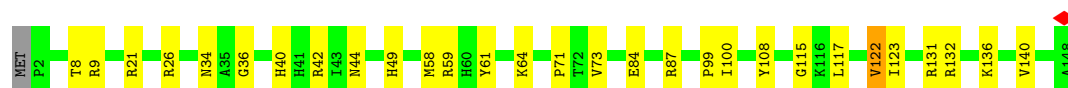
- Molecule 28: 60S ribosomal protein L27

Chain T2:  76% 23%



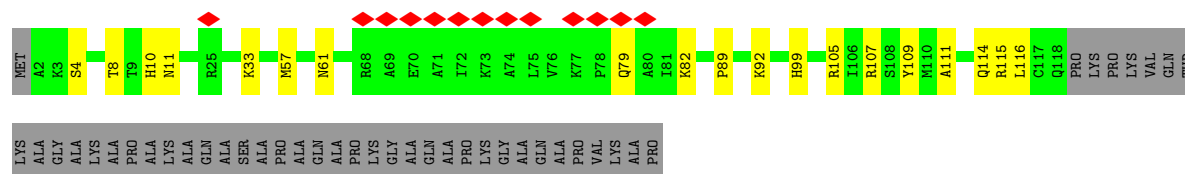
- Molecule 29: 60S ribosomal protein L27a

Chain U2:  80% 19%



- Molecule 30: 60S ribosomal protein L29

Chain V2:  8% 61% 12% 27%



- Molecule 31: 60S ribosomal protein L30

Chain W2:  63% 18% 18%



- Molecule 32: 60S ribosomal protein L31

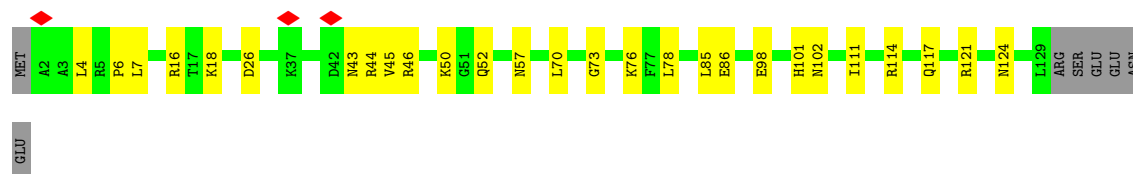
Chain X2:  66% 20% 14%



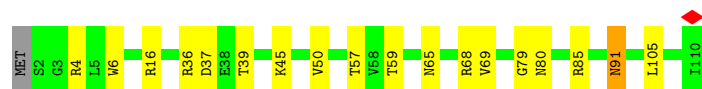
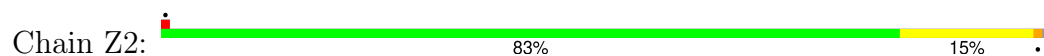
- Molecule 33: 60S ribosomal protein L32

Chain Y2:  75% 20% 5%

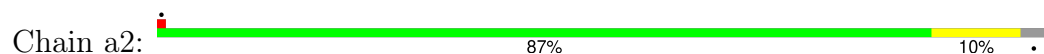




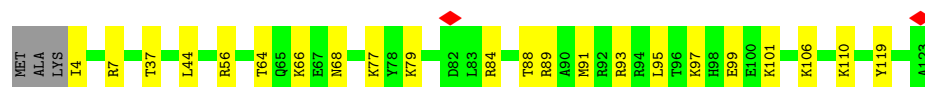
- Molecule 34: 60S ribosomal protein L35a



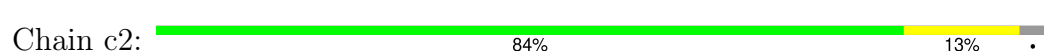
- Molecule 35: 60S ribosomal protein L34



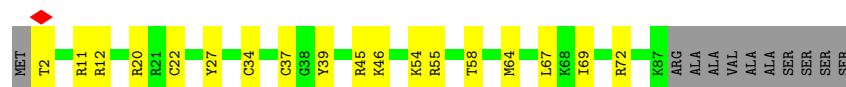
- Molecule 36: 60S ribosomal protein L35



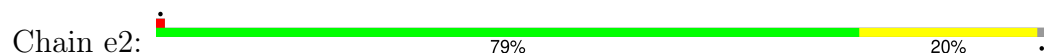
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



- Molecule 39: 60S ribosomal protein L38

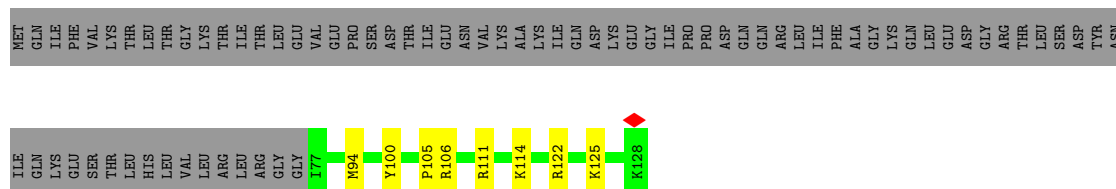




## • Molecule 40: 60S ribosomal protein L39

Chain f2:  71% 27%

## • Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain g2:  34% 6% 59%

## • Molecule 42: 60S ribosomal protein L41

Chain h2:  88% 8%

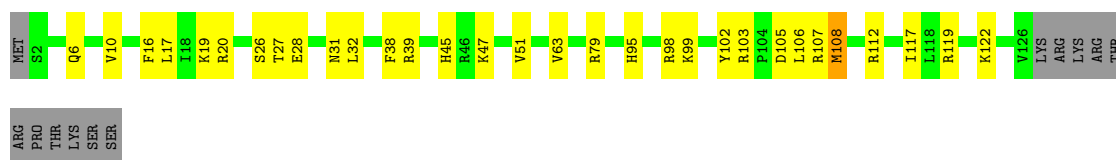
## • Molecule 43: 60S ribosomal protein L36a

Chain i2:  82% 15%

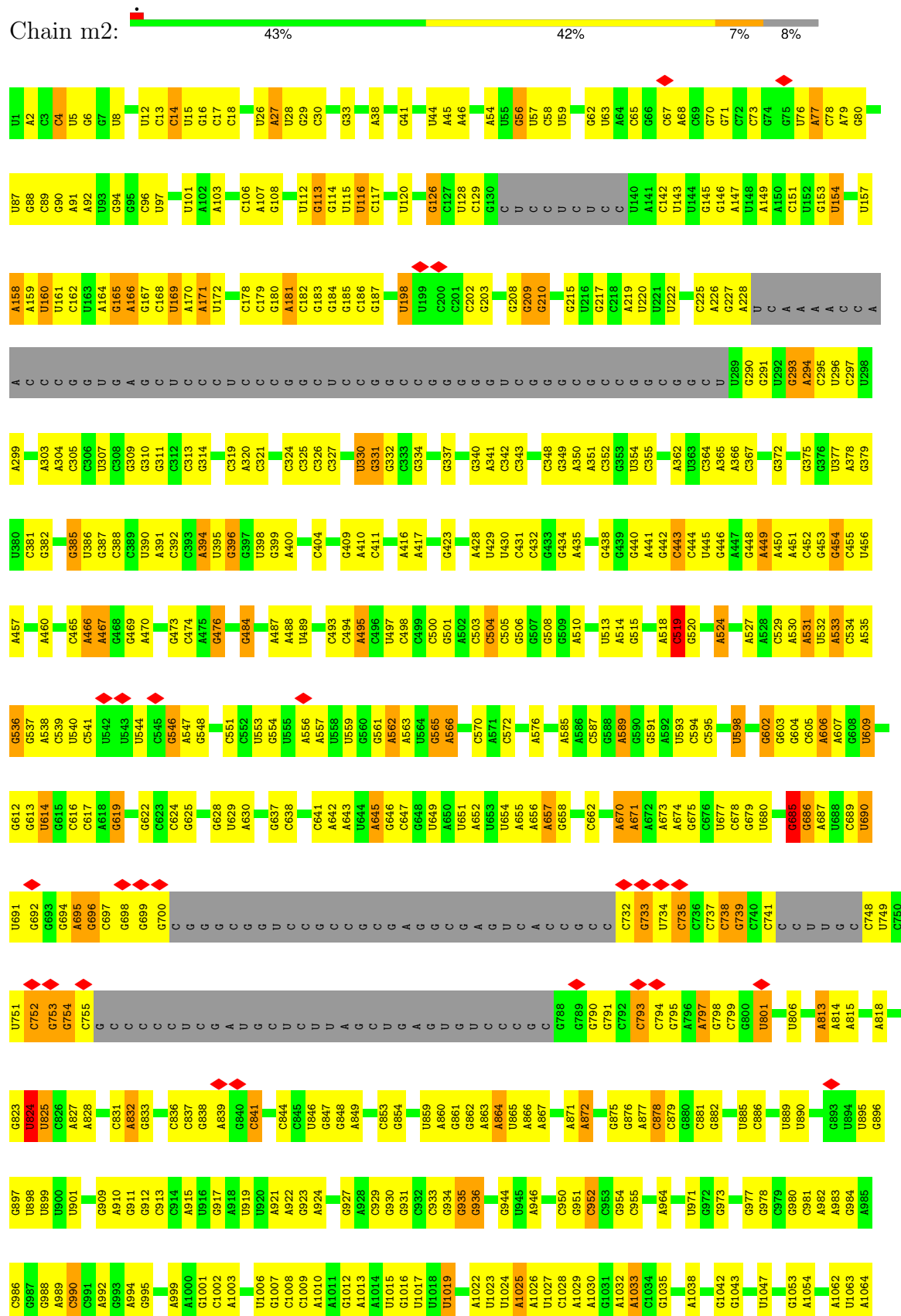
## • Molecule 44: 60S ribosomal protein L37a

Chain j2:  74% 22%

## • Molecule 45: 60S ribosomal protein L28

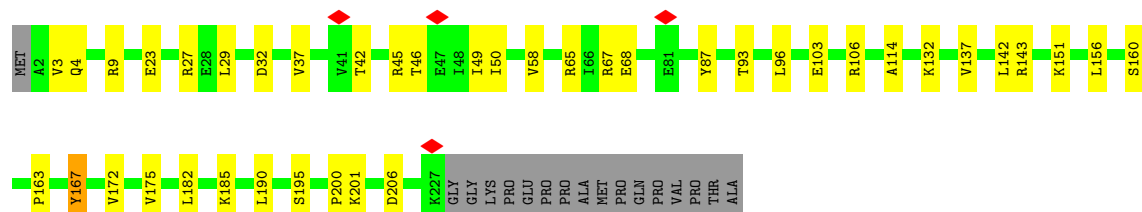
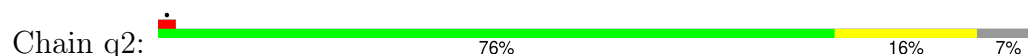
Chain k2:  69% 22% 9%

## ● Molecule 46: 18S rRNA

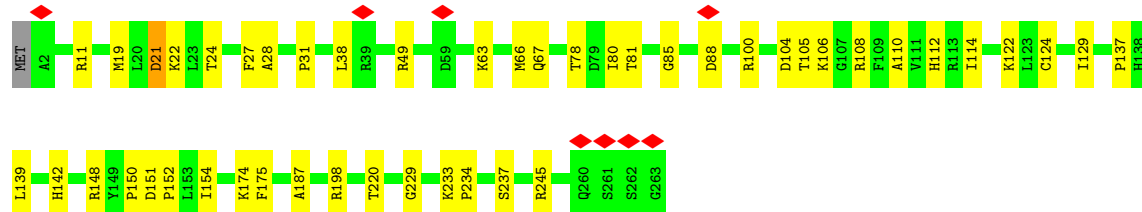
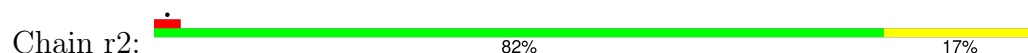




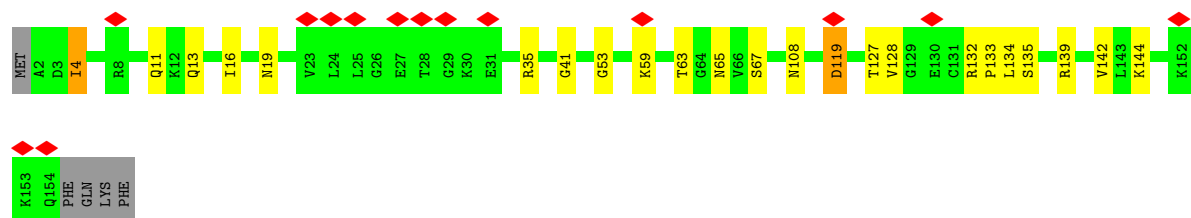
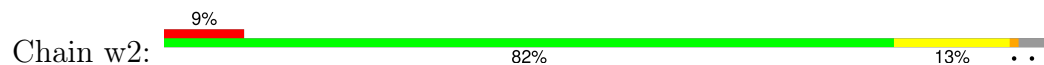
- Molecule 49: 40S ribosomal protein S3



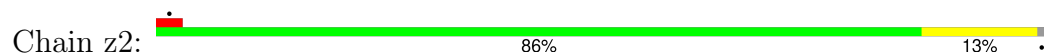
- Molecule 50: 40S ribosomal protein S4, X isoform

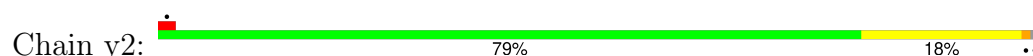


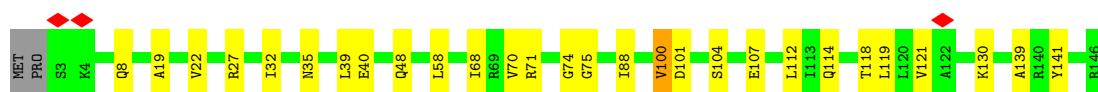
- Molecule 51: 40S ribosomal protein S11



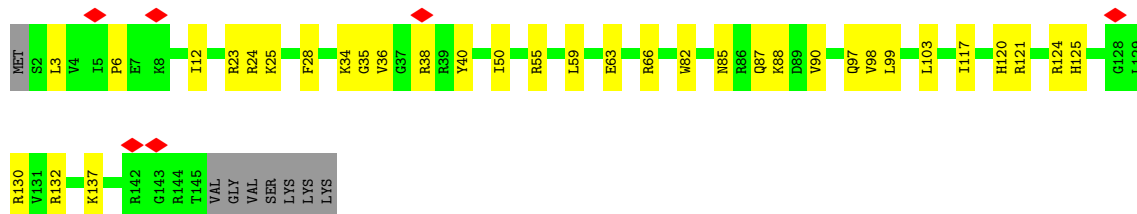
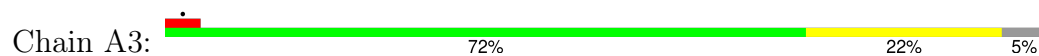
- Molecule 52: 40S ribosomal protein S17



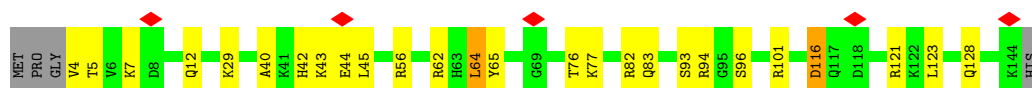
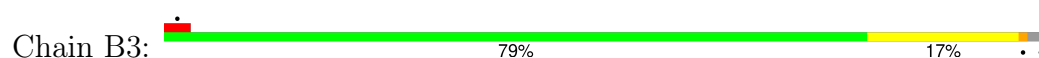




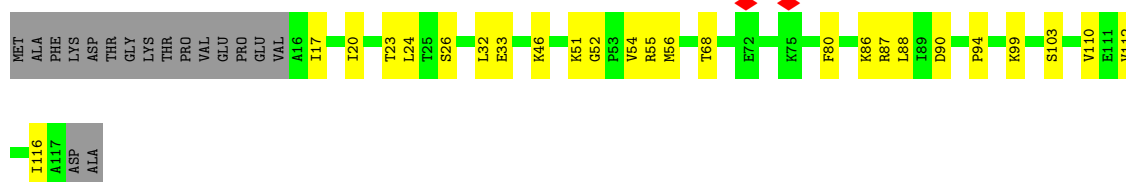
- Molecule 58: 40S ribosomal protein S18



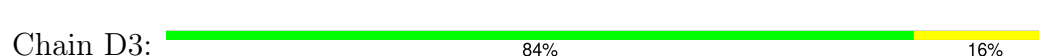
- Molecule 59: 40S ribosomal protein S19



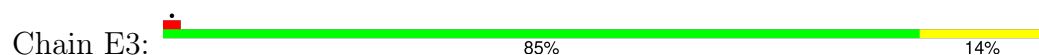
- Molecule 60: 40S ribosomal protein S20



- Molecule 61: 40S ribosomal protein S21



- Molecule 62: 40S ribosomal protein S23



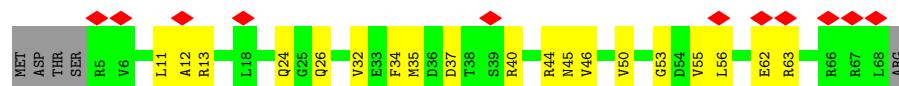
- Molecule 63: 40S ribosomal protein S26

Chain F3: 



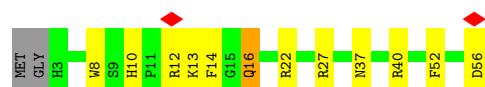
- Molecule 64: 40S ribosomal protein S28

Chain G3: 



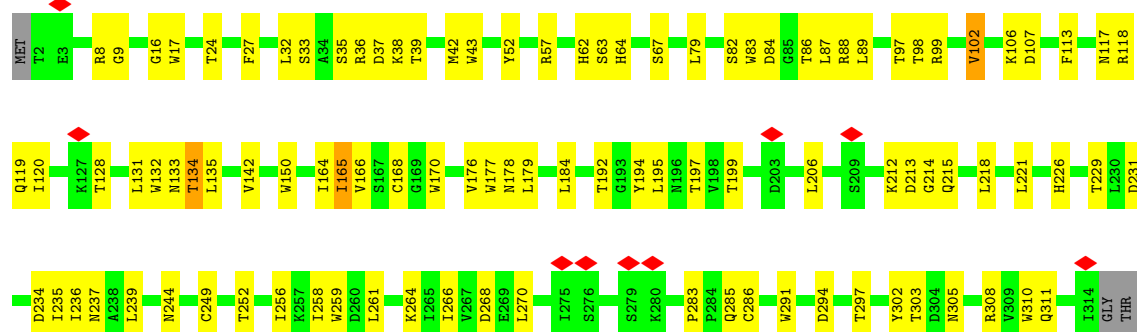
- Molecule 65: 40S ribosomal protein S29

Chain H3: 



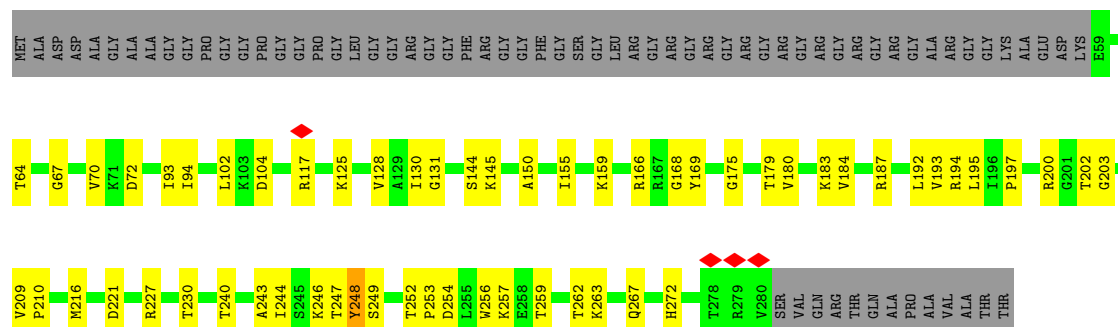
- Molecule 66: Receptor of activated protein C kinase 1

Chain I3: 



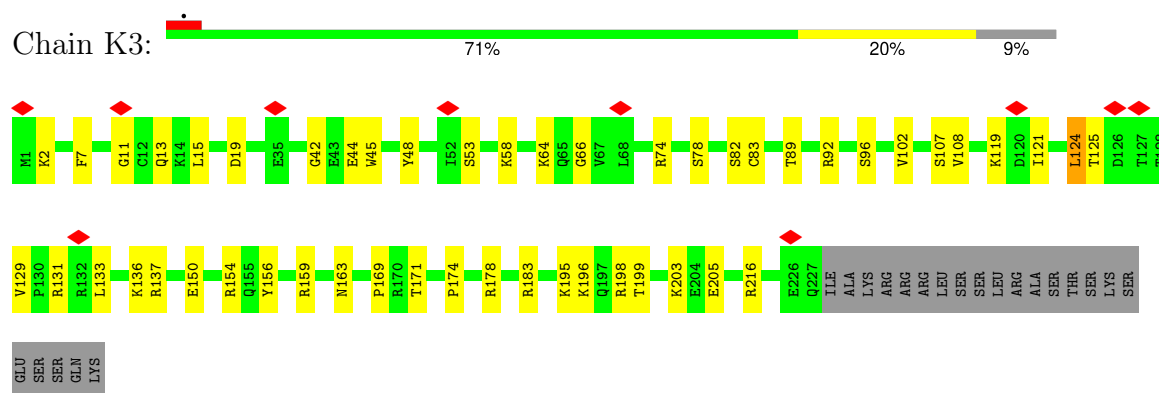
- Molecule 67: 40S ribosomal protein S2

Chain J3: 



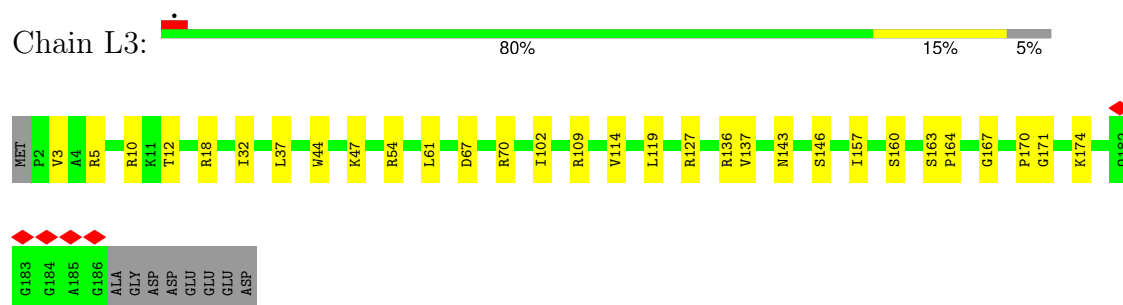
- Molecule 68: 40S ribosomal protein S6

Chain K3:



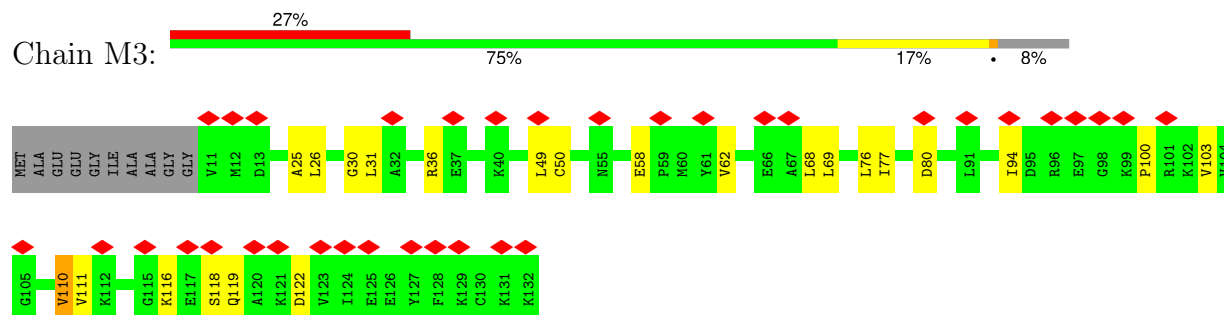
- Molecule 69: 40S ribosomal protein S9

Chain L3:



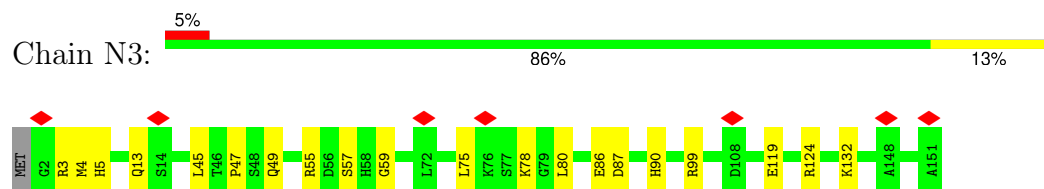
- Molecule 70: 40S ribosomal protein S12

Chain M3:



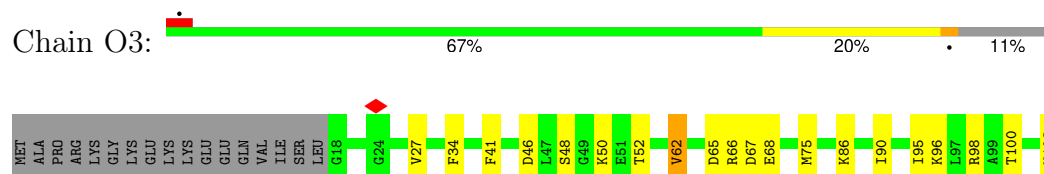
- Molecule 71: 40S ribosomal protein S13

Chain N3:

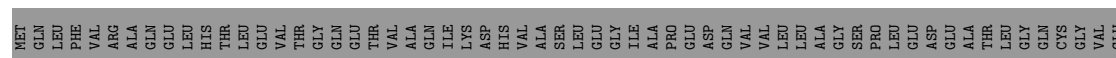


- Molecule 72: 40S ribosomal protein S14

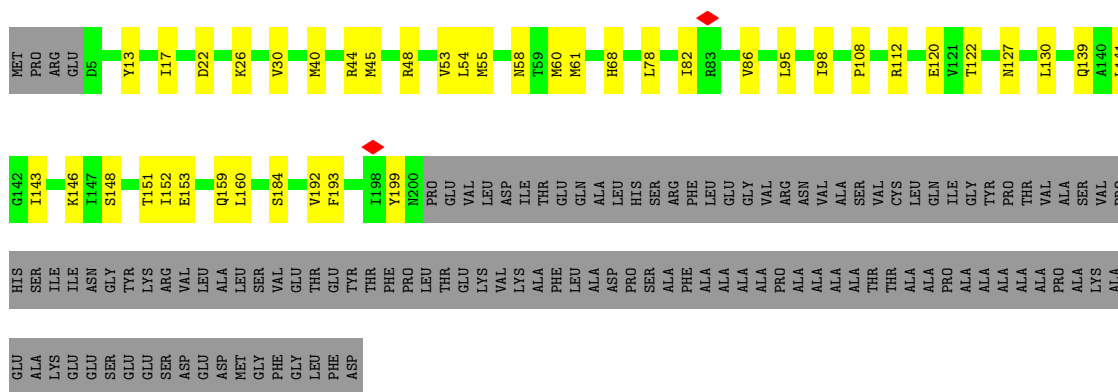
Chain O3:



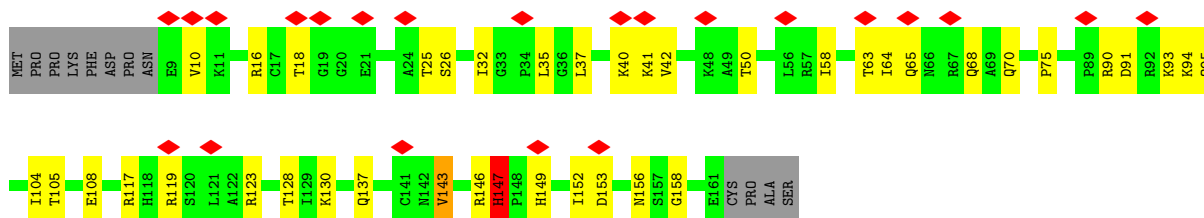




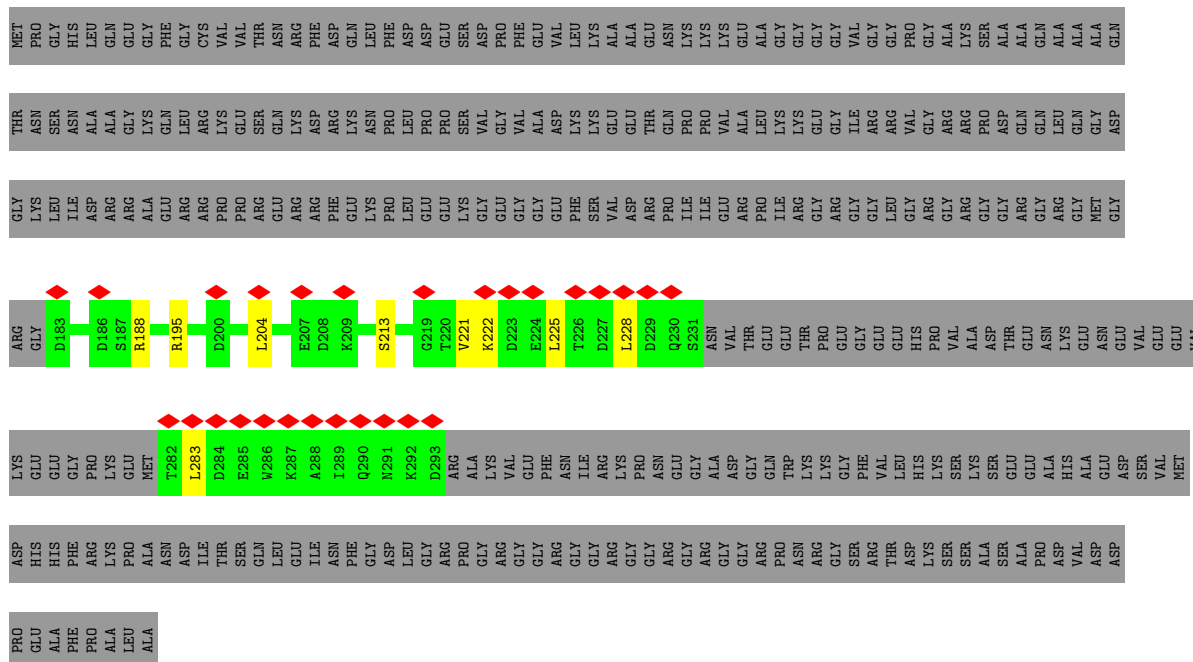




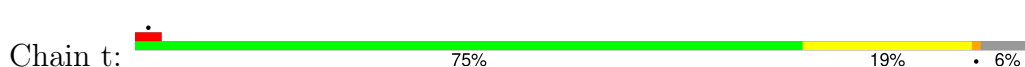
- Molecule 81: 60S ribosomal protein L12

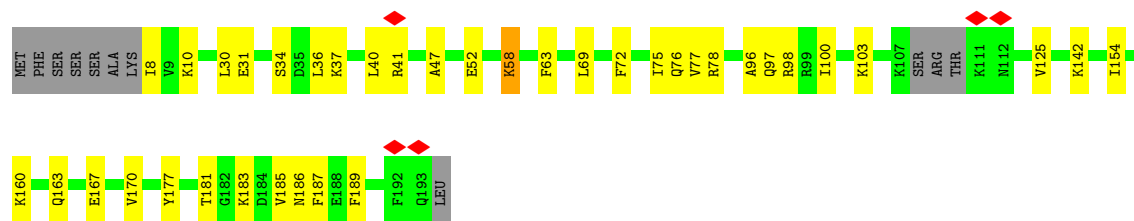


- Molecule 82: Isoform 3 of Plasminogen activator inhibitor 1 RNA-binding protein

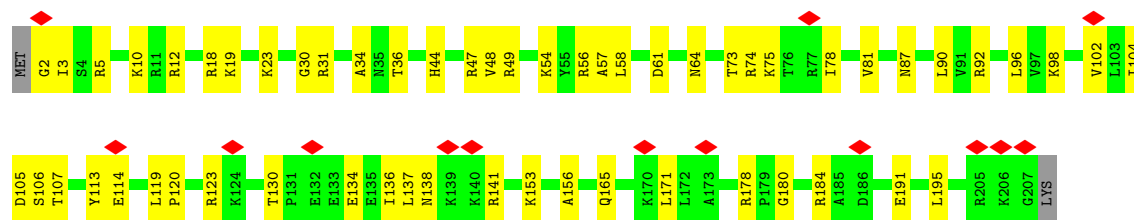


- Molecule 83: 40S ribosomal protein S7

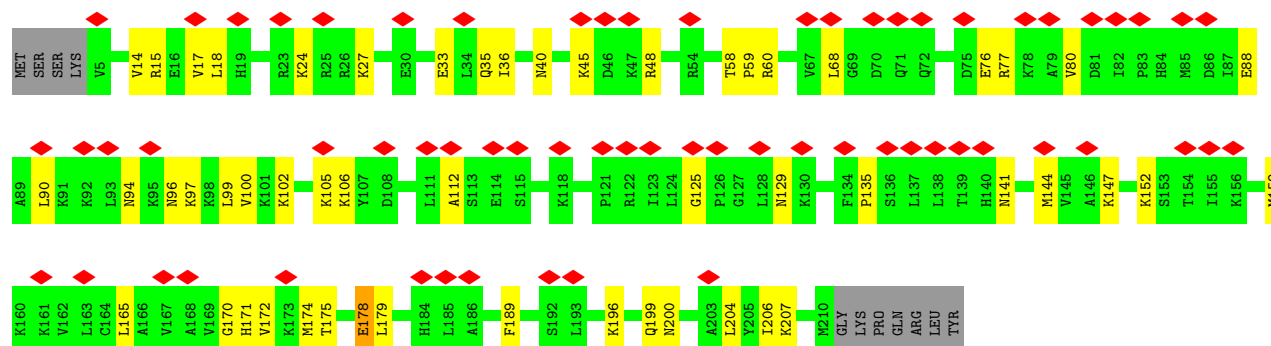
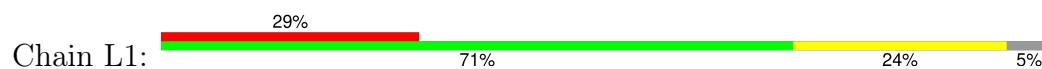




- Molecule 84: 40S ribosomal protein S8



- Molecule 85: 60S ribosomal protein L10a



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 23297                                   | 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 ( $e^-/\text{\AA}^2$ ) | 1.0                                     | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 30.264                                  | Depositor |
| Minimum map value                    | -17.005                                 | Depositor |
| Average map value                    | -0.003                                  | Depositor |
| Map value standard deviation         | 1.034                                   | Depositor |
| Recommended contour level            | 4                                       | Depositor |
| Map size ( $\text{\AA}$ )            | 814.07996, 814.07996, 814.07996         | wwPDB     |
| Map dimensions                       | 768, 768, 768                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E6G, 1MA, GDP, B9B, B8Q, P7G, OMU, B8N, MLZ, DDE, 5MC, I4U, 6MZ, B9H, 2MG, UR3, E7G, MG, A2M, 4AC, B8W, B8T, OMG, G7M, ZN, PSU, MHG, OMC

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   | A1    | 0.11         | 0/1888      | 0.27        | 0/2516      |
| 2   | B1    | 0.10         | 0/1898      | 0.24        | 0/2553      |
| 3   | C1    | 0.10         | 0/1537      | 0.25        | 0/2065      |
| 4   | D1    | 0.09         | 0/1728      | 0.22        | 0/2306      |
| 5   | E1    | 0.10         | 0/1420      | 0.27        | 0/1899      |
| 6   | F1    | 0.11         | 0/1707      | 0.26        | 0/2286      |
| 7   | G1    | 0.12         | 0/1165      | 0.24        | 0/1558      |
| 8   | H1    | 0.11         | 0/1746      | 0.24        | 0/2338      |
| 9   | A2    | 0.13         | 0/86883     | 0.24        | 0/135484    |
| 10  | B2    | 0.11         | 0/2858      | 0.23        | 0/4455      |
| 11  | C2    | 0.14         | 0/3679      | 0.25        | 0/5732      |
| 12  | D2    | 0.11         | 0/1959      | 0.26        | 0/2627      |
| 13  | E2    | 0.11         | 0/3305      | 0.27        | 0/4422      |
| 14  | F2    | 0.10         | 0/2971      | 0.24        | 0/3987      |
| 15  | G2    | 0.09         | 0/2431      | 0.22        | 0/3256      |
| 16  | H2    | 0.09         | 0/1822      | 0.23        | 0/2443      |
| 17  | I2    | 0.11         | 0/1670      | 0.26        | 0/2232      |
| 18  | J2    | 0.10         | 0/1268      | 0.26        | 0/1700      |
| 19  | K2    | 0.10         | 0/1535      | 0.25        | 0/2048      |
| 20  | L2    | 0.09         | 0/1558      | 0.21        | 0/2059      |
| 21  | M2    | 0.11         | 0/1490      | 0.27        | 0/2000      |
| 22  | N2    | 0.09         | 0/1326      | 0.21        | 0/1769      |
| 23  | O2    | 0.09         | 0/839       | 0.25        | 0/1126      |
| 24  | P2    | 0.09         | 0/983       | 0.23        | 0/1319      |
| 25  | Q2    | 0.10         | 0/909       | 0.26        | 0/1203      |
| 26  | R2    | 0.09         | 0/984       | 0.24        | 0/1323      |
| 27  | S2    | 0.09         | 0/1132      | 0.22        | 0/1504      |
| 28  | T2    | 0.09         | 0/1130      | 0.21        | 0/1507      |
| 29  | U2    | 0.10         | 0/1193      | 0.23        | 0/1593      |
| 30  | V2    | 0.10         | 0/963       | 0.24        | 0/1275      |
| 31  | W2    | 0.09         | 0/742       | 0.20        | 0/996       |

| Mol | Chain | Bond lengths |                | Bond angles |         |
|-----|-------|--------------|----------------|-------------|---------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5 |
| 32  | X2    | 0.10         | 0/903          | 0.25        | 0/1216  |
| 33  | Y2    | 0.10         | 0/1071         | 0.25        | 0/1429  |
| 34  | Z2    | 0.11         | 0/895          | 0.25        | 0/1198  |
| 35  | a2    | 0.09         | 0/916          | 0.23        | 0/1221  |
| 36  | b2    | 0.09         | 0/1009         | 0.22        | 0/1332  |
| 37  | c2    | 0.10         | 0/838          | 0.25        | 0/1111  |
| 38  | d2    | 0.10         | 0/720          | 0.25        | 0/952   |
| 39  | e2    | 0.08         | 0/574          | 0.22        | 0/760   |
| 40  | f2    | 0.10         | 0/454          | 0.22        | 0/599   |
| 41  | g2    | 0.09         | 0/425          | 0.25        | 0/561   |
| 42  | h2    | 0.09         | 0/231          | 0.18        | 0/294   |
| 43  | i2    | 0.10         | 0/855          | 0.24        | 0/1128  |
| 44  | j2    | 0.10         | 0/704          | 0.22        | 0/935   |
| 45  | k2    | 0.11         | 0/1016         | 0.27        | 0/1363  |
| 46  | m2    | 0.12         | 1/40772 (0.0%) | 0.23        | 0/63546 |
| 47  | n2    | 0.11         | 0/1795         | 0.26        | 0/2798  |
| 48  | p2    | 0.08         | 0/1765         | 0.23        | 0/2362  |
| 49  | q2    | 0.10         | 0/1784         | 0.24        | 0/2402  |
| 50  | r2    | 0.08         | 0/2118         | 0.24        | 0/2849  |
| 51  | w2    | 0.09         | 0/1268         | 0.24        | 0/1696  |
| 52  | z2    | 0.09         | 0/1094         | 0.24        | 0/1469  |
| 53  | o2    | 0.09         | 0/1731         | 0.23        | 0/2352  |
| 54  | s2    | 0.08         | 0/1517         | 0.23        | 0/2038  |
| 55  | v2    | 0.08         | 0/843          | 0.22        | 0/1137  |
| 56  | x2    | 0.08         | 0/1094         | 0.23        | 0/1460  |
| 57  | y2    | 0.10         | 0/1161         | 0.27        | 0/1553  |
| 58  | A3    | 0.08         | 0/1208         | 0.24        | 0/1618  |
| 59  | B3    | 0.08         | 0/1122         | 0.20        | 0/1503  |
| 60  | C3    | 0.08         | 0/817          | 0.22        | 0/1097  |
| 61  | D3    | 0.08         | 0/645          | 0.19        | 0/863   |
| 62  | E3    | 0.10         | 0/1116         | 0.27        | 0/1490  |
| 63  | F3    | 0.10         | 0/828          | 0.25        | 0/1109  |
| 64  | G3    | 0.08         | 0/508          | 0.24        | 0/680   |
| 65  | H3    | 0.10         | 0/466          | 0.29        | 0/618   |
| 66  | I3    | 0.09         | 0/2493         | 0.29        | 0/3394  |
| 67  | J3    | 0.10         | 0/1762         | 0.25        | 0/2382  |
| 68  | K3    | 0.08         | 0/1863         | 0.24        | 0/2481  |
| 69  | L3    | 0.08         | 0/1550         | 0.23        | 0/2069  |
| 70  | M3    | 0.07         | 0/952          | 0.22        | 0/1278  |
| 71  | N3    | 0.09         | 0/1232         | 0.21        | 0/1656  |
| 72  | O3    | 0.09         | 0/1015         | 0.23        | 0/1361  |
| 73  | P3    | 0.10         | 0/1051         | 0.27        | 0/1406  |
| 74  | Q3    | 0.08         | 0/1066         | 0.23        | 0/1415  |

| Mol | Chain | Bond lengths |                 | Bond angles |          |
|-----|-------|--------------|-----------------|-------------|----------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5  |
| 75  | R3    | 0.09         | 0/604           | 0.26        | 0/810    |
| 76  | S3    | 0.08         | 0/665           | 0.27        | 0/890    |
| 77  | T3    | 0.08         | 0/443           | 0.25        | 0/582    |
| 78  | U3    | 0.08         | 0/515           | 0.28        | 0/682    |
| 79  | m     | 0.10         | 0/6756          | 0.26        | 0/9122   |
| 80  | j     | 0.09         | 0/1530          | 0.24        | 0/2064   |
| 81  | k     | 0.10         | 0/1173          | 0.29        | 0/1581   |
| 82  | A     | 0.10         | 0/493           | 0.23        | 0/655    |
| 83  | t     | 0.09         | 0/1499          | 0.23        | 0/2007   |
| 84  | u     | 0.09         | 0/1715          | 0.25        | 0/2287   |
| 85  | L1    | 0.11         | 0/1686          | 0.31        | 0/2262   |
| All | All   | 0.12         | 1/241045 (0.0%) | 0.24        | 0/352704 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 46  | m2    | 670 | A2M  | O3'-P | 5.03 | 1.61        | 1.56     |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A1    | 1851  | 0        | 1988     | 35      | 0            |
| 2   | B1    | 1863  | 0        | 2003     | 23      | 0            |
| 3   | C1    | 1519  | 0        | 1603     | 30      | 0            |
| 4   | D1    | 1690  | 0        | 1745     | 22      | 0            |
| 5   | E1    | 1397  | 0        | 1425     | 20      | 0            |
| 6   | F1    | 1676  | 0        | 1777     | 34      | 0            |
| 7   | G1    | 1143  | 0        | 1217     | 21      | 0            |
| 8   | H1    | 1701  | 0        | 1749     | 30      | 0            |
| 9   | A2    | 79519 | 0        | 40066    | 1127    | 0            |
| 10  | B2    | 2558  | 0        | 1296     | 31      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | C2    | 3315  | 0        | 1685     | 52      | 0            |
| 12  | D2    | 1921  | 0        | 2022     | 45      | 0            |
| 13  | E2    | 3238  | 0        | 3380     | 63      | 0            |
| 14  | F2    | 2928  | 0        | 3110     | 46      | 0            |
| 15  | G2    | 2385  | 0        | 2409     | 34      | 0            |
| 16  | H2    | 1789  | 0        | 1932     | 23      | 0            |
| 17  | I2    | 1640  | 0        | 1790     | 34      | 0            |
| 18  | J2    | 1242  | 0        | 1274     | 18      | 0            |
| 19  | K2    | 1511  | 0        | 1636     | 32      | 0            |
| 20  | L2    | 1542  | 0        | 1698     | 22      | 0            |
| 21  | M2    | 1450  | 0        | 1488     | 17      | 0            |
| 22  | N2    | 1298  | 0        | 1365     | 25      | 0            |
| 23  | O2    | 825   | 0        | 850      | 8       | 0            |
| 24  | P2    | 969   | 0        | 1031     | 15      | 0            |
| 25  | Q2    | 895   | 0        | 948      | 11      | 0            |
| 26  | R2    | 967   | 0        | 1040     | 17      | 0            |
| 27  | S2    | 1115  | 0        | 1205     | 22      | 0            |
| 28  | T2    | 1107  | 0        | 1182     | 18      | 0            |
| 29  | U2    | 1164  | 0        | 1213     | 20      | 0            |
| 30  | V2    | 945   | 0        | 1037     | 13      | 0            |
| 31  | W2    | 732   | 0        | 769      | 13      | 0            |
| 32  | X2    | 888   | 0        | 929      | 16      | 0            |
| 33  | Y2    | 1053  | 0        | 1145     | 21      | 0            |
| 34  | Z2    | 876   | 0        | 912      | 14      | 0            |
| 35  | a2    | 906   | 0        | 997      | 11      | 0            |
| 36  | b2    | 1001  | 0        | 1138     | 17      | 0            |
| 37  | c2    | 827   | 0        | 895      | 11      | 0            |
| 38  | d2    | 705   | 0        | 737      | 15      | 0            |
| 39  | e2    | 568   | 0        | 635      | 9       | 0            |
| 40  | f2    | 444   | 0        | 483      | 10      | 0            |
| 41  | g2    | 430   | 0        | 465      | 9       | 0            |
| 42  | h2    | 230   | 0        | 276      | 2       | 0            |
| 43  | i2    | 842   | 0        | 912      | 11      | 0            |
| 44  | j2    | 694   | 0        | 738      | 17      | 0            |
| 45  | k2    | 1001  | 0        | 1066     | 23      | 0            |
| 46  | m2    | 36817 | 0        | 18599    | 578     | 0            |
| 47  | n2    | 1604  | 0        | 816      | 21      | 0            |
| 48  | p2    | 1738  | 0        | 1809     | 25      | 0            |
| 49  | q2    | 1756  | 0        | 1851     | 26      | 0            |
| 50  | r2    | 2076  | 0        | 2177     | 32      | 0            |
| 51  | w2    | 1247  | 0        | 1323     | 17      | 0            |
| 52  | z2    | 1080  | 0        | 1135     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 53  | o2    | 1694  | 0        | 1696     | 27      | 0            |
| 54  | s2    | 1496  | 0        | 1548     | 24      | 0            |
| 55  | v2    | 819   | 0        | 842      | 15      | 0            |
| 56  | x2    | 1073  | 0        | 1128     | 31      | 0            |
| 57  | y2    | 1143  | 0        | 1213     | 18      | 0            |
| 58  | A3    | 1190  | 0        | 1249     | 28      | 0            |
| 59  | B3    | 1104  | 0        | 1139     | 21      | 0            |
| 60  | C3    | 807   | 0        | 874      | 14      | 0            |
| 61  | D3    | 638   | 0        | 635      | 11      | 0            |
| 62  | E3    | 1098  | 0        | 1167     | 15      | 0            |
| 63  | F3    | 811   | 0        | 866      | 16      | 0            |
| 64  | G3    | 506   | 0        | 536      | 14      | 0            |
| 65  | H3    | 455   | 0        | 446      | 10      | 0            |
| 66  | I3    | 2436  | 0        | 2393     | 57      | 0            |
| 67  | J3    | 1725  | 0        | 1815     | 42      | 0            |
| 68  | K3    | 1840  | 0        | 1989     | 41      | 0            |
| 69  | L3    | 1525  | 0        | 1640     | 22      | 0            |
| 70  | M3    | 942   | 0        | 971      | 14      | 0            |
| 71  | N3    | 1208  | 0        | 1294     | 17      | 0            |
| 72  | O3    | 1002  | 0        | 1023     | 25      | 0            |
| 73  | P3    | 1034  | 0        | 1080     | 16      | 0            |
| 74  | Q3    | 1049  | 0        | 1122     | 24      | 0            |
| 75  | R3    | 598   | 0        | 656      | 9       | 0            |
| 76  | S3    | 652   | 0        | 676      | 11      | 0            |
| 77  | T3    | 438   | 0        | 484      | 8       | 0            |
| 78  | U3    | 505   | 0        | 506      | 6       | 0            |
| 79  | m     | 6649  | 0        | 6723     | 116     | 0            |
| 80  | j     | 1507  | 0        | 1564     | 25      | 0            |
| 81  | k     | 1159  | 0        | 1216     | 24      | 0            |
| 82  | A     | 486   | 0        | 441      | 10      | 0            |
| 83  | t     | 1477  | 0        | 1567     | 23      | 0            |
| 84  | u     | 1686  | 0        | 1772     | 42      | 0            |
| 85  | L1    | 1660  | 0        | 1768     | 33      | 0            |
| 86  | F3    | 1     | 0        | 0        | 0       | 0            |
| 86  | H3    | 1     | 0        | 0        | 0       | 0            |
| 86  | U3    | 1     | 0        | 0        | 0       | 0            |
| 86  | d2    | 1     | 0        | 0        | 0       | 0            |
| 86  | g2    | 1     | 0        | 0        | 0       | 0            |
| 86  | i2    | 1     | 0        | 0        | 0       | 0            |
| 86  | j2    | 1     | 0        | 0        | 0       | 0            |
| 87  | H3    | 1     | 0        | 0        | 0       | 0            |
| 88  | m     | 28    | 0        | 12       | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 89  | A2    | 1      | 0        | 0        | 0       | 0            |
| 89  | B1    | 1      | 0        | 0        | 0       | 0            |
| 89  | m2    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 227130 | 0        | 171022   | 3010    | 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 8.

All (3010) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A2:3837:B8W:C1' | 9:A2:3837:B8W:O4' | 1.67                     | 1.26              |
| 9:A2:2600:A:H61   | 9:A2:3499:C:N4    | 1.59                     | 1.01              |
| 46:m2:1745:G:N2   | 46:m2:1793:A:H62  | 1.60                     | 0.99              |
| 9:A2:2600:A:N6    | 9:A2:3499:C:H42   | 1.61                     | 0.98              |
| 83:t:72:PHE:O     | 83:t:76:GLN:HB2   | 1.64                     | 0.96              |
| 9:A2:2207:G:H21   | 9:A2:2262:A:H62   | 1.14                     | 0.96              |
| 46:m2:1658:G:H1   | 46:m2:1670:U:H3   | 1.15                     | 0.93              |
| 46:m2:1731:U:H3   | 46:m2:1807:G:H1   | 0.94                     | 0.92              |
| 46:m2:1745:G:H21  | 46:m2:1793:A:N6   | 1.65                     | 0.92              |
| 46:m2:1654:G:H1   | 46:m2:1674:U:H3   | 1.12                     | 0.92              |
| 9:A2:740:A:H62    | 9:A2:828:G:N2     | 1.67                     | 0.90              |
| 46:m2:1290:U:H3   | 46:m2:1313:C:H42  | 1.16                     | 0.89              |
| 9:A2:4253:U:H3    | 9:A2:4262:A:H62   | 1.18                     | 0.88              |
| 9:A2:740:A:N6     | 9:A2:828:G:H21    | 1.72                     | 0.87              |
| 9:A2:1541:G:N2    | 9:A2:1544:A:H61   | 1.72                     | 0.87              |
| 9:A2:1541:G:H21   | 9:A2:1544:A:N6    | 1.71                     | 0.86              |
| 9:A2:740:A:H62    | 9:A2:828:G:H21    | 0.91                     | 0.86              |
| 46:m2:1418:C:HO2' | 59:B3:4:VAL:N     | 1.73                     | 0.86              |
| 46:m2:1745:G:H21  | 46:m2:1793:A:H62  | 0.86                     | 0.85              |
| 9:A2:2600:A:H61   | 9:A2:3499:C:H42   | 0.86                     | 0.84              |
| 46:m2:1474:C:H42  | 46:m2:1478:A:H62  | 1.25                     | 0.83              |
| 9:A2:3996:U:H3    | 9:A2:4020:G:H1    | 1.24                     | 0.82              |
| 9:A2:464:G:H1     | 9:A2:699:A:N6     | 1.79                     | 0.80              |
| 46:m2:1750:G:H1   | 46:m2:1788:U:H3   | 1.26                     | 0.79              |
| 9:A2:3366:G:H22   | 9:A2:3398:G:H1'   | 1.47                     | 0.79              |
| 46:m2:1032:A:H2'  | 46:m2:1033:A2M:H8 | 1.66                     | 0.77              |
| 47:n2:9:U:N3      | 47:n2:15:A:N6     | 2.33                     | 0.76              |
| 9:A2:2240:U:H3    | 9:A2:2248:G:H1    | 1.34                     | 0.75              |
| 85:L1:196:LYS:HB3 | 85:L1:199:GLN:HB2 | 1.70                     | 0.73              |
| 46:m2:70:G:H21    | 46:m2:79:A:H62    | 1.35                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:m2:679:G:H21   | 46:m2:1030:A:H62  | 1.35                     | 0.73              |
| 9:A2:4639:G:H1    | 9:A2:4704:A:H2    | 1.37                     | 0.73              |
| 84:u:134:GLU:HA   | 84:u:138:ASN:HB2  | 1.71                     | 0.73              |
| 9:A2:1:C:H42      | 11:C2:156:U:H2'   | 1.54                     | 0.73              |
| 46:m2:15:U:O2'    | 46:m2:671:A:N6    | 2.22                     | 0.72              |
| 9:A2:2506:G:H2'   | 9:A2:2507:G:H8    | 1.54                     | 0.72              |
| 46:m2:824:PSU:N1  | 46:m2:827:A:N7    | 2.32                     | 0.72              |
| 9:A2:3297:U:OP2   | 9:A2:3302:A:N6    | 2.24                     | 0.71              |
| 46:m2:348:C:H5''  | 50:r2:38:LEU:HD22 | 1.71                     | 0.71              |
| 9:A2:4541:G:N1    | 9:A2:4570:U:N3    | 2.39                     | 0.70              |
| 9:A2:3353:U:H5''  | 9:A2:3354:G:H5'   | 1.73                     | 0.70              |
| 46:m2:1353:G:H1   | 46:m2:1362:U:H3   | 1.37                     | 0.70              |
| 10:B2:117:G:H5'   | 15:G2:256:LYS:HD2 | 1.74                     | 0.70              |
| 15:G2:37:VAL:HG12 | 15:G2:67:ALA:HB2  | 1.74                     | 0.70              |
| 46:m2:444:C:H42   | 46:m2:451:A:H62   | 1.40                     | 0.70              |
| 9:A2:1541:G:N2    | 9:A2:1544:A:N6    | 2.34                     | 0.69              |
| 46:m2:540:U:N3    | 46:m2:548:G:N1    | 2.41                     | 0.69              |
| 7:G1:56:GLN:HE22  | 9:A2:4515:OMG:H2' | 1.57                     | 0.69              |
| 9:A2:2207:G:N2    | 9:A2:2262:A:H62   | 1.88                     | 0.69              |
| 9:A2:1259:C:H42   | 9:A2:1901:A:H61   | 1.39                     | 0.69              |
| 9:A2:1354:U:H3    | 9:A2:1431:G:H1    | 1.41                     | 0.69              |
| 38:d2:54:LYS:O    | 38:d2:58:THR:HB   | 1.92                     | 0.69              |
| 82:A:225:LEU:HA   | 82:A:228:LEU:HD12 | 1.75                     | 0.69              |
| 79:m:598:HIS:HB3  | 79:m:709:HIS:HB2  | 1.75                     | 0.68              |
| 46:m2:1663:A:H8   | 65:H3:14:PHE:HB2  | 1.59                     | 0.68              |
| 9:A2:3600:G:H1    | 9:A2:3719:U:H3    | 1.42                     | 0.68              |
| 9:A2:3629:G:H5''  | 85:L1:27:LYS:HB2  | 1.76                     | 0.68              |
| 46:m2:160:U:H3    | 46:m2:470:A:HO2'  | 1.41                     | 0.68              |
| 46:m2:504:C:N3    | 50:r2:63:LYS:NZ   | 2.41                     | 0.68              |
| 39:e2:12:LEU:HB3  | 39:e2:16:ARG:HH21 | 1.59                     | 0.68              |
| 9:A2:1146:C:H2'   | 9:A2:1147:A:H8    | 1.57                     | 0.67              |
| 9:A2:1362:G:N2    | 9:A2:1392:C:O2    | 2.17                     | 0.67              |
| 9:A2:4193:G:N2    | 9:A2:4196:A:OP2   | 2.26                     | 0.67              |
| 9:A2:471:A:H61    | 9:A2:690:C:H42    | 1.43                     | 0.67              |
| 46:m2:651:U:H2'   | 46:m2:652:A:H8    | 1.59                     | 0.67              |
| 9:A2:1532:U:H4'   | 22:N2:100:LYS:HB2 | 1.75                     | 0.67              |
| 11:C2:83:C:H42    | 27:S2:50:ARG:HH22 | 1.43                     | 0.67              |
| 47:n2:26:G:O6     | 47:n2:44:A:N1     | 2.28                     | 0.67              |
| 50:r2:137:PRO:HG2 | 50:r2:150:PRO:HD2 | 1.77                     | 0.67              |
| 83:t:154:ILE:HB   | 83:t:185:VAL:HG12 | 1.77                     | 0.67              |
| 29:U2:59:ARG:NH2  | 29:U2:61:TYR:OH   | 2.28                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:m2:936:G:O6     | 46:m2:1010:A:N1   | 2.28                     | 0.67              |
| 46:m2:995:G:OP1    | 46:m2:1133:G:N2   | 2.26                     | 0.67              |
| 53:o2:137:ALA:HB1  | 53:o2:142:LEU:HB3 | 1.77                     | 0.66              |
| 9:A2:3452:U:HO2'   | 46:m2:1722:U:HO2' | 1.41                     | 0.66              |
| 46:m2:1240:U:H3    | 46:m2:1244:U:H5   | 1.44                     | 0.66              |
| 9:A2:1368:G:O6     | 44:j2:4:ARG:NH2   | 2.29                     | 0.66              |
| 9:A2:1367:A:H4'    | 44:j2:10:ILE:HG22 | 1.77                     | 0.66              |
| 9:A2:1657:G:O6     | 9:A2:1682:G:N2    | 2.29                     | 0.66              |
| 46:m2:198:U:H3     | 46:m2:203:G:H1    | 1.43                     | 0.66              |
| 79:m:579:ARG:HB2   | 79:m:740:MET:HB3  | 1.77                     | 0.66              |
| 46:m2:367:C:HO2'   | 46:m2:404:C:HO2'  | 1.41                     | 0.66              |
| 62:E3:39:ASN:HD21  | 62:E3:43:GLY:H    | 1.43                     | 0.66              |
| 79:m:18:ILE:HG13   | 79:m:360:PRO:HG2  | 1.76                     | 0.66              |
| 20:L2:172:ARG:HH12 | 46:m2:910:A:H5''  | 1.61                     | 0.66              |
| 9:A2:2392:U:HO2'   | 9:A2:2473:U:HO2'  | 1.44                     | 0.66              |
| 9:A2:2414:A:H62    | 9:A2:2430:G:N2    | 1.94                     | 0.66              |
| 46:m2:589:A:H5'    | 46:m2:594:C:H41   | 1.60                     | 0.66              |
| 13:E2:4:ARG:NH1    | 13:E2:6:PHE:O     | 2.29                     | 0.65              |
| 72:O3:103:ASN:HB3  | 72:O3:142:ARG:HG2 | 1.76                     | 0.65              |
| 79:m:428:ILE:HG22  | 79:m:484:ILE:HG12 | 1.78                     | 0.65              |
| 9:A2:2592:U:H5''   | 13:E2:249:ARG:HB2 | 1.77                     | 0.65              |
| 46:m2:73:C:O2'     | 46:m2:76:U:O4     | 2.15                     | 0.65              |
| 8:H1:120:TRP:HE1   | 8:H1:123:GLU:HB2  | 1.61                     | 0.65              |
| 46:m2:379:G:H5'    | 84:u:98:LYS:HB3   | 1.78                     | 0.65              |
| 9:A2:346:G:OP2     | 27:S2:13:LYS:NZ   | 2.26                     | 0.65              |
| 79:m:39:VAL:HG13   | 79:m:76:LEU:HD21  | 1.78                     | 0.65              |
| 5:E1:56:THR:HG22   | 5:E1:64:ARG:H     | 1.62                     | 0.65              |
| 22:N2:17:ARG:NH1   | 22:N2:45:MET:SD   | 2.70                     | 0.65              |
| 79:m:616:ILE:HG22  | 79:m:621:VAL:HB   | 1.77                     | 0.65              |
| 84:u:34:ALA:HB2    | 84:u:56:ARG:HH11  | 1.61                     | 0.65              |
| 9:A2:129:C:N4      | 9:A2:130:G:O6     | 2.30                     | 0.65              |
| 9:A2:295:A:OP2     | 43:i2:39:ARG:NH1  | 2.30                     | 0.65              |
| 9:A2:230:G:OP1     | 27:S2:15:ARG:NH1  | 2.30                     | 0.64              |
| 9:A2:323:C:H2'     | 9:A2:324:A:H8     | 1.61                     | 0.64              |
| 9:A2:2356:A:N6     | 9:A2:2499:A:OP2   | 2.28                     | 0.64              |
| 46:m2:1268:C:N3    | 46:m2:1519:G:N2   | 2.45                     | 0.64              |
| 46:m2:1590:A:H2'   | 46:m2:1591:A:H8   | 1.62                     | 0.64              |
| 9:A2:2073:G:N2     | 9:A2:2076:G:OP2   | 2.24                     | 0.64              |
| 66:I3:286:CYS:HA   | 66:I3:302:TYR:HA  | 1.80                     | 0.64              |
| 9:A2:4433:G:H22    | 9:A2:4499:G:H1    | 1.45                     | 0.64              |
| 34:Z2:57:THR:HG21  | 34:Z2:68:ARG:HD3  | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F1:16:LYS:NZ    | 9:A2:97:G:OP1     | 2.30                     | 0.64              |
| 46:m2:541:C:N3    | 46:m2:547:A:N6    | 2.46                     | 0.64              |
| 74:Q3:20:ARG:NH1  | 74:Q3:74:MET:SD   | 2.70                     | 0.64              |
| 9:A2:1763:G:N2    | 9:A2:1826:G:O2'   | 2.31                     | 0.64              |
| 9:A2:417:G:O2'    | 11:C2:16:G:N2     | 2.30                     | 0.64              |
| 46:m2:304:A:N3    | 84:u:64:ASN:ND2   | 2.45                     | 0.64              |
| 46:m2:1238:G:O6   | 58:A3:137:LYS:NZ  | 2.31                     | 0.64              |
| 46:m2:153:G:N3    | 68:K3:13:GLN:NE2  | 2.45                     | 0.64              |
| 46:m2:1403:A:H4'  | 60:C3:52:GLY:HA3  | 1.79                     | 0.64              |
| 79:m:113:GLU:HG2  | 79:m:531:PRO:HG3  | 1.79                     | 0.64              |
| 31:W2:37:MET:SD   | 31:W2:40:GLN:NE2  | 2.71                     | 0.63              |
| 49:q2:195:SER:HA  | 49:q2:201:LYS:HG3 | 1.78                     | 0.63              |
| 5:E1:20:LEU:HD11  | 5:E1:83:LEU:HB2   | 1.78                     | 0.63              |
| 9:A2:1386:G:OP1   | 20:L2:92:LYS:NZ   | 2.31                     | 0.63              |
| 9:A2:3356:C:O2'   | 9:A2:3430:A:N3    | 2.27                     | 0.63              |
| 9:A2:4351:U:OP2   | 41:g2:111:ARG:NH1 | 2.31                     | 0.63              |
| 10:B2:13:A:OP2    | 10:B2:66:G:N2     | 2.30                     | 0.63              |
| 47:n2:9:U:C2      | 47:n2:15:A:N6     | 2.66                     | 0.63              |
| 80:j:192:VAL:HB   | 80:j:199:TYR:HB3  | 1.80                     | 0.63              |
| 1:A1:267:ARG:NH2  | 9:A2:840:G:OP1    | 2.30                     | 0.63              |
| 46:m2:170:A:H5''  | 68:K3:136:LYS:HD3 | 1.80                     | 0.63              |
| 46:m2:546:G:H2'   | 46:m2:547:A:H8    | 1.63                     | 0.63              |
| 66:I3:8:ARG:HD2   | 66:I3:311:GLN:HG3 | 1.79                     | 0.63              |
| 9:A2:3626:G:O2'   | 85:L1:60:ARG:NH1  | 2.31                     | 0.63              |
| 22:N2:49:GLN:HA   | 22:N2:52:MET:HE3  | 1.81                     | 0.63              |
| 68:K3:2:LYS:HB3   | 68:K3:15:LEU:HD11 | 1.80                     | 0.63              |
| 9:A2:1622:C:H2'   | 9:A2:1623:G:H2'   | 1.79                     | 0.63              |
| 9:A2:2258:G:O2'   | 9:A2:2260:C:OP1   | 2.15                     | 0.63              |
| 46:m2:619:G:N7    | 62:E3:67:ARG:NH1  | 2.47                     | 0.63              |
| 9:A2:4563:C:H2'   | 9:A2:4564:G:H8    | 1.63                     | 0.63              |
| 46:m2:1270:C:O2   | 56:x2:97:TYR:OH   | 2.16                     | 0.63              |
| 8:H1:49:ARG:NH2   | 9:A2:152:U:OP2    | 2.26                     | 0.63              |
| 9:A2:1482:A:N3    | 9:A2:1654:U:O2'   | 2.30                     | 0.63              |
| 9:A2:2414:A:N6    | 9:A2:2430:G:N2    | 2.46                     | 0.63              |
| 40:f2:21:ARG:HH12 | 40:f2:24:PRO:HG3  | 1.64                     | 0.63              |
| 56:x2:123:TYR:OH  | 58:A3:124:ARG:NH1 | 2.30                     | 0.63              |
| 79:m:18:ILE:HG22  | 79:m:98:LEU:HD23  | 1.81                     | 0.63              |
| 79:m:365:LYS:HA   | 79:m:385:LYS:HG3  | 1.80                     | 0.63              |
| 9:A2:2532:G:H5''  | 9:A2:2533:G:H5'   | 1.81                     | 0.63              |
| 9:A2:4388:C:H2'   | 9:A2:4389:G:C8    | 2.34                     | 0.63              |
| 30:V2:8:THR:HG22  | 30:V2:10:HIS:H    | 1.62                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:j:44:ARG:NH2    | 80:j:53:VAL:O      | 2.32                     | 0.63              |
| 36:b2:4:ILE:O      | 36:b2:56:ARG:NH1   | 2.32                     | 0.62              |
| 13:E2:240:LEU:HD23 | 13:E2:244:THR:HG21 | 1.80                     | 0.62              |
| 16:H2:284:LEU:HB2  | 34:Z2:4:ARG:HB2    | 1.80                     | 0.62              |
| 46:m2:1016:G:H21   | 76:S3:51:GLN:HE21  | 1.46                     | 0.62              |
| 46:m2:1568:G:O6    | 59:B3:101:ARG:NH1  | 2.31                     | 0.62              |
| 46:m2:1652:A:N3    | 46:m2:1677:A:N6    | 2.47                     | 0.62              |
| 9:A2:282:C:O2      | 9:A2:306:A:N6      | 2.32                     | 0.62              |
| 9:A2:3890:G:H2'    | 9:A2:3891:A:H8     | 1.64                     | 0.62              |
| 60:C3:80:PHE:HB3   | 65:H3:52:PHE:HB3   | 1.81                     | 0.62              |
| 3:C1:137:SER:HB3   | 3:C1:143:GLU:HG3   | 1.81                     | 0.62              |
| 9:A2:1884:G:H5''   | 19:K2:12:LYS:HE2   | 1.82                     | 0.62              |
| 9:A2:4126:A:OP2    | 9:A2:4128:C:N4     | 2.30                     | 0.62              |
| 46:m2:1541:U:H5''  | 59:B3:43:LYS:HE3   | 1.82                     | 0.62              |
| 54:s2:28:VAL:HG21  | 54:s2:109:LEU:HB2  | 1.82                     | 0.62              |
| 79:m:372:TYR:HA    | 79:m:494:ARG:HG2   | 1.81                     | 0.62              |
| 9:A2:416:U:H4'     | 9:A2:2085:G:H4'    | 1.80                     | 0.62              |
| 20:L2:81:ARG:HB3   | 20:L2:88:ARG:HH21  | 1.64                     | 0.62              |
| 67:J3:102:LEU:HB3  | 67:J3:130:ILE:HD11 | 1.82                     | 0.62              |
| 79:m:261:GLY:HA3   | 79:m:263:ARG:HH21  | 1.65                     | 0.62              |
| 9:A2:112:C:OP2     | 36:b2:106:LYS:NZ   | 2.33                     | 0.62              |
| 9:A2:3416:A:N6     | 46:m2:1827:A:O2'   | 2.32                     | 0.62              |
| 9:A2:4626:C:N3     | 18:J2:69:ARG:NH2   | 2.44                     | 0.62              |
| 21:M2:95:ARG:NH1   | 21:M2:113:MET:SD   | 2.73                     | 0.62              |
| 56:x2:18:ARG:NH1   | 58:A3:88:LYS:O     | 2.32                     | 0.62              |
| 9:A2:1007:A:H2     | 9:A2:1017:G:H22    | 1.48                     | 0.62              |
| 9:A2:1310:A:N7     | 19:K2:180:ARG:NH1  | 2.47                     | 0.62              |
| 9:A2:3348:A:H62    | 9:A2:3479:G:H21    | 1.48                     | 0.62              |
| 79:m:222:PHE:HB3   | 79:m:343:LEU:HD13  | 1.81                     | 0.62              |
| 9:A2:1620:G:OP2    | 9:A2:1620:G:N2     | 2.29                     | 0.61              |
| 12:D2:51:ASP:OD2   | 12:D2:54:ARG:NH1   | 2.33                     | 0.61              |
| 12:D2:189:TYR:O    | 12:D2:192:LYS:C    | 2.43                     | 0.61              |
| 46:m2:1612:G:OP1   | 58:A3:121:ARG:NH2  | 2.33                     | 0.61              |
| 79:m:751:PRO:HA    | 79:m:780:MET:HA    | 1.80                     | 0.61              |
| 85:L1:36:ILE:HB    | 85:L1:165:LEU:HB3  | 1.82                     | 0.61              |
| 9:A2:1718:G:H21    | 9:A2:1870:C:H1'    | 1.65                     | 0.61              |
| 9:A2:2242:G:OP2    | 9:A2:2244:C:N4     | 2.33                     | 0.61              |
| 15:G2:152:ARG:NH1  | 15:G2:153:THR:O    | 2.33                     | 0.61              |
| 46:m2:1288:G:N2    | 46:m2:1314:G:O2'   | 2.30                     | 0.61              |
| 62:E3:100:VAL:HG12 | 62:E3:125:VAL:HG12 | 1.82                     | 0.61              |
| 66:I3:79:LEU:HD21  | 66:I3:87:LEU:HD23  | 1.80                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:A2:67:C:N4      | 9:A2:325:U:O2'     | 2.24                     | 0.61              |
| 13:E2:10:ARG:NH1  | 13:E2:11:HIS:O     | 2.33                     | 0.61              |
| 14:F2:218:ILE:O   | 14:F2:222:ARG:HB2  | 2.00                     | 0.61              |
| 46:m2:1580:U:O2   | 49:q2:9:ARG:NH2    | 2.33                     | 0.61              |
| 52:z2:90:ALA:O    | 52:z2:93:GLN:NE2   | 2.32                     | 0.61              |
| 79:m:771:GLU:HB3  | 79:m:784:LYS:HB2   | 1.82                     | 0.61              |
| 9:A2:1659:C:H2'   | 9:A2:1660:A:H8     | 1.65                     | 0.61              |
| 34:Z2:91:ASN:OD1  | 34:Z2:91:ASN:N     | 2.30                     | 0.61              |
| 45:k2:98:ARG:HH21 | 45:k2:107:ARG:HH12 | 1.47                     | 0.61              |
| 46:m2:690:U:H5''  | 83:t:103:LYS:HD2   | 1.82                     | 0.61              |
| 46:m2:1591:A:N3   | 46:m2:1655:U:O2'   | 2.31                     | 0.61              |
| 56:x2:100:LYS:HG3 | 56:x2:101:THR:HG23 | 1.81                     | 0.61              |
| 64:G3:24:GLN:OE1  | 64:G3:26:GLN:NE2   | 2.34                     | 0.61              |
| 9:A2:4287:A:H3'   | 9:A2:4288:PSU:H4'  | 1.82                     | 0.61              |
| 46:m2:1017:U:O2'  | 71:N3:55:ARG:NH1   | 2.33                     | 0.61              |
| 46:m2:1144:G:OP1  | 67:J3:187:ARG:NH2  | 2.34                     | 0.61              |
| 7:G1:5:ARG:HH21   | 7:G1:59:ASP:HB2    | 1.65                     | 0.61              |
| 9:A2:1409:U:O2'   | 18:J2:135:ARG:NH2  | 2.34                     | 0.61              |
| 44:j2:38:THR:HG22 | 44:j2:45:THR:HG22  | 1.83                     | 0.61              |
| 63:F3:51:ARG:NH1  | 64:G3:62:GLU:O     | 2.33                     | 0.61              |
| 9:A2:2155:G:H21   | 35:a2:6:THR:HG22   | 1.65                     | 0.61              |
| 30:V2:57:MET:O    | 30:V2:61:ASN:ND2   | 2.31                     | 0.61              |
| 32:X2:23:ARG:NH1  | 32:X2:121:ASN:OD1  | 2.34                     | 0.61              |
| 46:m2:449:A:OP1   | 84:u:49:ARG:NH1    | 2.34                     | 0.61              |
| 9:A2:3826:U:H2'   | 9:A2:3827:G:H8     | 1.65                     | 0.61              |
| 79:m:674:ILE:HD11 | 79:m:720:ILE:HG13  | 1.83                     | 0.61              |
| 10:B2:119:U:OP2   | 15:G2:259:ARG:NH2  | 2.33                     | 0.61              |
| 34:Z2:36:ARG:HG2  | 34:Z2:80:ASN:HA    | 1.83                     | 0.61              |
| 45:k2:28:GLU:HG2  | 45:k2:31:ASN:HB2   | 1.82                     | 0.61              |
| 9:A2:3991:A:O2'   | 19:K2:178:ARG:NH1  | 2.34                     | 0.60              |
| 19:K2:25:LEU:HD12 | 19:K2:28:LEU:HD11  | 1.82                     | 0.60              |
| 46:m2:184:G:H2'   | 46:m2:185:G:H8     | 1.65                     | 0.60              |
| 46:m2:1618:U:O2'  | 46:m2:1663:A:N3    | 2.34                     | 0.60              |
| 9:A2:1476:C:H1'   | 9:A2:2075:G:H21    | 1.66                     | 0.60              |
| 9:A2:4028:A:O2'   | 29:U2:42:ARG:NH2   | 2.33                     | 0.60              |
| 9:A2:4239:G:OP1   | 17:I2:61:ARG:NH1   | 2.34                     | 0.60              |
| 45:k2:39:ARG:NH1  | 45:k2:105:ASP:OD2  | 2.35                     | 0.60              |
| 51:w2:35:ARG:NH1  | 51:w2:53:GLY:O     | 2.34                     | 0.60              |
| 69:L3:163:SER:O   | 69:L3:167:GLY:N    | 2.33                     | 0.60              |
| 46:m2:1568:G:N7   | 59:B3:101:ARG:NH2  | 2.49                     | 0.60              |
| 53:o2:198:MET:HG2 | 53:o2:200:ASP:H    | 1.65                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:A2:4368:C:OP1   | 13:E2:276:HIS:ND1  | 2.35                     | 0.60              |
| 38:d2:64:MET:HB3  | 38:d2:67:LEU:HB2   | 1.83                     | 0.60              |
| 39:e2:33:LYS:HG2  | 39:e2:46:VAL:HG22  | 1.84                     | 0.60              |
| 46:m2:28:U:H2'    | 46:m2:29:G:H8      | 1.65                     | 0.60              |
| 49:q2:67:ARG:NH1  | 55:v2:93:THR:O     | 2.34                     | 0.60              |
| 66:I3:212:LYS:HA  | 66:I3:235:ILE:HG23 | 1.84                     | 0.60              |
| 9:A2:121:A:H62    | 9:A2:152:U:H3      | 1.50                     | 0.60              |
| 9:A2:3511:C:H2'   | 9:A2:3512:A:H8     | 1.67                     | 0.60              |
| 13:E2:57:VAL:HG22 | 13:E2:73:VAL:HG22  | 1.83                     | 0.60              |
| 46:m2:145:G:H2'   | 46:m2:146:G:C8     | 2.37                     | 0.60              |
| 46:m2:989:A:H5''  | 63:F3:70:LYS:HZ2   | 1.66                     | 0.60              |
| 51:w2:4:ILE:O     | 51:w2:11:GLN:NE2   | 2.33                     | 0.60              |
| 9:A2:1716:C:H4'   | 17:I2:89:PRO:HD3   | 1.83                     | 0.60              |
| 9:A2:3318:A:OP2   | 12:D2:156:LYS:NZ   | 2.33                     | 0.60              |
| 46:m2:1105:C:H2'  | 46:m2:1106:G:C8    | 2.36                     | 0.60              |
| 79:m:109:ASP:HB3  | 79:m:552:HIS:HB2   | 1.82                     | 0.60              |
| 9:A2:4198:A:N7    | 12:D2:215:ASN:ND2  | 2.48                     | 0.60              |
| 73:P3:82:GLN:OE1  | 73:P3:84:LYS:NZ    | 2.34                     | 0.60              |
| 46:m2:641:C:H2'   | 46:m2:642:A:H8     | 1.66                     | 0.60              |
| 56:x2:56:LEU:HD13 | 56:x2:78:THR:HG21  | 1.84                     | 0.60              |
| 9:A2:501:G:H5'    | 9:A2:505:G:H21     | 1.67                     | 0.60              |
| 9:A2:2159:A:H1'   | 38:d2:12:ARG:HH21  | 1.65                     | 0.60              |
| 9:A2:4252:G:N2    | 9:A2:4262:A:OP2    | 2.35                     | 0.60              |
| 9:A2:4274:A:H4'   | 13:E2:13:SER:HB2   | 1.83                     | 0.60              |
| 43:i2:26:TYR:HB3  | 43:i2:67:VAL:HB    | 1.82                     | 0.60              |
| 46:m2:1535:A:OP1  | 54:s2:164:ARG:NH2  | 2.34                     | 0.60              |
| 66:I3:119:GLN:HB2 | 66:I3:131:LEU:HD11 | 1.83                     | 0.60              |
| 83:t:98:ARG:HB3   | 83:t:125:VAL:HG22  | 1.84                     | 0.60              |
| 9:A2:423:G:OP1    | 18:J2:62:ARG:NH1   | 2.35                     | 0.60              |
| 9:A2:1189:C:OP1   | 14:F2:274:LYS:NZ   | 2.35                     | 0.60              |
| 9:A2:3344:U:OP2   | 12:D2:198:ARG:NH2  | 2.35                     | 0.60              |
| 13:E2:92:TYR:HB2  | 13:E2:159:VAL:HB   | 1.84                     | 0.60              |
| 27:S2:35:SER:HB3  | 27:S2:38:LEU:HD13  | 1.84                     | 0.60              |
| 46:m2:16:G:H5'    | 46:m2:671:A:H61    | 1.66                     | 0.60              |
| 46:m2:153:G:H22   | 46:m2:165:G:H1     | 1.49                     | 0.60              |
| 50:r2:104:ASP:HB3 | 50:r2:110:ALA:HB2  | 1.84                     | 0.60              |
| 9:A2:62:A:N3      | 9:A2:77:U:O2'      | 2.31                     | 0.59              |
| 9:A2:2519:A:H2'   | 9:A2:2520:A:H8     | 1.66                     | 0.59              |
| 9:A2:4129:A:H2'   | 9:A2:4130:G:H8     | 1.67                     | 0.59              |
| 36:b2:64:THR:O    | 36:b2:68:ASN:ND2   | 2.34                     | 0.59              |
| 46:m2:927:G:H1    | 46:m2:1019:U:H3    | 1.48                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:m2:1290:U:H3   | 46:m2:1313:C:N4    | 1.95                     | 0.59              |
| 85:L1:59:PRO:O    | 85:L1:171:HIS:ND1  | 2.34                     | 0.59              |
| 5:E1:145:LYS:NZ   | 9:A2:3892:G:OP1    | 2.35                     | 0.59              |
| 9:A2:20:U:H3'     | 9:A2:21:G:H8       | 1.66                     | 0.59              |
| 9:A2:501:G:H1'    | 9:A2:505:G:H3'     | 1.84                     | 0.59              |
| 9:A2:2646:U:OP2   | 20:L2:74:ARG:NH1   | 2.35                     | 0.59              |
| 9:A2:4388:C:H2'   | 9:A2:4389:G:H8     | 1.67                     | 0.59              |
| 9:A2:4628:A:OP1   | 18:J2:74:LYS:NZ    | 2.35                     | 0.59              |
| 11:C2:130:C:H2'   | 11:C2:131:G:H8     | 1.67                     | 0.59              |
| 46:m2:1453:G:OP1  | 52:z2:32:LYS:NZ    | 2.33                     | 0.59              |
| 54:s2:71:ARG:NH2  | 54:s2:148:ASN:OD1  | 2.35                     | 0.59              |
| 58:A3:85:ASN:H    | 58:A3:97:GLN:HG2   | 1.67                     | 0.59              |
| 79:m:82:GLU:O     | 79:m:86:ASN:ND2    | 2.35                     | 0.59              |
| 79:m:154:LEU:HB3  | 79:m:211:VAL:HG12  | 1.84                     | 0.59              |
| 9:A2:24:G:N7      | 38:d2:46:LYS:NZ    | 2.50                     | 0.59              |
| 21:M2:95:ARG:NH2  | 21:M2:112:ASP:OD2  | 2.35                     | 0.59              |
| 32:X2:26:THR:OG1  | 32:X2:85:ARG:NH1   | 2.36                     | 0.59              |
| 46:m2:1591:A:H4'  | 59:B3:82:ARG:HB2   | 1.84                     | 0.59              |
| 46:m2:1649:A:N6   | 46:m2:1678:U:OP2   | 2.34                     | 0.59              |
| 66:I3:38:LYS:HG2  | 66:I3:63:SER:HA    | 1.85                     | 0.59              |
| 84:u:138:ASN:O    | 84:u:141:ARG:NH1   | 2.36                     | 0.59              |
| 9:A2:1140:A2M:OP2 | 9:A2:4097:U:O2'    | 2.20                     | 0.59              |
| 9:A2:2614:G:N2    | 9:A2:3493:C:O2     | 2.34                     | 0.59              |
| 37:c2:48:CYS:SG   | 37:c2:49:GLY:N     | 2.76                     | 0.59              |
| 46:m2:1249:C:OP2  | 82:A:188:ARG:NH2   | 2.35                     | 0.59              |
| 49:q2:103:GLU:OE2 | 49:q2:106:ARG:NH2  | 2.35                     | 0.59              |
| 3:C1:31:ARG:NH1   | 3:C1:149:ASN:OD1   | 2.36                     | 0.59              |
| 9:A2:1785:A:N6    | 9:A2:1813:C:O3'    | 2.35                     | 0.59              |
| 9:A2:3891:A:H2'   | 9:A2:3892:G:C8     | 2.37                     | 0.59              |
| 9:A2:4639:G:O6    | 9:A2:4704:A:N1     | 2.35                     | 0.59              |
| 19:K2:39:THR:HG22 | 19:K2:41:SER:H     | 1.67                     | 0.59              |
| 19:K2:157:GLY:O   | 19:K2:188:ASN:ND2  | 2.35                     | 0.59              |
| 46:m2:1019:U:OP2  | 71:N3:55:ARG:NH1   | 2.36                     | 0.59              |
| 67:J3:244:ILE:O   | 67:J3:247:THR:OG1  | 2.17                     | 0.59              |
| 85:L1:94:ASN:O    | 85:L1:97:LYS:NZ    | 2.32                     | 0.59              |
| 9:A2:2330:U:O2    | 9:A2:2513:G:N2     | 2.30                     | 0.59              |
| 9:A2:3475:G:H2'   | 9:A2:3476:G:H8     | 1.67                     | 0.59              |
| 20:L2:15:LEU:HD13 | 20:L2:52:ARG:HB2   | 1.84                     | 0.59              |
| 46:m2:936:G:H1    | 46:m2:1010:A:H2    | 1.49                     | 0.59              |
| 9:A2:2192:C:H5'   | 26:R2:127:LEU:HD13 | 1.83                     | 0.59              |
| 24:P2:85:ARG:NH1  | 24:P2:99:GLU:O     | 2.36                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:m2:602:G:H2'   | 46:m2:603:G:C8     | 2.38                     | 0.59              |
| 66:I3:283:PRO:O   | 66:I3:285:GLN:NE2  | 2.35                     | 0.59              |
| 70:M3:119:GLN:NE2 | 70:M3:122:ASP:OD2  | 2.35                     | 0.59              |
| 79:m:44:ILE:HG22  | 79:m:45:ILE:HG13   | 1.85                     | 0.59              |
| 9:A2:440:U:O2'    | 34:Z2:91:ASN:O     | 2.21                     | 0.59              |
| 9:A2:1256:A:N1    | 9:A2:1904:G:O6     | 2.36                     | 0.59              |
| 9:A2:4342:G:H21   | 9:A2:4352:A:H62    | 1.50                     | 0.59              |
| 46:m2:1261:A:N6   | 46:m2:1521:U:O5'   | 2.34                     | 0.59              |
| 50:r2:122:LYS:NZ  | 50:r2:124:CYS:SG   | 2.75                     | 0.59              |
| 2:B1:154:LEU:HB3  | 2:B1:204:PHE:HB2   | 1.85                     | 0.59              |
| 9:A2:1166:C:OP2   | 19:K2:104:ARG:NH1  | 2.35                     | 0.59              |
| 9:A2:2088:G:H5''  | 14:F2:195:LYS:HE3  | 1.84                     | 0.59              |
| 9:A2:3378:G:H2'   | 9:A2:3379:A2M:H8   | 1.85                     | 0.59              |
| 9:A2:3501:A:OP2   | 13:E2:249:ARG:NH1  | 2.29                     | 0.59              |
| 9:A2:4177:C:OP1   | 13:E2:246:ARG:NH2  | 2.35                     | 0.59              |
| 10:B2:63:C:H5'    | 10:B2:64:G:H5''    | 1.85                     | 0.59              |
| 46:m2:455:C:O2'   | 68:K3:92:ARG:O     | 2.19                     | 0.59              |
| 46:m2:1474:C:N4   | 46:m2:1478:A:H62   | 1.98                     | 0.59              |
| 9:A2:3504:U:H2'   | 9:A2:3505:A:C8     | 2.38                     | 0.59              |
| 46:m2:1277:G:N2   | 46:m2:1508:A:OP2   | 2.36                     | 0.59              |
| 66:I3:79:LEU:HD22 | 66:I3:120:ILE:HD13 | 1.85                     | 0.59              |
| 6:F1:18:TRP:NE1   | 9:A2:1329:G:O2'    | 2.36                     | 0.58              |
| 9:A2:308:G:N2     | 9:A2:308:G:OP2     | 2.36                     | 0.58              |
| 9:A2:419:A:N3     | 9:A2:1146:C:O2'    | 2.36                     | 0.58              |
| 9:A2:2407:G:N2    | 44:j2:58:GLY:O     | 2.35                     | 0.58              |
| 9:A2:3577:U:OP1   | 12:D2:221:LYS:NZ   | 2.36                     | 0.58              |
| 28:T2:36:ARG:NH1  | 28:T2:38:TYR:OH    | 2.36                     | 0.58              |
| 46:m2:751:U:O2    | 46:m2:797:A:N6     | 2.36                     | 0.58              |
| 56:x2:44:ARG:NH2  | 56:x2:83:MET:SD    | 2.76                     | 0.58              |
| 9:A2:1692:G:N2    | 9:A2:1692:G:OP2    | 2.35                     | 0.58              |
| 10:B2:77:A:H62    | 10:B2:99:G:H21     | 1.51                     | 0.58              |
| 14:F2:334:THR:O   | 14:F2:338:ASN:ND2  | 2.33                     | 0.58              |
| 46:m2:70:G:N2     | 46:m2:79:A:H62     | 2.01                     | 0.58              |
| 46:m2:1132:G:N2   | 46:m2:1132:G:OP2   | 2.36                     | 0.58              |
| 48:p2:175:GLU:O   | 48:p2:179:ASN:ND2  | 2.35                     | 0.58              |
| 79:m:709:HIS:CE1  | 79:m:714:DDE:HD2   | 2.39                     | 0.58              |
| 81:k:90:ARG:HD3   | 81:k:95:GLN:HB2    | 1.83                     | 0.58              |
| 1:A1:264:ARG:HH22 | 9:A2:838:C:H5''    | 1.67                     | 0.58              |
| 9:A2:1071:G:O2'   | 9:A2:1079:A:N6     | 2.36                     | 0.58              |
| 9:A2:4412:G:OP1   | 17:I2:117:ARG:NH2  | 2.35                     | 0.58              |
| 24:P2:13:LYS:NZ   | 24:P2:59:ASP:OD1   | 2.36                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:m2:445:U:O2'   | 68:K3:89:THR:OG1   | 2.21                     | 0.58              |
| 46:m2:484:G:N1    | 46:m2:487:A:OP2    | 2.36                     | 0.58              |
| 9:A2:2054:G:OP2   | 14:F2:204:ARG:NH1  | 2.35                     | 0.58              |
| 9:A2:2333:G:N7    | 28:T2:17:ARG:NH1   | 2.52                     | 0.58              |
| 9:A2:3703:A:N3    | 85:L1:35:GLN:NE2   | 2.51                     | 0.58              |
| 9:A2:4520:G:H2'   | 21:M2:169:THR:HG22 | 1.86                     | 0.58              |
| 22:N2:75:ILE:HG12 | 22:N2:88:ARG:HG2   | 1.84                     | 0.58              |
| 46:m2:1572:G:HO2' | 46:m2:1616:A:HO2'  | 1.52                     | 0.58              |
| 53:o2:149:ASN:ND2 | 53:o2:165:ASN:OD1  | 2.34                     | 0.58              |
| 9:A2:32:G:H21     | 9:A2:50:C:H5       | 1.49                     | 0.58              |
| 9:A2:369:G:N2     | 9:A2:372:A:OP2     | 2.31                     | 0.58              |
| 9:A2:1084:G:N2    | 9:A2:1253:U:O2     | 2.35                     | 0.58              |
| 46:m2:1126:C:H5'' | 48:p2:150:ILE:HG12 | 1.85                     | 0.58              |
| 54:s2:201:LYS:HG3 | 54:s2:204:ARG:HH21 | 1.67                     | 0.58              |
| 58:A3:6:PRO:HD2   | 75:R3:49:LEU:HD13  | 1.85                     | 0.58              |
| 79:m:593:LYS:HG2  | 79:m:600:ARG:HG2   | 1.85                     | 0.58              |
| 4:D1:170:LYS:HA   | 4:D1:177:ASN:HA    | 1.85                     | 0.58              |
| 9:A2:3957:G:N7    | 22:N2:87:LYS:NZ    | 2.45                     | 0.58              |
| 54:s2:34:SER:HB3  | 64:G3:55:VAL:HB    | 1.86                     | 0.58              |
| 7:G1:41:PRO:HG3   | 7:G1:73:VAL:HG23   | 1.86                     | 0.58              |
| 9:A2:2017:G:OP2   | 45:k2:107:ARG:NH1  | 2.37                     | 0.58              |
| 9:A2:3526:C:H2'   | 9:A2:3527:A:H8     | 1.69                     | 0.58              |
| 9:A2:4137:C:O2'   | 41:g2:114:LYS:NZ   | 2.31                     | 0.58              |
| 9:A2:4498:C:N4    | 9:A2:4499:G:O6     | 2.36                     | 0.58              |
| 17:I2:27:VAL:O    | 17:I2:101:ARG:NH2  | 2.36                     | 0.58              |
| 21:M2:81:TRP:HB2  | 21:M2:128:LYS:HB3  | 1.86                     | 0.58              |
| 46:m2:1568:G:O2'  | 46:m2:1570:C:N4    | 2.33                     | 0.58              |
| 79:m:754:VAL:HG11 | 79:m:803:THR:HA    | 1.86                     | 0.58              |
| 9:A2:300:A:H2'    | 9:A2:301:G:H8      | 1.67                     | 0.58              |
| 9:A2:1365:G:O2'   | 9:A2:1387:B9B:N2   | 2.36                     | 0.58              |
| 9:A2:3267:A:O2'   | 84:u:92:ARG:NH2    | 2.37                     | 0.58              |
| 9:A2:4648:U:OP2   | 13:E2:385:LYS:NZ   | 2.31                     | 0.58              |
| 46:m2:529:C:O2    | 46:m2:561:G:N2     | 2.36                     | 0.58              |
| 52:z2:28:PHE:HA   | 52:z2:55:THR:HG21  | 1.86                     | 0.58              |
| 72:O3:34:PHE:HB3  | 72:O3:41:PHE:HB2   | 1.86                     | 0.58              |
| 3:C1:174:LYS:NZ   | 9:A2:4129:A:O2'    | 2.34                     | 0.58              |
| 6:F1:80:GLU:OE2   | 6:F1:102:ARG:NH2   | 2.37                     | 0.58              |
| 20:L2:62:ARG:O    | 20:L2:66:ASN:ND2   | 2.35                     | 0.58              |
| 22:N2:114:GLN:NE2 | 22:N2:118:GLU:OE2  | 2.37                     | 0.58              |
| 9:A2:1657:G:OP1   | 30:V2:4:SER:OG     | 2.18                     | 0.58              |
| 9:A2:3771:G:N7    | 44:j2:62:LYS:NZ    | 2.51                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:C2:19:C:H2'     | 11:C2:20:A:H8      | 1.69                     | 0.58              |
| 12:D2:180:LEU:HD22 | 44:j2:26:VAL:HG21  | 1.85                     | 0.58              |
| 39:e2:23:VAL:HG22  | 39:e2:36:VAL:HG12  | 1.86                     | 0.58              |
| 46:m2:128:U:OP2    | 46:m2:129:C:N4     | 2.37                     | 0.58              |
| 46:m2:1245:PSU:OP2 | 46:m2:1520:C:O2'   | 2.20                     | 0.58              |
| 50:r2:11:ARG:NH1   | 50:r2:21:ASP:O     | 2.36                     | 0.58              |
| 67:J3:64:THR:HG23  | 67:J3:67:GLY:H     | 1.69                     | 0.58              |
| 79:m:427:ARG:HG2   | 79:m:443:LEU:HG    | 1.86                     | 0.58              |
| 79:m:854:LEU:HD11  | 79:m:856:LYS:HE3   | 1.84                     | 0.58              |
| 9:A2:927:C:H2'     | 9:A2:928:G:C8      | 2.39                     | 0.57              |
| 9:A2:3328:G:OP2    | 9:A2:3328:G:N2     | 2.31                     | 0.57              |
| 9:A2:4631:U:O2     | 13:E2:174:ARG:NH1  | 2.37                     | 0.57              |
| 27:S2:19:PHE:O     | 27:S2:26:ARG:NH2   | 2.37                     | 0.57              |
| 28:T2:22:LYS:NZ    | 28:T2:129:TRP:O    | 2.36                     | 0.57              |
| 44:j2:7:LYS:NZ     | 46:m2:1182:C:OP2   | 2.33                     | 0.57              |
| 46:m2:1565:G:OP1   | 59:B3:121:ARG:NH1  | 2.36                     | 0.57              |
| 67:J3:183:LYS:HD3  | 67:J3:194:ARG:HH21 | 1.69                     | 0.57              |
| 9:A2:1561:G:H22    | 9:A2:1575:U:H3     | 1.52                     | 0.57              |
| 20:L2:173:ARG:NH2  | 46:m2:913:C:OP2    | 2.37                     | 0.57              |
| 46:m2:180:G:H3'    | 46:m2:181:A:H8     | 1.68                     | 0.57              |
| 46:m2:416:A:H2'    | 46:m2:417:A:H8     | 1.68                     | 0.57              |
| 46:m2:1158:U:O4    | 67:J3:194:ARG:NH1  | 2.37                     | 0.57              |
| 49:q2:143:ARG:NH2  | 82:A:213:SER:O     | 2.37                     | 0.57              |
| 53:o2:77:ILE:HG12  | 53:o2:99:ILE:HB    | 1.86                     | 0.57              |
| 81:k:50:THR:HG22   | 81:k:58:ILE:HG21   | 1.86                     | 0.57              |
| 9:A2:2414:A:N6     | 9:A2:2430:G:C2     | 2.72                     | 0.57              |
| 9:A2:4279:U:H4'    | 13:E2:373:LYS:HD2  | 1.86                     | 0.57              |
| 12:D2:225:ILE:HD13 | 12:D2:233:ARG:HH21 | 1.69                     | 0.57              |
| 14:F2:293:LEU:O    | 14:F2:299:GLN:NE2  | 2.37                     | 0.57              |
| 24:P2:21:PRO:HA    | 24:P2:54:ALA:HA    | 1.84                     | 0.57              |
| 66:I3:256:ILE:HB   | 66:I3:270:LEU:HB3  | 1.86                     | 0.57              |
| 80:j:122:THR:OG1   | 80:j:159:GLN:OE1   | 2.22                     | 0.57              |
| 85:L1:40:ASN:O     | 85:L1:200:ASN:ND2  | 2.36                     | 0.57              |
| 46:m2:1312:U:OP2   | 70:M3:36:ARG:NH1   | 2.37                     | 0.57              |
| 9:A2:955:U:H3      | 9:A2:1027:G:H1     | 1.52                     | 0.57              |
| 11:C2:47:C:H1'     | 11:C2:61:A:H2'     | 1.86                     | 0.57              |
| 46:m2:106:C:H2'    | 46:m2:107:A:H8     | 1.69                     | 0.57              |
| 46:m2:1476:A:H2'   | 46:m2:1477:G:C4    | 2.40                     | 0.57              |
| 52:z2:36:GLU:OE1   | 52:z2:47:ARG:NH1   | 2.37                     | 0.57              |
| 67:J3:192:LEU:HD21 | 67:J3:227:ARG:HD3  | 1.86                     | 0.57              |
| 77:T3:33:LYS:HG2   | 77:T3:36:MET:HE2   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 77:T3:51:LYS:HB3  | 77:T3:53:LYS:HE2   | 1.87                     | 0.57              |
| 81:k:75:PRO:O     | 81:k:119:ARG:NH2   | 2.37                     | 0.57              |
| 5:E1:147:ARG:NH2  | 10:B2:5:A:OP1      | 2.37                     | 0.57              |
| 8:H1:155:VAL:O    | 8:H1:162:ARG:NH2   | 2.38                     | 0.57              |
| 9:A2:866:A:N6     | 9:A2:1894:G:O3'    | 2.37                     | 0.57              |
| 9:A2:2057:C:O2'   | 33:Y2:102:ASN:O    | 2.22                     | 0.57              |
| 9:A2:3245:G:N2    | 9:A2:3246:G:O6     | 2.38                     | 0.57              |
| 9:A2:3336:U:OP1   | 12:D2:54:ARG:NH2   | 2.37                     | 0.57              |
| 9:A2:3575:C:OP1   | 12:D2:2:GLY:N      | 2.37                     | 0.57              |
| 49:q2:132:LYS:HG2 | 49:q2:156:LEU:HB3  | 1.87                     | 0.57              |
| 9:A2:1146:C:H2'   | 9:A2:1147:A:C8     | 2.40                     | 0.57              |
| 9:A2:3918:G:O2'   | 9:A2:3919:G:N2     | 2.38                     | 0.57              |
| 9:A2:4428:C:N4    | 9:A2:4429:G:O6     | 2.38                     | 0.57              |
| 13:E2:282:LYS:HZ3 | 13:E2:337:VAL:HG22 | 1.69                     | 0.57              |
| 30:V2:99:HIS:O    | 30:V2:107:ARG:NH2  | 2.38                     | 0.57              |
| 46:m2:865:U:H2'   | 46:m2:866:A:H8     | 1.69                     | 0.57              |
| 46:m2:1547:A:H5'' | 57:y2:74:GLY:HA2   | 1.87                     | 0.57              |
| 46:m2:1552:G:H3'  | 46:m2:1581:A:H61   | 1.69                     | 0.57              |
| 48:p2:35:ALA:HB2  | 48:p2:44:ILE:HD11  | 1.86                     | 0.57              |
| 6:F1:31:ARG:NH2   | 9:A2:338:A:OP1     | 2.37                     | 0.57              |
| 9:A2:4563:C:H2'   | 9:A2:4564:G:C8     | 2.40                     | 0.57              |
| 32:X2:63:ARG:NH1  | 32:X2:96:GLU:OE2   | 2.38                     | 0.57              |
| 9:A2:423:G:H21    | 18:J2:118:GLN:HE22 | 1.51                     | 0.57              |
| 9:A2:3334:G:OP2   | 12:D2:193:ARG:NH2  | 2.38                     | 0.57              |
| 15:G2:33:ARG:HH11 | 22:N2:27:LEU:HD22  | 1.70                     | 0.57              |
| 23:O2:22:THR:HG22 | 23:O2:71:THR:HG22  | 1.87                     | 0.57              |
| 46:m2:1238:G:O2'  | 56:x2:131:PRO:O    | 2.23                     | 0.57              |
| 54:s2:42:LYS:HE2  | 54:s2:44:LYS:HB3   | 1.87                     | 0.57              |
| 65:H3:22:ARG:HH21 | 65:H3:37:ASN:HB2   | 1.69                     | 0.57              |
| 80:j:22:ASP:OD1   | 80:j:68:HIS:NE2    | 2.37                     | 0.57              |
| 9:A2:1798:C:H5''  | 80:j:48:ARG:HH21   | 1.70                     | 0.57              |
| 9:A2:2279:U:H3    | 9:A2:2284:A:H2     | 1.52                     | 0.57              |
| 9:A2:4638:G:H2'   | 9:A2:4639:G:C8     | 2.39                     | 0.57              |
| 46:m2:598:U:O2'   | 46:m2:647:C:O2     | 2.22                     | 0.57              |
| 61:D3:16:LYS:NZ   | 67:J3:257:LYS:O    | 2.35                     | 0.57              |
| 66:I3:99:ARG:NH2  | 66:I3:134:THR:O    | 2.34                     | 0.57              |
| 9:A2:85:G:O2'     | 9:A2:97:G:O6       | 2.22                     | 0.56              |
| 9:A2:1779:C:N4    | 9:A2:1792:A:H61    | 2.01                     | 0.56              |
| 9:A2:1856:U:OP1   | 17:I2:18:ARG:NH1   | 2.38                     | 0.56              |
| 9:A2:2381:U:O4    | 23:O2:97:ARG:NH1   | 2.37                     | 0.56              |
| 9:A2:3629:G:H2'   | 9:A2:3630:G:C8     | 2.40                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:G2:91:GLY:O     | 15:G2:94:ASN:ND2   | 2.38                     | 0.56              |
| 46:m2:1679:U:OP1   | 54:s2:148:ASN:ND2  | 2.37                     | 0.56              |
| 51:w2:135:SER:O    | 51:w2:139:ARG:NH1  | 2.38                     | 0.56              |
| 9:A2:325:U:H2'     | 9:A2:326:C:C6      | 2.40                     | 0.56              |
| 46:m2:1866:U:H3'   | 63:F3:5:ARG:HH21   | 1.70                     | 0.56              |
| 81:k:104:ILE:H     | 81:k:143:VAL:HG12  | 1.70                     | 0.56              |
| 81:k:117:ARG:NH1   | 81:k:128:THR:OG1   | 2.37                     | 0.56              |
| 85:L1:18:LEU:HD13  | 85:L1:172:VAL:HB   | 1.87                     | 0.56              |
| 7:G1:114:LYS:HE2   | 9:A2:4574:C:H5''   | 1.86                     | 0.56              |
| 9:A2:1204:G:N2     | 9:A2:1207:G:OP2    | 2.37                     | 0.56              |
| 9:A2:1426:A:H5'    | 12:D2:183:GLY:HA2  | 1.88                     | 0.56              |
| 9:A2:4174:G:O2'    | 9:A2:4177:C:OP2    | 2.21                     | 0.56              |
| 11:C2:67:U:H2'     | 11:C2:68:G:H8      | 1.71                     | 0.56              |
| 13:E2:291:TYR:HB3  | 13:E2:298:LEU:HD11 | 1.87                     | 0.56              |
| 46:m2:56:G:OP1     | 74:Q3:111:LYS:NZ   | 2.35                     | 0.56              |
| 46:m2:1247:G:O2'   | 46:m2:1494:U:OP1   | 2.22                     | 0.56              |
| 46:m2:1389:G:N1    | 49:q2:206:ASP:OD2  | 2.38                     | 0.56              |
| 46:m2:1496:U:H4'   | 46:m2:1497:G:H5''  | 1.87                     | 0.56              |
| 50:r2:66:MET:SD    | 50:r2:78:THR:OG1   | 2.63                     | 0.56              |
| 60:C3:17:ILE:HG13  | 60:C3:94:PRO:HD3   | 1.88                     | 0.56              |
| 62:E3:67:ARG:HG3   | 62:E3:115:ILE:HG12 | 1.87                     | 0.56              |
| 70:M3:69:LEU:HD13  | 70:M3:76:LEU:HB3   | 1.87                     | 0.56              |
| 79:m:534:GLN:HB3   | 79:m:546:ALA:HB3   | 1.87                     | 0.56              |
| 83:t:31:GLU:HB3    | 83:t:37:LYS:HG3    | 1.87                     | 0.56              |
| 9:A2:2099:U:H2'    | 29:U2:9:ARG:HH22   | 1.69                     | 0.56              |
| 9:A2:2117:U:H2'    | 9:A2:2118:A2M:H8   | 1.88                     | 0.56              |
| 9:A2:2162:G:OP2    | 9:A2:2162:G:N2     | 2.28                     | 0.56              |
| 27:S2:1:MET:SD     | 27:S2:1:MET:N      | 2.77                     | 0.56              |
| 30:V2:89:PRO:HB2   | 30:V2:92:LYS:HB2   | 1.88                     | 0.56              |
| 50:r2:148:ARG:NH2  | 68:K3:205:GLU:OE2  | 2.38                     | 0.56              |
| 9:A2:1184:G:O6     | 14:F2:239:LYS:NZ   | 2.33                     | 0.56              |
| 9:A2:1779:C:H42    | 9:A2:1792:A:H61    | 1.54                     | 0.56              |
| 9:A2:1796:C:H2'    | 9:A2:1797:G:H8     | 1.71                     | 0.56              |
| 9:A2:2229:G:N2     | 9:A2:2257:G:O2'    | 2.38                     | 0.56              |
| 11:C2:22:U:OP1     | 27:S2:11:ARG:NH1   | 2.39                     | 0.56              |
| 46:m2:657:A:H4'    | 46:m2:658:G:H3'    | 1.88                     | 0.56              |
| 46:m2:1488:A:H2'   | 46:m2:1489:A:H8    | 1.71                     | 0.56              |
| 49:q2:142:LEU:HD21 | 49:q2:182:LEU:HD11 | 1.88                     | 0.56              |
| 71:N3:47:PRO:HD2   | 71:N3:86:GLU:HG2   | 1.88                     | 0.56              |
| 79:m:373:GLU:OE2   | 79:m:494:ARG:NH1   | 2.38                     | 0.56              |
| 4:D1:102:MET:N     | 4:D1:102:MET:SD    | 2.79                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:E1:9:GLU:HB3     | 5:E1:13:ARG:HB3   | 1.87                     | 0.56              |
| 6:F1:100:PRO:O     | 37:c2:25:ARG:NH2  | 2.39                     | 0.56              |
| 9:A2:311:G:H2'     | 9:A2:312:G:C8     | 2.40                     | 0.56              |
| 9:A2:806:C:H2'     | 9:A2:807:G:H8     | 1.70                     | 0.56              |
| 9:A2:3953:U:OP1    | 22:N2:78:LYS:NZ   | 2.35                     | 0.56              |
| 9:A2:4612:A:H5''   | 13:E2:126:LYS:HD2 | 1.86                     | 0.56              |
| 24:P2:87:SER:OG    | 25:Q2:19:ARG:NH2  | 2.39                     | 0.56              |
| 25:Q2:101:ARG:NH1  | 68:K3:156:TYR:OH  | 2.38                     | 0.56              |
| 46:m2:1149:C:OP1   | 63:F3:6:ARG:NH1   | 2.38                     | 0.56              |
| 46:m2:1488:A:H2'   | 46:m2:1489:A:C8   | 2.41                     | 0.56              |
| 59:B3:42:HIS:ND1   | 59:B3:93:SER:OG   | 2.37                     | 0.56              |
| 6:F1:44:ARG:NH1    | 9:A2:186:G:OP2    | 2.39                     | 0.56              |
| 9:A2:854:A:H1'     | 9:A2:1878:G:H5''  | 1.86                     | 0.56              |
| 9:A2:2166:C:H2'    | 9:A2:2167:A:H8    | 1.71                     | 0.56              |
| 9:A2:3534:C:N4     | 9:A2:4170:A:O4'   | 2.39                     | 0.56              |
| 15:G2:206:ASP:OD1  | 15:G2:209:ARG:NH2 | 2.39                     | 0.56              |
| 46:m2:17:C:O2'     | 46:m2:1196:A:N1   | 2.38                     | 0.56              |
| 50:r2:85:GLY:N     | 50:r2:88:ASP:OD2  | 2.38                     | 0.56              |
| 8:H1:13:LYS:NZ     | 9:A2:307:A:OP2    | 2.39                     | 0.56              |
| 9:A2:2591:A:N6     | 9:A2:3508:A:O2'   | 2.39                     | 0.56              |
| 26:R2:104:ALA:O    | 26:R2:134:LYS:NZ  | 2.39                     | 0.56              |
| 46:m2:954:G:OP1    | 48:p2:56:LYS:NZ   | 2.38                     | 0.56              |
| 49:q2:42:THR:OG1   | 49:q2:45:ARG:O    | 2.22                     | 0.56              |
| 79:m:26:HIS:HB2    | 79:m:138:THR:HG23 | 1.88                     | 0.56              |
| 80:j:48:ARG:HD2    | 81:k:123:ARG:HD2  | 1.88                     | 0.56              |
| 9:A2:1005:G:H22    | 9:A2:1019:G:H22   | 1.52                     | 0.56              |
| 9:A2:4109:U:OP1    | 24:P2:50:ASN:ND2  | 2.39                     | 0.56              |
| 15:G2:110:LEU:HD13 | 15:G2:116:ASP:HA  | 1.88                     | 0.56              |
| 45:k2:39:ARG:O     | 45:k2:103:ARG:NH2 | 2.38                     | 0.56              |
| 46:m2:65:C:N4      | 46:m2:169:U:O2'   | 2.39                     | 0.56              |
| 46:m2:1418:C:O2'   | 59:B3:4:VAL:N     | 2.35                     | 0.56              |
| 81:k:75:PRO:HG2    | 81:k:119:ARG:HE   | 1.70                     | 0.56              |
| 18:J2:45:THR:HG22  | 18:J2:49:LYS:HE2  | 1.87                     | 0.56              |
| 46:m2:1870:U:O2'   | 63:F3:100:ARG:NH1 | 2.39                     | 0.56              |
| 50:r2:175:PHE:HE2  | 50:r2:198:ARG:HD2 | 1.71                     | 0.56              |
| 81:k:153:ASP:O     | 81:k:158:GLY:N    | 2.38                     | 0.56              |
| 9:A2:1086:C:O2'    | 30:V2:115:ARG:NH2 | 2.39                     | 0.55              |
| 9:A2:1371:A:H2'    | 9:A2:1372:G:H8    | 1.71                     | 0.55              |
| 9:A2:1527:U:H2'    | 9:A2:1528:U:H6    | 1.71                     | 0.55              |
| 9:A2:1830:C:H2'    | 9:A2:1831:A:H8    | 1.71                     | 0.55              |
| 15:G2:23:ARG:NH1   | 15:G2:23:ARG:O    | 2.37                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:I2:35:VAL:HB    | 17:I2:104:VAL:HG12 | 1.88                     | 0.55              |
| 17:I2:125:LYS:HG2  | 17:I2:129:LEU:HD12 | 1.88                     | 0.55              |
| 46:m2:375:G:N2     | 46:m2:394:A:N1     | 2.54                     | 0.55              |
| 46:m2:691:U:H2'    | 46:m2:692:G:C8     | 2.41                     | 0.55              |
| 46:m2:930:G:H2'    | 46:m2:931:G:C8     | 2.40                     | 0.55              |
| 49:q2:163:PRO:O    | 49:q2:167:TYR:HB2  | 2.06                     | 0.55              |
| 50:r2:11:ARG:HA    | 50:r2:28:ALA:HB2   | 1.88                     | 0.55              |
| 57:y2:35:ASN:N     | 57:y2:70:VAL:O     | 2.38                     | 0.55              |
| 64:G3:44:ARG:NH1   | 64:G3:63:ARG:O     | 2.39                     | 0.55              |
| 66:I3:166:VAL:HG12 | 66:I3:176:VAL:HG22 | 1.89                     | 0.55              |
| 66:I3:249:CYS:SG   | 66:I3:291:TRP:NE1  | 2.74                     | 0.55              |
| 9:A2:1256:A:N6     | 9:A2:1905:G:O6     | 2.39                     | 0.55              |
| 46:m2:1840:U:H1'   | 72:O3:150:ARG:HG2  | 1.88                     | 0.55              |
| 48:p2:40:ASN:ND2   | 48:p2:76:ASN:OD1   | 2.40                     | 0.55              |
| 54:s2:179:ASN:ND2  | 54:s2:184:SER:OG   | 2.40                     | 0.55              |
| 55:v2:8:ARG:NH1    | 55:v2:12:TYR:OH    | 2.39                     | 0.55              |
| 68:K3:44:GLU:HA    | 68:K3:119:LYS:HE3  | 1.87                     | 0.55              |
| 9:A2:3526:C:O3'    | 13:E2:261:ARG:NH1  | 2.39                     | 0.55              |
| 9:A2:4413:G:OP1    | 17:I2:37:ARG:NH2   | 2.39                     | 0.55              |
| 46:m2:612:G:H2'    | 46:m2:613:G:H8     | 1.72                     | 0.55              |
| 66:I3:199:THR:OG1  | 66:I3:239:LEU:O    | 2.24                     | 0.55              |
| 5:E1:35:ARG:NH1    | 5:E1:122:SER:O     | 2.38                     | 0.55              |
| 9:A2:1124:C:H4'    | 34:Z2:16:ARG:HH12  | 1.71                     | 0.55              |
| 9:A2:1672:C:H2'    | 9:A2:1673:A2M:H8   | 1.89                     | 0.55              |
| 46:m2:497:U:OP1    | 50:r2:49:ARG:NH1   | 2.40                     | 0.55              |
| 46:m2:1543:G:N3    | 59:B3:12:GLN:NE2   | 2.53                     | 0.55              |
| 48:p2:52:THR:HG22  | 48:p2:58:ALA:H     | 1.72                     | 0.55              |
| 9:A2:1009:U:O2'    | 15:G2:286:SER:OG   | 2.25                     | 0.55              |
| 9:A2:3792:G:O6     | 9:A2:3794:G:N2     | 2.39                     | 0.55              |
| 9:A2:4588:C:H4'    | 16:H2:162:GLY:HA2  | 1.88                     | 0.55              |
| 79:m:751:PRO:HD2   | 79:m:806:GLN:HB3   | 1.87                     | 0.55              |
| 8:H1:172:ARG:NH1   | 9:A2:62:A:OP1      | 2.39                     | 0.55              |
| 9:A2:422:C:H2'     | 9:A2:423:G:H8      | 1.71                     | 0.55              |
| 9:A2:1848:G:C2     | 17:I2:60:LYS:HD3   | 2.42                     | 0.55              |
| 9:A2:3367:A:O2'    | 9:A2:3369:U:OP2    | 2.23                     | 0.55              |
| 46:m2:1105:C:H2'   | 46:m2:1106:G:H8    | 1.72                     | 0.55              |
| 61:D3:25:ALA:HB3   | 61:D3:28:ASP:HB2   | 1.89                     | 0.55              |
| 9:A2:1893:C:O2'    | 9:A2:1895:G:O2'    | 2.24                     | 0.55              |
| 9:A2:3379:A2M:H2'  | 9:A2:3380:A:H8     | 1.71                     | 0.55              |
| 9:A2:3415:A:H62    | 9:A2:3420:PSU:HN3  | 1.55                     | 0.55              |
| 10:B2:99:G:OP2     | 21:M2:55:LYS:NZ    | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:E2:50:LYS:HB2   | 13:E2:345:LEU:HD11 | 1.89                     | 0.55              |
| 46:m2:170:A:OP1    | 68:K3:137:ARG:N    | 2.38                     | 0.55              |
| 48:p2:124:HIS:HA   | 48:p2:137:LEU:O    | 2.07                     | 0.55              |
| 58:A3:63:GLU:OE1   | 58:A3:66:ARG:NH2   | 2.39                     | 0.55              |
| 67:J3:168:GLY:N    | 67:J3:179:THR:O    | 2.38                     | 0.55              |
| 79:m:303:ILE:HG21  | 79:m:335:LEU:HB2   | 1.89                     | 0.55              |
| 4:D1:21:ARG:O      | 4:D1:24:ARG:NE     | 2.39                     | 0.55              |
| 7:G1:13:ALA:HB1    | 7:G1:55:MET:HB2    | 1.88                     | 0.55              |
| 13:E2:213:GLN:NE2  | 13:E2:285:TYR:O    | 2.38                     | 0.55              |
| 46:m2:365:A:N1     | 46:m2:399:G:O2'    | 2.38                     | 0.55              |
| 46:m2:540:U:O4     | 46:m2:548:G:O6     | 2.25                     | 0.55              |
| 79:m:154:LEU:HB2   | 79:m:204:ILE:HD13  | 1.89                     | 0.55              |
| 1:A1:118:ARG:NH2   | 9:A2:1697:G:OP1    | 2.40                     | 0.55              |
| 6:F1:163:LYS:NZ    | 9:A2:511:U:OP1     | 2.40                     | 0.55              |
| 9:A2:318:A:H2'     | 9:A2:319:A:H8      | 1.72                     | 0.55              |
| 9:A2:3967:A:OP1    | 22:N2:69:GLN:NE2   | 2.35                     | 0.55              |
| 23:O2:62:THR:OG1   | 23:O2:73:THR:OG1   | 2.25                     | 0.55              |
| 46:m2:546:G:H2'    | 46:m2:547:A:C8     | 2.41                     | 0.55              |
| 46:m2:656:A:OP2    | 46:m2:657:A:O2'    | 2.19                     | 0.55              |
| 69:L3:67:ASP:HB3   | 69:L3:70:ARG:HB3   | 1.89                     | 0.55              |
| 6:F1:186:ARG:NH1   | 9:A2:1208:G:OP1    | 2.37                     | 0.55              |
| 9:A2:1040:C:H2'    | 9:A2:1041:G:H8     | 1.72                     | 0.55              |
| 9:A2:2199:U:O2'    | 11:C2:112:G:O2'    | 2.25                     | 0.55              |
| 9:A2:2590:A:O2'    | 13:E2:228:TYR:O    | 2.19                     | 0.55              |
| 9:A2:4690:A:H2'    | 9:A2:4691:G:H8     | 1.72                     | 0.55              |
| 46:m2:441:A:OP2    | 84:u:23:LYS:NZ     | 2.40                     | 0.55              |
| 46:m2:1077:C:H2'   | 46:m2:1078:G:H8    | 1.72                     | 0.55              |
| 46:m2:1402:U:O4    | 46:m2:1403:A:N6    | 2.41                     | 0.55              |
| 53:o2:41:ARG:HH21  | 53:o2:45:GLY:HA2   | 1.72                     | 0.55              |
| 53:o2:110:ASN:HB3  | 53:o2:113:GLN:HE22 | 1.72                     | 0.55              |
| 79:m:651:PHE:O     | 79:m:657:GLY:N     | 2.38                     | 0.55              |
| 79:m:726:ARG:HH12  | 79:m:855:ASP:HB2   | 1.72                     | 0.55              |
| 9:A2:284:G:H2'     | 9:A2:285:G:H8      | 1.72                     | 0.54              |
| 15:G2:83:LEU:HB3   | 15:G2:88:VAL:HB    | 1.89                     | 0.54              |
| 46:m2:1856:U:H2'   | 46:m2:1857:G:H8    | 1.71                     | 0.54              |
| 54:s2:102:LEU:HD11 | 75:R3:100:VAL:HG21 | 1.90                     | 0.54              |
| 56:x2:29:SER:OG    | 56:x2:32:GLN:OE1   | 2.24                     | 0.54              |
| 63:F3:44:ILE:HG12  | 63:F3:67:LEU:HG    | 1.87                     | 0.54              |
| 66:I3:32:LEU:HD13  | 66:I3:42:MET:HG2   | 1.88                     | 0.54              |
| 71:N3:99:ARG:NH2   | 71:N3:119:GLU:OE2  | 2.41                     | 0.54              |
| 2:B1:73:ARG:NE     | 9:A2:3726:G:OP1    | 2.38                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:A2:2611:C:O2    | 13:E2:242:ARG:NH2  | 2.40                     | 0.54              |
| 9:A2:3315:G:OP1   | 12:D2:241:ARG:NH1  | 2.37                     | 0.54              |
| 9:A2:3931:A:H5'   | 9:A2:3933:A:H1'    | 1.90                     | 0.54              |
| 11:C2:36:G:OP2    | 36:b2:88:THR:OG1   | 2.24                     | 0.54              |
| 33:Y2:44:ARG:NH1  | 33:Y2:52:GLN:OE1   | 2.40                     | 0.54              |
| 46:m2:1356:G:N1   | 46:m2:1359:A:OP2   | 2.33                     | 0.54              |
| 66:I3:33:SER:HB3  | 66:I3:43:TRP:HZ3   | 1.71                     | 0.54              |
| 66:I3:244:ASN:ND2 | 66:I3:294:ASP:O    | 2.40                     | 0.54              |
| 9:A2:1320:U:H2'   | 9:A2:1321:A:H8     | 1.71                     | 0.54              |
| 9:A2:2207:G:H21   | 9:A2:2262:A:N6     | 1.94                     | 0.54              |
| 9:A2:3910:C:H2'   | 9:A2:3911:C:H6     | 1.73                     | 0.54              |
| 9:A2:3931:A:O2'   | 15:G2:19:ARG:NH2   | 2.41                     | 0.54              |
| 9:A2:4253:U:H2'   | 9:A2:4254:A:H8     | 1.72                     | 0.54              |
| 9:A2:4513:G:O2'   | 9:A2:4517:2MG:OP1  | 2.25                     | 0.54              |
| 9:A2:4520:G:N2    | 17:I2:3:GLU:OE1    | 2.38                     | 0.54              |
| 27:S2:55:VAL:HG12 | 27:S2:106:ILE:HA   | 1.88                     | 0.54              |
| 46:m2:692:G:N2    | 83:t:181:THR:O     | 2.40                     | 0.54              |
| 53:o2:85:ARG:NH1  | 53:o2:201:LEU:O    | 2.40                     | 0.54              |
| 62:E3:51:VAL:HA   | 62:E3:72:VAL:HG22  | 1.88                     | 0.54              |
| 3:C1:114:ILE:HB   | 3:C1:124:ARG:HG3   | 1.90                     | 0.54              |
| 9:A2:3733:U:OP1   | 12:D2:123:ARG:NH1  | 2.40                     | 0.54              |
| 12:D2:147:ARG:HG2 | 12:D2:157:VAL:HG22 | 1.88                     | 0.54              |
| 18:J2:122:ALA:HB3 | 18:J2:143:PRO:HG2  | 1.90                     | 0.54              |
| 25:Q2:96:GLN:HB2  | 25:Q2:100:VAL:HB   | 1.89                     | 0.54              |
| 44:j2:10:ILE:HD11 | 44:j2:30:GLU:HB3   | 1.88                     | 0.54              |
| 46:m2:1547:A:H2'  | 46:m2:1548:G:C8    | 2.42                     | 0.54              |
| 47:n2:9:U:H3      | 47:n2:15:A:N6      | 2.05                     | 0.54              |
| 49:q2:32:ASP:OD2  | 49:q2:65:ARG:NH1   | 2.40                     | 0.54              |
| 4:D1:116:ARG:NH2  | 9:A2:3846:I4U:O2'  | 2.35                     | 0.54              |
| 9:A2:238:C:OP2    | 27:S2:45:ARG:NH2   | 2.40                     | 0.54              |
| 9:A2:2494:C:H4'   | 44:j2:52:VAL:HG21  | 1.90                     | 0.54              |
| 9:A2:3782:U:H3    | 9:A2:3804:G:H1     | 1.55                     | 0.54              |
| 9:A2:4711:U:O2    | 18:J2:75:GLN:NE2   | 2.40                     | 0.54              |
| 10:B2:64:G:H2'    | 10:B2:65:G:H8      | 1.72                     | 0.54              |
| 11:C2:134:G:H5''  | 26:R2:63:LYS:HD2   | 1.88                     | 0.54              |
| 41:g2:94:MET:HG2  | 41:g2:105:PRO:HA   | 1.88                     | 0.54              |
| 46:m2:931:G:N2    | 46:m2:1015:U:O2    | 2.41                     | 0.54              |
| 47:n2:13:G:H1     | 47:n2:23:C:H42     | 1.56                     | 0.54              |
| 47:n2:53:G:H2'    | 47:n2:54:A:H8      | 1.72                     | 0.54              |
| 1:A1:144:PHE:O    | 1:A1:227:ASN:ND2   | 2.41                     | 0.54              |
| 9:A2:870:G:OP1    | 9:A2:870:G:N2      | 2.40                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:3964:U:H4'    | 22:N2:51:GLY:HA2   | 1.90                     | 0.54              |
| 9:A2:4222:G:H2'    | 9:A2:4223:A2M:H8   | 1.90                     | 0.54              |
| 9:A2:4257:A:N6     | 79:m:800:ARG:O     | 2.40                     | 0.54              |
| 46:m2:146:G:H2'    | 46:m2:147:A:C8     | 2.43                     | 0.54              |
| 46:m2:853:C:H5''   | 46:m2:854:G:H5'    | 1.89                     | 0.54              |
| 46:m2:1562:U:H2'   | 46:m2:1563:G:H8    | 1.73                     | 0.54              |
| 66:I3:89:LEU:O     | 66:I3:98:THR:N     | 2.41                     | 0.54              |
| 84:u:119:LEU:HD12  | 84:u:120:PRO:HD2   | 1.90                     | 0.54              |
| 3:C1:120:GLU:HB2   | 9:A2:4264:C:C2     | 2.42                     | 0.54              |
| 7:G1:127:VAL:HG11  | 17:I2:178:ARG:HD2  | 1.90                     | 0.54              |
| 9:A2:2040:A:H2'    | 9:A2:2041:G:H8     | 1.73                     | 0.54              |
| 9:A2:2447:U:OP1    | 39:e2:33:LYS:NZ    | 2.40                     | 0.54              |
| 9:A2:4179:G:OP2    | 9:A2:4179:G:N2     | 2.39                     | 0.54              |
| 19:K2:172:ARG:HA   | 19:K2:176:ARG:HD2  | 1.89                     | 0.54              |
| 37:c2:68:ARG:HH21  | 37:c2:71:LYS:HD2   | 1.73                     | 0.54              |
| 46:m2:497:U:O2'    | 50:r2:27:PHE:O     | 2.23                     | 0.54              |
| 46:m2:1568:G:N2    | 46:m2:1571:A:OP2   | 2.40                     | 0.54              |
| 46:m2:1591:A:H61   | 46:m2:1674:U:H1'   | 1.73                     | 0.54              |
| 48:p2:198:GLU:OE2  | 48:p2:202:GLN:NE2  | 2.41                     | 0.54              |
| 75:R3:58:LEU:HD23  | 75:R3:62:VAL:HG21  | 1.88                     | 0.54              |
| 79:m:708:LEU:HD13  | 79:m:715:ARG:HD3   | 1.88                     | 0.54              |
| 9:A2:1771:G:OP1    | 80:j:112:ARG:NH1   | 2.41                     | 0.54              |
| 46:m2:388:C:H5''   | 84:u:10:LYS:HG3    | 1.90                     | 0.54              |
| 46:m2:1633:U:H3'   | 46:m2:1634:G:H8    | 1.73                     | 0.54              |
| 58:A3:124:ARG:NE   | 58:A3:130:ARG:O    | 2.35                     | 0.54              |
| 4:D1:139:ARG:NH2   | 4:D1:195:CYS:SG    | 2.81                     | 0.54              |
| 9:A2:3629:G:H2'    | 9:A2:3630:G:H8     | 1.72                     | 0.54              |
| 20:L2:105:LEU:HD22 | 20:L2:135:LYS:HG3  | 1.90                     | 0.54              |
| 29:U2:71:PRO:HG2   | 29:U2:108:TYR:HA   | 1.90                     | 0.54              |
| 61:D3:15:ARG:NH1   | 61:D3:33:GLN:OE1   | 2.40                     | 0.54              |
| 5:E1:35:ARG:HB2    | 5:E1:126:TYR:HE2   | 1.73                     | 0.54              |
| 9:A2:436:C:H2'     | 9:A2:437:G:H8      | 1.72                     | 0.54              |
| 9:A2:3744:G:H1     | 9:A2:3765:G:H22    | 1.56                     | 0.54              |
| 9:A2:4340:C:H2'    | 9:A2:4341:U:C6     | 2.43                     | 0.54              |
| 21:M2:115:ALA:O    | 21:M2:118:ARG:NH1  | 2.41                     | 0.54              |
| 46:m2:63:U:H1'     | 46:m2:171:A:H8     | 1.72                     | 0.54              |
| 46:m2:799:C:O2'    | 46:m2:801:U:OP1    | 2.20                     | 0.54              |
| 46:m2:837:C:O2     | 46:m2:841:C:N4     | 2.40                     | 0.54              |
| 9:A2:24:G:O2'      | 9:A2:26:C:N4       | 2.36                     | 0.53              |
| 19:K2:146:ARG:HG3  | 19:K2:148:VAL:HG22 | 1.90                     | 0.53              |
| 53:o2:145:ILE:HG12 | 53:o2:159:ILE:HB   | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:y2:58:LEU:HD21  | 57:y2:112:LEU:HD21 | 1.89                     | 0.53              |
| 64:G3:34:PHE:HB2   | 64:G3:40:ARG:HB3   | 1.90                     | 0.53              |
| 80:j:58:ASN:ND2    | 80:j:82:ILE:O      | 2.42                     | 0.53              |
| 4:D1:49:CYS:SG     | 4:D1:51:HIS:NE2    | 2.79                     | 0.53              |
| 9:A2:127:G:OP2     | 36:b2:77:LYS:NZ    | 2.40                     | 0.53              |
| 9:A2:857:A:O2'     | 9:A2:2018:A:N6     | 2.38                     | 0.53              |
| 9:A2:3573:A:H2'    | 9:A2:3574:G:H8     | 1.72                     | 0.53              |
| 9:A2:4652:U:H4'    | 9:A2:4653:A:H5'    | 1.90                     | 0.53              |
| 15:G2:104:LEU:HB2  | 15:G2:247:ILE:HD13 | 1.88                     | 0.53              |
| 15:G2:155:THR:HA   | 15:G2:179:ARG:HA   | 1.89                     | 0.53              |
| 25:Q2:80:ARG:NH2   | 68:K3:129:VAL:O    | 2.41                     | 0.53              |
| 31:W2:19:GLN:NE2   | 31:W2:84:ALA:O     | 2.41                     | 0.53              |
| 46:m2:1274:C:H1'   | 46:m2:1275:C:H5'   | 1.91                     | 0.53              |
| 66:I3:24:THR:OG1   | 66:I3:27:PHE:O     | 2.25                     | 0.53              |
| 71:N3:13:GLN:HE21  | 76:S3:21:LYS:HE3   | 1.73                     | 0.53              |
| 79:m:397:ILE:HG21  | 79:m:411:ALA:HB1   | 1.90                     | 0.53              |
| 85:L1:174:MET:HB3  | 85:L1:179:LEU:HD11 | 1.90                     | 0.53              |
| 16:H2:126:GLU:HG3  | 33:Y2:7:LEU:HD22   | 1.89                     | 0.53              |
| 31:W2:55:LEU:HD11  | 35:a2:92:LYS:HG3   | 1.90                     | 0.53              |
| 45:k2:28:GLU:OE2   | 45:k2:31:ASN:ND2   | 2.41                     | 0.53              |
| 46:m2:872:A:H5'    | 46:m2:917:G:H22    | 1.72                     | 0.53              |
| 59:B3:64:LEU:HB3   | 59:B3:123:LEU:HG   | 1.89                     | 0.53              |
| 73:P3:87:GLU:O     | 73:P3:91:ASN:ND2   | 2.42                     | 0.53              |
| 78:U3:90:LYS:NZ    | 78:U3:91:ASN:O     | 2.41                     | 0.53              |
| 3:C1:173:ARG:NH1   | 41:g2:125:LYS:O    | 2.41                     | 0.53              |
| 9:A2:2377:G:OP2    | 23:O2:84:LYS:NZ    | 2.41                     | 0.53              |
| 27:S2:50:ARG:HD2   | 27:S2:115:ARG:HD2  | 1.90                     | 0.53              |
| 46:m2:493:C:O2     | 46:m2:495:A:N6     | 2.42                     | 0.53              |
| 46:m2:1316:U:O2'   | 55:v2:3:MET:SD     | 2.66                     | 0.53              |
| 47:n2:6:G:H2'      | 47:n2:7:A:C8       | 2.44                     | 0.53              |
| 49:q2:49:ILE:HG22  | 49:q2:87:TYR:HB2   | 1.91                     | 0.53              |
| 54:s2:103:LEU:HD21 | 75:R3:67:LEU:HB2   | 1.90                     | 0.53              |
| 63:F3:44:ILE:O     | 72:O3:113:GLN:NE2  | 2.38                     | 0.53              |
| 79:m:120:VAL:O     | 79:m:414:ARG:NE    | 2.36                     | 0.53              |
| 9:A2:1147:A:H2'    | 9:A2:1148:A:H8     | 1.73                     | 0.53              |
| 9:A2:3926:A:H2'    | 9:A2:3927:G:H8     | 1.74                     | 0.53              |
| 14:F2:60:HIS:HA    | 14:F2:92:PHE:HE1   | 1.74                     | 0.53              |
| 16:H2:124:PRO:O    | 45:k2:112:ARG:NH1  | 2.41                     | 0.53              |
| 28:T2:11:VAL:HG22  | 28:T2:82:PRO:HA    | 1.90                     | 0.53              |
| 46:m2:101:U:H5''   | 84:u:19:LYS:HD2    | 1.90                     | 0.53              |
| 46:m2:679:G:N2     | 46:m2:1030:A:H62   | 2.04                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:1806:U:H2'   | 46:m2:1807:G:H8    | 1.72                     | 0.53              |
| 66:I3:16:GLY:N     | 66:I3:305:ASN:OD1  | 2.40                     | 0.53              |
| 66:I3:256:ILE:HD12 | 66:I3:270:LEU:HD23 | 1.89                     | 0.53              |
| 9:A2:176:G:OP1     | 36:b2:101:LYS:NZ   | 2.39                     | 0.53              |
| 9:A2:1468:C:O2     | 9:A2:4042:A:O2'    | 2.26                     | 0.53              |
| 45:k2:32:LEU:HD12  | 45:k2:106:LEU:HB3  | 1.91                     | 0.53              |
| 46:m2:87:U:H2'     | 46:m2:88:G:H8      | 1.73                     | 0.53              |
| 46:m2:398:U:OP1    | 51:w2:108:ASN:ND2  | 2.42                     | 0.53              |
| 79:m:606:ARG:NH2   | 79:m:702:ASP:OD2   | 2.37                     | 0.53              |
| 2:B1:100:HIS:HA    | 2:B1:103:ARG:HG3   | 1.91                     | 0.53              |
| 6:F1:2:ALA:HB1     | 9:A2:1327:U:H5''   | 1.90                     | 0.53              |
| 9:A2:364:G:O6      | 38:d2:55:ARG:NH2   | 2.37                     | 0.53              |
| 9:A2:1885:C:OP2    | 19:K2:14:ARG:NH2   | 2.42                     | 0.53              |
| 9:A2:2177:OMC:H2'  | 9:A2:2178:A:C4     | 2.44                     | 0.53              |
| 9:A2:4072:U:O4     | 9:A2:4127:G:N2     | 2.42                     | 0.53              |
| 46:m2:54:A:OP1     | 74:Q3:111:LYS:NZ   | 2.36                     | 0.53              |
| 50:r2:100:ARG:HB2  | 50:r2:114:ILE:HD13 | 1.90                     | 0.53              |
| 56:x2:41:GLN:HG3   | 56:x2:84:ILE:HD13  | 1.90                     | 0.53              |
| 79:m:321:LYS:O     | 79:m:341:ARG:NE    | 2.41                     | 0.53              |
| 79:m:560:LEU:HA    | 79:m:564:HIS:HB2   | 1.91                     | 0.53              |
| 84:u:87:ASN:HB3    | 84:u:90:LEU:HG     | 1.90                     | 0.53              |
| 4:D1:38:ARG:HG2    | 4:D1:41:ALA:HB2    | 1.90                     | 0.53              |
| 9:A2:3890:G:H2'    | 9:A2:3891:A:C8     | 2.44                     | 0.53              |
| 32:X2:46:LEU:HD11  | 32:X2:73:TRP:HE1   | 1.72                     | 0.53              |
| 45:k2:16:PHE:HB3   | 45:k2:27:THR:H     | 1.72                     | 0.53              |
| 45:k2:51:VAL:HG12  | 45:k2:117:ILE:HD12 | 1.91                     | 0.53              |
| 46:m2:1660:G:OP2   | 46:m2:1662:C:N4    | 2.42                     | 0.53              |
| 66:I3:165:ILE:HD11 | 66:I3:179:LEU:HD13 | 1.91                     | 0.53              |
| 69:L3:163:SER:O    | 69:L3:167:GLY:CA   | 2.56                     | 0.53              |
| 79:m:449:THR:OG1   | 79:m:460:ILE:O     | 2.25                     | 0.53              |
| 11:C2:8:U:H2'      | 11:C2:9:A:C8       | 2.44                     | 0.53              |
| 28:T2:25:ILE:HA    | 28:T2:43:VAL:HG12  | 1.91                     | 0.53              |
| 33:Y2:86:GLU:OE2   | 33:Y2:114:ARG:NE   | 2.37                     | 0.53              |
| 46:m2:1100:C:H2'   | 46:m2:1101:G:C8    | 2.44                     | 0.53              |
| 46:m2:1163:U:OP1   | 62:E3:12:LYS:NZ    | 2.42                     | 0.53              |
| 83:t:37:LYS:HE2    | 83:t:41:ARG:HH21   | 1.74                     | 0.53              |
| 6:F1:190:ARG:NH1   | 9:A2:4004:U:OP1    | 2.41                     | 0.53              |
| 9:A2:1406:A:H4'    | 9:A2:2594:U:H4'    | 1.90                     | 0.53              |
| 9:A2:3552:C:H1'    | 13:E2:268:ARG:HH22 | 1.73                     | 0.53              |
| 29:U2:99:PRO:HG2   | 29:U2:122:VAL:HG12 | 1.91                     | 0.53              |
| 35:a2:5:LEU:HD21   | 35:a2:30:ILE:HG22  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:m2:878:C:H2'   | 46:m2:879:C:C6    | 2.43                     | 0.53              |
| 71:N3:86:GLU:O    | 71:N3:90:HIS:ND1  | 2.41                     | 0.53              |
| 7:G1:8:GLU:OE2    | 7:G1:11:ARG:NH2   | 2.41                     | 0.52              |
| 9:A2:176:G:H2'    | 9:A2:177:G:C8     | 2.44                     | 0.52              |
| 9:A2:2386:U:OP2   | 23:O2:48:LYS:NZ   | 2.38                     | 0.52              |
| 9:A2:3360:U:N3    | 9:A2:3361:G:N7    | 2.57                     | 0.52              |
| 9:A2:4368:C:H2'   | 9:A2:4369:A:H8    | 1.75                     | 0.52              |
| 43:i2:17:LYS:NZ   | 43:i2:19:GLN:OE1  | 2.37                     | 0.52              |
| 46:m2:70:G:H21    | 46:m2:79:A:N6     | 2.03                     | 0.52              |
| 46:m2:1023:U:OP1  | 71:N3:132:LYS:NZ  | 2.41                     | 0.52              |
| 8:H1:75:VAL:HG21  | 8:H1:80:THR:HG22  | 1.92                     | 0.52              |
| 8:H1:204:ARG:OXT  | 14:F2:110:ARG:NH2 | 2.41                     | 0.52              |
| 9:A2:1851:G:H2'   | 9:A2:1852:OMG:H8  | 1.75                     | 0.52              |
| 9:A2:1911:G:H2'   | 9:A2:1912:A:C8    | 2.44                     | 0.52              |
| 9:A2:2162:G:O6    | 40:f2:2:SER:N     | 2.43                     | 0.52              |
| 9:A2:3261:C:OP2   | 20:L2:71:ARG:NH1  | 2.42                     | 0.52              |
| 9:A2:3480:A:H3'   | 9:A2:3481:A2M:H8  | 1.91                     | 0.52              |
| 9:A2:3801:C:OP1   | 28:T2:59:LYS:N    | 2.41                     | 0.52              |
| 9:A2:3956:A:OP1   | 22:N2:81:LYS:NZ   | 2.42                     | 0.52              |
| 9:A2:4394:G:H2'   | 9:A2:4395:G:H8    | 1.74                     | 0.52              |
| 13:E2:36:ASP:N    | 13:E2:36:ASP:OD1  | 2.42                     | 0.52              |
| 13:E2:216:MET:SD  | 13:E2:281:ASN:ND2 | 2.79                     | 0.52              |
| 14:F2:71:ARG:HB3  | 14:F2:73:VAL:HG22 | 1.90                     | 0.52              |
| 46:m2:16:G:H21    | 46:m2:1197:A:H62  | 1.55                     | 0.52              |
| 46:m2:446:G:N2    | 46:m2:449:A:OP2   | 2.33                     | 0.52              |
| 46:m2:524:A:H62   | 46:m2:645:A:H5'   | 1.74                     | 0.52              |
| 46:m2:553:U:H2'   | 46:m2:554:G:H8    | 1.74                     | 0.52              |
| 46:m2:698:G:O6    | 46:m2:732:C:O2'   | 2.23                     | 0.52              |
| 46:m2:946:A:H5''  | 72:O3:134:PRO:HB3 | 1.90                     | 0.52              |
| 46:m2:950:C:H2'   | 46:m2:951:G:C8    | 2.44                     | 0.52              |
| 54:s2:44:LYS:HE3  | 57:y2:114:GLN:HG2 | 1.91                     | 0.52              |
| 54:s2:59:LYS:HB3  | 54:s2:62:ARG:HB2  | 1.90                     | 0.52              |
| 60:C3:33:GLU:OE2  | 60:C3:87:ARG:NH2  | 2.42                     | 0.52              |
| 73:P3:3:ARG:HH12  | 73:P3:28:ARG:HE   | 1.55                     | 0.52              |
| 9:A2:2598:U:O2'   | 9:A2:4284:U:OP1   | 2.27                     | 0.52              |
| 9:A2:3546:A:N6    | 9:A2:4222:G:O2'   | 2.40                     | 0.52              |
| 9:A2:3612:G:N2    | 9:A2:3619:A:O2'   | 2.39                     | 0.52              |
| 9:A2:3776:C:H5''  | 9:A2:3777:A:H5''  | 1.90                     | 0.52              |
| 19:K2:151:HIS:ND1 | 19:K2:164:LYS:O   | 2.39                     | 0.52              |
| 35:a2:20:THR:HG22 | 35:a2:34:TYR:HA   | 1.90                     | 0.52              |
| 46:m2:290:G:H2'   | 46:m2:291:G:C8    | 2.45                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:1205:G:H2'   | 46:m2:1206:A:C8    | 2.44                     | 0.52              |
| 67:J3:144:SER:HB3  | 67:J3:150:ALA:HB2  | 1.90                     | 0.52              |
| 3:C1:92:MET:HG2    | 3:C1:181:VAL:HA    | 1.91                     | 0.52              |
| 6:F1:16:LYS:HG3    | 9:A2:46:U:H5''     | 1.92                     | 0.52              |
| 9:A2:310:G:H2'     | 9:A2:311:G:H8      | 1.74                     | 0.52              |
| 9:A2:382:G:N1      | 9:A2:385:A:OP2     | 2.35                     | 0.52              |
| 9:A2:1767:G:OP1    | 41:g2:106:ARG:NH2  | 2.43                     | 0.52              |
| 9:A2:2313:C:H2'    | 9:A2:2314:G:C8     | 2.44                     | 0.52              |
| 9:A2:3384:A:OP2    | 9:A2:3385:PSU:N1   | 2.42                     | 0.52              |
| 46:m2:154:U:O2     | 46:m2:165:G:N2     | 2.42                     | 0.52              |
| 46:m2:303:A:O2'    | 84:u:74:ARG:NH1    | 2.41                     | 0.52              |
| 46:m2:881:C:H2'    | 46:m2:882:G:H8     | 1.74                     | 0.52              |
| 46:m2:1102:A:H4'   | 52:z2:132:ARG:HD2  | 1.91                     | 0.52              |
| 46:m2:1452:G:H22   | 46:m2:1476:A:H61   | 1.57                     | 0.52              |
| 46:m2:1856:U:OP1   | 72:O3:150:ARG:NH2  | 2.36                     | 0.52              |
| 56:x2:17:TYR:HB3   | 56:x2:25:LEU:HD11  | 1.91                     | 0.52              |
| 60:C3:23:THR:HG22  | 60:C3:88:LEU:HG    | 1.90                     | 0.52              |
| 70:M3:119:GLN:HG3  | 70:M3:122:ASP:HB2  | 1.90                     | 0.52              |
| 71:N3:78:LYS:HD3   | 71:N3:80:LEU:HD22  | 1.92                     | 0.52              |
| 75:R3:64:ASN:O     | 75:R3:111:ARG:NH1  | 2.42                     | 0.52              |
| 9:A2:1120:C:H2'    | 9:A2:1121:A:C8     | 2.44                     | 0.52              |
| 9:A2:2535:C:H2'    | 9:A2:2536:G:H8     | 1.75                     | 0.52              |
| 9:A2:4515:OMG:O6   | 21:M2:157:ARG:NH1  | 2.42                     | 0.52              |
| 9:A2:4539:A:H4'    | 9:A2:4541:G:C6     | 2.45                     | 0.52              |
| 12:D2:189:TYR:O    | 12:D2:192:LYS:O    | 2.28                     | 0.52              |
| 18:J2:16:LYS:HG2   | 18:J2:149:ILE:HG12 | 1.92                     | 0.52              |
| 46:m2:833:G:N1     | 46:m2:846:U:N3     | 2.58                     | 0.52              |
| 50:r2:229:GLY:HA3  | 50:r2:234:PRO:HA   | 1.90                     | 0.52              |
| 56:x2:60:LEU:HB3   | 56:x2:89:MET:HE2   | 1.92                     | 0.52              |
| 61:D3:35:ASN:ND2   | 67:J3:267:GLN:OE1  | 2.42                     | 0.52              |
| 67:J3:246:LYS:HA   | 67:J3:249:SER:HB3  | 1.92                     | 0.52              |
| 9:A2:1129:C:N4     | 9:A2:1130:G:O6     | 2.42                     | 0.52              |
| 9:A2:1362:G:N1     | 9:A2:1392:C:N3     | 2.34                     | 0.52              |
| 9:A2:4124:G:O2'    | 41:g2:100:TYR:O    | 2.28                     | 0.52              |
| 9:A2:4169:A:OP2    | 13:E2:2:SER:N      | 2.43                     | 0.52              |
| 13:E2:163:ILE:HG12 | 13:E2:182:GLU:HG2  | 1.90                     | 0.52              |
| 22:N2:127:GLN:NE2  | 22:N2:129:LYS:O    | 2.37                     | 0.52              |
| 78:U3:109:ASP:HB3  | 78:U3:113:LYS:HB3  | 1.91                     | 0.52              |
| 7:G1:56:GLN:NE2    | 9:A2:4515:OMG:H2'  | 2.24                     | 0.52              |
| 9:A2:952:C:H2'     | 9:A2:953:G:H8      | 1.74                     | 0.52              |
| 9:A2:2329:G:H1     | 9:A2:2517:G:H1     | 1.58                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:J2:36:ILE:HA    | 18:J2:39:MET:HE2   | 1.92                     | 0.52              |
| 20:L2:25:ASP:OD1   | 20:L2:27:ASN:ND2   | 2.42                     | 0.52              |
| 46:m2:4:C:H1'      | 69:L3:18:ARG:HH22  | 1.75                     | 0.52              |
| 46:m2:576:A:O2'    | 74:Q3:99:LYS:NZ    | 2.42                     | 0.52              |
| 46:m2:695:A:H2'    | 46:m2:696:G:C5     | 2.45                     | 0.52              |
| 51:w2:65:ASN:HB3   | 51:w2:132:ARG:HH22 | 1.75                     | 0.52              |
| 64:G3:13:ARG:NH1   | 64:G3:53:GLY:O     | 2.43                     | 0.52              |
| 65:H3:8:TRP:HE1    | 65:H3:12:ARG:HD3   | 1.75                     | 0.52              |
| 69:L3:109:ARG:HE   | 69:L3:146:SER:HA   | 1.75                     | 0.52              |
| 69:L3:114:VAL:HG13 | 69:L3:119:LEU:HB2  | 1.91                     | 0.52              |
| 79:m:403:THR:OG1   | 79:m:405:ASP:OD1   | 2.28                     | 0.52              |
| 84:u:78:ILE:HA     | 84:u:104:ILE:HG22  | 1.92                     | 0.52              |
| 7:G1:40:GLY:HA3    | 7:G1:45:VAL:HB     | 1.92                     | 0.52              |
| 8:H1:67:ARG:HH12   | 9:A2:3328:G:H4'    | 1.75                     | 0.52              |
| 9:A2:1351:U:H2'    | 9:A2:1352:G:H8     | 1.74                     | 0.52              |
| 9:A2:2271:G:O2'    | 35:a2:62:LYS:NZ    | 2.43                     | 0.52              |
| 9:A2:2508:G:O2'    | 9:A2:2509:G:O4'    | 2.26                     | 0.52              |
| 9:A2:2536:G:O2'    | 40:f2:3:SER:O      | 2.28                     | 0.52              |
| 9:A2:4239:G:N2     | 13:E2:15:GLY:O     | 2.38                     | 0.52              |
| 12:D2:27:ALA:O     | 12:D2:128:ARG:NH2  | 2.43                     | 0.52              |
| 44:j2:44:LYS:HD2   | 44:j2:46:LYS:HE3   | 1.91                     | 0.52              |
| 84:u:114:GLU:OE2   | 84:u:123:ARG:NH1   | 2.43                     | 0.52              |
| 85:L1:112:ALA:HB2  | 85:L1:135:PRO:HB2  | 1.91                     | 0.52              |
| 6:F1:80:GLU:HA     | 6:F1:83:VAL:HG22   | 1.91                     | 0.52              |
| 9:A2:1291:C:H2'    | 9:A2:1292:G:H8     | 1.75                     | 0.52              |
| 9:A2:3309:A:N1     | 9:A2:3348:A:H4'    | 2.25                     | 0.52              |
| 19:K2:88:ASP:OD2   | 19:K2:108:ARG:NH1  | 2.43                     | 0.52              |
| 26:R2:129:ARG:NH2  | 26:R2:133:GLU:OE2  | 2.39                     | 0.52              |
| 46:m2:1590:A:H2'   | 46:m2:1591:A:C8    | 2.44                     | 0.52              |
| 46:m2:1622:A:OP1   | 56:x2:115:TYR:OH   | 2.28                     | 0.52              |
| 46:m2:1847:A:H2'   | 46:m2:1848:G:C8    | 2.45                     | 0.52              |
| 70:M3:94:ILE:HA    | 70:M3:100:PRO:HB3  | 1.92                     | 0.52              |
| 71:N3:57:SER:O     | 71:N3:59:GLY:N     | 2.42                     | 0.52              |
| 9:A2:418:A:H2'     | 9:A2:419:A:C8      | 2.45                     | 0.52              |
| 9:A2:1082:A:O2'    | 30:V2:105:ARG:NH2  | 2.37                     | 0.52              |
| 9:A2:1221:C:H42    | 9:A2:1224:G:H22    | 1.56                     | 0.52              |
| 9:A2:1626:G:H2'    | 9:A2:1627:A:C8     | 2.45                     | 0.52              |
| 22:N2:71:ALA:HA    | 22:N2:92:ARG:HA    | 1.91                     | 0.52              |
| 45:k2:38:PHE:O     | 45:k2:45:HIS:NE2   | 2.40                     | 0.52              |
| 46:m2:1146:A:H2'   | 46:m2:1147:A:C8    | 2.45                     | 0.52              |
| 46:m2:1359:A:OP1   | 67:J3:125:LYS:NZ   | 2.38                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:m2:1625:A:N1   | 58:A3:132:ARG:NH1  | 2.58                     | 0.52              |
| 83:t:160:LYS:HG2  | 83:t:189:PHE:HB3   | 1.92                     | 0.52              |
| 84:u:119:LEU:HD13 | 84:u:153:LYS:HE3   | 1.91                     | 0.52              |
| 85:L1:125:GLY:O   | 85:L1:129:ASN:HB2  | 2.10                     | 0.52              |
| 9:A2:418:A:H4'    | 9:A2:2066:C:H5'    | 1.92                     | 0.51              |
| 9:A2:1367:A:OP2   | 44:j2:4:ARG:NH1    | 2.41                     | 0.51              |
| 9:A2:1701:G:O2'   | 33:Y2:57:ASN:OD1   | 2.28                     | 0.51              |
| 9:A2:3320:G:H2'   | 9:A2:3321:G:H8     | 1.75                     | 0.51              |
| 9:A2:4039:C:OP2   | 9:A2:4184:U:O2'    | 2.27                     | 0.51              |
| 10:B2:28:C:H1'    | 10:B2:54:A:H61     | 1.74                     | 0.51              |
| 17:I2:186:GLU:HA  | 17:I2:189:ILE:HG22 | 1.92                     | 0.51              |
| 25:Q2:105:ARG:NH1 | 68:K3:150:GLU:OE1  | 2.43                     | 0.51              |
| 33:Y2:50:LYS:O    | 33:Y2:52:GLN:NE2   | 2.44                     | 0.51              |
| 56:x2:108:LYS:HD2 | 56:x2:111:MET:HE3  | 1.92                     | 0.51              |
| 6:F1:20:GLN:OE1   | 9:A2:340:C:N4      | 2.44                     | 0.51              |
| 9:A2:837:G:H2'    | 9:A2:838:C:C6      | 2.46                     | 0.51              |
| 9:A2:2141:U:H2'   | 9:A2:2142:G:H8     | 1.75                     | 0.51              |
| 9:A2:2197:G:OP1   | 35:a2:9:ARG:NH2    | 2.43                     | 0.51              |
| 9:A2:2235:G:H2'   | 9:A2:2236:G:H8     | 1.76                     | 0.51              |
| 9:A2:4613:A:OP1   | 13:E2:125:SER:OG   | 2.27                     | 0.51              |
| 17:I2:166:MET:HG2 | 17:I2:169:ARG:HH21 | 1.76                     | 0.51              |
| 46:m2:76:U:H2'    | 46:m2:77:A:C5      | 2.46                     | 0.51              |
| 46:m2:209:G:H3'   | 46:m2:210:G:H8     | 1.75                     | 0.51              |
| 46:m2:964:A:H5''  | 72:O3:66:ARG:HG3   | 1.91                     | 0.51              |
| 71:N3:13:GLN:O    | 76:S3:20:LYS:NZ    | 2.39                     | 0.51              |
| 72:O3:75:MET:HG3  | 72:O3:118:ALA:HB2  | 1.92                     | 0.51              |
| 9:A2:463:A:H2'    | 9:A2:464:G:C8      | 2.45                     | 0.51              |
| 9:A2:2030:G:H2'   | 9:A2:2031:A:C8     | 2.44                     | 0.51              |
| 9:A2:2654:C:OP1   | 20:L2:108:ARG:NH2  | 2.40                     | 0.51              |
| 9:A2:3504:U:H2'   | 9:A2:3505:A:H8     | 1.74                     | 0.51              |
| 9:A2:4346:G:OP1   | 9:A2:4346:G:N2     | 2.42                     | 0.51              |
| 46:m2:833:G:N2    | 46:m2:846:U:O2     | 2.43                     | 0.51              |
| 46:m2:1339:C:H2'  | 46:m2:1340:G:H8    | 1.74                     | 0.51              |
| 46:m2:1491:A:OP2  | 82:A:195:ARG:NH1   | 2.43                     | 0.51              |
| 50:r2:152:PRO:HG2 | 68:K3:216:ARG:HG2  | 1.92                     | 0.51              |
| 79:m:90:GLN:NE2   | 79:m:355:ILE:O     | 2.43                     | 0.51              |
| 80:j:108:PRO:HA   | 80:j:184:SER:HA    | 1.92                     | 0.51              |
| 2:B1:110:LYS:HD2  | 2:B1:113:ARG:HH12  | 1.76                     | 0.51              |
| 9:A2:1078:G:OP1   | 9:A2:1080:C:N4     | 2.39                     | 0.51              |
| 9:A2:3266:A:H2'   | 9:A2:3267:A:H8     | 1.76                     | 0.51              |
| 9:A2:3329:C:O2'   | 9:A2:3730:C:OP1    | 2.26                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:3430:A:H2'    | 9:A2:3431:A:C8     | 2.46                     | 0.51              |
| 9:A2:3625:G:H2'    | 9:A2:3626:G:C8     | 2.45                     | 0.51              |
| 9:A2:4324:A:OP1    | 24:P2:15:ARG:NH2   | 2.40                     | 0.51              |
| 25:Q2:80:ARG:HH22  | 68:K3:11:GLY:HA3   | 1.75                     | 0.51              |
| 32:X2:27:ILE:HB    | 32:X2:84:ILE:HG22  | 1.93                     | 0.51              |
| 46:m2:38:A:H5''    | 69:L3:5:ARG:HD3    | 1.92                     | 0.51              |
| 46:m2:534:C:H2'    | 46:m2:535:A:C8     | 2.46                     | 0.51              |
| 46:m2:680:U:OP2    | 46:m2:1028:C:N4    | 2.42                     | 0.51              |
| 46:m2:1103:U:H2'   | 46:m2:1104:G:H8    | 1.76                     | 0.51              |
| 46:m2:1747:A:H1'   | 68:K3:66:GLY:HA2   | 1.92                     | 0.51              |
| 66:I3:168:CYS:HB2  | 66:I3:195:LEU:HD13 | 1.92                     | 0.51              |
| 79:m:653:PRO:HD2   | 79:m:657:GLY:HA3   | 1.91                     | 0.51              |
| 3:C1:113:GLU:HG2   | 3:C1:125:ARG:HG2   | 1.92                     | 0.51              |
| 8:H1:65:ARG:NH2    | 9:A2:2212:G:OP1    | 2.43                     | 0.51              |
| 46:m2:390:U:H2'    | 46:m2:391:A:C8     | 2.45                     | 0.51              |
| 83:t:36:LEU:HD11   | 83:t:78:ARG:HD2    | 1.93                     | 0.51              |
| 9:A2:4541:G:N2     | 9:A2:4570:U:O2     | 2.44                     | 0.51              |
| 31:W2:38:ILE:HG21  | 31:W2:63:TYR:HB3   | 1.93                     | 0.51              |
| 46:m2:614:PSU:HO2' | 77:T3:11:LYS:HZ1   | 1.52                     | 0.51              |
| 46:m2:831:C:O2'    | 46:m2:847:G:N2     | 2.43                     | 0.51              |
| 51:w2:19:ASN:ND2   | 84:u:191:GLU:O     | 2.43                     | 0.51              |
| 1:A1:201:LEU:HD21  | 1:A1:226:ALA:HA    | 1.93                     | 0.51              |
| 3:C1:173:ARG:NH2   | 9:A2:4127:G:OP2    | 2.43                     | 0.51              |
| 6:F1:162:LYS:NZ    | 6:F1:164:GLU:OE1   | 2.43                     | 0.51              |
| 9:A2:1371:A:H2'    | 9:A2:1372:G:C8     | 2.46                     | 0.51              |
| 9:A2:3705:U:H2'    | 9:A2:3706:A:C8     | 2.46                     | 0.51              |
| 9:A2:4662:A:O3'    | 84:u:92:ARG:NH1    | 2.40                     | 0.51              |
| 13:E2:284:ILE:HA   | 13:E2:333:LEU:HD23 | 1.93                     | 0.51              |
| 23:O2:92:LYS:HG2   | 23:O2:97:ARG:HG3   | 1.93                     | 0.51              |
| 24:P2:13:LYS:HB2   | 24:P2:128:LEU:HD21 | 1.92                     | 0.51              |
| 39:e2:36:VAL:HG23  | 39:e2:43:TYR:HB2   | 1.93                     | 0.51              |
| 46:m2:1549:C:H1'   | 46:m2:1672:C:H4'   | 1.92                     | 0.51              |
| 46:m2:1721:A:N6    | 46:m2:1816:G:O2'   | 2.43                     | 0.51              |
| 60:C3:24:LEU:HG    | 60:C3:112:VAL:HG12 | 1.91                     | 0.51              |
| 1:A1:98:ARG:HD2    | 9:A2:736:G:H5''    | 1.93                     | 0.51              |
| 8:H1:35:ALA:HB2    | 8:H1:65:ARG:HH21   | 1.76                     | 0.51              |
| 9:A2:373:OMG:HM21  | 9:A2:1458:C:H4'    | 1.92                     | 0.51              |
| 9:A2:1389:G:O2'    | 9:A2:1391:U:O4'    | 2.29                     | 0.51              |
| 9:A2:2021:C:O2     | 45:k2:39:ARG:NH2   | 2.44                     | 0.51              |
| 9:A2:2504:C:H2'    | 9:A2:2505:G:H8     | 1.75                     | 0.51              |
| 9:A2:3495:G:N2     | 9:A2:3499:C:O2'    | 2.43                     | 0.51              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 9:A2:4004:U:H1'   | 29:U2:58:MET:HE1    | 1.92                     | 0.51              |
| 9:A2:4100:G:H5'   | 9:A2:4101:A:H5''    | 1.93                     | 0.51              |
| 9:A2:4119:A:O2'   | 9:A2:4162:A:N3      | 2.39                     | 0.51              |
| 9:A2:4294:U:H2'   | 9:A2:4295:G:H8      | 1.75                     | 0.51              |
| 9:A2:4676:U:H2'   | 9:A2:4677:G:H8      | 1.75                     | 0.51              |
| 16:H2:183:THR:HB  | 16:H2:193:LEU:HA    | 1.93                     | 0.51              |
| 34:Z2:59:THR:OG1  | 34:Z2:65:ASN:OD1    | 2.29                     | 0.51              |
| 46:m2:89:C:H2'    | 46:m2:90:G:C8       | 2.46                     | 0.51              |
| 46:m2:165:G:H4'   | 68:K3:53:SER:HB3    | 1.91                     | 0.51              |
| 46:m2:1201:A:H2'  | 46:m2:1202:A:C8     | 2.46                     | 0.51              |
| 46:m2:1707:C:H2'  | 46:m2:1708:G:C8     | 2.45                     | 0.51              |
| 50:r2:233:LYS:HD3 | 50:r2:234:PRO:HD2   | 1.93                     | 0.51              |
| 66:I3:35:SER:OG   | 66:I3:36:ARG:N      | 2.44                     | 0.51              |
| 1:A1:249:PHE:N    | 1:A1:255:ALA:O      | 2.43                     | 0.51              |
| 3:C1:107:GLU:HB2  | 3:C1:110:SER:HB3    | 1.92                     | 0.51              |
| 9:A2:424:U:H3     | 11:C2:10:G:H1       | 1.59                     | 0.51              |
| 9:A2:2230:G:N1    | 26:R2:51:THR:O      | 2.38                     | 0.51              |
| 9:A2:2238:G:H1    | 9:A2:2250:U:H3      | 1.57                     | 0.51              |
| 9:A2:3888:G:H4'   | 9:A2:3980:G:H4'     | 1.91                     | 0.51              |
| 9:A2:4410:C:H5''  | 17:I2:116:LYS:HE2   | 1.93                     | 0.51              |
| 9:A2:4634:U:H4'   | 9:A2:4635:U:H5      | 1.76                     | 0.51              |
| 14:F2:110:ARG:O   | 14:F2:113:ARG:NH1   | 2.44                     | 0.51              |
| 16:H2:58:VAL:HG12 | 16:H2:61:ILE:HB     | 1.93                     | 0.51              |
| 32:X2:64:ILE:HG23 | 32:X2:68:LEU:HD23   | 1.92                     | 0.51              |
| 46:m2:456:U:H2'   | 46:m2:457:A:H8      | 1.76                     | 0.51              |
| 46:m2:1129:C:H4'  | 76:S3:17:LYS:HE2    | 1.93                     | 0.51              |
| 53:o2:54:THR:HG22 | 53:o2:162:PRO:HG2   | 1.92                     | 0.51              |
| 79:m:40:CYS:SG    | 79:m:41:LYS:N       | 2.84                     | 0.51              |
| 80:j:141:LEU:HD23 | 80:j:143:ILE:HD11   | 1.93                     | 0.51              |
| 3:C1:43:VAL:HG12  | 3:C1:59:LYS:HD3     | 1.93                     | 0.51              |
| 9:A2:854:A:H62    | 9:A2:1097:G:H1'     | 1.76                     | 0.51              |
| 9:A2:1336:A:N3    | 9:A2:4041:C:O2'     | 2.43                     | 0.51              |
| 9:A2:1647:U:H2'   | 9:A2:1648:G:H8      | 1.76                     | 0.51              |
| 9:A2:3325:G:N2    | 9:A2:3328:G:OP2     | 2.44                     | 0.51              |
| 9:A2:4351:U:H1'   | 9:A2:4352:A:H5''    | 1.92                     | 0.51              |
| 46:m2:532:U:O4    | 46:m2:533:A:N6      | 2.44                     | 0.51              |
| 46:m2:642:A:H2'   | 46:m2:643:A:C8      | 2.46                     | 0.51              |
| 46:m2:1191:A:H2'  | 46:m2:1192:A:H8     | 1.76                     | 0.51              |
| 46:m2:1211:A:O3'  | 63:F3:85[A]:ARG:NH1 | 2.44                     | 0.51              |
| 46:m2:1211:A:O3'  | 63:F3:85[B]:ARG:NH1 | 2.44                     | 0.51              |
| 79:m:14:LYS:O     | 79:m:17:ASN:ND2     | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:m:427:ARG:HB3  | 79:m:441:LEU:HD11 | 1.93                     | 0.51              |
| 2:B1:225:ASN:O    | 2:B1:229:ARG:NH1  | 2.44                     | 0.50              |
| 9:A2:65:A:H61     | 9:A2:75:G:H1'     | 1.76                     | 0.50              |
| 9:A2:462:G:H2'    | 9:A2:463:A:C8     | 2.45                     | 0.50              |
| 9:A2:2334:G:N2    | 9:A2:2337:A:OP2   | 2.34                     | 0.50              |
| 9:A2:4271:U:O2'   | 9:A2:4272:OMU:H6  | 2.11                     | 0.50              |
| 46:m2:1858:C:H2'  | 46:m2:1859:G:H8   | 1.75                     | 0.50              |
| 58:A3:23:ARG:O    | 58:A3:55:ARG:NH1  | 2.41                     | 0.50              |
| 79:m:207:VAL:HG23 | 79:m:208:LEU:HD22 | 1.94                     | 0.50              |
| 79:m:819:LEU:HD12 | 79:m:820:PRO:HD2  | 1.93                     | 0.50              |
| 82:A:221:VAL:HG23 | 82:A:222:LYS:HG3  | 1.92                     | 0.50              |
| 85:L1:59:PRO:HB3  | 85:L1:170:GLY:H   | 1.76                     | 0.50              |
| 9:A2:1212:A:OP1   | 29:U2:136:LYS:NZ  | 2.40                     | 0.50              |
| 9:A2:2129:A:H2'   | 9:A2:2130:A:H8    | 1.77                     | 0.50              |
| 9:A2:2307:G:N2    | 9:A2:2522:U:O4    | 2.43                     | 0.50              |
| 9:A2:3309:A:OP1   | 12:D2:196:TRP:NE1 | 2.38                     | 0.50              |
| 9:A2:3343:A:O2'   | 12:D2:236:GLY:N   | 2.44                     | 0.50              |
| 9:A2:3926:A:H2'   | 9:A2:3927:G:C8    | 2.46                     | 0.50              |
| 9:A2:4274:A:H2'   | 9:A2:4275:OMG:H8  | 1.75                     | 0.50              |
| 9:A2:4622:U:N3    | 13:E2:342:LYS:O   | 2.44                     | 0.50              |
| 33:Y2:45:VAL:HG12 | 33:Y2:52:GLN:HB3  | 1.92                     | 0.50              |
| 38:d2:27:TYR:HA   | 38:d2:34:CYS:HA   | 1.92                     | 0.50              |
| 46:m2:395:U:O2'   | 46:m2:396:G:H8    | 1.94                     | 0.50              |
| 46:m2:508:G:OP1   | 74:Q3:108:LYS:NZ  | 2.39                     | 0.50              |
| 46:m2:981:C:H2'   | 46:m2:982:A:H8    | 1.76                     | 0.50              |
| 49:q2:65:ARG:HA   | 49:q2:68:GLU:HG2  | 1.94                     | 0.50              |
| 72:O3:86:LYS:HG3  | 72:O3:124:MET:HE1 | 1.93                     | 0.50              |
| 84:u:98:LYS:HG3   | 84:u:178:ARG:HG2  | 1.93                     | 0.50              |
| 4:D1:35:ASP:OD1   | 4:D1:86:HIS:NE2   | 2.44                     | 0.50              |
| 9:A2:2658:G:N2    | 9:A2:2659:U:O4    | 2.43                     | 0.50              |
| 9:A2:3772:G:O2'   | 35:a2:90:ARG:NH2  | 2.45                     | 0.50              |
| 9:A2:4651:G:N2    | 9:A2:4687:G:O2'   | 2.44                     | 0.50              |
| 11:C2:2:G:N2      | 11:C2:2:G:OP2     | 2.40                     | 0.50              |
| 11:C2:87:G:OP2    | 36:b2:7:ARG:NH2   | 2.43                     | 0.50              |
| 13:E2:74:GLU:OE1  | 13:E2:285:TYR:OH  | 2.30                     | 0.50              |
| 35:a2:8:ARG:HB2   | 35:a2:34:TYR:HE1  | 1.77                     | 0.50              |
| 46:m2:160:U:N3    | 46:m2:470:A:O2'   | 2.38                     | 0.50              |
| 46:m2:443:C:OP2   | 84:u:2:GLY:N      | 2.44                     | 0.50              |
| 46:m2:1248:A:OP2  | 82:A:188:ARG:NH1  | 2.42                     | 0.50              |
| 51:w2:13:GLN:HE22 | 51:w2:35:ARG:HE   | 1.57                     | 0.50              |
| 53:o2:31:ASP:HB3  | 53:o2:34:MET:HB2  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 84:u:113:TYR:OH    | 84:u:156:ALA:O    | 2.28                     | 0.50              |
| 9:A2:1632:G:H2'    | 9:A2:1633:G:C8    | 2.46                     | 0.50              |
| 9:A2:4322:C:O2'    | 9:A2:4324:A:OP2   | 2.27                     | 0.50              |
| 12:D2:102:LEU:HD12 | 12:D2:103:PRO:HD2 | 1.94                     | 0.50              |
| 12:D2:229:ALA:HB3  | 12:D2:234:LYS:HG2 | 1.92                     | 0.50              |
| 15:G2:50:ARG:NH2   | 15:G2:147:ASP:OD2 | 2.38                     | 0.50              |
| 22:N2:88:ARG:NH1   | 30:V2:33:LYS:O    | 2.45                     | 0.50              |
| 29:U2:36:GLY:HA3   | 29:U2:40:HIS:CE1  | 2.46                     | 0.50              |
| 46:m2:1412:C:N4    | 46:m2:1413:G:O6   | 2.44                     | 0.50              |
| 73:P3:69:LEU:HD21  | 73:P3:72:CYS:HB3  | 1.94                     | 0.50              |
| 9:A2:184:U:O2'     | 9:A2:186:G:OP1    | 2.30                     | 0.50              |
| 9:A2:1818:C:H2'    | 9:A2:1819:A:H8    | 1.76                     | 0.50              |
| 16:H2:115:LYS:HE3  | 16:H2:117:ARG:HB2 | 1.94                     | 0.50              |
| 46:m2:1865:A:OP2   | 63:F3:4:LYS:NZ    | 2.36                     | 0.50              |
| 48:p2:90:ASP:OD1   | 48:p2:91:VAL:N    | 2.44                     | 0.50              |
| 53:o2:110:ASN:ND2  | 53:o2:113:GLN:OE1 | 2.33                     | 0.50              |
| 55:v2:17:LYS:HG2   | 82:A:283:LEU:HB3  | 1.92                     | 0.50              |
| 66:I3:177:TRP:HA   | 66:I3:184:LEU:HA  | 1.94                     | 0.50              |
| 79:m:652:GLY:HA2   | 79:m:659:ASN:HB2  | 1.93                     | 0.50              |
| 2:B1:249:ARG:NH2   | 9:A2:3724:C:OP1   | 2.44                     | 0.50              |
| 4:D1:83:ASP:N      | 4:D1:83:ASP:OD1   | 2.45                     | 0.50              |
| 8:H1:3:ALA:O       | 8:H1:7:ILE:HG12   | 2.12                     | 0.50              |
| 8:H1:172:ARG:HG2   | 9:A2:29:G:H5''    | 1.92                     | 0.50              |
| 9:A2:1141:C:H2'    | 9:A2:1142:G:C8    | 2.46                     | 0.50              |
| 11:C2:135:C:OP1    | 26:R2:63:LYS:NZ   | 2.45                     | 0.50              |
| 31:W2:47:ILE:HD12  | 31:W2:94:LEU:HD11 | 1.92                     | 0.50              |
| 46:m2:168:C:O2'    | 68:K3:133:LEU:O   | 2.29                     | 0.50              |
| 46:m2:470:A:OP1    | 68:K3:74:ARG:NH1  | 2.45                     | 0.50              |
| 46:m2:553:U:H2'    | 46:m2:554:G:C8    | 2.46                     | 0.50              |
| 46:m2:1652:A:H5''  | 57:y2:139:ALA:HB2 | 1.93                     | 0.50              |
| 79:m:122:ASP:OD1   | 79:m:414:ARG:NH2  | 2.45                     | 0.50              |
| 79:m:589:LEU:HD23  | 79:m:604:LYS:HG3  | 1.93                     | 0.50              |
| 9:A2:866:A:N6      | 9:A2:1895:G:O4'   | 2.44                     | 0.50              |
| 9:A2:2343:C:OP1    | 9:A2:2523:C:O2'   | 2.29                     | 0.50              |
| 9:A2:2504:C:H2'    | 9:A2:2505:G:C8    | 2.47                     | 0.50              |
| 9:A2:3260:A:H2'    | 9:A2:3261:C:C6    | 2.47                     | 0.50              |
| 9:A2:3630:G:O3'    | 85:L1:24:LYS:NZ   | 2.45                     | 0.50              |
| 9:A2:4106:G:H2'    | 9:A2:4107:G:H8    | 1.77                     | 0.50              |
| 11:C2:67:U:H2'     | 11:C2:68:G:C8     | 2.47                     | 0.50              |
| 31:W2:51:ASN:ND2   | 31:W2:78:ASN:OD1  | 2.41                     | 0.50              |
| 49:q2:29:LEU:HB3   | 49:q2:32:ASP:HB2  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:m:585:GLU:OE2   | 79:m:606:ARG:NH1   | 2.44                     | 0.50              |
| 1:A1:206:ILE:HG23  | 1:A1:211:ASP:HB3   | 1.94                     | 0.50              |
| 2:B1:143:VAL:HG12  | 2:B1:203:ALA:HB2   | 1.92                     | 0.50              |
| 8:H1:116:LEU:HD22  | 8:H1:135:ILE:HD11  | 1.92                     | 0.50              |
| 9:A2:4:G:H2'       | 9:A2:5:A:H8        | 1.75                     | 0.50              |
| 9:A2:307:A:H2'     | 9:A2:308:G:C4      | 2.47                     | 0.50              |
| 9:A2:2282:A:P      | 20:L2:38:ARG:HH12  | 2.35                     | 0.50              |
| 9:A2:3272:U:H5'    | 9:A2:3273:G:H5'    | 1.93                     | 0.50              |
| 9:A2:3543:OMC:HM22 | 9:A2:3544:G:H5'    | 1.94                     | 0.50              |
| 9:A2:3985:C:O2     | 22:N2:8:ARG:NH1    | 2.45                     | 0.50              |
| 9:A2:4189:C:H2'    | 9:A2:4190:G:H8     | 1.76                     | 0.50              |
| 9:A2:4707:A:N6     | 13:E2:123:HIS:O    | 2.39                     | 0.50              |
| 24:P2:13:LYS:HD2   | 24:P2:128:LEU:HD11 | 1.94                     | 0.50              |
| 31:W2:22:MET:HE2   | 31:W2:85:CYS:HB2   | 1.92                     | 0.50              |
| 46:m2:935:G:H21    | 46:m2:1002:C:H3'   | 1.77                     | 0.50              |
| 53:o2:157:VAL:O    | 61:D3:65:SER:OG    | 2.30                     | 0.50              |
| 66:I3:259:TRP:HD1  | 66:I3:266:ILE:HA   | 1.77                     | 0.50              |
| 67:J3:169:TYR:OH   | 67:J3:175:GLY:O    | 2.27                     | 0.50              |
| 6:F1:62:PRO:HG3    | 9:A2:74:G:H1'      | 1.93                     | 0.50              |
| 6:F1:197:LYS:HD3   | 9:A2:4010:U:H4'    | 1.92                     | 0.50              |
| 9:A2:415:G:O6      | 11:C2:20:A:N6      | 2.44                     | 0.50              |
| 9:A2:1068:C:N4     | 9:A2:1082:A:N1     | 2.60                     | 0.50              |
| 9:A2:1697:G:O2'    | 9:A2:1709:A:N3     | 2.43                     | 0.50              |
| 9:A2:1801:A:N6     | 80:j:40:MET:SD     | 2.84                     | 0.50              |
| 9:A2:2275:C:H2'    | 9:A2:2276:G:H8     | 1.77                     | 0.50              |
| 9:A2:2586:G:H2'    | 9:A2:2587:A:H8     | 1.76                     | 0.50              |
| 9:A2:2625:A:OP2    | 9:A2:2634:A:N6     | 2.40                     | 0.50              |
| 12:D2:57:PRO:HG2   | 12:D2:78:ALA:HB3   | 1.93                     | 0.50              |
| 24:P2:107:ASN:OD1  | 24:P2:111:GLU:N    | 2.44                     | 0.50              |
| 46:m2:65:C:OP1     | 68:K3:136:LYS:NZ   | 2.44                     | 0.50              |
| 79:m:159:MET:HE1   | 79:m:213:PHE:HB3   | 1.93                     | 0.50              |
| 6:F1:32:LYS:NZ     | 9:A2:1176:G:OP2    | 2.43                     | 0.49              |
| 9:A2:1382:U:H2'    | 9:A2:1383:G:H8     | 1.77                     | 0.49              |
| 9:A2:1625:G:O2'    | 15:G2:44:TYR:O     | 2.28                     | 0.49              |
| 9:A2:2295:C:H2'    | 9:A2:2296:G:H8     | 1.77                     | 0.49              |
| 9:A2:3298:A:H1'    | 38:d2:2:THR:HB     | 1.94                     | 0.49              |
| 9:A2:3388:A:H2'    | 9:A2:3389:A:H8     | 1.76                     | 0.49              |
| 9:A2:3542:G:OP2    | 17:I2:90:HIS:NE2   | 2.45                     | 0.49              |
| 34:Z2:36:ARG:O     | 34:Z2:39:THR:OG1   | 2.28                     | 0.49              |
| 46:m2:944:G:OP1    | 48:p2:216:LYS:NZ   | 2.44                     | 0.49              |
| 64:G3:12:ALA:HB1   | 64:G3:32:VAL:HB    | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D1:47:PRO:HD2   | 4:D1:141:LYS:HA   | 1.94                     | 0.49              |
| 9:A2:1390:G:O2'   | 9:A2:1425:G:H4'   | 2.13                     | 0.49              |
| 9:A2:1543:G:O6    | 10:B2:103:A:O2'   | 2.26                     | 0.49              |
| 9:A2:2603:G:O2'   | 9:A2:3494:U:O4    | 2.24                     | 0.49              |
| 9:A2:4395:G:H2'   | 9:A2:4396:A:H8    | 1.76                     | 0.49              |
| 39:e2:37:ARG:HH11 | 39:e2:42:LEU:HB2  | 1.77                     | 0.49              |
| 46:m2:572:C:O2'   | 74:Q3:34:THR:O    | 2.30                     | 0.49              |
| 46:m2:1453:G:H21  | 46:m2:1477:G:H22  | 1.59                     | 0.49              |
| 48:p2:82:ARG:HH12 | 48:p2:191:ASP:HB2 | 1.77                     | 0.49              |
| 64:G3:46:VAL:HG21 | 64:G3:56:LEU:HD13 | 1.94                     | 0.49              |
| 79:m:25:ALA:HB2   | 79:m:127:VAL:HB   | 1.94                     | 0.49              |
| 79:m:393:LEU:HA   | 79:m:418:GLY:HA3  | 1.93                     | 0.49              |
| 1:A1:95:ARG:HD3   | 9:A2:737:G:C4     | 2.47                     | 0.49              |
| 2:B1:186:GLY:HA3  | 2:B1:189:ARG:HD3  | 1.94                     | 0.49              |
| 9:A2:1354:U:H5''  | 12:D2:21:LYS:HG2  | 1.93                     | 0.49              |
| 9:A2:2191:U:OP2   | 26:R2:135:LYS:NZ  | 2.43                     | 0.49              |
| 9:A2:3266:A:H2'   | 9:A2:3267:A:C8    | 2.47                     | 0.49              |
| 9:A2:4017:C:OP1   | 19:K2:184:ARG:NH2 | 2.46                     | 0.49              |
| 9:A2:4111:U:H2'   | 9:A2:4112:U:C6    | 2.47                     | 0.49              |
| 9:A2:4637:U:H2'   | 9:A2:4638:G:C8    | 2.47                     | 0.49              |
| 17:I2:9:LEU:HD23  | 17:I2:118:MET:HB2 | 1.94                     | 0.49              |
| 46:m2:562:A:H5'   | 69:L3:174:LYS:HB2 | 1.93                     | 0.49              |
| 46:m2:1006:U:H2'  | 46:m2:1007:G:H8   | 1.76                     | 0.49              |
| 53:o2:184:ARG:HD3 | 53:o2:191:ARG:HG3 | 1.93                     | 0.49              |
| 1:A1:116:ARG:HA   | 1:A1:162:ILE:HG22 | 1.94                     | 0.49              |
| 6:F1:107:THR:OG1  | 37:c2:18:THR:OG1  | 2.31                     | 0.49              |
| 8:H1:178:HIS:ND1  | 9:A2:68:U:OP1     | 2.34                     | 0.49              |
| 9:A2:490:C:N4     | 9:A2:671:G:O6     | 2.44                     | 0.49              |
| 9:A2:1147:A:H2'   | 9:A2:1148:A:C8    | 2.47                     | 0.49              |
| 9:A2:1870:C:OP1   | 34:Z2:85:ARG:NH2  | 2.45                     | 0.49              |
| 9:A2:3799:G:H2'   | 9:A2:3800:G:H8    | 1.78                     | 0.49              |
| 9:A2:4411:C:N4    | 9:A2:4412:G:O6    | 2.46                     | 0.49              |
| 14:F2:192:GLY:O   | 14:F2:195:LYS:NZ  | 2.41                     | 0.49              |
| 28:T2:46:ILE:HA   | 28:T2:70:SER:HA   | 1.93                     | 0.49              |
| 55:v2:32:HIS:HB3  | 55:v2:35:LEU:HB2  | 1.94                     | 0.49              |
| 56:x2:108:LYS:HG2 | 56:x2:110:GLU:H   | 1.77                     | 0.49              |
| 8:H1:53:TYR:HB2   | 8:H1:133:ILE:HD13 | 1.93                     | 0.49              |
| 9:A2:413:G:OP2    | 40:f2:36:ARG:NH2  | 2.40                     | 0.49              |
| 9:A2:1321:A:OP1   | 14:F2:110:ARG:NH2 | 2.46                     | 0.49              |
| 9:A2:2079:C:O2'   | 33:Y2:98:GLU:OE1  | 2.29                     | 0.49              |
| 9:A2:3589:G:H2'   | 9:A2:3590:G:H8    | 1.77                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:4172:G:N2     | 13:E2:253:CYS:SG   | 2.85                     | 0.49              |
| 16:H2:155:THR:HA   | 16:H2:207:LYS:HA   | 1.94                     | 0.49              |
| 36:b2:79:LYS:O     | 36:b2:84:ARG:NH2   | 2.43                     | 0.49              |
| 46:m2:500:C:H2'    | 46:m2:501:G:C8     | 2.47                     | 0.49              |
| 73:P3:54:ASP:HB3   | 83:t:142:LYS:HB2   | 1.93                     | 0.49              |
| 5:E1:120:ASP:HB3   | 5:E1:123:ILE:HB    | 1.93                     | 0.49              |
| 9:A2:1541:G:H5'    | 10:B2:102:U:H1'    | 1.94                     | 0.49              |
| 9:A2:1716:C:H3'    | 9:A2:1717:C:H2'    | 1.95                     | 0.49              |
| 9:A2:2241:G:H2'    | 9:A2:2242:G:C8     | 2.48                     | 0.49              |
| 9:A2:2469:G:H2'    | 9:A2:2470:G:H8     | 1.78                     | 0.49              |
| 9:A2:3567:C:H2'    | 9:A2:3568:U:H6     | 1.78                     | 0.49              |
| 9:A2:4239:G:O2'    | 13:E2:14:LEU:O     | 2.29                     | 0.49              |
| 32:X2:22:THR:OG1   | 32:X2:122:VAL:O    | 2.31                     | 0.49              |
| 33:Y2:78:LEU:HB3   | 45:k:20:ARG:HD3    | 1.93                     | 0.49              |
| 46:m2:57:U:OP1     | 46:m2:506:G:O2'    | 2.31                     | 0.49              |
| 46:m2:113:G:N1     | 46:m2:294:A:N7     | 2.59                     | 0.49              |
| 46:m2:1449:G:H2'   | 46:m2:1450:A:C8    | 2.47                     | 0.49              |
| 66:I3:214:GLY:HA2  | 66:I3:236:ILE:HG13 | 1.95                     | 0.49              |
| 73:P3:32:LYS:HA    | 73:P3:35:VAL:HG22  | 1.94                     | 0.49              |
| 9:A2:260:C:H2'     | 9:A2:261:G:C8      | 2.47                     | 0.49              |
| 9:A2:435:A:O2'     | 33:Y2:26:ASP:OD2   | 2.23                     | 0.49              |
| 9:A2:1274:C:H2'    | 9:A2:1275:A:H8     | 1.78                     | 0.49              |
| 9:A2:1830:C:H2'    | 9:A2:1831:A:C8     | 2.48                     | 0.49              |
| 9:A2:1893:C:H4'    | 9:A2:1894:G:H5'    | 1.94                     | 0.49              |
| 9:A2:4215:U:C2     | 9:A2:4216:A:C8     | 3.01                     | 0.49              |
| 38:d2:22:CYS:HB3   | 38:d2:37:CYS:SG    | 2.52                     | 0.49              |
| 46:m2:686:G:H2'    | 46:m2:687:A:C8     | 2.47                     | 0.49              |
| 46:m2:755:C:N4     | 46:m2:793:C:OP2    | 2.45                     | 0.49              |
| 46:m2:1206:A:OP1   | 67:J3:117:ARG:NH1  | 2.38                     | 0.49              |
| 46:m2:1343:C:OP1   | 46:m2:1689:C:O2'   | 2.30                     | 0.49              |
| 46:m2:1449:G:H2'   | 46:m2:1450:A:H8    | 1.76                     | 0.49              |
| 54:s2:100:ILE:HD11 | 54:s2:177:LEU:HD21 | 1.94                     | 0.49              |
| 60:C3:20:ILE:HG22  | 60:C3:116:ILE:HG22 | 1.94                     | 0.49              |
| 85:L1:48:ARG:NH2   | 85:L1:159:MET:O    | 2.39                     | 0.49              |
| 5:E1:113:ILE:HD13  | 5:E1:119:TYR:HB2   | 1.94                     | 0.49              |
| 9:A2:310:G:H2'     | 9:A2:311:G:C8      | 2.48                     | 0.49              |
| 9:A2:1752:U:O2'    | 21:M2:116:ARG:NH1  | 2.46                     | 0.49              |
| 9:A2:2366:A:H5'    | 9:A2:2443:G:H4'    | 1.95                     | 0.49              |
| 9:A2:3772:G:N2     | 28:T2:135:ARG:O    | 2.34                     | 0.49              |
| 9:A2:4542:G:N3     | 9:A2:4572:G:N2     | 2.61                     | 0.49              |
| 9:A2:4599:G:H2'    | 9:A2:4600:G:C8     | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A2:4701:G:N2    | 32:X2:118:GLN:OE1 | 2.44                     | 0.49              |
| 11:C2:102:G:H5'   | 38:d2:39:TYR:HE1  | 1.77                     | 0.49              |
| 14:F2:303:ARG:O   | 19:K2:38:ARG:NH2  | 2.38                     | 0.49              |
| 34:Z2:4:ARG:NH2   | 34:Z2:6:TRP:O     | 2.46                     | 0.49              |
| 46:m2:106:C:H2'   | 46:m2:107:A:C8    | 2.47                     | 0.49              |
| 46:m2:617:C:O2'   | 77:T3:8:ARG:NH1   | 2.45                     | 0.49              |
| 46:m2:815:A:O3'   | 50:r2:22:LYS:NZ   | 2.40                     | 0.49              |
| 46:m2:1019:U:H5'  | 71:N3:55:ARG:HD3  | 1.95                     | 0.49              |
| 46:m2:1242:A:OP1  | 56:x2:100:LYS:NZ  | 2.33                     | 0.49              |
| 46:m2:1525:C:H2'  | 46:m2:1526:G:H8   | 1.78                     | 0.49              |
| 53:o2:142:LEU:O   | 61:D3:60:ARG:NH2  | 2.45                     | 0.49              |
| 53:o2:144:THR:N   | 53:o2:158:ASP:OD2 | 2.43                     | 0.49              |
| 62:E3:99:GLU:OE2  | 62:E3:127:ASN:N   | 2.45                     | 0.49              |
| 79:m:329:LYS:HD3  | 79:m:333:PRO:HB2  | 1.94                     | 0.49              |
| 79:m:745:LEU:HD12 | 79:m:786:TYR:HE1  | 1.78                     | 0.49              |
| 9:A2:1802:G:O2'   | 9:A2:1803:G:N2    | 2.46                     | 0.49              |
| 9:A2:1881:G:H2'   | 9:A2:1882:U:C6    | 2.47                     | 0.49              |
| 9:A2:2378:A:H2'   | 9:A2:2379:G:H8    | 1.78                     | 0.49              |
| 10:B2:6:C:OP2     | 15:G2:22:ARG:NH2  | 2.46                     | 0.49              |
| 46:m2:1550:G:N1   | 46:m2:1588:U:O4   | 2.46                     | 0.49              |
| 46:m2:1625:A:N7   | 58:A3:132:ARG:HA  | 2.28                     | 0.49              |
| 79:m:433:TYR:HE1  | 79:m:441:LEU:HB2  | 1.76                     | 0.49              |
| 81:k:93:LYS:HE3   | 81:k:94:LYS:HE3   | 1.95                     | 0.49              |
| 9:A2:120:A:N1     | 9:A2:148:A:O2'    | 2.40                     | 0.49              |
| 9:A2:849:G:H2'    | 9:A2:850:G:H8     | 1.78                     | 0.49              |
| 9:A2:3263:U:OP1   | 20:L2:81:ARG:NH2  | 2.46                     | 0.49              |
| 29:U2:115:GLY:O   | 29:U2:136:LYS:NZ  | 2.41                     | 0.49              |
| 33:Y2:114:ARG:NH1 | 33:Y2:117:GLN:OE1 | 2.42                     | 0.49              |
| 46:m2:305:C:O2    | 84:u:184:ARG:NH1  | 2.46                     | 0.49              |
| 61:D3:50:PHE:HZ   | 67:J3:263:LYS:HE3 | 1.78                     | 0.49              |
| 79:m:63:GLN:OE1   | 79:m:455:ARG:NH2  | 2.46                     | 0.49              |
| 3:C1:106:GLN:HB2  | 3:C1:111:LEU:HB3  | 1.95                     | 0.48              |
| 9:A2:1316:A:H4'   | 9:A2:1317:G:H5'   | 1.94                     | 0.48              |
| 9:A2:2565:U:OP1   | 20:L2:70:ARG:NH2  | 2.46                     | 0.48              |
| 9:A2:3606:U:H2'   | 9:A2:3607:G:C8    | 2.48                     | 0.48              |
| 15:G2:107:ARG:NH2 | 15:G2:116:ASP:OD1 | 2.46                     | 0.48              |
| 20:L2:95:TRP:HZ3  | 20:L2:130:ASN:HB3 | 1.78                     | 0.48              |
| 46:m2:565:G:O2'   | 46:m2:566:A:OP1   | 2.29                     | 0.48              |
| 46:m2:977:G:H2'   | 46:m2:978:G:C8    | 2.49                     | 0.48              |
| 46:m2:1104:G:OP2  | 48:p2:151:ARG:NH2 | 2.45                     | 0.48              |
| 46:m2:1619:G:N1   | 46:m2:1622:A:OP2  | 2.36                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 66:I3:164:ILE:HG22 | 66:I3:178:ASN:HA  | 1.95                     | 0.48              |
| 67:J3:131:GLY:HA3  | 67:J3:216:MET:HB3 | 1.95                     | 0.48              |
| 75:R3:91:LEU:HD23  | 75:R3:97:ILE:HG13 | 1.94                     | 0.48              |
| 79:m:518:LYS:HB2   | 79:m:567:ILE:HD13 | 1.95                     | 0.48              |
| 80:j:146:LYS:NZ    | 80:j:153:GLU:OE1  | 2.39                     | 0.48              |
| 8:H1:179:LYS:O     | 9:A2:297:U:O2'    | 2.31                     | 0.48              |
| 9:A2:1322:C:H2'    | 9:A2:1323:G:H8    | 1.78                     | 0.48              |
| 9:A2:3594:G:O6     | 9:A2:3824:A:N6    | 2.45                     | 0.48              |
| 19:K2:168:ARG:HH21 | 19:K2:174:PHE:HE1 | 1.61                     | 0.48              |
| 46:m2:950:C:H2'    | 46:m2:951:G:H8    | 1.78                     | 0.48              |
| 46:m2:954:G:H2'    | 46:m2:955:C:C6    | 2.48                     | 0.48              |
| 59:B3:40:ALA:HB3   | 59:B3:43:LYS:HG3  | 1.95                     | 0.48              |
| 7:G1:117:LYS:NZ    | 9:A2:4574:C:OP1   | 2.45                     | 0.48              |
| 9:A2:1138:A:OP2    | 9:A2:1140:A2M:N6  | 2.43                     | 0.48              |
| 9:A2:1649:C:H2'    | 9:A2:1650:C:C6    | 2.48                     | 0.48              |
| 9:A2:1885:C:OP1    | 19:K2:12:LYS:NZ   | 2.45                     | 0.48              |
| 9:A2:3366:G:H2'    | 9:A2:3367:A:C4    | 2.48                     | 0.48              |
| 9:A2:3840:U:H2'    | 9:A2:3841:U:C6    | 2.49                     | 0.48              |
| 9:A2:4386:A:H2'    | 9:A2:4387:G:H8    | 1.78                     | 0.48              |
| 17:I2:3:GLU:O      | 17:I2:31:ARG:NH2  | 2.46                     | 0.48              |
| 60:C3:26:SER:HB3   | 60:C3:32:LEU:HD22 | 1.95                     | 0.48              |
| 68:K3:121:ILE:H    | 68:K3:125:THR:HB  | 1.77                     | 0.48              |
| 79:m:23:VAL:HG12   | 79:m:31:LYS:HG2   | 1.96                     | 0.48              |
| 8:H1:188:ARG:NH1   | 9:A2:48:G:O2'     | 2.45                     | 0.48              |
| 9:A2:1032:C:O4'    | 22:N2:142:ARG:NH2 | 2.41                     | 0.48              |
| 9:A2:2169:G:H2'    | 9:A2:2170:U:H6    | 1.78                     | 0.48              |
| 9:A2:2476:G:H2'    | 9:A2:2477:G:C8    | 2.48                     | 0.48              |
| 9:A2:2564:G:O2'    | 9:A2:4296:G:OP1   | 2.31                     | 0.48              |
| 9:A2:3346:U:H2'    | 9:A2:3347:G:O4'   | 2.13                     | 0.48              |
| 9:A2:3872:6MZ:OP2  | 9:A2:3872:6MZ:H8  | 2.13                     | 0.48              |
| 9:A2:3912:U:H2'    | 9:A2:3913:C:H6    | 1.79                     | 0.48              |
| 9:A2:4041:C:H2'    | 9:A2:4042:A:C8    | 2.48                     | 0.48              |
| 43:i2:19:GLN:NE2   | 43:i2:74:GLU:OE2  | 2.46                     | 0.48              |
| 46:m2:65:C:N4      | 46:m2:169:U:HO2'  | 2.09                     | 0.48              |
| 46:m2:183:G:H2'    | 46:m2:184:G:O4'   | 2.12                     | 0.48              |
| 46:m2:385:G:H4'    | 51:w2:132:ARG:HD2 | 1.96                     | 0.48              |
| 46:m2:513:U:H2'    | 46:m2:514:A:H8    | 1.77                     | 0.48              |
| 46:m2:619:G:H4'    | 62:E3:88:ASP:HB2  | 1.95                     | 0.48              |
| 46:m2:748:C:N4     | 46:m2:749:U:O4    | 2.47                     | 0.48              |
| 46:m2:977:G:OP1    | 72:O3:98:ARG:NH1  | 2.46                     | 0.48              |
| 46:m2:1459:U:H2'   | 46:m2:1460:G:H8   | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:s2:77:MET:HG2   | 54:s2:89:THR:HG21  | 1.95                     | 0.48              |
| 85:L1:96:ASN:HB3   | 85:L1:99:LEU:HD13  | 1.95                     | 0.48              |
| 4:D1:45:GLU:O      | 4:D1:141:LYS:NZ    | 2.44                     | 0.48              |
| 9:A2:1496:PSU:H2'  | 9:A2:1497:A:H8     | 1.78                     | 0.48              |
| 9:A2:3611:G:OP1    | 9:A2:3619:A:N6     | 2.46                     | 0.48              |
| 9:A2:4187:A:H2'    | 9:A2:4188:OMC:H6   | 1.78                     | 0.48              |
| 9:A2:4256:G:N2     | 9:A2:4259:A:OP2    | 2.47                     | 0.48              |
| 12:D2:200:ARG:NH1  | 12:D2:217:GLN:OE1  | 2.41                     | 0.48              |
| 16:H2:73:LYS:HE2   | 16:H2:75:LEU:HD21  | 1.94                     | 0.48              |
| 46:m2:57:U:O2      | 46:m2:501:G:O2'    | 2.32                     | 0.48              |
| 46:m2:325:C:N3     | 46:m2:330:U:O4     | 2.46                     | 0.48              |
| 46:m2:1515:C:H2'   | 46:m2:1516:G:H8    | 1.77                     | 0.48              |
| 47:n2:23:C:N4      | 47:n2:24:G:O6      | 2.46                     | 0.48              |
| 67:J3:184:VAL:HG12 | 67:J3:195:LEU:HB2  | 1.94                     | 0.48              |
| 9:A2:4394:G:H2'    | 9:A2:4395:G:C8     | 2.48                     | 0.48              |
| 14:F2:7:LEU:HG     | 14:F2:21:ASN:HB3   | 1.95                     | 0.48              |
| 31:W2:48:LEU:HD11  | 31:W2:60:ILE:HG21  | 1.96                     | 0.48              |
| 42:h2:18:ARG:NH2   | 46:m2:1184:A:OP1   | 2.47                     | 0.48              |
| 84:u:61:ASP:OD1    | 84:u:61:ASP:N      | 2.47                     | 0.48              |
| 1:A1:75:LYS:NZ     | 1:A1:79:TYR:OH     | 2.46                     | 0.48              |
| 9:A2:718:A:H2'     | 9:A2:719:C:C6      | 2.49                     | 0.48              |
| 9:A2:1175:G:H2'    | 9:A2:1176:G:H8     | 1.79                     | 0.48              |
| 9:A2:1316:A:H1'    | 9:A2:1317:G:C8     | 2.48                     | 0.48              |
| 9:A2:1880:C:H2'    | 9:A2:1881:G:C8     | 2.49                     | 0.48              |
| 9:A2:2081:G:OP2    | 33:Y2:101:HIS:ND1  | 2.33                     | 0.48              |
| 9:A2:3263:U:H2'    | 9:A2:3264:A:C8     | 2.49                     | 0.48              |
| 9:A2:3309:A:N6     | 9:A2:3347:G:O2'    | 2.47                     | 0.48              |
| 9:A2:4499:G:H2'    | 9:A2:4500:G:C8     | 2.49                     | 0.48              |
| 15:G2:64:ILE:HG13  | 15:G2:105:LEU:HD21 | 1.95                     | 0.48              |
| 24:P2:86:LYS:NZ    | 24:P2:87:SER:O     | 2.45                     | 0.48              |
| 46:m2:806:U:H5''   | 73:P3:82:GLN:HG2   | 1.96                     | 0.48              |
| 48:p2:179:ASN:HB3  | 48:p2:183:GLU:HB2  | 1.93                     | 0.48              |
| 51:w2:59:LYS:HB3   | 51:w2:134:LEU:HD21 | 1.95                     | 0.48              |
| 74:Q3:91:LEU:HB3   | 74:Q3:96:LEU:HB2   | 1.96                     | 0.48              |
| 79:m:40:CYS:O      | 79:m:45:ILE:N      | 2.47                     | 0.48              |
| 9:A2:1534:C:H2'    | 9:A2:1535:G:C8     | 2.49                     | 0.48              |
| 9:A2:2157:G:O2'    | 35:a2:10:ARG:O     | 2.32                     | 0.48              |
| 9:A2:2235:G:H2'    | 9:A2:2236:G:C8     | 2.49                     | 0.48              |
| 13:E2:83:PRO:O     | 13:E2:167:GLN:NE2  | 2.38                     | 0.48              |
| 46:m2:225:C:H2'    | 46:m2:226:A:C8     | 2.49                     | 0.48              |
| 46:m2:1526:G:O2'   | 47:n2:30:G:OP1     | 2.25                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:m2:1564:C:H2'  | 46:m2:1565:G:H8    | 1.79                     | 0.48              |
| 46:m2:1731:U:O4   | 46:m2:1807:G:O6    | 2.31                     | 0.48              |
| 46:m2:1860:G:H2'  | 46:m2:1861:A:H8    | 1.79                     | 0.48              |
| 47:n2:22:G:H2'    | 47:n2:23:C:C6      | 2.49                     | 0.48              |
| 50:r2:151:ASP:HB3 | 50:r2:154:ILE:HG13 | 1.96                     | 0.48              |
| 54:s2:30:ILE:HG22 | 54:s2:32:ASP:H     | 1.78                     | 0.48              |
| 74:Q3:14:THR:HG22 | 74:Q3:21:LYS:HG2   | 1.96                     | 0.48              |
| 79:m:12:MET:HE2   | 79:m:464:PRO:HD2   | 1.95                     | 0.48              |
| 2:B1:160:ASP:OD1  | 2:B1:160:ASP:N     | 2.44                     | 0.48              |
| 9:A2:425:U:H2'    | 9:A2:426:A:H8      | 1.79                     | 0.48              |
| 9:A2:1005:G:H1    | 9:A2:1019:G:H1     | 1.61                     | 0.48              |
| 9:A2:1015:C:H2'   | 9:A2:1016:A:C8     | 2.49                     | 0.48              |
| 9:A2:2336:A:O2'   | 9:A2:2337:A:O4'    | 2.29                     | 0.48              |
| 9:A2:4273:C:H2'   | 9:A2:4274:A:H8     | 1.77                     | 0.48              |
| 9:A2:4356:C:H2'   | 9:A2:4357:A:H8     | 1.79                     | 0.48              |
| 17:I2:130:LYS:HB2 | 17:I2:133:ARG:HG2  | 1.96                     | 0.48              |
| 26:R2:82:THR:HG21 | 36:b2:37:THR:HG22  | 1.94                     | 0.48              |
| 27:S2:54:GLU:HB2  | 27:S2:108:ARG:HB3  | 1.96                     | 0.48              |
| 46:m2:1562:U:H2'  | 46:m2:1563:G:C8    | 2.49                     | 0.48              |
| 46:m2:1564:C:H2'  | 46:m2:1565:G:C8    | 2.48                     | 0.48              |
| 46:m2:1694:U:H2'  | 46:m2:1695:G:C8    | 2.49                     | 0.48              |
| 46:m2:1847:A:H2'  | 46:m2:1848:G:H8    | 1.77                     | 0.48              |
| 60:C3:51:LYS:HB3  | 60:C3:90:ASP:HB3   | 1.95                     | 0.48              |
| 80:j:127:ASN:OD1  | 80:j:148:SER:OG    | 2.31                     | 0.48              |
| 3:C1:163:GLN:NE2  | 9:A2:4338:G:N3     | 2.45                     | 0.48              |
| 9:A2:153:G:H2'    | 9:A2:154:G:H8      | 1.78                     | 0.48              |
| 9:A2:161:G:H2'    | 9:A2:162:A:H8      | 1.79                     | 0.48              |
| 9:A2:3317:G:H4'   | 9:A2:3318:A:H5'    | 1.95                     | 0.48              |
| 9:A2:3524:G:H22   | 9:A2:3556:G:H1'    | 1.79                     | 0.48              |
| 9:A2:3747:G:H2'   | 9:A2:3748:A:H8     | 1.78                     | 0.48              |
| 11:C2:28:C:H2'    | 11:C2:29:G:C8      | 2.48                     | 0.48              |
| 13:E2:101:THR:O   | 13:E2:101:THR:OG1  | 2.29                     | 0.48              |
| 46:m2:1026:A:H2'  | 46:m2:1027:U:C6    | 2.48                     | 0.48              |
| 46:m2:1095:A:H2'  | 46:m2:1096:C:C6    | 2.49                     | 0.48              |
| 54:s2:27:ASP:OD1  | 54:s2:107:ASN:ND2  | 2.47                     | 0.48              |
| 67:J3:70:VAL:HG21 | 67:J3:93:ILE:HG23  | 1.96                     | 0.48              |
| 6:F1:42:LYS:O     | 6:F1:46:ILE:HG12   | 2.14                     | 0.47              |
| 8:H1:2:GLY:N      | 9:A2:116:G:OP2     | 2.47                     | 0.47              |
| 9:A2:218:A:H1'    | 9:A2:219:G:C8      | 2.49                     | 0.47              |
| 9:A2:857:A:C8     | 16:H2:130:ARG:HG2  | 2.49                     | 0.47              |
| 9:A2:1155:U:H2'   | 9:A2:1156:A:H8     | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:2480:A:N6     | 20:L2:88:ARG:O     | 2.47                     | 0.47              |
| 9:A2:2494:C:O2     | 12:D2:174:ARG:NH1  | 2.47                     | 0.47              |
| 11:C2:59:A:H5'     | 11:C2:61:A:C8      | 2.49                     | 0.47              |
| 13:E2:165:HIS:ND1  | 13:E2:166:THR:O    | 2.47                     | 0.47              |
| 46:m2:126:G:OP1    | 68:K3:198:ARG:NH1  | 2.42                     | 0.47              |
| 46:m2:536:G:H2'    | 46:m2:537:G:H8     | 1.79                     | 0.47              |
| 46:m2:641:C:H2'    | 46:m2:642:A:C8     | 2.48                     | 0.47              |
| 46:m2:1167:G:OP2   | 62:E3:23:HIS:ND1   | 2.47                     | 0.47              |
| 46:m2:1205:G:H2'   | 46:m2:1206:A:H8    | 1.78                     | 0.47              |
| 46:m2:1858:C:H2'   | 46:m2:1859:G:C8    | 2.48                     | 0.47              |
| 47:n2:6:G:H2'      | 47:n2:7:A:H8       | 1.78                     | 0.47              |
| 50:r2:129:ILE:HG12 | 50:r2:139:LEU:HD22 | 1.96                     | 0.47              |
| 2:B1:141:ASN:ND2   | 9:A2:151:G:N7      | 2.61                     | 0.47              |
| 9:A2:308:G:C8      | 9:A2:310:G:H1'     | 2.49                     | 0.47              |
| 9:A2:2254:C:OP1    | 26:R2:39:LYS:NZ    | 2.40                     | 0.47              |
| 9:A2:3529:G:H2'    | 9:A2:3530:G:C8     | 2.48                     | 0.47              |
| 13:E2:207:VAL:HG21 | 13:E2:331:ILE:HD11 | 1.96                     | 0.47              |
| 33:Y2:70:LEU:HD21  | 33:Y2:76:LYS:HB2   | 1.95                     | 0.47              |
| 45:k2:17:LEU:HD21  | 45:k2:19:LYS:HZ2   | 1.78                     | 0.47              |
| 46:m2:911:G:H2'    | 46:m2:912:G:C8     | 2.49                     | 0.47              |
| 46:m2:1615:G:H2'   | 46:m2:1616:A:C8    | 2.49                     | 0.47              |
| 46:m2:1622:A:O2'   | 56:x2:40:ARG:NH1   | 2.47                     | 0.47              |
| 57:y2:8:GLN:OE1    | 57:y2:27:ARG:NH1   | 2.47                     | 0.47              |
| 61:D3:10:ASP:OD1   | 61:D3:11:LEU:N     | 2.46                     | 0.47              |
| 66:I3:84:ASP:OD2   | 66:I3:86:THR:OG1   | 2.31                     | 0.47              |
| 66:I3:258:ILE:HB   | 66:I3:268:ASP:HB3  | 1.96                     | 0.47              |
| 3:C1:111:LEU:HD11  | 3:C1:125:ARG:HB3   | 1.96                     | 0.47              |
| 5:E1:17:ILE:HA     | 5:E1:134:LEU:HD12  | 1.95                     | 0.47              |
| 9:A2:1284:U:H2'    | 9:A2:1285:C:H6     | 1.79                     | 0.47              |
| 9:A2:2275:C:O2'    | 9:A2:2395:G:N3     | 2.44                     | 0.47              |
| 9:A2:3507:U:H3'    | 9:A2:3508:A:H8     | 1.79                     | 0.47              |
| 9:A2:3626:G:HO2'   | 85:L1:60:ARG:NH1   | 2.12                     | 0.47              |
| 9:A2:4076:A:O4'    | 41:g2:125:LYS:NZ   | 2.39                     | 0.47              |
| 9:A2:4144:U:O2'    | 9:A2:4164:U:O2     | 2.28                     | 0.47              |
| 9:A2:4330:G:N2     | 9:A2:4365:G:H1'    | 2.29                     | 0.47              |
| 13:E2:188:GLY:O    | 13:E2:193:LYS:NZ   | 2.47                     | 0.47              |
| 16:H2:185:PRO:HB3  | 16:H2:265:LEU:HD11 | 1.96                     | 0.47              |
| 42:h2:7:LYS:NZ     | 46:m2:1845:G:OP1   | 2.35                     | 0.47              |
| 46:m2:5:U:H2'      | 46:m2:6:G:H8       | 1.78                     | 0.47              |
| 46:m2:112:U:H3     | 46:m2:351:A:H61    | 1.62                     | 0.47              |
| 46:m2:982:A:H2'    | 46:m2:983:A:H8     | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:I3:83:TRP:HA    | 66:I3:107:ASP:HA   | 1.96                     | 0.47              |
| 76:S3:64:CYS:HB3   | 76:S3:73:LEU:HG    | 1.96                     | 0.47              |
| 79:m:375:PRO:HD3   | 79:m:491:HIS:HB2   | 1.97                     | 0.47              |
| 82:A:195:ARG:HB3   | 82:A:204:LEU:HD21  | 1.96                     | 0.47              |
| 84:u:134:GLU:OE1   | 84:u:134:GLU:N     | 2.47                     | 0.47              |
| 3:C1:48:LEU:HD23   | 3:C1:56:ARG:HG3    | 1.96                     | 0.47              |
| 5:E1:99:PHE:O      | 5:E1:159:LYS:NZ    | 2.47                     | 0.47              |
| 6:F1:92:ARG:HH22   | 9:A2:109:G:H5'     | 1.78                     | 0.47              |
| 6:F1:92:ARG:HE     | 6:F1:98:VAL:HB     | 1.78                     | 0.47              |
| 9:A2:1597:A:N3     | 10:B2:79:U:O2'     | 2.47                     | 0.47              |
| 10:B2:47:G:H2'     | 10:B2:48:G:C8      | 2.50                     | 0.47              |
| 13:E2:276:HIS:O    | 13:E2:277:ARG:NH1  | 2.44                     | 0.47              |
| 13:E2:285:TYR:N    | 13:E2:332:MET:O    | 2.48                     | 0.47              |
| 15:G2:65:ALA:HB2   | 15:G2:74:ILE:HD13  | 1.96                     | 0.47              |
| 46:m2:983:A:H2'    | 46:m2:984:G:C8     | 2.50                     | 0.47              |
| 46:m2:1012:G:H2'   | 46:m2:1013:A:C8    | 2.49                     | 0.47              |
| 58:A3:24:ARG:HH21  | 58:A3:28:PHE:HB3   | 1.79                     | 0.47              |
| 66:I3:226:HIS:NE2  | 66:I3:229:THR:OG1  | 2.36                     | 0.47              |
| 79:m:544:ILE:HD12  | 79:m:574:PRO:HB3   | 1.95                     | 0.47              |
| 79:m:674:ILE:HD13  | 79:m:715:ARG:HG2   | 1.97                     | 0.47              |
| 9:A2:65:A:N6       | 9:A2:75:G:H1'      | 2.29                     | 0.47              |
| 9:A2:1626:G:H2'    | 9:A2:1627:A:H8     | 1.79                     | 0.47              |
| 9:A2:2050:C:O2'    | 14:F2:45:ARG:NH1   | 2.45                     | 0.47              |
| 11:C2:9:A:H2'      | 11:C2:10:G:H8      | 1.79                     | 0.47              |
| 14:F2:236:ASN:HD21 | 14:F2:238:LEU:HB2  | 1.79                     | 0.47              |
| 44:j2:46:LYS:HD2   | 44:j2:59:SER:HB2   | 1.96                     | 0.47              |
| 46:m2:1611:C:OP1   | 58:A3:132:ARG:N    | 2.41                     | 0.47              |
| 56:x2:75:VAL:HG12  | 56:x2:93:MET:HB3   | 1.96                     | 0.47              |
| 69:L3:47:LYS:HB3   | 69:L3:102:ILE:HD12 | 1.97                     | 0.47              |
| 70:M3:26:LEU:HA    | 70:M3:30:GLY:HA2   | 1.95                     | 0.47              |
| 72:O3:95:ILE:HB    | 72:O3:129:ILE:HG12 | 1.97                     | 0.47              |
| 9:A2:4114:C:H42    | 9:A2:4166:G:H1     | 1.62                     | 0.47              |
| 9:A2:4176:G:C2     | 13:E2:252:ALA:HB1  | 2.49                     | 0.47              |
| 11:C2:121:G:H2'    | 11:C2:122:G:C8     | 2.50                     | 0.47              |
| 17:I2:15:LEU:HD12  | 17:I2:18:ARG:HH12  | 1.79                     | 0.47              |
| 31:W2:24:SER:OG    | 31:W2:101:ASP:OD1  | 2.32                     | 0.47              |
| 46:m2:909:G:H2'    | 46:m2:910:A:C8     | 2.49                     | 0.47              |
| 46:m2:1324:G:N2    | 46:m2:1324:G:OP2   | 2.48                     | 0.47              |
| 68:K3:42:GLY:HA3   | 68:K3:45:TRP:HD1   | 1.79                     | 0.47              |
| 84:u:105:ASP:OD1   | 84:u:105:ASP:N     | 2.47                     | 0.47              |
| 8:H1:189:ARG:NH2   | 9:A2:30:C:H41      | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A2:156:G:N2     | 9:A2:157:U:O4     | 2.48                     | 0.47              |
| 9:A2:288:G:H2'    | 9:A2:289:C:C6     | 2.50                     | 0.47              |
| 9:A2:318:A:H2'    | 9:A2:319:A:C8     | 2.49                     | 0.47              |
| 9:A2:1254:C:N4    | 9:A2:1907:A:H61   | 2.11                     | 0.47              |
| 9:A2:1262:C:OP2   | 19:K2:134:ARG:NH2 | 2.46                     | 0.47              |
| 9:A2:1312:C:OP1   | 19:K2:150:ARG:NH2 | 2.47                     | 0.47              |
| 9:A2:1891:G:O4'   | 9:A2:1893:C:N4    | 2.48                     | 0.47              |
| 9:A2:2381:U:C5    | 23:O2:92:LYS:HG3  | 2.50                     | 0.47              |
| 9:A2:3309:A:C2    | 9:A2:3348:A:H4'   | 2.50                     | 0.47              |
| 9:A2:3410:G:O6    | 9:A2:3427:C:N4    | 2.47                     | 0.47              |
| 9:A2:3549:C:H2'   | 9:A2:3550:A:H8    | 1.80                     | 0.47              |
| 10:B2:15:C:H2'    | 10:B2:16:A:H8     | 1.80                     | 0.47              |
| 11:C2:28:C:H2'    | 11:C2:29:G:H8     | 1.80                     | 0.47              |
| 15:G2:41:LYS:NZ   | 22:N2:30:TYR:O    | 2.36                     | 0.47              |
| 18:J2:7:ASP:OD1   | 18:J2:7:ASP:N     | 2.45                     | 0.47              |
| 18:J2:40:HIS:NE2  | 18:J2:110:ASP:O   | 2.45                     | 0.47              |
| 46:m2:456:U:H2'   | 46:m2:457:A:C8    | 2.50                     | 0.47              |
| 46:m2:813:A:H2'   | 46:m2:814:A:H8    | 1.80                     | 0.47              |
| 48:p2:86:LEU:HB3  | 48:p2:98:THR:HB   | 1.96                     | 0.47              |
| 57:y2:40:GLU:O    | 57:y2:48:GLN:NE2  | 2.48                     | 0.47              |
| 60:C3:99:LYS:O    | 60:C3:103:SER:HB2 | 2.14                     | 0.47              |
| 79:m:26:HIS:ND1   | 79:m:137:GLN:HB2  | 2.29                     | 0.47              |
| 85:L1:40:ASN:N    | 85:L1:40:ASN:OD1  | 2.48                     | 0.47              |
| 85:L1:175:THR:OG1 | 85:L1:178:GLU:OE1 | 2.29                     | 0.47              |
| 1:A1:204:PHE:HB3  | 1:A1:222:ARG:HG2  | 1.96                     | 0.47              |
| 1:A1:206:ILE:HD11 | 1:A1:215:GLU:HG3  | 1.96                     | 0.47              |
| 1:A1:265:LEU:HD11 | 1:A1:269:MET:HE3  | 1.96                     | 0.47              |
| 9:A2:16:G:H5'     | 26:R2:60:TYR:HE1  | 1.80                     | 0.47              |
| 9:A2:1132:C:OP2   | 29:U2:21:ARG:NH2  | 2.41                     | 0.47              |
| 9:A2:2276:G:H4'   | 35:a2:26:PRO:HD2  | 1.97                     | 0.47              |
| 9:A2:2354:G:N2    | 9:A2:2502:U:O4    | 2.48                     | 0.47              |
| 9:A2:2365:G:H2'   | 9:A2:2366:A:H8    | 1.80                     | 0.47              |
| 9:A2:2377:G:H2'   | 9:A2:2378:A:C8    | 2.50                     | 0.47              |
| 9:A2:2430:G:N1    | 31:W2:33:GLN:OE1  | 2.46                     | 0.47              |
| 9:A2:4542:G:O6    | 9:A2:4568:U:O4    | 2.32                     | 0.47              |
| 46:m2:305:C:H4'   | 84:u:75:LYS:HD3   | 1.96                     | 0.47              |
| 46:m2:377:U:O4    | 46:m2:378:A:N6    | 2.47                     | 0.47              |
| 46:m2:385:G:H21   | 51:w2:133:PRO:HG2 | 1.79                     | 0.47              |
| 46:m2:563:A:OP1   | 69:L3:171:GLY:N   | 2.46                     | 0.47              |
| 46:m2:654:U:H2'   | 46:m2:655:A:C8    | 2.49                     | 0.47              |
| 67:J3:253:PRO:HA  | 67:J3:256:TRP:CE2 | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:1083:A:OP2    | 30:V2:109:TYR:OH   | 2.32                     | 0.47              |
| 9:A2:1529:U:H2'    | 9:A2:1530:U:C6     | 2.50                     | 0.47              |
| 9:A2:1678:U:H2'    | 9:A2:1679:G:H8     | 1.79                     | 0.47              |
| 9:A2:1864:C:O2'    | 21:M2:111:ARG:NH2  | 2.41                     | 0.47              |
| 9:A2:1877:G:OP1    | 14:F2:312:ARG:NH2  | 2.47                     | 0.47              |
| 9:A2:2214:G:N2     | 9:A2:2217:U:OP2    | 2.48                     | 0.47              |
| 9:A2:4130:G:N2     | 9:A2:4260:G:O2'    | 2.48                     | 0.47              |
| 9:A2:4541:G:O2'    | 9:A2:4542:G:O4'    | 2.30                     | 0.47              |
| 14:F2:10:VAL:HG13  | 14:F2:153:VAL:HG12 | 1.97                     | 0.47              |
| 29:U2:84:GLU:OE2   | 29:U2:87:ARG:NH2   | 2.48                     | 0.47              |
| 46:m2:17:C:H2'     | 46:m2:18:C:C6      | 2.50                     | 0.47              |
| 46:m2:806:U:H3     | 46:m2:861:G:H1     | 1.63                     | 0.47              |
| 46:m2:933:C:H2'    | 46:m2:934:G:C8     | 2.50                     | 0.47              |
| 46:m2:1035:G:N1    | 46:m2:1082:A:O2'   | 2.41                     | 0.47              |
| 46:m2:1173:G:O2'   | 46:m2:1189:G:O6    | 2.30                     | 0.47              |
| 67:J3:256:TRP:CD2  | 73:P3:68:ARG:HD3   | 2.50                     | 0.47              |
| 71:N3:4:MET:HG2    | 71:N3:5:HIS:CD2    | 2.50                     | 0.47              |
| 81:k:41:LYS:NZ     | 81:k:68:GLN:OE1    | 2.48                     | 0.47              |
| 84:u:57:ALA:H      | 84:u:180:GLY:HA2   | 1.79                     | 0.47              |
| 9:A2:3912:U:H2'    | 9:A2:3913:C:C6     | 2.49                     | 0.47              |
| 9:A2:4189:C:H2'    | 9:A2:4190:G:C8     | 2.50                     | 0.47              |
| 9:A2:4415:U:O2'    | 21:M2:174:THR:OG1  | 2.25                     | 0.47              |
| 14:F2:24:LEU:HD12  | 14:F2:25:PRO:HD2   | 1.97                     | 0.47              |
| 46:m2:382:G:H5''   | 84:u:31:ARG:HH11   | 1.80                     | 0.47              |
| 46:m2:1349:U:H2'   | 46:m2:1350:G:N3    | 2.30                     | 0.47              |
| 46:m2:1654:G:O6    | 46:m2:1674:U:O4    | 2.33                     | 0.47              |
| 46:m2:1677:A:H2'   | 46:m2:1678:U:C6    | 2.50                     | 0.47              |
| 54:s2:50:PRO:HB3   | 54:s2:69:VAL:HG12  | 1.97                     | 0.47              |
| 85:L1:141:ASN:HB3  | 85:L1:147:LYS:HD2  | 1.97                     | 0.47              |
| 3:C1:104:VAL:HB    | 3:C1:113:GLU:HB2   | 1.96                     | 0.46              |
| 9:A2:1678:U:H2'    | 9:A2:1679:G:C8     | 2.49                     | 0.46              |
| 9:A2:2352:G:H2'    | 9:A2:2353:A:C8     | 2.50                     | 0.46              |
| 9:A2:3720:U:H2'    | 9:A2:3721:U:C6     | 2.50                     | 0.46              |
| 9:A2:4656:U:H2'    | 9:A2:4657:A:C8     | 2.49                     | 0.46              |
| 45:k2:119:ARG:HD2  | 45:k2:122:LYS:HE2  | 1.97                     | 0.46              |
| 46:m2:488:A:H1'    | 46:m2:515:G:H22    | 1.79                     | 0.46              |
| 46:m2:986:C:O2'    | 72:O3:138:ASP:OD2  | 2.31                     | 0.46              |
| 50:r2:31:PRO:HA    | 50:r2:81:THR:HB    | 1.96                     | 0.46              |
| 58:A3:34:LYS:HB3   | 58:A3:103:LEU:HD23 | 1.97                     | 0.46              |
| 59:B3:5:THR:HG23   | 59:B3:7:LYS:H      | 1.80                     | 0.46              |
| 67:J3:193:VAL:HG11 | 67:J3:240:THR:HG22 | 1.95                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:m:104:SER:HB2   | 79:m:114:VAL:HG22  | 1.97                     | 0.46              |
| 79:m:752:GLU:HA    | 79:m:781:PHE:HE2   | 1.80                     | 0.46              |
| 4:D1:87:ILE:HG12   | 4:D1:138:ILE:HG12  | 1.97                     | 0.46              |
| 9:A2:1627:A:H2'    | 9:A2:1628:G:C8     | 2.51                     | 0.46              |
| 9:A2:1851:G:H2'    | 9:A2:1852:OMG:C8   | 2.50                     | 0.46              |
| 9:A2:2202:U:H2'    | 9:A2:2203:G:H8     | 1.79                     | 0.46              |
| 9:A2:3263:U:H2'    | 9:A2:3264:A:H8     | 1.80                     | 0.46              |
| 12:D2:189:TYR:HA   | 12:D2:192:LYS:HB2  | 1.97                     | 0.46              |
| 13:E2:161:ARG:HG2  | 13:E2:184:GLN:HA   | 1.97                     | 0.46              |
| 14:F2:219:LYS:HG2  | 14:F2:222:ARG:HH12 | 1.80                     | 0.46              |
| 14:F2:230:LEU:HD21 | 14:F2:239:LYS:HD2  | 1.98                     | 0.46              |
| 14:F2:278:ASN:OD1  | 14:F2:279:LEU:N    | 2.48                     | 0.46              |
| 33:Y2:6:PRO:HG3    | 33:Y2:73:GLY:HA3   | 1.96                     | 0.46              |
| 46:m2:1062:A:N6    | 46:m2:1832:UR3:OP1 | 2.48                     | 0.46              |
| 46:m2:1369:U:O2'   | 46:m2:1468:G:O2'   | 2.22                     | 0.46              |
| 46:m2:1538:G:H2'   | 46:m2:1539:A:C8    | 2.51                     | 0.46              |
| 46:m2:1545:U:OP2   | 59:B3:62:ARG:NH2   | 2.41                     | 0.46              |
| 46:m2:1685:C:O2    | 64:G3:24:GLN:NE2   | 2.48                     | 0.46              |
| 62:E3:134:TYR:O    | 77:T3:13:ARG:NH2   | 2.35                     | 0.46              |
| 68:K3:48:TYR:OH    | 68:K3:119:LYS:O    | 2.26                     | 0.46              |
| 79:m:208:LEU:O     | 79:m:356:HIS:NE2   | 2.48                     | 0.46              |
| 83:t:177:TYR:HE2   | 83:t:183:LYS:HB2   | 1.80                     | 0.46              |
| 9:A2:424:U:H2'     | 9:A2:425:U:C6      | 2.51                     | 0.46              |
| 9:A2:1164:C:O2     | 14:F2:119:GLN:NE2  | 2.48                     | 0.46              |
| 9:A2:1500:U:H2'    | 9:A2:1501:G:C8     | 2.50                     | 0.46              |
| 9:A2:2258:G:N2     | 9:A2:3734:G:O4'    | 2.48                     | 0.46              |
| 9:A2:4700:C:H5''   | 9:A2:4701:G:H5'    | 1.98                     | 0.46              |
| 27:S2:17:ARG:O     | 27:S2:21:ALA:HB2   | 2.14                     | 0.46              |
| 46:m2:1184:A:C5    | 46:m2:1185:A:H1'   | 2.51                     | 0.46              |
| 46:m2:1519:G:H2'   | 46:m2:1520:C:O4'   | 2.15                     | 0.46              |
| 53:o2:154:LEU:HD22 | 53:o2:157:VAL:HG11 | 1.98                     | 0.46              |
| 79:m:620:GLU:OE2   | 79:m:633:TYR:OH    | 2.23                     | 0.46              |
| 81:k:10:VAL:HG22   | 81:k:65:GLN:HG3    | 1.97                     | 0.46              |
| 3:C1:174:LYS:HZ2   | 9:A2:4255:C:H4'    | 1.80                     | 0.46              |
| 9:A2:178:C:N4      | 9:A2:179:G:O6      | 2.49                     | 0.46              |
| 9:A2:2500:A:H2'    | 9:A2:2501:A:H8     | 1.80                     | 0.46              |
| 12:D2:189:TYR:CG   | 12:D2:196:TRP:HB2  | 2.50                     | 0.46              |
| 19:K2:59:PRO:HG3   | 19:K2:143:ARG:HA   | 1.98                     | 0.46              |
| 27:S2:30:MET:HB3   | 27:S2:101:PRO:HG3  | 1.97                     | 0.46              |
| 36:b2:97:LYS:HE3   | 36:b2:101:LYS:HE3  | 1.98                     | 0.46              |
| 46:m2:350:A:H2'    | 46:m2:351:A:C8     | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:1124:A:N3    | 48:p2:146:ARG:NH1  | 2.63                     | 0.46              |
| 46:m2:1258:G:H5''  | 65:H3:40:ARG:HE    | 1.80                     | 0.46              |
| 46:m2:1490:C:H3'   | 46:m2:1491:A:H4'   | 1.96                     | 0.46              |
| 79:m:183:ASN:OD1   | 80:j:139:GLN:NE2   | 2.47                     | 0.46              |
| 7:G1:90:ARG:HA     | 7:G1:93:LYS:HD3    | 1.98                     | 0.46              |
| 9:A2:1446:G:C6     | 12:D2:207:VAL:HG21 | 2.50                     | 0.46              |
| 9:A2:1553:A:H2'    | 9:A2:1554:G:H8     | 1.80                     | 0.46              |
| 19:K2:67:ILE:HD11  | 19:K2:95:VAL:HG13  | 1.96                     | 0.46              |
| 46:m2:613:G:H2'    | 46:m2:614:PSU:H6   | 1.80                     | 0.46              |
| 46:m2:1365:C:N3    | 46:m2:1378:A:N6    | 2.61                     | 0.46              |
| 46:m2:1670:U:OP2   | 57:y2:141:TYR:OH   | 2.21                     | 0.46              |
| 49:q2:3:VAL:HG23   | 49:q2:4:GLN:HG2    | 1.96                     | 0.46              |
| 49:q2:23:GLU:OE2   | 49:q2:27:ARG:NE    | 2.48                     | 0.46              |
| 66:I3:37:ASP:OD2   | 66:I3:39:THR:OG1   | 2.33                     | 0.46              |
| 70:M3:31:LEU:HB2   | 70:M3:111:VAL:HA   | 1.98                     | 0.46              |
| 79:m:406:LYS:HD2   | 79:m:525:ARG:HG2   | 1.97                     | 0.46              |
| 83:t:63:PHE:HB3    | 83:t:97:GLN:HG3    | 1.97                     | 0.46              |
| 4:D1:193:ASP:OD1   | 4:D1:193:ASP:N     | 2.49                     | 0.46              |
| 9:A2:1648:G:H2'    | 9:A2:1649:C:C6     | 2.50                     | 0.46              |
| 9:A2:3392:A:H2'    | 9:A2:3393:A:H8     | 1.80                     | 0.46              |
| 9:A2:3549:C:H2'    | 9:A2:3550:A:C8     | 2.50                     | 0.46              |
| 11:C2:141:C:H2'    | 11:C2:142:U:C6     | 2.51                     | 0.46              |
| 14:F2:195:LYS:HG2  | 14:F2:200:ARG:HG3  | 1.97                     | 0.46              |
| 14:F2:291:ARG:HA   | 14:F2:294:LYS:HG2  | 1.96                     | 0.46              |
| 16:H2:100:THR:HG22 | 16:H2:113:VAL:HG22 | 1.97                     | 0.46              |
| 16:H2:285:THR:H    | 16:H2:288:MET:HG3  | 1.81                     | 0.46              |
| 46:m2:1145:A:O3'   | 46:m2:1357:C:N4    | 2.48                     | 0.46              |
| 46:m2:1675:U:H2'   | 46:m2:1676:G:O4'   | 2.15                     | 0.46              |
| 46:m2:1688:G:H2'   | 46:m2:1689:C:H6    | 1.80                     | 0.46              |
| 66:I3:9:GLY:HA3    | 66:I3:52:TYR:HB2   | 1.98                     | 0.46              |
| 74:Q3:13:MET:SD    | 74:Q3:22:GLN:NE2   | 2.87                     | 0.46              |
| 75:R3:102:LYS:HA   | 75:R3:107:VAL:HG13 | 1.96                     | 0.46              |
| 79:m:765:LYS:NZ    | 79:m:798:ASP:OD2   | 2.41                     | 0.46              |
| 80:j:17:ILE:HD13   | 80:j:54:LEU:HD23   | 1.98                     | 0.46              |
| 8:H1:157:LYS:HE3   | 9:A2:56:A:H5''     | 1.96                     | 0.46              |
| 9:A2:110:C:O3'     | 36:b2:110:LYS:NZ   | 2.49                     | 0.46              |
| 9:A2:1480:G:N1     | 9:A2:2036:U:OP2    | 2.38                     | 0.46              |
| 9:A2:1800:A:N6     | 80:j:55:MET:SD     | 2.89                     | 0.46              |
| 9:A2:4506:G:H2'    | 9:A2:4507:G:H8     | 1.81                     | 0.46              |
| 27:S2:43:ASN:OD1   | 27:S2:126:ARG:NE   | 2.48                     | 0.46              |
| 28:T2:50:PRO:HD3   | 28:T2:68:ILE:HG23  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:m2:27:A2M:HM'3  | 46:m2:27:A2M:H1'  | 1.80                     | 0.46              |
| 46:m2:519:OMC:HM22 | 46:m2:520:G:H5'   | 1.97                     | 0.46              |
| 46:m2:865:U:H2'    | 46:m2:866:A:C8    | 2.49                     | 0.46              |
| 46:m2:1181:G:N2    | 46:m2:1184:A:OP2  | 2.44                     | 0.46              |
| 46:m2:1261:A:H62   | 46:m2:1520:C:H3'  | 1.80                     | 0.46              |
| 46:m2:1297:A:H2'   | 46:m2:1298:U:H6   | 1.81                     | 0.46              |
| 48:p2:130:THR:OG1  | 48:p2:180:ASP:OD1 | 2.31                     | 0.46              |
| 50:r2:105:THR:HG23 | 50:r2:106:LYS:HG3 | 1.97                     | 0.46              |
| 55:v2:91:PRO:HD2   | 55:v2:94:LEU:HD23 | 1.97                     | 0.46              |
| 67:J3:183:LYS:HA   | 67:J3:195:LEU:O   | 2.15                     | 0.46              |
| 79:m:582:VAL:HG22  | 79:m:699:VAL:HG12 | 1.97                     | 0.46              |
| 83:t:163:GLN:O     | 83:t:167:GLU:HB2  | 2.15                     | 0.46              |
| 9:A2:38:A:H61      | 9:A2:41:C:H3'     | 1.81                     | 0.46              |
| 9:A2:88:A:N7       | 19:K2:173:LYS:NZ  | 2.64                     | 0.46              |
| 9:A2:188:G:N2      | 9:A2:190:G:N7     | 2.63                     | 0.46              |
| 9:A2:418:A:H2'     | 9:A2:419:A:H8     | 1.79                     | 0.46              |
| 9:A2:500:G:OP1     | 9:A2:503:C:N4     | 2.44                     | 0.46              |
| 9:A2:952:C:H2'     | 9:A2:953:G:C8     | 2.51                     | 0.46              |
| 9:A2:1196:G:H2'    | 9:A2:1197:G:H8    | 1.81                     | 0.46              |
| 9:A2:1482:A:OP1    | 30:V2:11:ASN:ND2  | 2.41                     | 0.46              |
| 9:A2:1882:U:H2'    | 9:A2:1883:C:C6    | 2.51                     | 0.46              |
| 9:A2:2149:G:O4'    | 9:A2:2152:G:N2    | 2.47                     | 0.46              |
| 9:A2:2451:A:N1     | 39:e2:24:LYS:NZ   | 2.45                     | 0.46              |
| 9:A2:3250:C:H1'    | 9:A2:3253:G:H22   | 1.81                     | 0.46              |
| 9:A2:3454:U:N3     | 9:A2:3457:U:OP2   | 2.36                     | 0.46              |
| 10:B2:57:C:H2'     | 10:B2:58:A:H8     | 1.79                     | 0.46              |
| 16:H2:220:THR:H    | 16:H2:223:TYR:HB3 | 1.81                     | 0.46              |
| 28:T2:64:LYS:HA    | 28:T2:67:LYS:HE3  | 1.97                     | 0.46              |
| 48:p2:82:ARG:HH22  | 48:p2:191:ASP:HB2 | 1.81                     | 0.46              |
| 56:x2:118:GLU:O    | 58:A3:120:HIS:N   | 2.47                     | 0.46              |
| 66:I3:67:SER:H     | 66:I3:82:SER:HA   | 1.81                     | 0.46              |
| 79:m:151:LYS:HD3   | 79:m:358:PRO:HD3  | 1.97                     | 0.46              |
| 79:m:692:CYS:SG    | 79:m:693:GLU:N    | 2.89                     | 0.46              |
| 1:A1:95:ARG:HH22   | 9:A2:734:C:H5''   | 1.80                     | 0.46              |
| 1:A1:129:LYS:HA    | 1:A1:132:GLN:HE21 | 1.80                     | 0.46              |
| 9:A2:429:A:H2'     | 9:A2:430:G:C8     | 2.51                     | 0.46              |
| 9:A2:1771:G:N1     | 9:A2:1821:C:N3    | 2.64                     | 0.46              |
| 9:A2:1876:C:H2'    | 9:A2:1877:G:H8    | 1.80                     | 0.46              |
| 9:A2:2276:G:H5'    | 9:A2:2395:G:H1'   | 1.98                     | 0.46              |
| 9:A2:3499:C:OP1    | 24:P2:51:ARG:NE   | 2.48                     | 0.46              |
| 34:Z2:45:LYS:HD2   | 34:Z2:105:LEU:HA  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:1591:A:H2'   | 46:m2:1592:C:C6    | 2.51                     | 0.46              |
| 46:m2:1702:C:O2    | 46:m2:1836:A:N6    | 2.49                     | 0.46              |
| 51:w2:13:GLN:HB2   | 51:w2:16:ILE:HG12  | 1.98                     | 0.46              |
| 66:I3:170:TRP:HA   | 66:I3:194:TYR:HB2  | 1.97                     | 0.46              |
| 67:J3:128:VAL:HG11 | 67:J3:155:ILE:HG12 | 1.97                     | 0.46              |
| 74:Q3:118:ARG:HA   | 74:Q3:118:ARG:HD2  | 1.73                     | 0.46              |
| 2:B1:162:ASP:HB2   | 2:B1:163:PRO:HD3   | 1.97                     | 0.46              |
| 9:A2:40:G:N2       | 9:A2:4032:A:H62    | 2.14                     | 0.46              |
| 9:A2:1354:U:H1'    | 9:A2:2203:G:H21    | 1.80                     | 0.46              |
| 9:A2:4002:C:H2'    | 9:A2:4003:U:H6     | 1.81                     | 0.46              |
| 11:C2:75:G:OP2     | 27:S2:74:TYR:OH    | 2.31                     | 0.46              |
| 11:C2:78:G:H2'     | 11:C2:79:G:C8      | 2.51                     | 0.46              |
| 29:U2:117:LEU:HB2  | 29:U2:140:VAL:HG21 | 1.98                     | 0.46              |
| 46:m2:94:G:O2'     | 46:m2:510:A:O2'    | 2.29                     | 0.46              |
| 46:m2:1027:U:O2'   | 46:m2:1091:G:N2    | 2.49                     | 0.46              |
| 46:m2:1520:C:H5'   | 46:m2:1521:U:H5''  | 1.98                     | 0.46              |
| 46:m2:1658:G:O6    | 46:m2:1670:U:O4    | 2.34                     | 0.46              |
| 70:M3:68:LEU:HD23  | 78:U3:114:ILE:HD13 | 1.98                     | 0.46              |
| 74:Q3:91:LEU:HA    | 74:Q3:94:HIS:CE1   | 2.51                     | 0.46              |
| 81:k:93:LYS:HG3    | 81:k:94:LYS:HG3    | 1.98                     | 0.46              |
| 84:u:36:THR:HB     | 84:u:96:LEU:HB2    | 1.98                     | 0.46              |
| 6:F1:59:VAL:HG22   | 9:A2:74:G:H5'      | 1.98                     | 0.45              |
| 9:A2:284:G:H2'     | 9:A2:285:G:C8      | 2.50                     | 0.45              |
| 9:A2:854:A:N6      | 9:A2:1097:G:H1'    | 2.31                     | 0.45              |
| 9:A2:1680:G:H2'    | 9:A2:1681:C:C6     | 2.51                     | 0.45              |
| 9:A2:2130:A:H2'    | 9:A2:2131:A:H8     | 1.80                     | 0.45              |
| 9:A2:2305:G:H2'    | 9:A2:2306:A:C8     | 2.51                     | 0.45              |
| 9:A2:4176:G:N3     | 13:E2:252:ALA:HB1  | 2.31                     | 0.45              |
| 9:A2:4214:C:H2'    | 9:A2:4215:U:H6     | 1.80                     | 0.45              |
| 17:I2:15:LEU:HD12  | 17:I2:18:ARG:HH22  | 1.80                     | 0.45              |
| 17:I2:181:ALA:O    | 17:I2:185:VAL:HG22 | 2.16                     | 0.45              |
| 31:W2:38:ILE:HD11  | 31:W2:46:VAL:HG21  | 1.98                     | 0.45              |
| 46:m2:28:U:H2'     | 46:m2:29:G:C8      | 2.47                     | 0.45              |
| 46:m2:1142:G:H2'   | 46:m2:1143:G:C8    | 2.51                     | 0.45              |
| 67:J3:202:THR:N    | 67:J3:221:ASP:OD2  | 2.49                     | 0.45              |
| 84:u:106:SER:HB3   | 84:u:171:LEU:HG    | 1.97                     | 0.45              |
| 1:A1:108:GLU:HG3   | 22:N2:135:PRO:HB3  | 1.98                     | 0.45              |
| 8:H1:166:SER:OG    | 9:A2:330:G:OP2     | 2.21                     | 0.45              |
| 9:A2:209:U:H3      | 9:A2:233:U:H3      | 1.65                     | 0.45              |
| 9:A2:1112:C:H2'    | 9:A2:1113:G:H8     | 1.80                     | 0.45              |
| 9:A2:1155:U:H2'    | 9:A2:1156:A:C8     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A2:1274:C:H2'   | 9:A2:1275:A:C8    | 2.51                     | 0.45              |
| 9:A2:1784:G:H5''  | 9:A2:1812:A:H4'   | 1.96                     | 0.45              |
| 9:A2:2515:G:O2'   | 9:A2:2516:U:O4'   | 2.34                     | 0.45              |
| 9:A2:3871:A:C6    | 9:A2:3872:6MZ:H9  | 2.51                     | 0.45              |
| 9:A2:4274:A:H2'   | 9:A2:4275:OMG:C8  | 2.50                     | 0.45              |
| 9:A2:4375:A:H2'   | 9:A2:4376:A:C8    | 2.51                     | 0.45              |
| 9:A2:4693:C:O2'   | 9:A2:4696:C:OP2   | 2.34                     | 0.45              |
| 12:D2:106:THR:O   | 44:j2:90:LYS:NZ   | 2.47                     | 0.45              |
| 13:E2:383:GLU:OE1 | 13:E2:386:LYS:NZ  | 2.36                     | 0.45              |
| 36:b2:95:LEU:HB3  | 36:b2:99:GLU:HG3  | 1.99                     | 0.45              |
| 46:m2:5:U:OP2     | 67:J3:230:THR:OG1 | 2.27                     | 0.45              |
| 46:m2:77:A:H3'    | 68:K3:154:ARG:HB3 | 1.98                     | 0.45              |
| 46:m2:434:G:H2'   | 46:m2:435:A:C8    | 2.51                     | 0.45              |
| 46:m2:1574:C:H2'  | 46:m2:1575:G:C8   | 2.51                     | 0.45              |
| 46:m2:1600:G:O6   | 75:R3:85:ARG:NH2  | 2.48                     | 0.45              |
| 66:I3:197:THR:OG1 | 66:I3:237:ASN:O   | 2.33                     | 0.45              |
| 67:J3:72:ASP:OD2  | 67:J3:272:HIS:NE2 | 2.50                     | 0.45              |
| 68:K3:163:ASN:HA  | 68:K3:169:PRO:HB3 | 1.97                     | 0.45              |
| 73:P3:101:PHE:HA  | 73:P3:113:HIS:CE1 | 2.51                     | 0.45              |
| 76:S3:33:MET:HE1  | 76:S3:73:LEU:HD11 | 1.98                     | 0.45              |
| 81:k:32:ILE:HG21  | 81:k:42:VAL:HG21  | 1.99                     | 0.45              |
| 3:C1:89:ARG:HG3   | 3:C1:145:ILE:HG23 | 1.97                     | 0.45              |
| 9:A2:721:G:H2'    | 9:A2:722:G:H8     | 1.81                     | 0.45              |
| 9:A2:1153:U:H2'   | 9:A2:1154:C:C6    | 2.52                     | 0.45              |
| 9:A2:1327:U:H2'   | 9:A2:1328:A:C8    | 2.52                     | 0.45              |
| 9:A2:1560:G:H2'   | 9:A2:1561:G:C8    | 2.51                     | 0.45              |
| 9:A2:2116:G:O2'   | 9:A2:3515:G:O6    | 2.32                     | 0.45              |
| 9:A2:3339:C:OP1   | 12:D2:132:ASN:ND2 | 2.49                     | 0.45              |
| 9:A2:3523:A2M:H2' | 9:A2:3524:G:C8    | 2.51                     | 0.45              |
| 9:A2:3838:A:H2'   | 9:A2:3839:G:C8    | 2.51                     | 0.45              |
| 9:A2:4230:G:H2'   | 9:A2:4231:U:C6    | 2.52                     | 0.45              |
| 9:A2:4257:A:H2    | 79:m:108:VAL:HG21 | 1.82                     | 0.45              |
| 39:e2:47:ILE:HG13 | 39:e2:49:ASP:H    | 1.80                     | 0.45              |
| 46:m2:107:A:H2'   | 46:m2:108:G:H8    | 1.81                     | 0.45              |
| 46:m2:1115:A:H2'  | 46:m2:1116:U:C6   | 2.52                     | 0.45              |
| 46:m2:1624:U:OP1  | 58:A3:120:HIS:ND1 | 2.48                     | 0.45              |
| 54:s2:123:GLU:HG2 | 54:s2:138:ALA:HB1 | 1.97                     | 0.45              |
| 6:F1:72:ALA:HA    | 6:F1:157:ILE:HD12 | 1.99                     | 0.45              |
| 8:H1:17:ASP:HA    | 8:H1:20:ARG:HG2   | 1.97                     | 0.45              |
| 9:A2:406:C:O2'    | 9:A2:407:A:OP1    | 2.30                     | 0.45              |
| 9:A2:2158:A:OP1   | 35:a2:10:ARG:NH1  | 2.49                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:3748:A:H2'    | 9:A2:3749:G:C8     | 2.51                     | 0.45              |
| 9:A2:3810:C:H2'    | 9:A2:3811:C:H6     | 1.81                     | 0.45              |
| 9:A2:4300:A:H2'    | 9:A2:4301:G:H8     | 1.82                     | 0.45              |
| 9:A2:4438:C:H2'    | 9:A2:4439:G:C8     | 2.50                     | 0.45              |
| 16:H2:148:ARG:N    | 16:H2:198:GLN:OE1  | 2.50                     | 0.45              |
| 17:I2:54:TYR:OH    | 17:I2:73:PHE:O     | 2.35                     | 0.45              |
| 33:Y2:4:LEU:O      | 33:Y2:121:ARG:NH1  | 2.50                     | 0.45              |
| 45:k2:47:LYS:HB2   | 45:k2:102:TYR:CZ   | 2.51                     | 0.45              |
| 46:m2:930:G:H2'    | 46:m2:931:G:H8     | 1.81                     | 0.45              |
| 48:p2:89:GLU:OE2   | 48:p2:220:LYS:NZ   | 2.46                     | 0.45              |
| 48:p2:111:CYS:HA   | 48:p2:114:VAL:HG12 | 1.99                     | 0.45              |
| 49:q2:106:ARG:HG3  | 49:q2:175:VAL:HG22 | 1.99                     | 0.45              |
| 53:o2:108:PHE:N    | 53:o2:136:GLU:OE2  | 2.38                     | 0.45              |
| 56:x2:20:VAL:HG11  | 56:x2:28:MET:HE1   | 1.99                     | 0.45              |
| 66:I3:113:PHE:HB3  | 66:I3:117:ASN:HD22 | 1.81                     | 0.45              |
| 67:J3:256:TRP:CE2  | 73:P3:68:ARG:HB3   | 2.51                     | 0.45              |
| 79:m:578:TYR:N     | 79:m:694:GLU:OE1   | 2.47                     | 0.45              |
| 1:A1:224:LYS:NZ    | 9:A2:1642:G:OP2    | 2.49                     | 0.45              |
| 6:F1:130:LYS:HE3   | 6:F1:132:SER:HB2   | 1.97                     | 0.45              |
| 9:A2:187:U:O4      | 9:A2:1180:G:N1     | 2.43                     | 0.45              |
| 9:A2:938:U:H2'     | 9:A2:939:C:C6      | 2.52                     | 0.45              |
| 9:A2:1175:G:H2'    | 9:A2:1176:G:C8     | 2.52                     | 0.45              |
| 9:A2:1496:PSU:H5'' | 29:U2:44:ASN:HB2   | 1.99                     | 0.45              |
| 9:A2:1793:A:H2'    | 9:A2:1794:U:O4'    | 2.16                     | 0.45              |
| 9:A2:2275:C:OP2    | 9:A2:2285:U:N3     | 2.48                     | 0.45              |
| 9:A2:4041:C:H2'    | 9:A2:4042:A:H8     | 1.81                     | 0.45              |
| 43:i2:12:CYS:HB3   | 43:i2:15:CYS:HB2   | 1.98                     | 0.45              |
| 46:m2:5:U:H2'      | 46:m2:6:G:C8       | 2.51                     | 0.45              |
| 46:m2:91:A:H5''    | 46:m2:92:A:H5''    | 1.98                     | 0.45              |
| 46:m2:1263:C:O2    | 65:H3:10:HIS:NE2   | 2.32                     | 0.45              |
| 46:m2:1595:C:H2'   | 46:m2:1596:A:H8    | 1.81                     | 0.45              |
| 50:r2:124:CYS:HA   | 50:r2:142:HIS:HE1  | 1.81                     | 0.45              |
| 54:s2:119:SER:HA   | 54:s2:193:LYS:HE2  | 1.98                     | 0.45              |
| 59:B3:44:GLU:HG2   | 59:B3:45:LEU:HG    | 1.98                     | 0.45              |
| 66:I3:206:LEU:HB3  | 66:I3:218:LEU:HD12 | 1.99                     | 0.45              |
| 72:O3:86:LYS:NZ    | 72:O3:122:SER:O    | 2.35                     | 0.45              |
| 74:Q3:55:ILE:HG13  | 74:Q3:75:ILE:HG12  | 1.98                     | 0.45              |
| 2:B1:176:LYS:HE3   | 37:c2:43:MET:HE1   | 1.97                     | 0.45              |
| 9:A2:85:G:H3'      | 19:K2:168:ARG:HD2  | 1.98                     | 0.45              |
| 9:A2:3379:A2M:H2'  | 9:A2:3380:A:C8     | 2.50                     | 0.45              |
| 9:A2:3491:C:H2'    | 9:A2:3492:A:C8     | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A2:4086:C:H2'   | 9:A2:4087:U:C6    | 2.51                     | 0.45              |
| 16:H2:76:TYR:CE2  | 16:H2:77:LYS:HG3  | 2.52                     | 0.45              |
| 24:P2:99:GLU:HB3  | 25:Q2:24:THR:HG23 | 1.99                     | 0.45              |
| 46:m2:319:C:H2'   | 46:m2:320:A:C8    | 2.51                     | 0.45              |
| 46:m2:1841:U:O4   | 63:F3:28:ARG:NH2  | 2.49                     | 0.45              |
| 72:O3:27:VAL:HB   | 72:O3:90:ILE:HA   | 1.98                     | 0.45              |
| 79:m:33:THR:HG21  | 88:m:900:GDP:H2'  | 1.98                     | 0.45              |
| 84:u:81:VAL:HG22  | 84:u:102:VAL:HG12 | 1.98                     | 0.45              |
| 9:A2:450:G:H2'    | 9:A2:451:C:C6     | 2.52                     | 0.45              |
| 9:A2:464:G:N1     | 9:A2:699:A:N6     | 2.58                     | 0.45              |
| 9:A2:1382:U:H2'   | 9:A2:1383:G:C8    | 2.52                     | 0.45              |
| 9:A2:1592:U:OP2   | 22:N2:13:TYR:OH   | 2.24                     | 0.45              |
| 9:A2:2519:A:H2'   | 9:A2:2520:A:C8    | 2.49                     | 0.45              |
| 9:A2:4430:U:H2'   | 9:A2:4431:C:C6    | 2.52                     | 0.45              |
| 11:C2:27:U:H2'    | 11:C2:28:C:C6     | 2.52                     | 0.45              |
| 11:C2:49:G:H1'    | 36:b2:44:LEU:HD13 | 1.99                     | 0.45              |
| 11:C2:130:C:H2'   | 11:C2:131:G:C8    | 2.49                     | 0.45              |
| 11:C2:148:A:H2'   | 11:C2:149:G:C8    | 2.52                     | 0.45              |
| 17:I2:85:ARG:O    | 17:I2:90:HIS:ND1  | 2.48                     | 0.45              |
| 24:P2:20:LEU:O    | 24:P2:55:ALA:N    | 2.50                     | 0.45              |
| 39:e2:26:LYS:HB2  | 39:e2:69:LEU:HD12 | 1.98                     | 0.45              |
| 45:k2:95:HIS:O    | 45:k2:99:LYS:HB2  | 2.16                     | 0.45              |
| 46:m2:859:U:H2'   | 46:m2:860:A:C8    | 2.51                     | 0.45              |
| 46:m2:866:A:H2'   | 46:m2:867:A:C8    | 2.52                     | 0.45              |
| 46:m2:1436:C:H5'' | 46:m2:1437:C:C4   | 2.52                     | 0.45              |
| 46:m2:1586:G:OP1  | 59:B3:77:LYS:NZ   | 2.50                     | 0.45              |
| 56:x2:98:ASN:ND2  | 56:x2:121:ILE:O   | 2.49                     | 0.45              |
| 58:A3:3:LEU:HB2   | 58:A3:6:PRO:HG3   | 1.98                     | 0.45              |
| 80:j:13:TYR:OH    | 80:j:61:MET:SD    | 2.70                     | 0.45              |
| 83:t:31:GLU:HG2   | 83:t:40:LEU:HB3   | 1.98                     | 0.45              |
| 83:t:100:ILE:HG12 | 83:t:125:VAL:HG21 | 1.99                     | 0.45              |
| 83:t:170:VAL:HG13 | 83:t:187:PHE:HB2  | 1.99                     | 0.45              |
| 5:E1:147:ARG:NH1  | 10:B2:26:C:O2'    | 2.49                     | 0.45              |
| 9:A2:1140:A2M:H2' | 9:A2:1141:C:C6    | 2.52                     | 0.45              |
| 9:A2:1416:C:H2'   | 9:A2:1417:G:H8    | 1.82                     | 0.45              |
| 9:A2:1553:A:H2'   | 9:A2:1554:G:C8    | 2.52                     | 0.45              |
| 9:A2:1851:G:O2'   | 9:A2:3540:U:O2'   | 2.35                     | 0.45              |
| 9:A2:3762:C:H2'   | 9:A2:3763:U:H6    | 1.82                     | 0.45              |
| 9:A2:3836:G:H5'   | 12:D2:233:ARG:HG2 | 1.99                     | 0.45              |
| 11:C2:96:C:H5''   | 36:b2:66:LYS:HG2  | 1.99                     | 0.45              |
| 46:m2:923:G:C6    | 73:P3:28:ARG:HG3  | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:1625:A:C5    | 58:A3:132:ARG:HG3  | 2.52                     | 0.45              |
| 54:s2:193:LYS:HE3  | 54:s2:193:LYS:HB3  | 1.77                     | 0.45              |
| 69:L3:163:SER:O    | 69:L3:167:GLY:HA3  | 2.17                     | 0.45              |
| 74:Q3:102:THR:HG23 | 74:Q3:107:ARG:HH11 | 1.81                     | 0.45              |
| 79:m:498:PHE:HE2   | 79:m:532:MET:HB2   | 1.82                     | 0.45              |
| 80:j:26:LYS:HB3    | 80:j:95:LEU:HD21   | 1.98                     | 0.45              |
| 5:E1:28:GLU:HB2    | 5:E1:32:ARG:HG2    | 1.99                     | 0.45              |
| 7:G1:126:GLU:HB3   | 17:I2:181:ALA:HB1  | 1.98                     | 0.45              |
| 9:A2:1040:C:H2'    | 9:A2:1041:G:C8     | 2.52                     | 0.45              |
| 9:A2:1562:G:H2'    | 9:A2:1563:G:C8     | 2.52                     | 0.45              |
| 9:A2:3527:A:H2'    | 9:A2:3528:A:C8     | 2.51                     | 0.45              |
| 9:A2:4272:OMU:HM23 | 9:A2:4272:OMU:H1'  | 1.55                     | 0.45              |
| 9:A2:4555:A:C4     | 17:I2:156:LEU:HD23 | 2.52                     | 0.45              |
| 10:B2:23:A:N3      | 10:B2:118:C:O2'    | 2.47                     | 0.45              |
| 11:C2:90:C:H2'     | 11:C2:91:A:C8      | 2.52                     | 0.45              |
| 11:C2:109:C:H2'    | 38:d2:20:ARG:HH22  | 1.82                     | 0.45              |
| 29:U2:131:ARG:HH21 | 29:U2:132:ARG:HD3  | 1.82                     | 0.45              |
| 40:f2:15:LYS:NZ    | 40:f2:19:GLN:OE1   | 2.50                     | 0.45              |
| 46:m2:827:A:H2'    | 46:m2:828:A:C8     | 2.51                     | 0.45              |
| 46:m2:981:C:H2'    | 46:m2:982:A:C8     | 2.51                     | 0.45              |
| 46:m2:1038:A:H4'   | 46:m2:1857:G:N2    | 2.32                     | 0.45              |
| 46:m2:1111:C:H2'   | 46:m2:1112:G:O4'   | 2.17                     | 0.45              |
| 52:z2:59:LYS:O     | 52:z2:62:GLN:HG3   | 2.17                     | 0.45              |
| 69:L3:170:PRO:HB3  | 69:L3:174:LYS:HD3  | 1.99                     | 0.45              |
| 4:D1:48:LEU:HB2    | 4:D1:142:LEU:HD23  | 1.98                     | 0.45              |
| 9:A2:70:A:OP2      | 29:U2:64:LYS:NZ    | 2.33                     | 0.45              |
| 9:A2:878:2MG:HM23  | 9:A2:879:C:H1'     | 1.98                     | 0.45              |
| 9:A2:1154:C:H2'    | 9:A2:1155:U:C6     | 2.52                     | 0.45              |
| 9:A2:1729:U:OP1    | 9:A2:1751:U:O2'    | 2.22                     | 0.45              |
| 9:A2:2256:C:N4     | 9:A2:2257:G:O6     | 2.50                     | 0.45              |
| 9:A2:2602:G:H3'    | 9:A2:2603:G:C8     | 2.52                     | 0.45              |
| 9:A2:3502:C:H2'    | 9:A2:3503:C:H6     | 1.82                     | 0.45              |
| 15:G2:55:VAL:HG22  | 15:G2:60:ILE:HD12  | 1.98                     | 0.45              |
| 33:Y2:43:ASN:HD22  | 33:Y2:46:ARG:HB2   | 1.82                     | 0.45              |
| 33:Y2:124:ASN:OD1  | 33:Y2:124:ASN:N    | 2.49                     | 0.45              |
| 46:m2:753:G:O2'    | 46:m2:793:C:O2     | 2.32                     | 0.45              |
| 46:m2:1025:A:OP2   | 71:N3:124:ARG:NH2  | 2.50                     | 0.45              |
| 46:m2:1470:C:H2'   | 46:m2:1471:A:H8    | 1.81                     | 0.45              |
| 46:m2:1515:C:H2'   | 46:m2:1516:G:C8    | 2.52                     | 0.45              |
| 46:m2:1543:G:OP1   | 59:B3:56:ARG:NE    | 2.45                     | 0.45              |
| 46:m2:1606:G:OP1   | 58:A3:38:ARG:NH1   | 2.48                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:n2:16:G:H2'    | 47:n2:17:C:C6     | 2.52                     | 0.45              |
| 74:Q3:87:PRO:HG2  | 74:Q3:90:ARG:HB2  | 1.99                     | 0.45              |
| 79:m:609:PRO:HG2  | 79:m:612:LEU:HB2  | 1.99                     | 0.45              |
| 9:A2:158:A:H5''   | 9:A2:159:C:H2'    | 1.99                     | 0.44              |
| 9:A2:325:U:H2'    | 9:A2:326:C:H6     | 1.82                     | 0.44              |
| 9:A2:2652:G:H2'   | 9:A2:2653:G:H8    | 1.82                     | 0.44              |
| 9:A2:3884:U:C2    | 43:i2:5:PRO:HD3   | 2.52                     | 0.44              |
| 9:A2:4554:A:OP1   | 17:I2:163:LYS:NZ  | 2.50                     | 0.44              |
| 46:m2:116:OMU:H2' | 46:m2:117:C:C6    | 2.52                     | 0.44              |
| 46:m2:390:U:H2'   | 46:m2:391:A:H8    | 1.81                     | 0.44              |
| 46:m2:438:G:O6    | 46:m2:460:A:N6    | 2.50                     | 0.44              |
| 46:m2:534:C:H2'   | 46:m2:535:A:H8    | 1.80                     | 0.44              |
| 46:m2:982:A:H2'   | 46:m2:983:A:C8    | 2.52                     | 0.44              |
| 46:m2:1239:C:H2'  | 46:m2:1240:U:C6   | 2.51                     | 0.44              |
| 46:m2:1279:C:H2'  | 46:m2:1280:A:H8   | 1.82                     | 0.44              |
| 46:m2:1472:C:O2'  | 46:m2:1473:C:H5'  | 2.17                     | 0.44              |
| 46:m2:1558:A:H1'  | 65:H3:13:LYS:HE2  | 1.99                     | 0.44              |
| 46:m2:1650:G:N2   | 46:m2:1677:A:OP2  | 2.39                     | 0.44              |
| 48:p2:65:ARG:HH21 | 72:O3:48:SER:HB3  | 1.81                     | 0.44              |
| 48:p2:65:ARG:NH2  | 72:O3:46:ASP:OD2  | 2.50                     | 0.44              |
| 50:r2:19:MET:SD   | 50:r2:108:ARG:NH1 | 2.90                     | 0.44              |
| 55:v2:38:LYS:HB3  | 55:v2:40:VAL:HG23 | 1.99                     | 0.44              |
| 57:y2:104:SER:HA  | 57:y2:107:GLU:HG2 | 1.97                     | 0.44              |
| 9:A2:422:C:H2'    | 9:A2:423:G:C8     | 2.52                     | 0.44              |
| 9:A2:819:C:H5''   | 21:M2:74:ARG:HD3  | 1.99                     | 0.44              |
| 9:A2:1116:U:H4'   | 33:Y2:18:LYS:HG2  | 1.99                     | 0.44              |
| 9:A2:1416:C:H2'   | 9:A2:1417:G:C8    | 2.52                     | 0.44              |
| 9:A2:3838:A:H2'   | 9:A2:3839:G:H8    | 1.82                     | 0.44              |
| 38:d2:46:LYS:HD2  | 38:d2:54:LYS:HE3  | 2.00                     | 0.44              |
| 46:m2:617:C:O2    | 77:T3:11:LYS:NZ   | 2.35                     | 0.44              |
| 46:m2:825:PSU:N3  | 69:L3:143:ASN:OD1 | 2.45                     | 0.44              |
| 46:m2:1339:C:H2'  | 46:m2:1340:G:C8   | 2.52                     | 0.44              |
| 46:m2:1570:C:OP1  | 59:B3:96:SER:OG   | 2.35                     | 0.44              |
| 46:m2:1824:A:H2'  | 46:m2:1825:A:C8   | 2.52                     | 0.44              |
| 47:n2:53:G:H2'    | 47:n2:54:A:C8     | 2.52                     | 0.44              |
| 58:A3:50:ILE:HG21 | 58:A3:59:LEU:HD21 | 1.98                     | 0.44              |
| 74:Q3:41:ARG:HH22 | 74:Q3:94:HIS:HD2  | 1.64                     | 0.44              |
| 74:Q3:41:ARG:HH22 | 74:Q3:94:HIS:CD2  | 2.35                     | 0.44              |
| 83:t:186:ASN:OD1  | 83:t:187:PHE:N    | 2.50                     | 0.44              |
| 6:F1:39:ARG:NH1   | 9:A2:1176:G:OP1   | 2.44                     | 0.44              |
| 7:G1:53:LYS:HD2   | 21:M2:160:ARG:HG3 | 2.00                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:G1:91:TRP:HE1    | 9:A2:4515:OMG:H3' | 1.82                     | 0.44              |
| 9:A2:464:G:H1      | 9:A2:699:A:H61    | 1.62                     | 0.44              |
| 9:A2:720:C:H2'     | 9:A2:721:G:H8     | 1.82                     | 0.44              |
| 9:A2:850:G:H2'     | 9:A2:851:C:C6     | 2.53                     | 0.44              |
| 9:A2:1088:A:O2'    | 9:A2:1089:G:H8    | 2.01                     | 0.44              |
| 9:A2:1256:A:H2     | 9:A2:1904:G:H1    | 1.62                     | 0.44              |
| 9:A2:1756:U:H2'    | 9:A2:1757:G:H8    | 1.82                     | 0.44              |
| 9:A2:3625:G:N2     | 85:L1:33:GLU:OE2  | 2.44                     | 0.44              |
| 9:A2:3703:A:H2'    | 9:A2:3704:C:C6    | 2.53                     | 0.44              |
| 9:A2:3748:A:H2'    | 9:A2:3749:G:H8    | 1.82                     | 0.44              |
| 10:B2:7:G:H5''     | 15:G2:22:ARG:HD3  | 1.99                     | 0.44              |
| 46:m2:434:G:H2'    | 46:m2:435:A:H8    | 1.81                     | 0.44              |
| 46:m2:1223:G:H2'   | 46:m2:1224:G:C8   | 2.52                     | 0.44              |
| 47:n2:69:U:H2'     | 47:n2:70:G:H8     | 1.82                     | 0.44              |
| 75:R3:46:ASN:HB2   | 75:R3:80:ARG:HE   | 1.81                     | 0.44              |
| 81:k:146:ARG:O     | 81:k:147:HIS:ND1  | 2.49                     | 0.44              |
| 9:A2:181:C:H2'     | 9:A2:182:G:C8     | 2.52                     | 0.44              |
| 9:A2:1322:C:H2'    | 9:A2:1323:G:C8    | 2.52                     | 0.44              |
| 9:A2:1541:G:C2     | 9:A2:1544:A:N6    | 2.85                     | 0.44              |
| 9:A2:3708:U:H2'    | 9:A2:3709:C:H6    | 1.83                     | 0.44              |
| 9:A2:4648:U:H2'    | 9:A2:4649:U:C6    | 2.52                     | 0.44              |
| 11:C2:8:U:H2'      | 11:C2:9:A:H8      | 1.82                     | 0.44              |
| 11:C2:70:G:N2      | 11:C2:87:G:O2'    | 2.40                     | 0.44              |
| 28:T2:47:ASP:N     | 28:T2:69:LYS:O    | 2.45                     | 0.44              |
| 28:T2:92:ASP:OD1   | 28:T2:94:THR:OG1  | 2.33                     | 0.44              |
| 37:c2:2:ALA:O      | 37:c2:4:ARG:N     | 2.50                     | 0.44              |
| 46:m2:351:A:H2'    | 46:m2:352:C:C6    | 2.53                     | 0.44              |
| 46:m2:529:C:H2'    | 46:m2:530:A:C8    | 2.53                     | 0.44              |
| 46:m2:813:A:H2'    | 46:m2:814:A:C8    | 2.52                     | 0.44              |
| 47:n2:67:U:H2'     | 47:n2:68:C:H6     | 1.83                     | 0.44              |
| 53:o2:76:VAL:HG13  | 53:o2:123:VAL:HB  | 1.97                     | 0.44              |
| 56:x2:25:LEU:HA    | 56:x2:28:MET:HE3  | 2.00                     | 0.44              |
| 59:B3:65:TYR:HE1   | 59:B3:128:GLN:HG3 | 1.83                     | 0.44              |
| 67:J3:180:VAL:HG23 | 67:J3:197:PRO:HG3 | 2.00                     | 0.44              |
| 84:u:12:ARG:HA     | 84:u:18:ARG:HH21  | 1.82                     | 0.44              |
| 1:A1:111:LEU:HD11  | 1:A1:144:PHE:HB3  | 1.99                     | 0.44              |
| 9:A2:1210:G:HO2'   | 9:A2:1281:C:HO2'  | 1.65                     | 0.44              |
| 9:A2:1527:U:H2'    | 9:A2:1528:U:C6    | 2.50                     | 0.44              |
| 9:A2:3242:G:O2'    | 9:A2:3243:C:O4'   | 2.34                     | 0.44              |
| 9:A2:3884:U:H1'    | 9:A2:3885:A:C2    | 2.53                     | 0.44              |
| 9:A2:4015:A:H5''   | 43:i2:36:GLN:HG2  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:4126:A:H5''   | 41:g2:125:LYS:HD2  | 1.99                     | 0.44              |
| 10:B2:58:A:H2'     | 10:B2:59:G:H8      | 1.81                     | 0.44              |
| 15:G2:193:GLU:HA   | 15:G2:196:ARG:HG2  | 1.99                     | 0.44              |
| 46:m2:107:A:H2'    | 46:m2:108:G:C8     | 2.52                     | 0.44              |
| 46:m2:603:G:H2'    | 46:m2:604:G:C8     | 2.52                     | 0.44              |
| 46:m2:1137:C:H2'   | 46:m2:1138:U:C6    | 2.52                     | 0.44              |
| 46:m2:1522:G:H21   | 56:x2:126:VAL:HG11 | 1.82                     | 0.44              |
| 46:m2:1682:G:H2'   | 46:m2:1683:U:C6    | 2.52                     | 0.44              |
| 53:o2:110:ASN:HD21 | 53:o2:112:ILE:HB   | 1.81                     | 0.44              |
| 56:x2:115:TYR:HB2  | 56:x2:118:GLU:HG3  | 1.98                     | 0.44              |
| 74:Q3:90:ARG:HD3   | 74:Q3:93:ARG:HD2   | 2.00                     | 0.44              |
| 79:m:57:ASP:OD1    | 79:m:57:ASP:N      | 2.45                     | 0.44              |
| 79:m:215:SER:OG    | 79:m:220:TRP:NE1   | 2.51                     | 0.44              |
| 1:A1:245:LYS:HE3   | 9:A2:1709:A:H4'    | 1.99                     | 0.44              |
| 6:F1:124:LEU:HD11  | 36:b2:119:TYR:HB2  | 1.99                     | 0.44              |
| 9:A2:1149:G:H21    | 14:F2:95:MET:HB2   | 1.82                     | 0.44              |
| 9:A2:1795:C:H5'    | 81:k:137:GLN:HE22  | 1.82                     | 0.44              |
| 9:A2:4276:A:H2'    | 9:A2:4277:C:C6     | 2.52                     | 0.44              |
| 9:A2:4312:G:N1     | 9:A2:4313:G:O6     | 2.51                     | 0.44              |
| 9:A2:4413:G:H2'    | 9:A2:4414:A:C8     | 2.52                     | 0.44              |
| 11:C2:72:A:OP1     | 27:S2:51:LYS:N     | 2.51                     | 0.44              |
| 13:E2:218:ASP:OD2  | 13:E2:348:ARG:NH1  | 2.51                     | 0.44              |
| 14:F2:190:ARG:HB2  | 14:F2:202:ILE:HG23 | 1.99                     | 0.44              |
| 45:k2:108:MET:O    | 45:k2:112:ARG:HG2  | 2.18                     | 0.44              |
| 46:m2:219:A:H4'    | 46:m2:343:C:H4'    | 1.99                     | 0.44              |
| 46:m2:609:U:O4     | 49:q2:114:ALA:N    | 2.50                     | 0.44              |
| 46:m2:752:C:O2'    | 46:m2:754:G:O4'    | 2.36                     | 0.44              |
| 46:m2:1388:A:OP2   | 49:q2:160:SER:OG   | 2.31                     | 0.44              |
| 46:m2:1530:G:O2'   | 46:m2:1668:C:OP1   | 2.26                     | 0.44              |
| 46:m2:1599:C:H4'   | 46:m2:1605:G:H1    | 1.82                     | 0.44              |
| 46:m2:1691:C:H2'   | 46:m2:1692:U:C6    | 2.53                     | 0.44              |
| 48:p2:75:GLN:HG3   | 48:p2:78:GLU:HG3   | 2.00                     | 0.44              |
| 55:v2:14:LEU:HD22  | 55:v2:35:LEU:HD21  | 1.98                     | 0.44              |
| 56:x2:34:MET:HB3   | 56:x2:42:ARG:HG3   | 2.00                     | 0.44              |
| 57:y2:101:ASP:OD1  | 57:y2:101:ASP:N    | 2.50                     | 0.44              |
| 58:A3:121:ARG:O    | 58:A3:125:HIS:ND1  | 2.34                     | 0.44              |
| 66:I3:215:GLN:HG3  | 66:I3:231:ASP:HB2  | 1.99                     | 0.44              |
| 68:K3:159:ARG:NH2  | 68:K3:171:THR:O    | 2.51                     | 0.44              |
| 85:L1:77:ARG:HG2   | 85:L1:144:MET:HE1  | 1.99                     | 0.44              |
| 1:A1:126:LYS:NZ    | 9:A2:1599:E7G:OP1  | 2.50                     | 0.44              |
| 2:B1:33:GLU:O      | 9:A2:3778:A:O2'    | 2.36                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C1:71:ARG:HG2    | 9:A2:4343:A:H4'    | 1.99                     | 0.44              |
| 6:F1:116:ARG:NH2   | 6:F1:155:MET:O     | 2.47                     | 0.44              |
| 9:A2:268:G:H2'     | 9:A2:269:G:H8      | 1.83                     | 0.44              |
| 9:A2:1093:A:O2'    | 14:F2:323:ARG:NH1  | 2.51                     | 0.44              |
| 9:A2:1144:A:H5''   | 9:A2:3521:A:H5''   | 1.99                     | 0.44              |
| 9:A2:1339:G:H2'    | 9:A2:1340:A:H8     | 1.83                     | 0.44              |
| 9:A2:3345:G:O2'    | 9:A2:3474:U:OP2    | 2.36                     | 0.44              |
| 9:A2:3898:G:H2'    | 9:A2:3899:G:H8     | 1.83                     | 0.44              |
| 9:A2:4176:G:OP1    | 9:A2:4211:A:N6     | 2.44                     | 0.44              |
| 9:A2:4582:U:H4'    | 9:A2:4583:U:OP1    | 2.17                     | 0.44              |
| 10:B2:13:A:O2'     | 15:G2:24:ARG:NH2   | 2.51                     | 0.44              |
| 13:E2:10:ARG:HH21  | 13:E2:14:LEU:HD21  | 1.82                     | 0.44              |
| 21:M2:165:PRO:O    | 21:M2:167:PHE:N    | 2.50                     | 0.44              |
| 46:m2:96:C:H1'     | 46:m2:476:G:H5'    | 2.00                     | 0.44              |
| 46:m2:116:OMU:O5'  | 46:m2:116:OMU:H6   | 2.17                     | 0.44              |
| 46:m2:733:G:OP1    | 46:m2:735:C:N4     | 2.51                     | 0.44              |
| 46:m2:1008:C:H2'   | 46:m2:1009:C:C6    | 2.53                     | 0.44              |
| 46:m2:1267:A:O2'   | 46:m2:1329:G:OP2   | 2.29                     | 0.44              |
| 61:D3:16:LYS:HG2   | 61:D3:23:ILE:HD13  | 2.00                     | 0.44              |
| 66:I3:234:ASP:HB3  | 66:I3:252:THR:HB   | 2.00                     | 0.44              |
| 67:J3:200:ARG:O    | 69:L3:54:ARG:NH1   | 2.39                     | 0.44              |
| 70:M3:25:ALA:O     | 70:M3:30:GLY:N     | 2.46                     | 0.44              |
| 79:m:126:VAL:HG21  | 79:m:142:LEU:HD13  | 1.99                     | 0.44              |
| 8:H1:94:PHE:CE2    | 8:H1:96:ARG:HB2    | 2.53                     | 0.44              |
| 9:A2:227:A:N6      | 9:A2:242:U:O4'     | 2.51                     | 0.44              |
| 9:A2:1207:G:O2'    | 9:A2:4004:U:OP1    | 2.30                     | 0.44              |
| 9:A2:1621:G:O2'    | 9:A2:1622:C:O4'    | 2.35                     | 0.44              |
| 9:A2:1744:A:H2'    | 9:A2:1745:A:C8     | 2.53                     | 0.44              |
| 9:A2:2241:G:H2'    | 9:A2:2242:G:H8     | 1.82                     | 0.44              |
| 9:A2:2587:A:H2'    | 9:A2:2588:A:C8     | 2.52                     | 0.44              |
| 9:A2:3523:A2M:H1'  | 9:A2:3523:A2M:HM'3 | 1.72                     | 0.44              |
| 9:A2:4194:U:O2'    | 12:D2:220:GLY:O    | 2.35                     | 0.44              |
| 9:A2:4420:G:OP1    | 17:I2:168:TYR:OH   | 2.25                     | 0.44              |
| 14:F2:134:PRO:HB3  | 14:F2:150:LEU:HD11 | 2.00                     | 0.44              |
| 18:J2:119:VAL:HG12 | 18:J2:146:ILE:HG12 | 1.99                     | 0.44              |
| 43:i2:33:LEU:HA    | 43:i2:38:LYS:HG2   | 1.99                     | 0.44              |
| 46:m2:416:A:H2'    | 46:m2:417:A:C8     | 2.51                     | 0.44              |
| 46:m2:832:A:OP2    | 46:m2:848:G:N2     | 2.51                     | 0.44              |
| 46:m2:1203:U:H2'   | 46:m2:1204:U:C6    | 2.53                     | 0.44              |
| 46:m2:1507:U:H5'   | 46:m2:1508:A:H5'   | 1.99                     | 0.44              |
| 46:m2:1538:G:H2'   | 46:m2:1539:A:H8    | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:1806:U:H2'   | 46:m2:1807:G:C8    | 2.52                     | 0.44              |
| 49:q2:37:VAL:HG12  | 49:q2:50:ILE:HA    | 1.99                     | 0.44              |
| 51:w2:35:ARG:HH21  | 51:w2:63:THR:HG21  | 1.83                     | 0.44              |
| 67:J3:252:THR:OG1  | 67:J3:254:ASP:OD1  | 2.29                     | 0.44              |
| 76:S3:64:CYS:HA    | 76:S3:73:LEU:HA    | 2.00                     | 0.44              |
| 4:D1:3:ARG:NH2     | 9:A2:4083:U:OP2    | 2.51                     | 0.44              |
| 8:H1:32:GLN:NE2    | 9:A2:3728:C:OP1    | 2.50                     | 0.44              |
| 9:A2:162:A:H2'     | 9:A2:163:A:C8      | 2.53                     | 0.44              |
| 9:A2:287:U:H2'     | 9:A2:288:G:C8      | 2.53                     | 0.44              |
| 9:A2:1681:C:H2'    | 9:A2:1682:G:O4'    | 2.17                     | 0.44              |
| 9:A2:2229:G:O4'    | 26:R2:47:ARG:NH2   | 2.51                     | 0.44              |
| 9:A2:3469:A:N3     | 9:A2:4190:G:O2'    | 2.45                     | 0.44              |
| 9:A2:3955:C:H3'    | 9:A2:3957:G:H21    | 1.83                     | 0.44              |
| 9:A2:4238:G:O6     | 9:A2:4369:A:N6     | 2.51                     | 0.44              |
| 25:Q2:82:ILE:HA    | 68:K3:131:ARG:HB3  | 1.99                     | 0.44              |
| 46:m2:126:G:OP2    | 68:K3:195:LYS:NZ   | 2.51                     | 0.44              |
| 46:m2:951:G:H2'    | 46:m2:952:C:O4'    | 2.18                     | 0.44              |
| 46:m2:1027:U:O2    | 46:m2:1162:U:O2'   | 2.27                     | 0.44              |
| 46:m2:1138:U:H2'   | 46:m2:1139:U:C6    | 2.53                     | 0.44              |
| 46:m2:1229:G:H21   | 46:m2:1637:C:H4'   | 1.83                     | 0.44              |
| 46:m2:1718:C:H2'   | 46:m2:1719:C:H6    | 1.83                     | 0.44              |
| 57:y2:112:LEU:HD22 | 57:y2:119:LEU:HD13 | 1.99                     | 0.44              |
| 63:F3:29:CYS:HB3   | 72:O3:146:ARG:HG3  | 1.99                     | 0.44              |
| 68:K3:7:PHE:HB2    | 68:K3:124:LEU:HD13 | 1.99                     | 0.44              |
| 68:K3:78:SER:HB3   | 68:K3:92:ARG:HG2   | 1.99                     | 0.44              |
| 71:N3:75:LEU:HD22  | 71:N3:80:LEU:HD21  | 2.00                     | 0.44              |
| 79:m:438:LYS:HG2   | 79:m:441:LEU:HD23  | 2.00                     | 0.44              |
| 79:m:774:GLN:HG3   | 79:m:781:PHE:HB3   | 2.00                     | 0.44              |
| 1:A1:187:LYS:NZ    | 9:A2:1885:C:O2'    | 2.50                     | 0.43              |
| 9:A2:1320:U:H2'    | 9:A2:1321:A:C8     | 2.51                     | 0.43              |
| 9:A2:1561:G:H2'    | 9:A2:1562:G:C8     | 2.52                     | 0.43              |
| 9:A2:1778:G:O2'    | 9:A2:1779:C:OP1    | 2.35                     | 0.43              |
| 9:A2:3739:G:H2'    | 9:A2:3740:G:C8     | 2.53                     | 0.43              |
| 9:A2:4290:U:H2'    | 9:A2:4291:G:N3     | 2.33                     | 0.43              |
| 9:A2:4332:G:H2'    | 9:A2:4333:A:C8     | 2.53                     | 0.43              |
| 12:D2:102:LEU:HB3  | 12:D2:107:MET:HE3  | 1.99                     | 0.43              |
| 12:D2:137:ILE:HD11 | 12:D2:149:LYS:HB2  | 1.99                     | 0.43              |
| 12:D2:181:LYS:HB3  | 12:D2:184:ARG:HB2  | 2.00                     | 0.43              |
| 20:L2:36:ASN:N     | 20:L2:40:GLN:OE1   | 2.42                     | 0.43              |
| 24:P2:45:ILE:HG21  | 24:P2:53:PRO:HB3   | 2.00                     | 0.43              |
| 38:d2:37:CYS:HA    | 38:d2:45:ARG:HB3   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:m2:114:G:OP2    | 51:w2:67:SER:OG    | 2.34                     | 0.43              |
| 46:m2:1597:U:H2'   | 46:m2:1598:U:C6    | 2.53                     | 0.43              |
| 46:m2:1716:U:H2'   | 46:m2:1717:A:C8    | 2.53                     | 0.43              |
| 57:y2:22:VAL:HB    | 57:y2:71:ARG:HG3   | 2.00                     | 0.43              |
| 57:y2:68:ILE:HG21  | 57:y2:88:ILE:HG22  | 2.00                     | 0.43              |
| 58:A3:82:TRP:O     | 58:A3:87:GLN:NE2   | 2.51                     | 0.43              |
| 66:I3:133:ASN:OD1  | 66:I3:134:THR:N    | 2.48                     | 0.43              |
| 66:I3:285:GLN:O    | 66:I3:303:THR:N    | 2.50                     | 0.43              |
| 70:M3:58:GLU:H     | 70:M3:58:GLU:HG2   | 1.51                     | 0.43              |
| 72:O3:100:THR:OG1  | 72:O3:105:THR:O    | 2.36                     | 0.43              |
| 3:C1:174:LYS:HB3   | 3:C1:174:LYS:HE2   | 1.78                     | 0.43              |
| 9:A2:138:C:H2'     | 9:A2:139:G:C8      | 2.53                     | 0.43              |
| 9:A2:141:C:H2'     | 9:A2:142:G:C8      | 2.53                     | 0.43              |
| 9:A2:932:C:H2'     | 9:A2:933:G:C8      | 2.53                     | 0.43              |
| 9:A2:1621:G:H2'    | 9:A2:1622:C:C6     | 2.53                     | 0.43              |
| 16:H2:185:PRO:HG2  | 16:H2:188:ILE:HD12 | 2.01                     | 0.43              |
| 18:J2:127:ARG:HB2  | 18:J2:139:TYR:HB3  | 1.99                     | 0.43              |
| 32:X2:43:PRO:HA    | 32:X2:46:LEU:HD12  | 2.00                     | 0.43              |
| 33:Y2:85:LEU:HD22  | 33:Y2:111:ILE:HG23 | 2.00                     | 0.43              |
| 46:m2:622:G:N2     | 46:m2:649:U:OP1    | 2.51                     | 0.43              |
| 46:m2:1316:U:H2'   | 55:v2:2:LEU:HD12   | 1.99                     | 0.43              |
| 46:m2:1612:G:OP2   | 46:m2:1625:A:N6    | 2.46                     | 0.43              |
| 46:m2:1618:U:OP2   | 56:x2:43:ARG:NH2   | 2.45                     | 0.43              |
| 50:r2:80:ILE:HG13  | 50:r2:81:THR:HG23  | 2.00                     | 0.43              |
| 68:K3:74:ARG:HG2   | 68:K3:96:SER:HB3   | 2.00                     | 0.43              |
| 69:L3:44:TRP:HA    | 69:L3:47:LYS:HG2   | 1.99                     | 0.43              |
| 74:Q3:114:MET:HA   | 74:Q3:117:VAL:HG22 | 2.00                     | 0.43              |
| 79:m:396:TYR:HB3   | 79:m:416:PHE:HE2   | 1.83                     | 0.43              |
| 83:t:30:LEU:O      | 83:t:34:SER:HB3    | 2.18                     | 0.43              |
| 83:t:69:LEU:HD22   | 83:t:96:ALA:HB2    | 1.99                     | 0.43              |
| 84:u:165:GLN:HE22  | 84:u:195:LEU:HD11  | 1.83                     | 0.43              |
| 2:B1:190:LEU:HB3   | 2:B1:199:CYS:HB3   | 2.00                     | 0.43              |
| 6:F1:92:ARG:HH12   | 9:A2:109:G:H5'     | 1.84                     | 0.43              |
| 9:A2:819:C:H5''    | 21:M2:74:ARG:NH1   | 2.33                     | 0.43              |
| 9:A2:1881:G:H2'    | 9:A2:1882:U:H6     | 1.83                     | 0.43              |
| 9:A2:2040:A:H2'    | 9:A2:2041:G:C8     | 2.51                     | 0.43              |
| 9:A2:3526:C:H2'    | 9:A2:3527:A:C8     | 2.50                     | 0.43              |
| 9:A2:3697:A:O5'    | 85:L1:105:LYS:NZ   | 2.48                     | 0.43              |
| 9:A2:3888:G:H1     | 9:A2:3941:U:H3     | 1.65                     | 0.43              |
| 9:A2:4381:A:OP2    | 9:A2:4714:G:N1     | 2.40                     | 0.43              |
| 17:I2:196:LEU:HD23 | 17:I2:202:LEU:HD23 | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:j2:56:HIS:ND1   | 44:j2:63:THR:HG22  | 2.33                     | 0.43              |
| 46:m2:540:U:O2     | 46:m2:548:G:N2     | 2.51                     | 0.43              |
| 46:m2:818:A:OP2    | 69:L3:10:ARG:NH2   | 2.40                     | 0.43              |
| 46:m2:1523:C:H5'   | 56:x2:126:VAL:HB   | 2.00                     | 0.43              |
| 49:q2:42:THR:H     | 49:q2:46:THR:HG22  | 1.83                     | 0.43              |
| 60:C3:54:VAL:O     | 60:C3:87:ARG:HA    | 2.19                     | 0.43              |
| 68:K3:137:ARG:HD2  | 68:K3:178:ARG:HD3  | 1.99                     | 0.43              |
| 81:k:91:ASP:OD1    | 81:k:91:ASP:N      | 2.52                     | 0.43              |
| 2:B1:44:ASP:OD1    | 2:B1:45:ILE:N      | 2.48                     | 0.43              |
| 3:C1:68:ALA:O      | 3:C1:72:THR:HG23   | 2.18                     | 0.43              |
| 9:A2:18:C:H2'      | 9:A2:19:G:C8       | 2.53                     | 0.43              |
| 9:A2:1437:G:H21    | 9:A2:1455:A:H1'    | 1.83                     | 0.43              |
| 9:A2:2169:G:H2'    | 9:A2:2170:U:C6     | 2.52                     | 0.43              |
| 9:A2:3481:A2M:HM'3 | 9:A2:3481:A2M:H1'  | 1.80                     | 0.43              |
| 9:A2:3563:G:O2'    | 9:A2:3565:OMC:N4   | 2.51                     | 0.43              |
| 9:A2:3595:G:O2'    | 9:A2:3726:G:N1     | 2.42                     | 0.43              |
| 9:A2:4693:C:OP2    | 9:A2:4696:C:N4     | 2.50                     | 0.43              |
| 9:A2:4700:C:H4'    | 9:A2:4701:G:C8     | 2.54                     | 0.43              |
| 11:C2:69:U:H2'     | 11:C2:70:G:O4'     | 2.18                     | 0.43              |
| 27:S2:82:ILE:HB    | 27:S2:85:VAL:HB    | 2.00                     | 0.43              |
| 46:m2:14:C:H2'     | 46:m2:15:U:C6      | 2.53                     | 0.43              |
| 46:m2:444:C:N4     | 46:m2:451:A:H62    | 2.11                     | 0.43              |
| 46:m2:607:A:N3     | 46:m2:641:C:H1'    | 2.33                     | 0.43              |
| 46:m2:1283:G:N2    | 46:m2:1319:C:O2    | 2.52                     | 0.43              |
| 59:B3:116:ASP:OD1  | 59:B3:116:ASP:N    | 2.51                     | 0.43              |
| 79:m:375:PRO:HG3   | 79:m:491:HIS:H     | 1.83                     | 0.43              |
| 1:A1:173:ASN:HD21  | 9:A2:841:A:H62     | 1.67                     | 0.43              |
| 7:G1:118:MET:HE3   | 7:G1:122:ILE:HD11  | 2.00                     | 0.43              |
| 8:H1:140:LYS:HA    | 8:H1:143:ARG:HG2   | 1.99                     | 0.43              |
| 9:A2:86:U:H2'      | 9:A2:87:A:C8       | 2.53                     | 0.43              |
| 9:A2:434:A:H3'     | 9:A2:435:A:H8      | 1.83                     | 0.43              |
| 9:A2:1434:A:H5''   | 9:A2:2206:A:H5'    | 1.99                     | 0.43              |
| 9:A2:1659:C:H2'    | 9:A2:1660:A:C8     | 2.49                     | 0.43              |
| 9:A2:2395:G:H2'    | 9:A2:2396:A:C8     | 2.53                     | 0.43              |
| 9:A2:2429:A:N6     | 44:j2:41:PHE:O     | 2.50                     | 0.43              |
| 9:A2:3491:C:H2'    | 9:A2:3492:A:H8     | 1.83                     | 0.43              |
| 9:A2:3709:C:H2'    | 9:A2:3710:U:C6     | 2.54                     | 0.43              |
| 9:A2:4048:A:N7     | 9:A2:4099:5MC:N4   | 2.67                     | 0.43              |
| 9:A2:4612:A:H5'    | 13:E2:128:LYS:HD2  | 2.00                     | 0.43              |
| 11:C2:106:G:H4'    | 11:C2:137:A:H5'    | 1.99                     | 0.43              |
| 16:H2:171:PHE:HA   | 16:H2:182:VAL:HG12 | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:S2:54:GLU:OE1   | 27:S2:108:ARG:NH1  | 2.43                     | 0.43              |
| 44:j2:7:LYS:HE2    | 44:j2:7:LYS:HB3    | 1.82                     | 0.43              |
| 46:m2:116:OMU:HM23 | 46:m2:116:OMU:H1'  | 1.56                     | 0.43              |
| 46:m2:159:A:H2     | 46:m2:469:G:H21    | 1.66                     | 0.43              |
| 46:m2:527:A:O3'    | 77:T3:31:ARG:NH2   | 2.50                     | 0.43              |
| 46:m2:1239:C:H42   | 46:m2:1522:G:H1    | 1.66                     | 0.43              |
| 46:m2:1708:G:O2'   | 46:m2:1852:A:O3'   | 2.36                     | 0.43              |
| 64:G3:37:ASP:OD1   | 64:G3:37:ASP:N     | 2.49                     | 0.43              |
| 64:G3:45:ASN:OD1   | 64:G3:45:ASN:N     | 2.51                     | 0.43              |
| 65:H3:16:GLN:HE21  | 65:H3:16:GLN:HB2   | 1.62                     | 0.43              |
| 5:E1:50:PHE:HD1    | 5:E1:70:VAL:HG12   | 1.83                     | 0.43              |
| 9:A2:162:A:H2'     | 9:A2:163:A:H8      | 1.84                     | 0.43              |
| 9:A2:372:A:O2'     | 38:d2:45:ARG:NH2   | 2.52                     | 0.43              |
| 9:A2:1160:C:H2'    | 9:A2:1161:G:H8     | 1.84                     | 0.43              |
| 9:A2:1389:G:HO2'   | 9:A2:1391:U:H6     | 1.66                     | 0.43              |
| 9:A2:1905:G:H2'    | 9:A2:1906:G:C8     | 2.53                     | 0.43              |
| 9:A2:2299:G:H1     | 11:C2:124:U:H4'    | 1.83                     | 0.43              |
| 9:A2:2652:G:H2'    | 9:A2:2653:G:C8     | 2.53                     | 0.43              |
| 10:B2:15:C:H2'     | 10:B2:16:A:C8      | 2.53                     | 0.43              |
| 10:B2:79:U:H3      | 10:B2:97:G:H1      | 1.66                     | 0.43              |
| 14:F2:294:LYS:HA   | 14:F2:299:GLN:HE21 | 1.82                     | 0.43              |
| 30:V2:111:ALA:O    | 30:V2:115:ARG:HG2  | 2.18                     | 0.43              |
| 46:m2:690:U:H1'    | 46:m2:691:U:C5     | 2.54                     | 0.43              |
| 46:m2:1268:C:C4    | 46:m2:1519:G:N2    | 2.86                     | 0.43              |
| 46:m2:1281:C:H2'   | 46:m2:1282:G:C8    | 2.53                     | 0.43              |
| 46:m2:1819:G:H2'   | 46:m2:1820:A:C8    | 2.54                     | 0.43              |
| 53:o2:5:LEU:HD13   | 61:D3:41:ARG:HA    | 2.00                     | 0.43              |
| 58:A3:25:LYS:HD2   | 58:A3:55:ARG:HG2   | 2.00                     | 0.43              |
| 60:C3:46:LYS:HD2   | 60:C3:46:LYS:HA    | 1.90                     | 0.43              |
| 63:F3:49:ALA:HB2   | 72:O3:117:ARG:HG2  | 1.99                     | 0.43              |
| 66:I3:270:LEU:HD21 | 66:I3:310:TRP:CE2  | 2.54                     | 0.43              |
| 69:L3:32:ILE:HG12  | 69:L3:37:LEU:HB2   | 2.00                     | 0.43              |
| 72:O3:62:VAL:HG21  | 72:O3:67:ASP:HB2   | 2.01                     | 0.43              |
| 73:P3:60:LYS:NZ    | 76:S3:23:ARG:O     | 2.51                     | 0.43              |
| 79:m:608:PHE:HE1   | 79:m:700:ARG:HB2   | 1.83                     | 0.43              |
| 9:A2:11:G:H2'      | 9:A2:12:A:C8       | 2.54                     | 0.43              |
| 9:A2:262:G:H2'     | 9:A2:263:G:C8      | 2.54                     | 0.43              |
| 9:A2:1037:C:H2'    | 9:A2:1038:G:C8     | 2.54                     | 0.43              |
| 9:A2:1317:G:H2'    | 9:A2:1318:C:C6     | 2.53                     | 0.43              |
| 9:A2:1434:A:H2'    | 9:A2:1435:U:C6     | 2.54                     | 0.43              |
| 9:A2:1880:C:H2'    | 9:A2:1881:G:H8     | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:3314:C:H2'    | 9:A2:3315:G:H8     | 1.83                     | 0.43              |
| 9:A2:4294:U:H2'    | 9:A2:4295:G:C8     | 2.54                     | 0.43              |
| 11:C2:19:C:H2'     | 11:C2:20:A:C8      | 2.50                     | 0.43              |
| 20:L2:130:ASN:O    | 20:L2:130:ASN:ND2  | 2.51                     | 0.43              |
| 26:R2:82:THR:HA    | 26:R2:87:MET:HE3   | 2.00                     | 0.43              |
| 26:R2:100:VAL:HG23 | 26:R2:134:LYS:HB3  | 2.00                     | 0.43              |
| 27:S2:34:LEU:HD21  | 27:S2:47:MET:HG2   | 1.99                     | 0.43              |
| 28:T2:18:TYR:HA    | 28:T2:21:ARG:HH11  | 1.83                     | 0.43              |
| 46:m2:738:C:H2'    | 46:m2:739:G:C5     | 2.54                     | 0.43              |
| 46:m2:1167:G:OP2   | 46:m2:1167:G:N2    | 2.31                     | 0.43              |
| 46:m2:1242:A:N1    | 56:x2:100:LYS:N    | 2.67                     | 0.43              |
| 46:m2:1242:A:H2'   | 46:m2:1243:A:C4    | 2.54                     | 0.43              |
| 48:p2:57:ILE:HB    | 48:p2:60:ASP:HB2   | 2.01                     | 0.43              |
| 50:r2:112:HIS:NE2  | 50:r2:237:SER:OG   | 2.45                     | 0.43              |
| 81:k:105:THR:HG23  | 81:k:108:GLU:H     | 1.84                     | 0.43              |
| 84:u:73:THR:O      | 84:u:74:ARG:NH1    | 2.40                     | 0.43              |
| 85:L1:58:THR:HG21  | 85:L1:152:LYS:HE2  | 2.01                     | 0.43              |
| 1:A1:149:LYS:HB2   | 22:N2:133:ALA:HB3  | 2.01                     | 0.43              |
| 2:B1:180:PRO:HG3   | 2:B1:219:VAL:HG13  | 2.00                     | 0.43              |
| 3:C1:142:ASP:N     | 3:C1:142:ASP:OD1   | 2.52                     | 0.43              |
| 9:A2:168:C:H2'     | 9:A2:169:A:H8      | 1.84                     | 0.43              |
| 9:A2:1153:U:OP1    | 29:U2:8:THR:OG1    | 2.33                     | 0.43              |
| 9:A2:1652:A:N3     | 9:A2:2038:G:O2'    | 2.46                     | 0.43              |
| 9:A2:1695:C:O2'    | 9:A2:1738:C:N3     | 2.48                     | 0.43              |
| 9:A2:1801:A:O2'    | 9:A2:1802:G:O4'    | 2.20                     | 0.43              |
| 9:A2:2211:G:H2'    | 9:A2:2212:G:C8     | 2.53                     | 0.43              |
| 9:A2:3379:A2M:OP2  | 37:c2:68:ARG:NH1   | 2.52                     | 0.43              |
| 9:A2:3567:C:H2'    | 9:A2:3568:U:C6     | 2.53                     | 0.43              |
| 9:A2:3572:G:H2'    | 9:A2:3573:A:C8     | 2.53                     | 0.43              |
| 9:A2:3826:U:H2'    | 9:A2:3827:G:C8     | 2.50                     | 0.43              |
| 9:A2:4244:C:N3     | 9:A2:4271:U:O4     | 2.51                     | 0.43              |
| 13:E2:200:ARG:HH21 | 13:E2:205:VAL:HG12 | 1.84                     | 0.43              |
| 46:m2:929:C:H2'    | 46:m2:930:G:C8     | 2.54                     | 0.43              |
| 46:m2:1042:G:H2'   | 46:m2:1043:G:H8    | 1.84                     | 0.43              |
| 46:m2:1191:A:H2'   | 46:m2:1192:A:C8    | 2.52                     | 0.43              |
| 47:n2:12:C:H2'     | 47:n2:13:G:C8      | 2.53                     | 0.43              |
| 53:o2:38:ILE:HD13  | 53:o2:47:TYR:HB3   | 2.01                     | 0.43              |
| 66:I3:302:TYR:HE1  | 66:I3:308:ARG:HB2  | 1.83                     | 0.43              |
| 6:F1:36:ARG:HH21   | 9:A2:1178:U:H5''   | 1.82                     | 0.43              |
| 6:F1:103:ARG:NH1   | 9:A2:75:G:O6       | 2.52                     | 0.43              |
| 8:H1:90:ASN:HB2    | 9:A2:3584:A:H5''   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:H1:135:ILE:HG23 | 8:H1:142:ILE:HD13  | 1.99                     | 0.43              |
| 9:A2:221:C:H2'    | 9:A2:222:C:C6      | 2.53                     | 0.43              |
| 9:A2:849:G:H2'    | 9:A2:850:G:C8      | 2.54                     | 0.43              |
| 9:A2:1303:G:H2'   | 9:A2:1304:A:H8     | 1.82                     | 0.43              |
| 9:A2:1458:C:H2'   | 9:A2:1459:A:C8     | 2.53                     | 0.43              |
| 9:A2:2414:A:N6    | 9:A2:2430:G:H21    | 2.16                     | 0.43              |
| 9:A2:3938:C:H2'   | 9:A2:3939:G:C8     | 2.54                     | 0.43              |
| 9:A2:4128:C:O2'   | 9:A2:4130:G:OP2    | 2.31                     | 0.43              |
| 9:A2:4258:G:H22   | 79:m:800:ARG:HB3   | 1.84                     | 0.43              |
| 9:A2:4541:G:HO2'  | 9:A2:4542:G:H8     | 1.66                     | 0.43              |
| 14:F2:211:TYR:HE1 | 14:F2:229:LEU:HB3  | 1.84                     | 0.43              |
| 15:G2:45:ASN:OD1  | 15:G2:68:ARG:NH2   | 2.52                     | 0.43              |
| 15:G2:237:GLU:HG2 | 15:G2:241:LYS:HE2  | 2.01                     | 0.43              |
| 33:Y2:26:ASP:OD1  | 33:Y2:26:ASP:N     | 2.47                     | 0.43              |
| 34:Z2:36:ARG:NE   | 34:Z2:79:GLY:O     | 2.51                     | 0.43              |
| 46:m2:184:G:H2'   | 46:m2:185:G:C8     | 2.50                     | 0.43              |
| 46:m2:319:C:OP2   | 68:K3:183:ARG:NH1  | 2.51                     | 0.43              |
| 46:m2:530:A:H2'   | 46:m2:531:A:C8     | 2.53                     | 0.43              |
| 46:m2:862:G:H21   | 73:P3:107:SER:HB2  | 1.84                     | 0.43              |
| 46:m2:1176:U:H2'  | 46:m2:1177:G:H8    | 1.84                     | 0.43              |
| 50:r2:21:ASP:N    | 50:r2:21:ASP:OD1   | 2.50                     | 0.43              |
| 62:E3:68:LYS:HB3  | 62:E3:91:LEU:HD22  | 2.01                     | 0.43              |
| 68:K3:64:LYS:NZ   | 68:K3:82:SER:H     | 2.17                     | 0.43              |
| 71:N3:45:LEU:HB3  | 71:N3:49:GLN:HG3   | 2.00                     | 0.43              |
| 4:D1:57:TYR:HD1   | 4:D1:130:HIS:HA    | 1.84                     | 0.43              |
| 5:E1:158:SER:HB2  | 5:E1:161:GLU:HG2   | 2.01                     | 0.43              |
| 8:H1:202:ARG:HD2  | 14:F2:112:HIS:CE1  | 2.54                     | 0.43              |
| 9:A2:347:A:H2'    | 9:A2:348:G:C8      | 2.54                     | 0.43              |
| 9:A2:498:G:N2     | 9:A2:499:U:O4      | 2.48                     | 0.43              |
| 9:A2:1287:C:H2'   | 9:A2:1288:G:C8     | 2.54                     | 0.43              |
| 9:A2:2016:G:O2'   | 9:A2:2017:G:O4'    | 2.30                     | 0.43              |
| 9:A2:2168:U:H2'   | 9:A2:2169:G:C8     | 2.54                     | 0.43              |
| 9:A2:4110:C:H2'   | 9:A2:4111:U:C6     | 2.53                     | 0.43              |
| 12:D2:193:ARG:HE  | 12:D2:193:ARG:H    | 1.66                     | 0.43              |
| 40:f2:6:THR:H     | 40:f2:9:ILE:HD11   | 1.84                     | 0.43              |
| 46:m2:26:U:H2'    | 46:m2:27:A2M:H8    | 2.01                     | 0.43              |
| 46:m2:65:C:H41    | 46:m2:169:U:HO2'   | 1.65                     | 0.43              |
| 46:m2:1840:U:O2   | 72:O3:150:ARG:NE   | 2.50                     | 0.43              |
| 51:w2:127:THR:HB  | 51:w2:144:LYS:HB3  | 2.00                     | 0.43              |
| 54:s2:142:SER:HB3 | 64:G3:50:VAL:HG22  | 2.00                     | 0.43              |
| 61:D3:16:LYS:H    | 67:J3:259:THR:HG21 | 1.84                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:E3:100:VAL:HB   | 62:E3:122:VAL:HG13 | 2.01                     | 0.43              |
| 69:L3:137:VAL:HG22 | 69:L3:157:ILE:HG12 | 2.01                     | 0.43              |
| 83:t:47:ALA:HB3    | 83:t:63:PHE:HD2    | 1.84                     | 0.43              |
| 2:B1:89:ARG:NH1    | 11:C2:155:C:OP2    | 2.52                     | 0.42              |
| 3:C1:93:ARG:HD3    | 3:C1:143:GLU:HB3   | 2.00                     | 0.42              |
| 4:D1:200:ILE:HG21  | 4:D1:212:LEU:HD11  | 2.01                     | 0.42              |
| 9:A2:159:C:H5'     | 37:c2:25:ARG:HH21  | 1.84                     | 0.42              |
| 9:A2:286:U:H2'     | 9:A2:287:U:C6      | 2.54                     | 0.42              |
| 9:A2:1082:A:O2'    | 30:V2:109:TYR:OH   | 2.30                     | 0.42              |
| 9:A2:1886:C:O2     | 19:K2:45:GLN:NE2   | 2.43                     | 0.42              |
| 9:A2:2103:G:OP1    | 9:A2:2106:C:N4     | 2.52                     | 0.42              |
| 9:A2:2125:A:C8     | 32:X2:39:LYS:HE3   | 2.54                     | 0.42              |
| 9:A2:2414:A:N6     | 9:A2:2428:G:O4'    | 2.52                     | 0.42              |
| 9:A2:4295:G:H2'    | 9:A2:4296:G:H8     | 1.83                     | 0.42              |
| 9:A2:4313:G:H2'    | 9:A2:4314:C:C6     | 2.54                     | 0.42              |
| 16:H2:260:VAL:HA   | 16:H2:263:GLN:HE21 | 1.85                     | 0.42              |
| 45:k2:6:GLN:O      | 45:k2:10:VAL:HG22  | 2.20                     | 0.42              |
| 46:m2:921:A:O2'    | 46:m2:1022:A:N1    | 2.48                     | 0.42              |
| 57:y2:100:VAL:HG12 | 57:y2:101:ASP:H    | 1.84                     | 0.42              |
| 58:A3:35:GLY:HA3   | 58:A3:99:LEU:HA    | 2.01                     | 0.42              |
| 58:A3:36:VAL:HG13  | 58:A3:40:TYR:HD2   | 1.84                     | 0.42              |
| 66:I3:17:TRP:HB2   | 66:I3:36:ARG:HG2   | 2.01                     | 0.42              |
| 84:u:136:ILE:HG22  | 84:u:137:LEU:HG    | 2.00                     | 0.42              |
| 85:L1:68:LEU:HD11  | 85:L1:90:LEU:HD11  | 2.01                     | 0.42              |
| 4:D1:205:PRO:HG2   | 4:D1:208:LYS:HG2   | 2.01                     | 0.42              |
| 9:A2:750:G:H2'     | 9:A2:751:G:C8      | 2.55                     | 0.42              |
| 9:A2:847:G:H2'     | 9:A2:848:G:H8      | 1.83                     | 0.42              |
| 9:A2:2084:U:H2'    | 9:A2:2085:G:O4'    | 2.19                     | 0.42              |
| 9:A2:2366:A:H2'    | 9:A2:2367:G:H8     | 1.85                     | 0.42              |
| 9:A2:2505:G:H2'    | 9:A2:2506:G:C8     | 2.54                     | 0.42              |
| 9:A2:2598:U:H2'    | 9:A2:2599:A:C8     | 2.54                     | 0.42              |
| 9:A2:3314:C:H2'    | 9:A2:3315:G:C8     | 2.54                     | 0.42              |
| 9:A2:3379:A2M:HM'3 | 9:A2:3379:A2M:H1'  | 1.80                     | 0.42              |
| 9:A2:3831:G:H2'    | 9:A2:3832:G:H8     | 1.85                     | 0.42              |
| 9:A2:4215:U:H2'    | 9:A2:4216:A:H8     | 1.84                     | 0.42              |
| 9:A2:4661:G:O2'    | 9:A2:4680:A:N6     | 2.52                     | 0.42              |
| 10:B2:110:G:H2'    | 10:B2:111:C:C6     | 2.54                     | 0.42              |
| 13:E2:222:VAL:O    | 13:E2:343:ARG:NH1  | 2.51                     | 0.42              |
| 16:H2:186:LEU:HD22 | 16:H2:257:GLN:HG2  | 2.01                     | 0.42              |
| 26:R2:80:PRO:HA    | 26:R2:98:PHE:HA    | 2.00                     | 0.42              |
| 27:S2:115:ARG:HA   | 27:S2:118:ILE:HG22 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:U2:100:ILE:HG12 | 29:U2:123:ILE:HB   | 2.00                     | 0.42              |
| 46:m2:126:G:C8     | 68:K3:199:THR:HG21 | 2.54                     | 0.42              |
| 46:m2:1095:A:H2'   | 46:m2:1096:C:H6    | 1.84                     | 0.42              |
| 46:m2:1547:A:N3    | 46:m2:1673:G:O2'   | 2.44                     | 0.42              |
| 47:n2:27:C:H2'     | 47:n2:28:U:H6      | 1.84                     | 0.42              |
| 55:v2:58:VAL:HG11  | 55:v2:69:TRP:HB3   | 2.01                     | 0.42              |
| 67:J3:209:VAL:HB   | 67:J3:210:PRO:HD3  | 2.01                     | 0.42              |
| 79:m:100:ASN:HB2   | 79:m:468:ILE:HD11  | 2.00                     | 0.42              |
| 80:j:45:MET:HA     | 80:j:48:ARG:HG2    | 2.00                     | 0.42              |
| 9:A2:260:C:H2'     | 9:A2:261:G:H8      | 1.84                     | 0.42              |
| 9:A2:1084:G:H1'    | 9:A2:1909:G:H21    | 1.85                     | 0.42              |
| 9:A2:1112:C:H2'    | 9:A2:1113:G:C8     | 2.54                     | 0.42              |
| 9:A2:1365:G:N2     | 9:A2:1387:B9B:O2'  | 2.51                     | 0.42              |
| 9:A2:1613:G:H2'    | 9:A2:1614:C:H6     | 1.85                     | 0.42              |
| 9:A2:2006:C:H4'    | 9:A2:2007:G:C8     | 2.54                     | 0.42              |
| 9:A2:2202:U:H1'    | 9:A2:2499:A:H2     | 1.83                     | 0.42              |
| 9:A2:3945:PSU:N1   | 9:A2:3981:G:O2'    | 2.42                     | 0.42              |
| 11:C2:141:C:H2'    | 11:C2:142:U:H6     | 1.84                     | 0.42              |
| 14:F2:170:LEU:HD23 | 14:F2:221:PHE:HZ   | 1.83                     | 0.42              |
| 31:W2:47:ILE:HB    | 31:W2:94:LEU:HG    | 2.01                     | 0.42              |
| 32:X2:33:ILE:HD11  | 32:X2:41:ARG:HB3   | 2.02                     | 0.42              |
| 45:k2:26:SER:OG    | 45:k2:28:GLU:OE1   | 2.30                     | 0.42              |
| 46:m2:533:A:H2'    | 46:m2:534:C:C6     | 2.54                     | 0.42              |
| 46:m2:1674:U:H2'   | 46:m2:1675:U:C6    | 2.54                     | 0.42              |
| 49:q2:190:LEU:HD12 | 49:q2:200:PRO:HG3  | 2.01                     | 0.42              |
| 53:o2:34:MET:HE1   | 53:o2:162:PRO:HB3  | 2.00                     | 0.42              |
| 55:v2:3:MET:SD     | 55:v2:3:MET:N      | 2.92                     | 0.42              |
| 57:y2:19:ALA:HB2   | 57:y2:75:GLY:HA3   | 2.01                     | 0.42              |
| 66:I3:99:ARG:NE    | 66:I3:135:LEU:O    | 2.52                     | 0.42              |
| 67:J3:144:SER:OG   | 67:J3:145:LYS:N    | 2.52                     | 0.42              |
| 74:Q3:16:ARG:O     | 74:Q3:19:GLN:NE2   | 2.52                     | 0.42              |
| 78:U3:105:TYR:HB3  | 78:U3:117:LEU:HB2  | 2.00                     | 0.42              |
| 85:L1:15:ARG:HD2   | 85:L1:15:ARG:HA    | 1.79                     | 0.42              |
| 3:C1:92:MET:HE3    | 3:C1:92:MET:HB2    | 1.90                     | 0.42              |
| 7:G1:17:PHE:HB3    | 9:A2:1723:C:C4     | 2.54                     | 0.42              |
| 7:G1:56:GLN:HG2    | 9:A2:4515:OMG:C5   | 2.55                     | 0.42              |
| 8:H1:9:GLU:HB2     | 37:c2:44:ILE:HG13  | 2.01                     | 0.42              |
| 9:A2:207:G:H2'     | 9:A2:208:A:C8      | 2.55                     | 0.42              |
| 9:A2:717:G:H2'     | 9:A2:718:A:H8      | 1.84                     | 0.42              |
| 9:A2:1318:C:H2'    | 9:A2:1319:G:C8     | 2.54                     | 0.42              |
| 9:A2:1347:A2M:HM'1 | 38:d2:11:ARG:HG2   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:A2:1360:A:H2     | 9:A2:2568:A:H8      | 1.67                     | 0.42              |
| 9:A2:2537:U:OP2    | 40:f2:10:LYS:NZ     | 2.52                     | 0.42              |
| 9:A2:3509:U:O2'    | 9:A2:4625:A:N3      | 2.53                     | 0.42              |
| 9:A2:3527:A:H2'    | 9:A2:3528:A:H8      | 1.84                     | 0.42              |
| 9:A2:4325:U:OP2    | 24:P2:15:ARG:NH2    | 2.47                     | 0.42              |
| 11:C2:60:G:O6      | 11:C2:96:C:O2'      | 2.28                     | 0.42              |
| 31:W2:28:VAL:HG21  | 31:W2:37:MET:HE3    | 2.02                     | 0.42              |
| 46:m2:12:U:H2'     | 46:m2:13:C:H6       | 1.84                     | 0.42              |
| 46:m2:466:A:H5'    | 46:m2:467:A:C8      | 2.54                     | 0.42              |
| 46:m2:677:U:H2'    | 46:m2:678:C:H6      | 1.84                     | 0.42              |
| 46:m2:1212:G:OP1   | 63:F3:85[B]:ARG:NH2 | 2.43                     | 0.42              |
| 46:m2:1678:U:H2'   | 46:m2:1679:U:O4'    | 2.19                     | 0.42              |
| 50:r2:11:ARG:HH12  | 50:r2:24:THR:HB     | 1.84                     | 0.42              |
| 66:I3:164:ILE:HD11 | 66:I3:221:LEU:HG    | 2.01                     | 0.42              |
| 68:K3:58:LYS:HA    | 68:K3:107:SER:HB2   | 2.00                     | 0.42              |
| 73:P3:80:ASP:OD1   | 73:P3:80:ASP:N      | 2.43                     | 0.42              |
| 76:S3:19:HIS:CD2   | 76:S3:21:LYS:H      | 2.38                     | 0.42              |
| 79:m:759:TYR:OH    | 79:m:772:GLU:OE1    | 2.37                     | 0.42              |
| 81:k:16:ARG:HH22   | 81:k:18:THR:HB      | 1.84                     | 0.42              |
| 1:A1:177:TYR:HB3   | 14:F2:318:PRO:HG2   | 2.02                     | 0.42              |
| 4:D1:4:ARG:NH1     | 9:A2:1668:UR3:O5'   | 2.48                     | 0.42              |
| 9:A2:7:C:H2'       | 9:A2:8:U:C6         | 2.54                     | 0.42              |
| 9:A2:132:G:N2      | 9:A2:136:C:N3       | 2.65                     | 0.42              |
| 9:A2:1026:G:H2'    | 9:A2:1027:G:H8      | 1.84                     | 0.42              |
| 9:A2:1291:C:H2'    | 9:A2:1292:G:C8      | 2.54                     | 0.42              |
| 9:A2:1314:C:H2'    | 19:K2:68:ARG:HH11   | 1.84                     | 0.42              |
| 9:A2:1774:G:O2'    | 9:A2:1775:G:H5'     | 2.19                     | 0.42              |
| 9:A2:3388:A:H2'    | 9:A2:3389:A:C8      | 2.55                     | 0.42              |
| 9:A2:3450:C:H2'    | 9:A2:3451:A:H8      | 1.84                     | 0.42              |
| 9:A2:3487:U:H2'    | 9:A2:3488:U:H6      | 1.85                     | 0.42              |
| 9:A2:3615:U:O2     | 9:A2:3616:A:N6      | 2.52                     | 0.42              |
| 9:A2:3721:U:H2'    | 9:A2:3722:C:C6      | 2.54                     | 0.42              |
| 10:B2:75:G:N2      | 10:B2:100:A:OP2     | 2.41                     | 0.42              |
| 13:E2:152:SER:HA   | 13:E2:155:LYS:HG2   | 2.01                     | 0.42              |
| 15:G2:103:LEU:HD11 | 15:G2:248:ARG:HH21  | 1.84                     | 0.42              |
| 32:X2:123:ASP:OD1  | 32:X2:124:GLU:N     | 2.52                     | 0.42              |
| 46:m2:164:A:H5'    | 68:K3:83:CYS:H      | 1.85                     | 0.42              |
| 46:m2:293:G:H1'    | 51:w2:41:GLY:HA3    | 2.01                     | 0.42              |
| 46:m2:563:A:H5''   | 69:L3:164:PRO:HG2   | 2.00                     | 0.42              |
| 46:m2:1440:A:H2'   | 46:m2:1441:A:C8     | 2.53                     | 0.42              |
| 46:m2:1520:C:P     | 46:m2:1521:U:H2'    | 2.59                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:m2:1525:C:H2'  | 46:m2:1526:G:C8   | 2.54                     | 0.42              |
| 46:m2:1595:C:H2'  | 46:m2:1596:A:C8   | 2.55                     | 0.42              |
| 53:o2:74:VAL:HG12 | 53:o2:121:LEU:HB3 | 2.01                     | 0.42              |
| 79:m:11:ILE:HD12  | 79:m:11:ILE:HA    | 1.95                     | 0.42              |
| 79:m:455:ARG:H    | 79:m:455:ARG:HD2  | 1.85                     | 0.42              |
| 80:j:127:ASN:ND2  | 80:j:151:THR:OG1  | 2.45                     | 0.42              |
| 84:u:48:VAL:HG21  | 84:u:54:LYS:HE3   | 2.02                     | 0.42              |
| 5:E1:33:LEU:HD23  | 5:E1:33:LEU:H     | 1.85                     | 0.42              |
| 6:F1:101:ARG:HH21 | 9:A2:76:A:H5'     | 1.84                     | 0.42              |
| 9:A2:417:G:HO2'   | 11:C2:16:G:H22    | 1.61                     | 0.42              |
| 9:A2:475:G:H2'    | 9:A2:476:G:H8     | 1.84                     | 0.42              |
| 9:A2:507:C:H2'    | 9:A2:508:G:C8     | 2.55                     | 0.42              |
| 9:A2:2377:G:H2'   | 9:A2:2378:A:H8    | 1.83                     | 0.42              |
| 9:A2:3563:G:N3    | 9:A2:3565:OMC:C4  | 2.87                     | 0.42              |
| 9:A2:3708:U:H2'   | 9:A2:3709:C:C6    | 2.55                     | 0.42              |
| 11:C2:50:C:H2'    | 40:f2:26:TRP:CH2  | 2.54                     | 0.42              |
| 12:D2:196:TRP:O   | 12:D2:198:ARG:N   | 2.53                     | 0.42              |
| 33:Y2:16:ARG:NE   | 33:Y2:18:LYS:O    | 2.52                     | 0.42              |
| 46:m2:15:U:H2'    | 46:m2:16:G:O4'    | 2.20                     | 0.42              |
| 46:m2:59:U:H5''   | 46:m2:505:C:N4    | 2.34                     | 0.42              |
| 46:m2:1630:C:H2'  | 46:m2:1631:C:C6   | 2.55                     | 0.42              |
| 54:s2:42:LYS:HG3  | 54:s2:44:LYS:H    | 1.85                     | 0.42              |
| 79:m:218:HIS:HB2  | 79:m:220:TRP:CD1  | 2.55                     | 0.42              |
| 79:m:696:MET:HE2  | 79:m:699:VAL:HG21 | 2.02                     | 0.42              |
| 80:j:120:GLU:HB2  | 80:j:159:GLN:HE22 | 1.85                     | 0.42              |
| 9:A2:20:U:H3'     | 9:A2:21:G:C8      | 2.51                     | 0.42              |
| 9:A2:321:U:H2'    | 9:A2:322:C:C6     | 2.55                     | 0.42              |
| 9:A2:757:U:C2     | 9:A2:758:G:C8     | 3.07                     | 0.42              |
| 9:A2:806:C:H2'    | 9:A2:807:G:C8     | 2.52                     | 0.42              |
| 9:A2:1430:G:H1'   | 9:A2:2268:A:N6    | 2.34                     | 0.42              |
| 9:A2:1667:G:N2    | 9:A2:1670:A:OP2   | 2.37                     | 0.42              |
| 9:A2:2041:G:H2'   | 9:A2:2042:G:C8    | 2.55                     | 0.42              |
| 9:A2:2110:G:O2'   | 11:C2:15:G:O2'    | 2.24                     | 0.42              |
| 9:A2:2127:U:H2'   | 9:A2:2128:C:C6    | 2.55                     | 0.42              |
| 9:A2:2129:A:H2'   | 9:A2:2130:A:C8    | 2.53                     | 0.42              |
| 9:A2:3488:U:H2'   | 9:A2:3489:C:H6    | 1.85                     | 0.42              |
| 9:A2:3942:U:H5'   | 43:i2:9:ARG:O     | 2.19                     | 0.42              |
| 9:A2:4298:U:OP1   | 20:L2:59:SER:N    | 2.38                     | 0.42              |
| 9:A2:4542:G:O6    | 9:A2:4568:U:C4    | 2.73                     | 0.42              |
| 10:B2:113:G:N2    | 15:G2:72:ASP:O    | 2.40                     | 0.42              |
| 13:E2:35:ASP:OD1  | 13:E2:184:GLN:NE2 | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:m2:1266:C:OP2  | 65:H3:27:ARG:NH2  | 2.46                     | 0.42              |
| 70:M3:49:LEU:HD11 | 70:M3:77:ILE:HG13 | 2.02                     | 0.42              |
| 84:u:3:ILE:O      | 84:u:30:GLY:N     | 2.44                     | 0.42              |
| 84:u:19:LYS:HE3   | 84:u:19:LYS:HB2   | 1.88                     | 0.42              |
| 9:A2:161:G:H2'    | 9:A2:162:A:C8     | 2.55                     | 0.42              |
| 9:A2:302:C:H2'    | 9:A2:303:C:C6     | 2.55                     | 0.42              |
| 9:A2:866:A:H61    | 9:A2:1895:G:P     | 2.43                     | 0.42              |
| 9:A2:2352:G:H2'   | 9:A2:2353:A:H8    | 1.84                     | 0.42              |
| 9:A2:2403:G:H2'   | 9:A2:2404:G:H8    | 1.83                     | 0.42              |
| 9:A2:3255:A:H2'   | 9:A2:3256:G:C8    | 2.54                     | 0.42              |
| 9:A2:3915:C:H2'   | 9:A2:3916:G:O4'   | 2.19                     | 0.42              |
| 16:H2:70:TYR:CE1  | 16:H2:75:LEU:HB2  | 2.55                     | 0.42              |
| 18:J2:84:PRO:HB2  | 18:J2:87:SER:HB2  | 2.01                     | 0.42              |
| 46:m2:375:G:H1    | 46:m2:394:A:H61   | 1.67                     | 0.42              |
| 46:m2:431:C:H2'   | 46:m2:432:C:C6    | 2.54                     | 0.42              |
| 46:m2:616:C:N4    | 46:m2:628:G:OP2   | 2.48                     | 0.42              |
| 46:m2:1482:A:O2'  | 65:H3:56:ASP:OXT  | 2.34                     | 0.42              |
| 46:m2:1603:A:N6   | 46:m2:1638:G:OP2  | 2.47                     | 0.42              |
| 52:z2:44:LYS:HB3  | 52:z2:44:LYS:HE2  | 1.78                     | 0.42              |
| 66:I3:106:LYS:NZ  | 66:I3:107:ASP:OD2 | 2.43                     | 0.42              |
| 67:J3:203:GLY:O   | 67:J3:221:ASP:HA  | 2.19                     | 0.42              |
| 74:Q3:118:ARG:HG3 | 74:Q3:119:GLY:H   | 1.85                     | 0.42              |
| 79:m:136:VAL:HG11 | 79:m:805:GLY:HA3  | 2.01                     | 0.42              |
| 79:m:478:LEU:HD11 | 79:m:482:GLY:HA3  | 2.01                     | 0.42              |
| 4:D1:77:VAL:HG13  | 4:D1:82:LYS:HG2   | 2.02                     | 0.42              |
| 7:G1:70:GLN:HA    | 7:G1:73:VAL:HG22  | 2.02                     | 0.42              |
| 9:A2:48:G:O6      | 9:A2:289:C:O2'    | 2.37                     | 0.42              |
| 9:A2:198:A:O2'    | 9:A2:221:C:O2     | 2.33                     | 0.42              |
| 9:A2:475:G:H2'    | 9:A2:476:G:C8     | 2.54                     | 0.42              |
| 9:A2:1475:C:H2'   | 9:A2:1476:C:H6    | 1.84                     | 0.42              |
| 9:A2:1505:C:O3'   | 19:K2:143:ARG:NH1 | 2.51                     | 0.42              |
| 9:A2:1790:G:H2'   | 9:A2:1791:G:C8    | 2.55                     | 0.42              |
| 9:A2:2142:G:H2'   | 9:A2:2143:A:H8    | 1.85                     | 0.42              |
| 9:A2:2260:C:H5''  | 9:A2:2261:G:C2    | 2.55                     | 0.42              |
| 9:A2:2413:G:O2'   | 9:A2:2414:A:N7    | 2.52                     | 0.42              |
| 9:A2:2422:C:OP1   | 20:L2:100:ARG:NE  | 2.49                     | 0.42              |
| 9:A2:3475:G:H2'   | 9:A2:3476:G:C8    | 2.52                     | 0.42              |
| 9:A2:4106:G:H2'   | 9:A2:4107:G:C8    | 2.55                     | 0.42              |
| 9:A2:4603:C:H2'   | 9:A2:4604:C:C6    | 2.55                     | 0.42              |
| 13:E2:143:LYS:HE3 | 13:E2:143:LYS:HB2 | 1.93                     | 0.42              |
| 32:X2:29:ILE:HD11 | 32:X2:84:ILE:HB   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:m2:180:G:H3'    | 46:m2:181:A:C8    | 2.51                     | 0.42              |
| 46:m2:1497:G:H2'   | 46:m2:1498:U:C6   | 2.55                     | 0.42              |
| 46:m2:1535:A:H62   | 46:m2:1604:U:H3   | 1.68                     | 0.42              |
| 49:q2:58:VAL:O     | 49:q2:65:ARG:HB3  | 2.20                     | 0.42              |
| 49:q2:172:VAL:HG22 | 49:q2:185:LYS:HG2 | 2.01                     | 0.42              |
| 53:o2:50:ASN:O     | 53:o2:54:THR:HG23 | 2.19                     | 0.42              |
| 59:B3:76:THR:HB    | 59:B3:94:ARG:HG2  | 2.01                     | 0.42              |
| 66:I3:88:ARG:HH11  | 66:I3:97:THR:HG21 | 1.85                     | 0.42              |
| 70:M3:80:ASP:OD1   | 70:M3:80:ASP:N    | 2.38                     | 0.42              |
| 79:m:591:LEU:HA    | 79:m:601:LEU:O    | 2.20                     | 0.42              |
| 84:u:44:HIS:CD2    | 84:u:58:LEU:HD23  | 2.55                     | 0.42              |
| 9:A2:507:C:H2'     | 9:A2:508:G:H8     | 1.85                     | 0.42              |
| 9:A2:1468:C:OP2    | 29:U2:26:ARG:NH1  | 2.53                     | 0.42              |
| 9:A2:1753:G:H1     | 9:A2:1834:U:H3    | 1.68                     | 0.42              |
| 9:A2:2403:G:H2'    | 9:A2:2404:G:C8    | 2.55                     | 0.42              |
| 9:A2:2513:G:H2'    | 9:A2:2514:G:C5    | 2.55                     | 0.42              |
| 9:A2:2660:C:H2'    | 9:A2:2661:G:C8    | 2.55                     | 0.42              |
| 9:A2:3392:A:H2'    | 9:A2:3393:A:C8    | 2.55                     | 0.42              |
| 9:A2:3808:G:H5''   | 9:A2:3809:A:H2'   | 2.00                     | 0.42              |
| 11:C2:59:A:O3'     | 26:R2:70:LYS:HG2  | 2.20                     | 0.42              |
| 12:D2:80:GLU:HB2   | 12:D2:170:ALA:HA  | 2.02                     | 0.42              |
| 14:F2:11:TYR:CZ    | 14:F2:148:PRO:HB2 | 2.55                     | 0.42              |
| 16:H2:51:CYS:SG    | 16:H2:52:SER:N    | 2.93                     | 0.42              |
| 25:Q2:101:ARG:O    | 25:Q2:104:GLN:NE2 | 2.53                     | 0.42              |
| 46:m2:619:G:OP2    | 62:E3:68:LYS:NZ   | 2.45                     | 0.42              |
| 46:m2:685:OMG:N1   | 46:m2:1024:U:OP2  | 2.47                     | 0.42              |
| 46:m2:1369:U:H2'   | 46:m2:1370:U:C6   | 2.55                     | 0.42              |
| 46:m2:1645:U:H2'   | 46:m2:1646:C:C6   | 2.55                     | 0.42              |
| 50:r2:63:LYS:HE3   | 50:r2:67:GLN:HE21 | 1.85                     | 0.42              |
| 67:J3:104:ASP:OD1  | 67:J3:104:ASP:N   | 2.49                     | 0.42              |
| 67:J3:202:THR:OG1  | 69:L3:54:ARG:NH2  | 2.53                     | 0.42              |
| 85:L1:45:LYS:HD3   | 85:L1:45:LYS:HA   | 1.95                     | 0.42              |
| 2:B1:161:VAL:HG12  | 2:B1:163:PRO:HD2  | 2.02                     | 0.41              |
| 9:A2:735:C:H3'     | 9:A2:736:G:H3'    | 2.02                     | 0.41              |
| 9:A2:1141:C:H2'    | 9:A2:1142:G:H8    | 1.83                     | 0.41              |
| 9:A2:1756:U:H2'    | 9:A2:1757:G:C8    | 2.55                     | 0.41              |
| 9:A2:1905:G:H2'    | 9:A2:1906:G:H8    | 1.85                     | 0.41              |
| 9:A2:2088:G:OP1    | 11:C2:20:A:O2'    | 2.38                     | 0.41              |
| 9:A2:2419:G:H4'    | 9:A2:2432:G:H4'   | 2.01                     | 0.41              |
| 9:A2:2511:G:H2'    | 9:A2:2512:A:C8    | 2.54                     | 0.41              |
| 9:A2:3444:C:N4     | 9:A2:3468:C:O4'   | 2.53                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:A2:3973:U:H2'    | 9:A2:3974:G:C8    | 2.55                     | 0.41              |
| 9:A2:4223:A2M:HM'3 | 9:A2:4223:A2M:H1' | 1.89                     | 0.41              |
| 9:A2:4360:A:N3     | 9:A2:4361:U:H5'   | 2.35                     | 0.41              |
| 9:A2:4416:A:OP1    | 21:M2:156:HIS:ND1 | 2.52                     | 0.41              |
| 9:A2:4580:C:H2'    | 9:A2:4581:G:C8    | 2.54                     | 0.41              |
| 9:A2:4600:G:H2'    | 9:A2:4601:A:C8    | 2.54                     | 0.41              |
| 14:F2:28:PHE:HA    | 14:F2:129:ALA:HA  | 2.01                     | 0.41              |
| 46:m2:158:A:H2     | 46:m2:465:C:H1'   | 1.85                     | 0.41              |
| 46:m2:679:G:H21    | 46:m2:1030:A:N6   | 2.11                     | 0.41              |
| 46:m2:1098:G:H1    | 46:m2:1138:U:H3   | 1.67                     | 0.41              |
| 46:m2:1192:A:N3    | 46:m2:1716:U:O2'  | 2.52                     | 0.41              |
| 54:s2:179:ASN:ND2  | 54:s2:186:ASN:HB2 | 2.35                     | 0.41              |
| 59:B3:83:GLN:HB2   | 59:B3:93:SER:HB3  | 2.02                     | 0.41              |
| 60:C3:55:ARG:HE    | 60:C3:87:ARG:HH21 | 1.67                     | 0.41              |
| 66:I3:42:MET:HB2   | 66:I3:57:ARG:HG2  | 2.02                     | 0.41              |
| 66:I3:118:ARG:O    | 66:I3:134:THR:OG1 | 2.37                     | 0.41              |
| 66:I3:150:TRP:HB2  | 66:I3:170:TRP:CD1 | 2.55                     | 0.41              |
| 74:Q3:120:THR:O    | 74:Q3:124:ASN:ND2 | 2.51                     | 0.41              |
| 1:A1:212:LEU:HD21  | 1:A1:230:LEU:HD21 | 2.01                     | 0.41              |
| 6:F1:163:LYS:NZ    | 9:A2:512:C:OP2    | 2.51                     | 0.41              |
| 9:A2:288:G:H2'     | 9:A2:289:C:H6     | 1.85                     | 0.41              |
| 9:A2:835:U:H2'     | 9:A2:836:C:C6     | 2.56                     | 0.41              |
| 9:A2:1532:U:H2'    | 9:A2:1533:C:C6    | 2.55                     | 0.41              |
| 9:A2:1911:G:H2'    | 9:A2:1912:A:H8    | 1.84                     | 0.41              |
| 9:A2:2038:G:H2'    | 9:A2:2039:G:H8    | 1.85                     | 0.41              |
| 9:A2:2041:G:H2'    | 9:A2:2042:G:H8    | 1.85                     | 0.41              |
| 9:A2:2136:A:H1'    | 9:A2:2138:C:P     | 2.60                     | 0.41              |
| 9:A2:3315:G:H2'    | 9:A2:3316:C:C6    | 2.55                     | 0.41              |
| 9:A2:3430:A:H2'    | 9:A2:3431:A:H8    | 1.85                     | 0.41              |
| 9:A2:4642:C:OP1    | 32:X2:32:ARG:NH1  | 2.50                     | 0.41              |
| 10:B2:72:U:H2'     | 10:B2:73:U:O4'    | 2.20                     | 0.41              |
| 13:E2:55:HIS:NE2   | 25:Q2:16:GLY:HA3  | 2.35                     | 0.41              |
| 13:E2:93:VAL:HG12  | 13:E2:102:PHE:HB2 | 2.02                     | 0.41              |
| 14:F2:228:THR:OG1  | 14:F2:248:ARG:NH2 | 2.53                     | 0.41              |
| 38:d2:69:ILE:HD13  | 38:d2:72:ARG:HH12 | 1.85                     | 0.41              |
| 46:m2:733:G:H5''   | 46:m2:735:C:H41   | 1.85                     | 0.41              |
| 46:m2:954:G:N2     | 72:O3:52:THR:OG1  | 2.49                     | 0.41              |
| 46:m2:1245:PSU:H2' | 46:m2:1246:U:O4'  | 2.20                     | 0.41              |
| 46:m2:1671:G:H5''  | 57:y2:130:LYS:HB3 | 2.02                     | 0.41              |
| 46:m2:1750:G:H2'   | 46:m2:1751:G:C8   | 2.55                     | 0.41              |
| 66:I3:128:THR:OG1  | 66:I3:142:VAL:O   | 2.32                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:I3:197:THR:HG21 | 66:I3:239:LEU:H    | 1.85                     | 0.41              |
| 67:J3:166:ARG:HB2  | 67:J3:248:TYR:CG   | 2.54                     | 0.41              |
| 80:j:82:ILE:HA     | 80:j:86:VAL:HG21   | 2.01                     | 0.41              |
| 80:j:130:LEU:HB2   | 80:j:152:ILE:HD12  | 2.01                     | 0.41              |
| 81:k:25:THR:OG1    | 81:k:26:SER:N      | 2.53                     | 0.41              |
| 81:k:35:LEU:HD21   | 81:k:37:LEU:HD12   | 2.01                     | 0.41              |
| 3:C1:18:ILE:HG22   | 3:C1:27:VAL:HG22   | 2.02                     | 0.41              |
| 9:A2:142:G:H2'     | 9:A2:144:G:H8      | 1.84                     | 0.41              |
| 9:A2:1360:A:C2     | 9:A2:2568:A:H8     | 2.38                     | 0.41              |
| 9:A2:1852:OMG:HN22 | 17:I2:87:MET:HA    | 1.85                     | 0.41              |
| 9:A2:2052:E7G:O2'  | 9:A2:2053:U:O4'    | 2.38                     | 0.41              |
| 9:A2:2211:G:H2'    | 9:A2:2212:G:H8     | 1.85                     | 0.41              |
| 9:A2:3840:U:H2'    | 9:A2:3841:U:H6     | 1.85                     | 0.41              |
| 9:A2:4391:C:H5''   | 9:A2:4392:G:H5''   | 2.02                     | 0.41              |
| 9:A2:4631:U:H4'    | 13:E2:175:GLN:HG3  | 2.02                     | 0.41              |
| 15:G2:41:LYS:NZ    | 22:N2:32:ARG:O     | 2.41                     | 0.41              |
| 18:J2:129:THR:HG23 | 18:J2:137:ASN:HB3  | 2.02                     | 0.41              |
| 22:N2:14:MET:HG3   | 22:N2:15:PHE:HD1   | 1.85                     | 0.41              |
| 37:c2:35:ASN:OD1   | 37:c2:36:HIS:N     | 2.53                     | 0.41              |
| 45:k2:98:ARG:HH21  | 45:k2:107:ARG:NH1  | 2.17                     | 0.41              |
| 46:m2:30:C:H1'     | 46:m2:598:U:H5'    | 2.01                     | 0.41              |
| 46:m2:1025:A:N1    | 46:m2:1026:A:N6    | 2.68                     | 0.41              |
| 46:m2:1053:G:H2'   | 46:m2:1054:A:H8    | 1.86                     | 0.41              |
| 46:m2:1794:G:H2'   | 46:m2:1795:A:C8    | 2.55                     | 0.41              |
| 49:q2:137:VAL:HG22 | 49:q2:151:LYS:HB2  | 2.03                     | 0.41              |
| 52:z2:84:TYR:OH    | 53:o2:213:GLU:OE1  | 2.26                     | 0.41              |
| 56:x2:49:LEU:HB2   | 56:x2:54:HIS:CE1   | 2.55                     | 0.41              |
| 70:M3:116:LYS:HG2  | 70:M3:118:SER:H    | 1.86                     | 0.41              |
| 79:m:228:ALA:HB1   | 79:m:255:MET:HB3   | 2.01                     | 0.41              |
| 80:j:60:MET:HE3    | 80:j:60:MET:HB2    | 1.98                     | 0.41              |
| 85:L1:76:GLU:O     | 85:L1:80:VAL:HG23  | 2.20                     | 0.41              |
| 3:C1:43:VAL:O      | 9:A2:4416:A:O2'    | 2.33                     | 0.41              |
| 3:C1:64:ARG:NH1    | 9:A2:4345:C:OP1    | 2.43                     | 0.41              |
| 5:E1:32:ARG:HE     | 5:E1:126:TYR:HE1   | 1.67                     | 0.41              |
| 9:A2:423:G:H2'     | 9:A2:424:U:C6      | 2.55                     | 0.41              |
| 9:A2:1116:U:H3'    | 9:A2:1117:A:C8     | 2.55                     | 0.41              |
| 9:A2:1635:G:N2     | 9:A2:1637:G:O4'    | 2.54                     | 0.41              |
| 9:A2:1802:G:O3'    | 9:A2:1803:G:N2     | 2.50                     | 0.41              |
| 9:A2:2559:OMC:H1'  | 9:A2:2559:OMC:HM23 | 1.83                     | 0.41              |
| 9:A2:2654:C:OP2    | 20:L2:108:ARG:NH1  | 2.45                     | 0.41              |
| 9:A2:3600:G:N2     | 9:A2:3719:U:O2     | 2.41                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:4264:C:H2'    | 9:A2:4265:C:H6     | 1.84                     | 0.41              |
| 9:A2:4439:G:H2'    | 9:A2:4440:C:C6     | 2.56                     | 0.41              |
| 11:C2:74:U:O4      | 27:S2:72:GLN:NE2   | 2.54                     | 0.41              |
| 12:D2:107:MET:HE2  | 12:D2:166:VAL:HG22 | 2.02                     | 0.41              |
| 14:F2:35:ASP:OD1   | 14:F2:35:ASP:N     | 2.51                     | 0.41              |
| 17:I2:182:GLU:O    | 17:I2:186:GLU:HG3  | 2.21                     | 0.41              |
| 18:J2:10:ASN:HD21  | 18:J2:13:LYS:HB2   | 1.83                     | 0.41              |
| 19:K2:124:ASP:OD1  | 19:K2:124:ASP:N    | 2.51                     | 0.41              |
| 34:Z2:50:VAL:HG22  | 34:Z2:69:VAL:HG22  | 2.01                     | 0.41              |
| 46:m2:27:A2M:H2'   | 46:m2:28:U:C6      | 2.55                     | 0.41              |
| 46:m2:1168:G:H2'   | 46:m2:1169:G:H8    | 1.85                     | 0.41              |
| 47:n2:43:G:H2'     | 47:n2:44:A:C8      | 2.55                     | 0.41              |
| 49:q2:93:THR:HB    | 49:q2:96:LEU:HD23  | 2.03                     | 0.41              |
| 50:r2:31:PRO:HG2   | 50:r2:38:LEU:HB2   | 2.01                     | 0.41              |
| 56:x2:111:MET:HE2  | 58:A3:117:ILE:HB   | 2.01                     | 0.41              |
| 69:L3:136:ARG:HG2  | 69:L3:160:SER:HA   | 2.01                     | 0.41              |
| 1:A1:81:LYS:NZ     | 9:A2:1046:G:OP1    | 2.40                     | 0.41              |
| 2:B1:184:ILE:HD13  | 2:B1:184:ILE:HA    | 1.94                     | 0.41              |
| 7:G1:101:LYS:HA    | 7:G1:104:MET:HG3   | 2.02                     | 0.41              |
| 7:G1:124:LYS:HE2   | 7:G1:124:LYS:HB2   | 1.94                     | 0.41              |
| 9:A2:273:U:H2'     | 9:A2:274:C:C6      | 2.55                     | 0.41              |
| 9:A2:307:A:H2'     | 9:A2:308:G:N3      | 2.35                     | 0.41              |
| 9:A2:686:C:H2'     | 9:A2:687:G:C8      | 2.55                     | 0.41              |
| 9:A2:1140:A2M:HM'3 | 9:A2:1140:A2M:HI'  | 1.74                     | 0.41              |
| 9:A2:1231:C:H2'    | 9:A2:1232:G:O4'    | 2.21                     | 0.41              |
| 9:A2:1303:G:H2'    | 9:A2:1304:A:C8     | 2.55                     | 0.41              |
| 9:A2:1475:C:H2'    | 9:A2:1476:C:C6     | 2.54                     | 0.41              |
| 9:A2:1795:C:H41    | 9:A2:1804:A:H5''   | 1.84                     | 0.41              |
| 9:A2:2198:G:OP2    | 9:A2:2271:G:N2     | 2.50                     | 0.41              |
| 9:A2:3289:C:H2'    | 9:A2:3290:G:C8     | 2.55                     | 0.41              |
| 9:A2:3589:G:H2'    | 9:A2:3590:G:C8     | 2.54                     | 0.41              |
| 9:A2:4021:A:O2'    | 43:i2:64:LYS:NZ    | 2.53                     | 0.41              |
| 9:A2:4690:A:H2'    | 9:A2:4691:G:C8     | 2.54                     | 0.41              |
| 12:D2:5:ILE:HD13   | 12:D2:210:PRO:HD3  | 2.02                     | 0.41              |
| 13:E2:171:LEU:HB3  | 13:E2:173:LEU:HD13 | 2.01                     | 0.41              |
| 14:F2:317:ASN:HD21 | 14:F2:319:LEU:HB2  | 1.85                     | 0.41              |
| 17:I2:27:VAL:HG12  | 17:I2:98:ALA:HB1   | 2.01                     | 0.41              |
| 28:T2:41:ALA:HB2   | 28:T2:77:TYR:HE1   | 1.86                     | 0.41              |
| 28:T2:87:VAL:HG12  | 28:T2:89:ILE:HG13  | 2.02                     | 0.41              |
| 40:f2:8:ARG:O      | 40:f2:11:ARG:HG2   | 2.19                     | 0.41              |
| 46:m2:382:G:HI'    | 84:u:5:ARG:HD3     | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:m2:565:G:HO2'  | 46:m2:566:A:P      | 2.43                     | 0.41              |
| 46:m2:1210:A:H2'  | 46:m2:1211:A:H8    | 1.85                     | 0.41              |
| 48:p2:68:GLU:OE2  | 72:O3:96:LYS:NZ    | 2.37                     | 0.41              |
| 50:r2:174:LYS:HE3 | 50:r2:174:LYS:HB3  | 1.87                     | 0.41              |
| 55:v2:41:PRO:HG2  | 55:v2:44:HIS:CG    | 2.55                     | 0.41              |
| 66:I3:86:THR:HG22 | 66:I3:102:VAL:HG13 | 2.03                     | 0.41              |
| 83:t:47:ALA:HB3   | 83:t:63:PHE:CD2    | 2.56                     | 0.41              |
| 1:A1:184:ILE:HG22 | 1:A1:185:ASN:HD22  | 1.85                     | 0.41              |
| 9:A2:93:G:H2'     | 9:A2:94:A:C8       | 2.56                     | 0.41              |
| 9:A2:489:G:H2'    | 9:A2:490:C:O4'     | 2.20                     | 0.41              |
| 9:A2:689:G:H2'    | 9:A2:690:C:C6      | 2.56                     | 0.41              |
| 9:A2:1543:G:O2'   | 15:G2:10:LYS:NZ    | 2.53                     | 0.41              |
| 9:A2:1650:C:H2'   | 9:A2:1651:U:O4'    | 2.21                     | 0.41              |
| 9:A2:1708:U:H2'   | 9:A2:1709:A:C8     | 2.55                     | 0.41              |
| 9:A2:2295:C:H2'   | 9:A2:2296:G:C8     | 2.56                     | 0.41              |
| 9:A2:2427:C:H2'   | 9:A2:2428:G:H21    | 1.86                     | 0.41              |
| 9:A2:2539:C:H2'   | 9:A2:2540:C:H6     | 1.86                     | 0.41              |
| 9:A2:2551:G:H5'   | 40:f2:45:ARG:NH1   | 2.36                     | 0.41              |
| 9:A2:3264:A:H2'   | 9:A2:3265:G:C8     | 2.56                     | 0.41              |
| 9:A2:4112:U:H2'   | 9:A2:4113:C:C6     | 2.56                     | 0.41              |
| 9:A2:4125:A:O2'   | 41:g2:122:ARG:NH2  | 2.52                     | 0.41              |
| 46:m2:96:C:H2'    | 46:m2:97:U:C6      | 2.56                     | 0.41              |
| 46:m2:220:U:O2    | 84:u:184:ARG:NH1   | 2.53                     | 0.41              |
| 46:m2:1691:C:H2'  | 46:m2:1692:U:H6    | 1.85                     | 0.41              |
| 47:n2:18:G:N7     | 47:n2:58:A:C6      | 2.88                     | 0.41              |
| 52:z2:32:LYS:HE2  | 52:z2:32:LYS:HB3   | 1.78                     | 0.41              |
| 54:s2:125:SER:HA  | 54:s2:138:ALA:HA   | 2.02                     | 0.41              |
| 66:I3:192:THR:N   | 66:I3:213:ASP:OD2  | 2.52                     | 0.41              |
| 74:Q3:17:LEU:H    | 74:Q3:17:LEU:HD12  | 1.85                     | 0.41              |
| 76:S3:56:CYS:HB3  | 76:S3:59:CYS:HB3   | 2.02                     | 0.41              |
| 79:m:688:GLU:O    | 79:m:729:TYR:OH    | 2.24                     | 0.41              |
| 79:m:691:LEU:HD11 | 79:m:737:PRO:HB2   | 2.02                     | 0.41              |
| 83:t:8:ILE:HG13   | 83:t:41:ARG:HA     | 2.03                     | 0.41              |
| 1:A1:154:MET:O    | 1:A1:158:VAL:HG22  | 2.20                     | 0.41              |
| 3:C1:41:ILE:HG22  | 3:C1:43:VAL:HG13   | 2.03                     | 0.41              |
| 8:H1:120:TRP:NE1  | 8:H1:123:GLU:HB2   | 2.34                     | 0.41              |
| 9:A2:308:G:H8     | 9:A2:310:G:H1'     | 1.86                     | 0.41              |
| 9:A2:324:A:H2'    | 9:A2:325:U:C6      | 2.55                     | 0.41              |
| 9:A2:944:G:H2'    | 9:A2:945:G:H8      | 1.86                     | 0.41              |
| 9:A2:1269:B8Q:O2' | 19:K2:73:PRO:O     | 2.37                     | 0.41              |
| 9:A2:1751:U:H2'   | 9:A2:1752:U:C6     | 2.55                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:A2:2177:OMC:O2   | 9:A2:2584:U:H1'   | 2.21                     | 0.41              |
| 9:A2:3272:U:H4'    | 9:A2:3273:G:C4    | 2.56                     | 0.41              |
| 9:A2:3321:G:O3'    | 12:D2:227:ARG:NH1 | 2.53                     | 0.41              |
| 9:A2:3727:A:N1     | 9:A2:3823:C:N4    | 2.66                     | 0.41              |
| 9:A2:3971:C:H2'    | 9:A2:3972:G:H8    | 1.85                     | 0.41              |
| 9:A2:4273:C:H2'    | 9:A2:4274:A:C8    | 2.55                     | 0.41              |
| 11:C2:7:U:H2'      | 11:C2:8:U:C6      | 2.55                     | 0.41              |
| 17:I2:120:VAL:HG22 | 21:M2:167:PHE:HD1 | 1.86                     | 0.41              |
| 26:R2:113:VAL:O    | 26:R2:117:TYR:HB2 | 2.19                     | 0.41              |
| 36:b2:88:THR:HG23  | 36:b2:91:MET:H    | 1.85                     | 0.41              |
| 46:m2:354:U:H2'    | 46:m2:355:C:C6    | 2.55                     | 0.41              |
| 46:m2:391:A:H2'    | 46:m2:392:C:C6    | 2.56                     | 0.41              |
| 46:m2:518:A:N1     | 46:m2:645:A:O2'   | 2.47                     | 0.41              |
| 46:m2:1614:G:OP1   | 56:x2:18:ARG:NH2  | 2.49                     | 0.41              |
| 46:m2:1688:G:H2'   | 46:m2:1689:C:C6   | 2.55                     | 0.41              |
| 46:m2:1694:U:H2'   | 46:m2:1695:G:H8   | 1.85                     | 0.41              |
| 63:F3:12:LYS:HE2   | 63:F3:12:LYS:HB3  | 1.93                     | 0.41              |
| 67:J3:94:ILE:HG13  | 67:J3:159:LYS:O   | 2.21                     | 0.41              |
| 68:K3:19:ASP:OD1   | 68:K3:19:ASP:N    | 2.54                     | 0.41              |
| 68:K3:203:LYS:HE3  | 68:K3:203:LYS:HB3 | 1.81                     | 0.41              |
| 73:P3:88:LYS:HA    | 73:P3:91:ASN:HD21 | 1.85                     | 0.41              |
| 79:m:22:SER:HA     | 79:m:102:ILE:HG13 | 2.02                     | 0.41              |
| 81:k:149:HIS:O     | 81:k:152:ILE:HG13 | 2.20                     | 0.41              |
| 9:A2:184:U:H5''    | 9:A2:253:G:H22    | 1.86                     | 0.41              |
| 9:A2:666:G:H2'     | 9:A2:667:G:H8     | 1.85                     | 0.41              |
| 9:A2:883:C:H2'     | 9:A2:884:C:O4'    | 2.20                     | 0.41              |
| 9:A2:1104:G:H2'    | 9:A2:1105:G:C8    | 2.56                     | 0.41              |
| 9:A2:1138:A:O2'    | 9:A2:1140:A2M:OP1 | 2.26                     | 0.41              |
| 9:A2:1149:G:N2     | 14:F2:95:MET:HB2  | 2.36                     | 0.41              |
| 9:A2:1284:U:H2'    | 9:A2:1285:C:C6    | 2.55                     | 0.41              |
| 9:A2:2388:U:H2'    | 9:A2:2389:C:C6    | 2.55                     | 0.41              |
| 9:A2:3483:G:O2'    | 9:A2:3485:G:OP2   | 2.33                     | 0.41              |
| 9:A2:3696:A:N6     | 9:A2:3697:A:H62   | 2.18                     | 0.41              |
| 9:A2:4187:A:H2'    | 9:A2:4188:OMC:C6  | 2.55                     | 0.41              |
| 9:A2:4402:G:H2'    | 9:A2:4403:G:C8    | 2.55                     | 0.41              |
| 9:A2:4650:C:H2'    | 9:A2:4651:G:O4'   | 2.19                     | 0.41              |
| 12:D2:233:ARG:HA   | 12:D2:233:ARG:HD2 | 1.88                     | 0.41              |
| 13:E2:317:LEU:HD12 | 13:E2:317:LEU:HA  | 1.95                     | 0.41              |
| 18:J2:96:LYS:HA    | 18:J2:99:GLU:HG2  | 2.02                     | 0.41              |
| 27:S2:31:SER:HA    | 27:S2:48:PRO:HA   | 2.03                     | 0.41              |
| 28:T2:31:ASP:OD1   | 28:T2:31:ASP:N    | 2.48                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:Z2:37:ASP:OD1   | 34:Z2:37:ASP:N     | 2.52                     | 0.41              |
| 46:m2:1077:C:H2'   | 46:m2:1078:G:C8    | 2.55                     | 0.41              |
| 46:m2:1408:G:H2'   | 46:m2:1409:U:H6    | 1.86                     | 0.41              |
| 46:m2:1493:G:H2'   | 46:m2:1494:U:C6    | 2.56                     | 0.41              |
| 46:m2:1713:U:H2'   | 46:m2:1714:A:C8    | 2.56                     | 0.41              |
| 46:m2:1731:U:O2    | 46:m2:1807:G:N2    | 2.37                     | 0.41              |
| 51:w2:119:ASP:OD1  | 51:w2:119:ASP:N    | 2.52                     | 0.41              |
| 57:y2:32:ILE:HG21  | 57:y2:39:LEU:HD22  | 2.03                     | 0.41              |
| 62:E3:32:LEU:HD23  | 62:E3:32:LEU:HA    | 1.92                     | 0.41              |
| 76:S3:8:LEU:HD23   | 76:S3:8:LEU:H      | 1.86                     | 0.41              |
| 85:L1:14:VAL:HA    | 85:L1:17:VAL:HG22  | 2.02                     | 0.41              |
| 1:A1:95:ARG:HD3    | 9:A2:737:G:C5      | 2.56                     | 0.41              |
| 1:A1:120:ILE:HD13  | 19:K2:3:VAL:HG13   | 2.03                     | 0.41              |
| 1:A1:173:ASN:ND2   | 9:A2:841:A:N7      | 2.68                     | 0.41              |
| 2:B1:103:ARG:NH2   | 2:B1:192:HIS:O     | 2.53                     | 0.41              |
| 3:C1:63:ASN:ND2    | 3:C1:66:GLU:OE2    | 2.53                     | 0.41              |
| 4:D1:206:LEU:HD23  | 4:D1:210:ARG:HH21  | 1.86                     | 0.41              |
| 5:E1:18:ARG:HG3    | 5:E1:135:GLY:HA3   | 2.02                     | 0.41              |
| 6:F1:7:GLY:O       | 29:U2:49:HIS:NE2   | 2.42                     | 0.41              |
| 9:A2:1098:G:O2'    | 9:A2:1099:U:O5'    | 2.37                     | 0.41              |
| 9:A2:1118:C:H2'    | 9:A2:1119:C:H6     | 1.85                     | 0.41              |
| 9:A2:1118:C:H2'    | 9:A2:1119:C:C6     | 2.55                     | 0.41              |
| 9:A2:1244:C:H2'    | 9:A2:1245:G:O4'    | 2.21                     | 0.41              |
| 9:A2:1263:C:H2'    | 9:A2:1264:G:O4'    | 2.21                     | 0.41              |
| 9:A2:1380:U:H2'    | 9:A2:1381:C:C6     | 2.55                     | 0.41              |
| 9:A2:1480:G:H21    | 9:A2:2037:A:H62    | 1.69                     | 0.41              |
| 9:A2:1535:G:N3     | 9:A2:3866:A:H2'    | 2.35                     | 0.41              |
| 9:A2:1581:U:H2'    | 9:A2:1582:A:C8     | 2.56                     | 0.41              |
| 9:A2:1726:C:H2'    | 9:A2:1727:G:C8     | 2.55                     | 0.41              |
| 9:A2:1811:A:H5''   | 79:m:755:VAL:HB    | 2.03                     | 0.41              |
| 9:A2:3744:G:H22    | 9:A2:3765:G:N2     | 2.19                     | 0.41              |
| 9:A2:3892:G:H2'    | 9:A2:3893:C:C6     | 2.56                     | 0.41              |
| 9:A2:4152:PSU:H2'  | 9:A2:4153:U:H6     | 1.84                     | 0.41              |
| 9:A2:4241:A:N1     | 9:A2:4273:C:O2'    | 2.47                     | 0.41              |
| 10:B2:23:A:H2      | 10:B2:118:C:H1'    | 1.86                     | 0.41              |
| 10:B2:64:G:H2'     | 10:B2:65:G:C8      | 2.52                     | 0.41              |
| 14:F2:209:ILE:HB   | 14:F2:229:LEU:HD13 | 2.02                     | 0.41              |
| 15:G2:275:GLN:OE1  | 15:G2:275:GLN:N    | 2.54                     | 0.41              |
| 17:I2:177:LEU:HD23 | 17:I2:177:LEU:HA   | 1.94                     | 0.41              |
| 19:K2:80:ALA:HB3   | 19:K2:100:VAL:HG12 | 2.01                     | 0.41              |
| 21:M2:83:ARG:HD2   | 22:N2:156:TYR:HB2  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:T2:76:ASN:OD1   | 28:T2:77:TYR:N    | 2.54                     | 0.41              |
| 46:m2:91:A:OP1     | 46:m2:448:G:N2    | 2.47                     | 0.41              |
| 46:m2:96:C:H2'     | 46:m2:97:U:H6     | 1.86                     | 0.41              |
| 46:m2:178:C:H2'    | 46:m2:179:C:C6    | 2.56                     | 0.41              |
| 46:m2:186:C:H2'    | 46:m2:187:G:C8    | 2.56                     | 0.41              |
| 46:m2:340:G:O2'    | 46:m2:341:A:O4'   | 2.38                     | 0.41              |
| 46:m2:381:C:H5''   | 84:u:56:ARG:HH12  | 1.85                     | 0.41              |
| 46:m2:454:G:H2'    | 46:m2:455:C:C6    | 2.56                     | 0.41              |
| 46:m2:605:C:H1'    | 46:m2:606:A:N7    | 2.36                     | 0.41              |
| 46:m2:864:A:H8     | 73:P3:105:THR:HB  | 1.85                     | 0.41              |
| 46:m2:881:C:H2'    | 46:m2:882:G:C8    | 2.56                     | 0.41              |
| 46:m2:1281:C:H2'   | 46:m2:1282:G:H8   | 1.85                     | 0.41              |
| 46:m2:1375:C:OP1   | 52:z2:7:LYS:HB2   | 2.21                     | 0.41              |
| 46:m2:1520:C:OP1   | 46:m2:1522:G:H8   | 2.03                     | 0.41              |
| 46:m2:1552:G:O2'   | 46:m2:1560:C:O2   | 2.29                     | 0.41              |
| 48:p2:230:GLU:O    | 48:p2:234:GLU:HB2 | 2.21                     | 0.41              |
| 55:v2:17:LYS:HG3   | 82:A:283:LEU:HD23 | 2.02                     | 0.41              |
| 63:F3:10:ARG:HD2   | 63:F3:34:LYS:HE2  | 2.03                     | 0.41              |
| 67:J3:184:VAL:HG13 | 67:J3:243:ALA:HB1 | 2.03                     | 0.41              |
| 79:m:61:ASP:OD1    | 79:m:61:ASP:N     | 2.44                     | 0.41              |
| 79:m:76:LEU:HD13   | 79:m:78:TYR:CE2   | 2.56                     | 0.41              |
| 79:m:590:CYS:O     | 79:m:602:TYR:HA   | 2.21                     | 0.41              |
| 79:m:606:ARG:HH21  | 79:m:700:ARG:CZ   | 2.33                     | 0.41              |
| 80:j:78:LEU:HD21   | 80:j:193:PHE:HB2  | 2.03                     | 0.41              |
| 85:L1:88:GLU:H     | 85:L1:88:GLU:HG3  | 1.74                     | 0.41              |
| 6:F1:74:ARG:HH12   | 9:A2:76:A:H8      | 1.68                     | 0.41              |
| 9:A2:146:G:H2'     | 9:A2:147:A:H8     | 1.85                     | 0.41              |
| 9:A2:453:G:H1      | 9:A2:1107:G:N2    | 2.19                     | 0.41              |
| 9:A2:690:C:H2'     | 9:A2:691:G:O4'    | 2.21                     | 0.41              |
| 9:A2:1401:U:H2'    | 9:A2:1402:C:C6    | 2.56                     | 0.41              |
| 9:A2:1442:G:H1     | 12:D2:208:GLU:HG2 | 1.85                     | 0.41              |
| 9:A2:2220:C:H2'    | 9:A2:2221:G:O4'   | 2.21                     | 0.41              |
| 9:A2:2240:U:H2'    | 9:A2:2241:G:C8    | 2.56                     | 0.41              |
| 9:A2:2598:U:H2'    | 9:A2:2599:A:H8    | 1.84                     | 0.41              |
| 9:A2:3528:A:H2'    | 9:A2:3529:G:H8    | 1.86                     | 0.41              |
| 9:A2:3624:U:H2'    | 9:A2:3625:G:C8    | 2.56                     | 0.41              |
| 9:A2:3924:G:OP2    | 9:A2:3924:G:N2    | 2.54                     | 0.41              |
| 9:A2:4236:A:H2'    | 9:A2:4237:U:O4'   | 2.21                     | 0.41              |
| 9:A2:4325:U:H2'    | 9:A2:4326:C:H6    | 1.85                     | 0.41              |
| 13:E2:170:LEU:O    | 13:E2:328:ASN:ND2 | 2.54                     | 0.41              |
| 14:F2:150:LEU:HB2  | 14:F2:151:PRO:HD3 | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:K2:88:ASP:HB2   | 19:K2:109:ALA:HB2  | 2.03                     | 0.41              |
| 19:K2:165:PRO:HG3  | 19:K2:180:ARG:HH22 | 1.85                     | 0.41              |
| 46:m2:1428:U:H2'   | 46:m2:1429:C:C6    | 2.55                     | 0.41              |
| 47:n2:9:U:O4       | 47:n2:15:A:N7      | 2.54                     | 0.41              |
| 64:G3:11:LEU:HB2   | 64:G3:35:MET:HE2   | 2.03                     | 0.41              |
| 72:O3:65:ASP:HA    | 72:O3:68:GLU:HG3   | 2.03                     | 0.41              |
| 78:U3:132:MET:HG2  | 78:U3:141:CYS:HB2  | 2.02                     | 0.41              |
| 79:m:330:GLU:HA    | 79:m:334:LEU:HD22  | 2.03                     | 0.41              |
| 83:t:52:GLU:HG3    | 83:t:58:LYS:HG3    | 2.03                     | 0.41              |
| 85:L1:102:LYS:HE2  | 85:L1:106:LYS:HE2  | 2.03                     | 0.41              |
| 9:A2:94:A:H5''     | 29:U2:34:ASN:HB2   | 2.03                     | 0.40              |
| 9:A2:506:G:H2'     | 9:A2:507:C:C6      | 2.55                     | 0.40              |
| 9:A2:721:G:H2'     | 9:A2:722:G:C8      | 2.56                     | 0.40              |
| 9:A2:1796:C:H4'    | 81:k:130:LYS:HE3   | 2.03                     | 0.40              |
| 9:A2:2485:U:H2'    | 9:A2:2486:C:C6     | 2.56                     | 0.40              |
| 9:A2:3267:A:H2'    | 9:A2:3268:C:C6     | 2.55                     | 0.40              |
| 9:A2:3517:A:H2'    | 9:A2:3518:A:H8     | 1.86                     | 0.40              |
| 9:A2:4395:G:H2'    | 9:A2:4396:A:C8     | 2.55                     | 0.40              |
| 15:G2:95:TYR:HA    | 15:G2:158:LYS:HG2  | 2.02                     | 0.40              |
| 32:X2:57:MET:HA    | 32:X2:90:ARG:HH21  | 1.86                     | 0.40              |
| 36:b2:89:ARG:O     | 36:b2:93:ARG:HG2   | 2.21                     | 0.40              |
| 46:m2:87:U:H2'     | 46:m2:88:G:C8      | 2.55                     | 0.40              |
| 46:m2:443:C:H2'    | 46:m2:444:C:C6     | 2.56                     | 0.40              |
| 46:m2:637:G:H2'    | 46:m2:638:C:C6     | 2.56                     | 0.40              |
| 46:m2:977:G:N2     | 72:O3:50:LYS:O     | 2.55                     | 0.40              |
| 46:m2:1613:G:O2'   | 58:A3:87:GLN:O     | 2.36                     | 0.40              |
| 64:G3:24:GLN:H     | 64:G3:26:GLN:NE2   | 2.19                     | 0.40              |
| 67:J3:155:ILE:HG22 | 67:J3:159:LYS:HE2  | 2.02                     | 0.40              |
| 70:M3:50:CYS:HB2   | 70:M3:110:VAL:HG13 | 2.03                     | 0.40              |
| 74:Q3:111:LYS:HE3  | 74:Q3:111:LYS:HB3  | 1.84                     | 0.40              |
| 79:m:596:ASN:O     | 79:m:598:HIS:ND1   | 2.54                     | 0.40              |
| 79:m:740:MET:HG3   | 79:m:816:TRP:HB3   | 2.03                     | 0.40              |
| 1:A1:127:VAL:HG13  | 1:A1:158:VAL:HG12  | 2.03                     | 0.40              |
| 2:B1:44:ASP:HA     | 12:D2:64:ARG:HH22  | 1.85                     | 0.40              |
| 2:B1:146:LEU:HB3   | 2:B1:152:ALA:HB2   | 2.03                     | 0.40              |
| 2:B1:211:ASP:N     | 2:B1:211:ASP:OD1   | 2.54                     | 0.40              |
| 3:C1:128:MET:SD    | 3:C1:157:SER:HB3   | 2.62                     | 0.40              |
| 9:A2:271:C:H2'     | 9:A2:272:U:C6      | 2.56                     | 0.40              |
| 9:A2:444:G:H2'     | 9:A2:445:U:C6      | 2.56                     | 0.40              |
| 9:A2:683:C:H2'     | 9:A2:684:G:H8      | 1.86                     | 0.40              |
| 9:A2:1393:C:H2'    | 9:A2:1394:G:O4'    | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:A2:1410:G:N3     | 9:A2:1412:A:N6     | 2.69                     | 0.40              |
| 9:A2:1676:A:O4'    | 9:A2:3865:A:N6     | 2.54                     | 0.40              |
| 9:A2:1730:C:N3     | 17:I2:133:ARG:NH2  | 2.69                     | 0.40              |
| 9:A2:2276:G:H2'    | 9:A2:2277:G7M:H8   | 2.03                     | 0.40              |
| 9:A2:2413:G:O2'    | 9:A2:2430:G:N2     | 2.54                     | 0.40              |
| 9:A2:3573:A:H2'    | 9:A2:3574:G:C8     | 2.54                     | 0.40              |
| 9:A2:3884:U:H5'    | 43:i2:3:ASN:HB3    | 2.03                     | 0.40              |
| 9:A2:4362:C:H2'    | 9:A2:4363:C:C6     | 2.55                     | 0.40              |
| 12:D2:116:LEU:O    | 12:D2:126:LEU:HB3  | 2.21                     | 0.40              |
| 14:F2:37:VAL:HG13  | 14:F2:237:ILE:HD11 | 2.03                     | 0.40              |
| 14:F2:162:LYS:NZ   | 14:F2:215:ASN:O    | 2.39                     | 0.40              |
| 20:L2:105:LEU:HD23 | 20:L2:138:LEU:HD23 | 2.03                     | 0.40              |
| 28:T2:90:PRO:O     | 28:T2:117:LYS:NZ   | 2.53                     | 0.40              |
| 30:V2:116:LEU:HD23 | 30:V2:116:LEU:HA   | 1.95                     | 0.40              |
| 37:c2:63:VAL:HG23  | 37:c2:65:LYS:HG2   | 2.04                     | 0.40              |
| 46:m2:70:G:N2      | 46:m2:71:G:O6      | 2.54                     | 0.40              |
| 46:m2:537:G:H2'    | 46:m2:538:A:C8     | 2.56                     | 0.40              |
| 47:n2:69:U:H2'     | 47:n2:70:G:C8      | 2.56                     | 0.40              |
| 66:I3:261:LEU:HA   | 66:I3:264:LYS:HD3  | 2.03                     | 0.40              |
| 69:L3:127:ARG:HD3  | 77:T3:31:ARG:HD3   | 2.04                     | 0.40              |
| 71:N3:87:ASP:OD1   | 71:N3:87:ASP:N     | 2.52                     | 0.40              |
| 79:m:9:ARG:HE      | 79:m:460:ILE:HG13  | 1.86                     | 0.40              |
| 79:m:751:PRO:HD3   | 79:m:780:MET:HE3   | 2.03                     | 0.40              |
| 81:k:63:THR:HG23   | 81:k:70:GLN:HE21   | 1.86                     | 0.40              |
| 1:A1:147:LEU:HD23  | 1:A1:147:LEU:HA    | 1.86                     | 0.40              |
| 9:A2:462:G:H2'     | 9:A2:463:A:H8      | 1.85                     | 0.40              |
| 9:A2:724:U:H2'     | 9:A2:725:C:C6      | 2.57                     | 0.40              |
| 9:A2:1317:G:H2'    | 9:A2:1318:C:H6     | 1.86                     | 0.40              |
| 9:A2:1379:C:H2'    | 9:A2:1380:U:C6     | 2.56                     | 0.40              |
| 9:A2:1645:A:H2'    | 9:A2:1646:G:C8     | 2.55                     | 0.40              |
| 9:A2:2018:A:H5''   | 45:k2:108:MET:SD   | 2.60                     | 0.40              |
| 9:A2:2566:G:H2'    | 9:A2:2568:A:H2     | 1.86                     | 0.40              |
| 9:A2:4623:A:OP1    | 13:E2:225:GLY:N    | 2.39                     | 0.40              |
| 13:E2:245:HIS:CE1  | 13:E2:246:ARG:HG3  | 2.56                     | 0.40              |
| 16:H2:174:GLN:HE21 | 16:H2:178:GLY:HA2  | 1.86                     | 0.40              |
| 26:R2:71:LEU:HD12  | 26:R2:71:LEU:HA    | 1.93                     | 0.40              |
| 44:j2:30:GLU:HA    | 44:j2:33:GLN:HG2   | 2.02                     | 0.40              |
| 45:k2:63:VAL:HG22  | 45:k2:79:ARG:HB3   | 2.03                     | 0.40              |
| 46:m2:89:C:H2'     | 46:m2:90:G:H8      | 1.86                     | 0.40              |
| 46:m2:1568:G:H21   | 46:m2:1570:C:H6    | 1.69                     | 0.40              |
| 51:w2:128:VAL:HG12 | 51:w2:142:VAL:HA   | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:z2:9:VAL:HG21   | 52:z2:49:LYS:HE3   | 2.02                     | 0.40              |
| 55:v2:16:PHE:HB3   | 82:A:283:LEU:HD22  | 2.03                     | 0.40              |
| 56:x2:18:ARG:N     | 58:A3:90:VAL:O     | 2.45                     | 0.40              |
| 60:C3:56:MET:HG3   | 60:C3:86:LYS:NZ    | 2.36                     | 0.40              |
| 62:E3:77:ASN:OD1   | 62:E3:77:ASN:N     | 2.54                     | 0.40              |
| 79:m:714:DDE:HAA3  | 79:m:714:DDE:HAU3  | 1.76                     | 0.40              |
| 81:k:35:LEU:HD13   | 81:k:64:ILE:HG23   | 2.03                     | 0.40              |
| 85:L1:171:HIS:CE1  | 85:L1:174:MET:HB2  | 2.57                     | 0.40              |
| 1:A1:114:VAL:HG13  | 1:A1:162:ILE:HD13  | 2.03                     | 0.40              |
| 5:E1:72:CYS:SG     | 5:E1:73:THR:N      | 2.95                     | 0.40              |
| 5:E1:95:ARG:HG2    | 5:E1:175:LEU:HG    | 2.04                     | 0.40              |
| 7:G1:5:ARG:HA      | 7:G1:11:ARG:HH12   | 1.85                     | 0.40              |
| 9:A2:1201:A:N6     | 9:A2:1211:A:OP2    | 2.43                     | 0.40              |
| 9:A2:1254:C:H42    | 9:A2:1907:A:H61    | 1.70                     | 0.40              |
| 9:A2:1541:G:H2'    | 9:A2:1542:C:C6     | 2.57                     | 0.40              |
| 9:A2:1635:G:OP1    | 22:N2:120:LYS:NZ   | 2.51                     | 0.40              |
| 9:A2:1813:C:H3'    | 9:A2:1814:A:H8     | 1.86                     | 0.40              |
| 9:A2:2177:OMC:HM22 | 9:A2:2178:A:C8     | 2.57                     | 0.40              |
| 9:A2:2308:A:OP2    | 9:A2:2329:G:O2'    | 2.33                     | 0.40              |
| 9:A2:3549:C:O2'    | 9:A2:4625:A:N1     | 2.48                     | 0.40              |
| 9:A2:3631:C:P      | 85:L1:24:LYS:HZ1   | 2.44                     | 0.40              |
| 9:A2:4183:PSU:H6   | 9:A2:4183:PSU:H2'  | 1.73                     | 0.40              |
| 9:A2:4388:C:H4'    | 9:A2:4714:G:C4     | 2.57                     | 0.40              |
| 10:B2:67:C:H2'     | 10:B2:68:C:C6      | 2.57                     | 0.40              |
| 13:E2:85:VAL:HB    | 13:E2:165:HIS:CD2  | 2.57                     | 0.40              |
| 14:F2:41:HIS:NE2   | 14:F2:242:PRO:O    | 2.55                     | 0.40              |
| 22:N2:68:THR:OG1   | 22:N2:71:ALA:O     | 2.37                     | 0.40              |
| 46:m2:12:U:H2'     | 46:m2:13:C:C6      | 2.56                     | 0.40              |
| 46:m2:179:C:H2'    | 46:m2:180:G:O4'    | 2.21                     | 0.40              |
| 46:m2:678:C:H2'    | 46:m2:679:G:O4'    | 2.22                     | 0.40              |
| 46:m2:1012:G:H2'   | 46:m2:1013:A:H8    | 1.86                     | 0.40              |
| 46:m2:1200:G:H2'   | 46:m2:1201:A:H8    | 1.86                     | 0.40              |
| 46:m2:1846:U:H2'   | 46:m2:1847:A:C8    | 2.56                     | 0.40              |
| 55:v2:41:PRO:HG2   | 55:v2:44:HIS:HB2   | 2.02                     | 0.40              |
| 57:y2:118:THR:HA   | 57:y2:121:VAL:HG22 | 2.03                     | 0.40              |
| 67:J3:243:ALA:O    | 67:J3:247:THR:HG23 | 2.21                     | 0.40              |
| 71:N3:3:ARG:HD3    | 71:N3:3:ARG:HA     | 1.92                     | 0.40              |
| 74:Q3:120:THR:HG23 | 74:Q3:124:ASN:HD21 | 1.87                     | 0.40              |
| 78:U3:109:ASP:OD1  | 78:U3:110:GLU:N    | 2.55                     | 0.40              |
| 79:m:315:ILE:HG23  | 79:m:320:ILE:HG13  | 2.03                     | 0.40              |
| 4:D1:39:LYS:HA     | 4:D1:86:HIS:CD2    | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:A2:102:G:O2'    | 9:A2:1195:U:O2'    | 2.34                     | 0.40              |
| 9:A2:178:C:H2'    | 9:A2:179:G:C8      | 2.56                     | 0.40              |
| 9:A2:1286:U:H2'   | 9:A2:1287:C:C6     | 2.56                     | 0.40              |
| 9:A2:2160:G:O2'   | 9:A2:2546:C:O2'    | 2.38                     | 0.40              |
| 9:A2:2438:C:H2'   | 9:A2:2439:C:H6     | 1.87                     | 0.40              |
| 9:A2:3583:U:H2'   | 9:A2:3584:A:H8     | 1.87                     | 0.40              |
| 9:A2:4197:G:H2'   | 9:A2:4198:A:H8     | 1.86                     | 0.40              |
| 9:A2:4204:U:H2'   | 9:A2:4205:A:C8     | 2.56                     | 0.40              |
| 9:A2:4230:G:H2'   | 9:A2:4231:U:H6     | 1.86                     | 0.40              |
| 9:A2:4232:U:O2'   | 13:E2:182:GLU:OE2  | 2.30                     | 0.40              |
| 10:B2:5:A:H1'     | 15:G2:63:GLN:HE22  | 1.85                     | 0.40              |
| 11:C2:59:A:H5''   | 11:C2:60:G:H3'     | 2.03                     | 0.40              |
| 19:K2:92:ILE:O    | 19:K2:112:ARG:NH2  | 2.41                     | 0.40              |
| 23:O2:90:TYR:O    | 23:O2:94:ASN:ND2   | 2.36                     | 0.40              |
| 25:Q2:11:TYR:OH   | 25:Q2:51:TRP:O     | 2.27                     | 0.40              |
| 32:X2:84:ILE:HD12 | 32:X2:84:ILE:HA    | 1.97                     | 0.40              |
| 46:m2:59:U:H5''   | 46:m2:505:C:H41    | 1.87                     | 0.40              |
| 46:m2:65:C:C6     | 68:K3:174:PRO:HB3  | 2.57                     | 0.40              |
| 46:m2:126:G:O6    | 68:K3:196:LYS:HG2  | 2.21                     | 0.40              |
| 46:m2:331:G:H2'   | 46:m2:332:G:C8     | 2.57                     | 0.40              |
| 46:m2:988:G:OP2   | 46:m2:990:C:N4     | 2.54                     | 0.40              |
| 46:m2:1235:G:N3   | 46:m2:1254:C:O2'   | 2.49                     | 0.40              |
| 46:m2:1251:C:OP2  | 46:m2:1252:A:O2'   | 2.34                     | 0.40              |
| 46:m2:1804:C:H2'  | 46:m2:1805:U:C6    | 2.56                     | 0.40              |
| 50:r2:187:ALA:O   | 50:r2:245:ARG:NH1  | 2.40                     | 0.40              |
| 52:z2:85:VAL:HG22 | 53:o2:201:LEU:HD13 | 2.04                     | 0.40              |
| 53:o2:107:THR:N   | 53:o2:136:GLU:OE2  | 2.54                     | 0.40              |
| 68:K3:42:GLY:HA3  | 68:K3:45:TRP:CD1   | 2.57                     | 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 |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | A1    | 221/270 (82%) | 214 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 2   | B1    | 227/266 (85%) | 220 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 3   | C1    | 188/192 (98%) | 185 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 4   | D1    | 204/214 (95%) | 201 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 5   | E1    | 172/178 (97%) | 167 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 6   | F1    | 205/211 (97%) | 194 (95%)  | 11 (5%) | 0        | 100         | 100 |
| 7   | G1    | 137/217 (63%) | 133 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 8   | H1    | 201/204 (98%) | 198 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 12  | D2    | 249/257 (97%) | 234 (94%)  | 15 (6%) | 0        | 100         | 100 |
| 13  | E2    | 400/403 (99%) | 397 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 14  | F2    | 364/419 (87%) | 359 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 15  | G2    | 291/297 (98%) | 284 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 16  | H2    | 215/296 (73%) | 208 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 17  | I2    | 199/203 (98%) | 195 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 18  | J2    | 151/184 (82%) | 146 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 19  | K2    | 184/188 (98%) | 181 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 20  | L2    | 182/196 (93%) | 181 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 21  | M2    | 173/176 (98%) | 166 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 22  | N2    | 157/160 (98%) | 155 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 23  | O2    | 99/128 (77%)  | 97 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 24  | P2    | 127/140 (91%) | 125 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 25  | Q2    | 106/157 (68%) | 104 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 26  | R2    | 116/156 (74%) | 114 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 27  | S2    | 132/145 (91%) | 131 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 28  | T2    | 133/136 (98%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 29  | U2    | 145/148 (98%) | 139 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 30  | V2    | 115/160 (72%) | 110 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 31  | W2    | 92/115 (80%)  | 86 (94%)   | 6 (6%)  | 0        | 100         | 100 |
| 32  | X2    | 105/125 (84%) | 104 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 33  | Y2    | 126/135 (93%) | 125 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 34  | Z2    | 107/110 (97%) | 106 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 35  | a2    | 112/117 (96%) | 110 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 36  | b2    | 118/123 (96%) | 115 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 37  | c2    | 100/105 (95%) | 97 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 38  | d2    | 84/97 (87%)   | 82 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 39  | e2    | 67/70 (96%)   | 67 (100%)  | 0       | 0        | 100         | 100 |
| 40  | f2    | 48/51 (94%)   | 45 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 41  | g2    | 49/128 (38%)  | 48 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 42  | h2    | 22/25 (88%)   | 22 (100%)  | 0       | 0        | 100         | 100 |
| 43  | i2    | 101/106 (95%) | 95 (94%)   | 6 (6%)  | 0        | 100         | 100 |
| 44  | j2    | 87/92 (95%)   | 83 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 45  | k2    | 123/137 (90%) | 119 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 48  | p2    | 212/264 (80%) | 210 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 49  | q2    | 224/243 (92%) | 217 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 50  | r2    | 260/263 (99%) | 252 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 51  | w2    | 151/158 (96%) | 144 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 52  | z2    | 132/135 (98%) | 128 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 53  | o2    | 212/295 (72%) | 211 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 54  | s2    | 187/204 (92%) | 182 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 55  | v2    | 95/165 (58%)  | 93 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 56  | x2    | 128/145 (88%) | 124 (97%)  | 3 (2%)  | 1 (1%)   | 16          | 47  |
| 57  | y2    | 142/146 (97%) | 139 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 58  | A3    | 142/152 (93%) | 138 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 59  | B3    | 139/145 (96%) | 139 (100%) | 0       | 0        | 100         | 100 |
| 60  | C3    | 100/119 (84%) | 97 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 61  | D3    | 81/83 (98%)   | 80 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 62  | E3    | 139/143 (97%) | 135 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 63  | F3    | 99/115 (86%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 64  | G3    | 62/69 (90%)   | 61 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 65  | H3    | 52/56 (93%)   | 50 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 66  | I3    | 311/317 (98%) | 295 (95%)  | 16 (5%) | 0        | 100         | 100 |
| 67  | J3    | 220/293 (75%) | 217 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 68  | K3    | 225/249 (90%) | 223 (99%)  | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 69  | L3    | 183/194 (94%)     | 181 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 70  | M3    | 120/132 (91%)     | 114 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 71  | N3    | 148/151 (98%)     | 144 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 72  | O3    | 132/151 (87%)     | 126 (96%)   | 6 (4%)   | 0        | 100         | 100 |
| 73  | P3    | 127/130 (98%)     | 124 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 74  | Q3    | 127/133 (96%)     | 122 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 75  | R3    | 73/125 (58%)      | 73 (100%)   | 0        | 0        | 100         | 100 |
| 76  | S3    | 81/84 (96%)       | 80 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 77  | T3    | 53/133 (40%)      | 50 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| 78  | U3    | 60/156 (38%)      | 59 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 79  | m     | 846/858 (99%)     | 823 (97%)   | 23 (3%)  | 0        | 100         | 100 |
| 80  | j     | 194/317 (61%)     | 191 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 81  | k     | 151/165 (92%)     | 144 (95%)   | 6 (4%)   | 1 (1%)   | 18          | 49  |
| 82  | A     | 57/386 (15%)      | 57 (100%)   | 0        | 0        | 100         | 100 |
| 83  | t     | 179/194 (92%)     | 174 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 84  | u     | 204/208 (98%)     | 195 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 85  | L1    | 204/217 (94%)     | 187 (92%)   | 16 (8%)  | 1 (0%)   | 24          | 57  |
| All | All   | 12686/14730 (86%) | 12350 (97%) | 333 (3%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | k     | 147 | HIS  |
| 56  | x2    | 108 | LYS  |
| 85  | L1    | 207 | LYS  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A1    | 194/234 (83%)  | 194 (100%) | 0        | 100         | 100 |
| 2   | B1    | 198/223 (89%)  | 198 (100%) | 0        | 100         | 100 |
| 3   | C1    | 169/171 (99%)  | 169 (100%) | 0        | 100         | 100 |
| 4   | D1    | 177/180 (98%)  | 176 (99%)  | 1 (1%)   | 78          | 83  |
| 5   | E1    | 147/149 (99%)  | 145 (99%)  | 2 (1%)   | 59          | 76  |
| 6   | F1    | 174/178 (98%)  | 171 (98%)  | 3 (2%)   | 53          | 74  |
| 7   | G1    | 118/157 (75%)  | 118 (100%) | 0        | 100         | 100 |
| 8   | H1    | 171/172 (99%)  | 170 (99%)  | 1 (1%)   | 78          | 83  |
| 12  | D2    | 193/199 (97%)  | 191 (99%)  | 2 (1%)   | 68          | 79  |
| 13  | E2    | 347/348 (100%) | 340 (98%)  | 7 (2%)   | 48          | 72  |
| 14  | F2    | 307/347 (88%)  | 305 (99%)  | 2 (1%)   | 76          | 82  |
| 15  | G2    | 245/249 (98%)  | 244 (100%) | 1 (0%)   | 84          | 86  |
| 16  | H2    | 198/256 (77%)  | 195 (98%)  | 3 (2%)   | 57          | 75  |
| 17  | I2    | 172/173 (99%)  | 171 (99%)  | 1 (1%)   | 78          | 83  |
| 18  | J2    | 134/164 (82%)  | 131 (98%)  | 3 (2%)   | 45          | 71  |
| 19  | K2    | 164/165 (99%)  | 163 (99%)  | 1 (1%)   | 78          | 83  |
| 20  | L2    | 163/175 (93%)  | 161 (99%)  | 2 (1%)   | 63          | 78  |
| 21  | M2    | 155/156 (99%)  | 154 (99%)  | 1 (1%)   | 78          | 83  |
| 22  | N2    | 138/139 (99%)  | 137 (99%)  | 1 (1%)   | 76          | 82  |
| 23  | O2    | 91/114 (80%)   | 91 (100%)  | 0        | 100         | 100 |
| 24  | P2    | 100/107 (94%)  | 99 (99%)   | 1 (1%)   | 68          | 79  |
| 25  | Q2    | 90/126 (71%)   | 90 (100%)  | 0        | 100         | 100 |
| 26  | R2    | 106/133 (80%)  | 106 (100%) | 0        | 100         | 100 |
| 27  | S2    | 124/135 (92%)  | 124 (100%) | 0        | 100         | 100 |
| 28  | T2    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 29  | U2    | 120/121 (99%)  | 118 (98%)  | 2 (2%)   | 53          | 74  |
| 30  | V2    | 98/124 (79%)   | 95 (97%)   | 3 (3%)   | 35          | 64  |
| 31  | W2    | 79/97 (81%)    | 78 (99%)   | 1 (1%)   | 61          | 77  |
| 32  | X2    | 98/110 (89%)   | 98 (100%)  | 0        | 100         | 100 |
| 33  | Y2    | 114/121 (94%)  | 114 (100%) | 0        | 100         | 100 |
| 34  | Z2    | 88/89 (99%)    | 87 (99%)   | 1 (1%)   | 65          | 78  |
| 35  | a2    | 98/100 (98%)   | 98 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 36  | b2    | 108/110 (98%)  | 108 (100%) | 0        | 100         | 100 |
| 37  | c2    | 86/90 (96%)    | 86 (100%)  | 0        | 100         | 100 |
| 38  | d2    | 73/80 (91%)    | 73 (100%)  | 0        | 100         | 100 |
| 39  | e2    | 64/65 (98%)    | 64 (100%)  | 0        | 100         | 100 |
| 40  | f2    | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 41  | g2    | 47/115 (41%)   | 47 (100%)  | 0        | 100         | 100 |
| 42  | h2    | 23/24 (96%)    | 23 (100%)  | 0        | 100         | 100 |
| 43  | i2    | 91/94 (97%)    | 90 (99%)   | 1 (1%)   | 65          | 78  |
| 44  | j2    | 73/75 (97%)    | 69 (94%)   | 4 (6%)   | 19          | 50  |
| 45  | k2    | 109/121 (90%)  | 108 (99%)  | 1 (1%)   | 70          | 80  |
| 48  | p2    | 195/229 (85%)  | 195 (100%) | 0        | 100         | 100 |
| 49  | q2    | 189/202 (94%)  | 188 (100%) | 1 (0%)   | 81          | 85  |
| 50  | r2    | 224/225 (100%) | 222 (99%)  | 2 (1%)   | 70          | 80  |
| 51  | w2    | 137/142 (96%)  | 135 (98%)  | 2 (2%)   | 57          | 75  |
| 52  | z2    | 120/121 (99%)  | 118 (98%)  | 2 (2%)   | 53          | 74  |
| 53  | o2    | 179/242 (74%)  | 178 (99%)  | 1 (1%)   | 78          | 83  |
| 54  | s2    | 159/170 (94%)  | 158 (99%)  | 1 (1%)   | 78          | 83  |
| 55  | v2    | 88/136 (65%)   | 87 (99%)   | 1 (1%)   | 65          | 78  |
| 56  | x2    | 116/130 (89%)  | 112 (97%)  | 4 (3%)   | 32          | 63  |
| 57  | y2    | 119/121 (98%)  | 118 (99%)  | 1 (1%)   | 73          | 81  |
| 58  | A3    | 125/132 (95%)  | 123 (98%)  | 2 (2%)   | 55          | 75  |
| 59  | B3    | 112/115 (97%)  | 109 (97%)  | 3 (3%)   | 39          | 67  |
| 60  | C3    | 93/107 (87%)   | 91 (98%)   | 2 (2%)   | 45          | 71  |
| 61  | D3    | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 62  | E3    | 113/115 (98%)  | 112 (99%)  | 1 (1%)   | 70          | 80  |
| 63  | F3    | 88/98 (90%)    | 85 (97%)   | 3 (3%)   | 32          | 63  |
| 64  | G3    | 57/62 (92%)    | 57 (100%)  | 0        | 100         | 100 |
| 65  | H3    | 48/49 (98%)    | 47 (98%)   | 1 (2%)   | 47          | 71  |
| 66  | I3    | 272/275 (99%)  | 265 (97%)  | 7 (3%)   | 40          | 68  |
| 67  | J3    | 188/224 (84%)  | 186 (99%)  | 2 (1%)   | 65          | 78  |
| 68  | K3    | 198/218 (91%)  | 195 (98%)  | 3 (2%)   | 57          | 75  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 69  | L3    | 161/168 (96%)     | 158 (98%)   | 3 (2%)   | 50          | 73  |
| 70  | M3    | 102/108 (94%)     | 99 (97%)    | 3 (3%)   | 37          | 66  |
| 71  | N3    | 130/131 (99%)     | 130 (100%)  | 0        | 100         | 100 |
| 72  | O3    | 104/119 (87%)     | 100 (96%)   | 4 (4%)   | 29          | 60  |
| 73  | P3    | 112/113 (99%)     | 112 (100%)  | 0        | 100         | 100 |
| 74  | Q3    | 111/115 (96%)     | 111 (100%)  | 0        | 100         | 100 |
| 75  | R3    | 66/103 (64%)      | 64 (97%)    | 2 (3%)   | 36          | 65  |
| 76  | S3    | 75/76 (99%)       | 74 (99%)    | 1 (1%)   | 61          | 77  |
| 77  | T3    | 45/106 (42%)      | 44 (98%)    | 1 (2%)   | 45          | 71  |
| 78  | U3    | 55/140 (39%)      | 50 (91%)    | 5 (9%)   | 9           | 32  |
| 79  | m     | 725/729 (100%)    | 719 (99%)   | 6 (1%)   | 73          | 81  |
| 80  | j     | 164/255 (64%)     | 161 (98%)   | 3 (2%)   | 51          | 73  |
| 81  | k     | 126/137 (92%)     | 122 (97%)   | 4 (3%)   | 34          | 64  |
| 82  | A     | 52/304 (17%)      | 52 (100%)   | 0        | 100         | 100 |
| 83  | t     | 164/174 (94%)     | 160 (98%)   | 4 (2%)   | 43          | 69  |
| 84  | u     | 178/180 (99%)     | 175 (98%)   | 3 (2%)   | 53          | 74  |
| 85  | L1    | 187/197 (95%)     | 182 (97%)   | 5 (3%)   | 39          | 67  |
| All | All   | 11052/12487 (88%) | 10924 (99%) | 128 (1%) | 61          | 78  |

All (128) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D1    | 31  | ILE  |
| 5   | E1    | 22  | LEU  |
| 5   | E1    | 115 | LEU  |
| 6   | F1    | 59  | VAL  |
| 6   | F1    | 63  | THR  |
| 6   | F1    | 67  | HIS  |
| 8   | H1    | 174 | LEU  |
| 12  | D2    | 5   | ILE  |
| 12  | D2    | 44  | ILE  |
| 13  | E2    | 36  | ASP  |
| 13  | E2    | 39  | LYS  |
| 13  | E2    | 95  | THR  |
| 13  | E2    | 101 | THR  |
| 13  | E2    | 167 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | E2    | 285 | TYR  |
| 13  | E2    | 292 | LEU  |
| 14  | F2    | 115 | VAL  |
| 14  | F2    | 257 | PHE  |
| 15  | G2    | 37  | VAL  |
| 16  | H2    | 46  | LYS  |
| 16  | H2    | 119 | MET  |
| 16  | H2    | 201 | VAL  |
| 17  | I2    | 190 | CYS  |
| 18  | J2    | 118 | GLN  |
| 18  | J2    | 136 | ILE  |
| 18  | J2    | 145 | HIS  |
| 19  | K2    | 137 | VAL  |
| 20  | L2    | 74  | ARG  |
| 20  | L2    | 88  | ARG  |
| 21  | M2    | 32  | ILE  |
| 22  | N2    | 76  | VAL  |
| 24  | P2    | 72  | LEU  |
| 29  | U2    | 73  | VAL  |
| 29  | U2    | 122 | VAL  |
| 30  | V2    | 79  | GLN  |
| 30  | V2    | 82  | LYS  |
| 30  | V2    | 114 | GLN  |
| 31  | W2    | 71  | VAL  |
| 34  | Z2    | 91  | ASN  |
| 43  | i2    | 85  | ILE  |
| 44  | j2    | 13  | LYS  |
| 44  | j2    | 16  | THR  |
| 44  | j2    | 29  | ILE  |
| 44  | j2    | 52  | VAL  |
| 45  | k2    | 108 | MET  |
| 49  | q2    | 167 | TYR  |
| 50  | r2    | 21  | ASP  |
| 50  | r2    | 220 | THR  |
| 51  | w2    | 4   | ILE  |
| 51  | w2    | 119 | ASP  |
| 52  | z2    | 66  | VAL  |
| 52  | z2    | 117 | LEU  |
| 53  | o2    | 123 | VAL  |
| 54  | s2    | 63  | LYS  |
| 55  | v2    | 58  | VAL  |
| 56  | x2    | 37  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | x2    | 64  | LYS  |
| 56  | x2    | 78  | THR  |
| 56  | x2    | 84  | ILE  |
| 57  | y2    | 100 | VAL  |
| 58  | A3    | 12  | ILE  |
| 58  | A3    | 98  | VAL  |
| 59  | B3    | 29  | LYS  |
| 59  | B3    | 64  | LEU  |
| 59  | B3    | 116 | ASP  |
| 60  | C3    | 68  | THR  |
| 60  | C3    | 110 | VAL  |
| 62  | E3    | 105 | PHE  |
| 63  | F3    | 45  | VAL  |
| 63  | F3    | 74  | CYS  |
| 63  | F3    | 87  | ARG  |
| 65  | H3    | 16  | GLN  |
| 66  | I3    | 62  | HIS  |
| 66  | I3    | 64  | HIS  |
| 66  | I3    | 102 | VAL  |
| 66  | I3    | 132 | TRP  |
| 66  | I3    | 134 | THR  |
| 66  | I3    | 165 | ILE  |
| 66  | I3    | 297 | THR  |
| 67  | J3    | 248 | TYR  |
| 67  | J3    | 262 | THR  |
| 68  | K3    | 102 | VAL  |
| 68  | K3    | 108 | VAL  |
| 68  | K3    | 124 | LEU  |
| 69  | L3    | 3   | VAL  |
| 69  | L3    | 12  | THR  |
| 69  | L3    | 61  | LEU  |
| 70  | M3    | 62  | VAL  |
| 70  | M3    | 103 | VAL  |
| 70  | M3    | 110 | VAL  |
| 72  | O3    | 62  | VAL  |
| 72  | O3    | 138 | ASP  |
| 72  | O3    | 142 | ARG  |
| 72  | O3    | 151 | LEU  |
| 75  | R3    | 91  | LEU  |
| 75  | R3    | 107 | VAL  |
| 76  | S3    | 6   | ASP  |
| 77  | T3    | 46  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | U3    | 108 | VAL  |
| 78  | U3    | 113 | LYS  |
| 78  | U3    | 116 | ARG  |
| 78  | U3    | 117 | LEU  |
| 78  | U3    | 118 | ARG  |
| 79  | m     | 29  | HIS  |
| 79  | m     | 76  | LEU  |
| 79  | m     | 77  | PHE  |
| 79  | m     | 372 | TYR  |
| 79  | m     | 474 | VAL  |
| 79  | m     | 755 | VAL  |
| 80  | j     | 30  | VAL  |
| 80  | j     | 98  | ILE  |
| 80  | j     | 160 | LEU  |
| 81  | k     | 40  | LYS  |
| 81  | k     | 143 | VAL  |
| 81  | k     | 147 | HIS  |
| 81  | k     | 156 | ASN  |
| 83  | t     | 10  | LYS  |
| 83  | t     | 58  | LYS  |
| 83  | t     | 75  | ILE  |
| 83  | t     | 77  | VAL  |
| 84  | u     | 47  | ARG  |
| 84  | u     | 107 | THR  |
| 84  | u     | 130 | THR  |
| 85  | L1    | 100 | VAL  |
| 85  | L1    | 178 | GLU  |
| 85  | L1    | 189 | PHE  |
| 85  | L1    | 204 | LEU  |
| 85  | L1    | 206 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 173 | ASN  |
| 4   | D1    | 73  | ASN  |
| 4   | D1    | 166 | HIS  |
| 5   | E1    | 46  | GLN  |
| 5   | E1    | 97  | ASN  |
| 5   | E1    | 155 | HIS  |
| 7   | G1    | 34  | ASN  |
| 8   | H1    | 87  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | F2    | 38  | ASN  |
| 14  | F2    | 236 | ASN  |
| 14  | F2    | 329 | ASN  |
| 15  | G2    | 63  | GLN  |
| 15  | G2    | 225 | GLN  |
| 15  | G2    | 244 | HIS  |
| 16  | H2    | 263 | GLN  |
| 17  | I2    | 50  | ASN  |
| 18  | J2    | 25  | HIS  |
| 18  | J2    | 34  | GLN  |
| 26  | R2    | 93  | ASN  |
| 28  | T2    | 97  | ASN  |
| 29  | U2    | 14  | HIS  |
| 29  | U2    | 40  | HIS  |
| 29  | U2    | 66  | ASN  |
| 30  | V2    | 6   | ASN  |
| 31  | W2    | 19  | GLN  |
| 31  | W2    | 72  | HIS  |
| 32  | X2    | 116 | ASN  |
| 33  | Y2    | 43  | ASN  |
| 34  | Z2    | 21  | GLN  |
| 35  | a2    | 112 | GLN  |
| 37  | c2    | 15  | HIS  |
| 38  | d2    | 48  | ASN  |
| 40  | f2    | 17  | GLN  |
| 41  | g2    | 90  | ASN  |
| 45  | k2    | 31  | ASN  |
| 45  | k2    | 36  | ASN  |
| 48  | p2    | 43  | ASN  |
| 49  | q2    | 145 | GLN  |
| 50  | r2    | 67  | GLN  |
| 51  | w2    | 19  | ASN  |
| 52  | z2    | 26  | ASN  |
| 52  | z2    | 29  | HIS  |
| 52  | z2    | 116 | ASN  |
| 54  | s2    | 74  | ASN  |
| 54  | s2    | 107 | ASN  |
| 54  | s2    | 110 | GLN  |
| 54  | s2    | 114 | ASN  |
| 54  | s2    | 168 | ASN  |
| 54  | s2    | 179 | ASN  |
| 55  | v2    | 42  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | v2    | 44  | HIS  |
| 56  | x2    | 79  | HIS  |
| 57  | y2    | 80  | GLN  |
| 58  | A3    | 42  | HIS  |
| 58  | A3    | 105 | ASN  |
| 60  | C3    | 47  | ASN  |
| 60  | C3    | 92  | HIS  |
| 61  | D3    | 35  | ASN  |
| 62  | E3    | 39  | ASN  |
| 62  | E3    | 61  | GLN  |
| 62  | E3    | 73  | GLN  |
| 63  | F3    | 43  | ASN  |
| 64  | G3    | 7   | GLN  |
| 66  | I3    | 15  | ASN  |
| 66  | I3    | 188 | HIS  |
| 67  | J3    | 113 | GLN  |
| 67  | J3    | 267 | GLN  |
| 68  | K3    | 81  | HIS  |
| 68  | K3    | 202 | ASN  |
| 73  | P3    | 91  | ASN  |
| 74  | Q3    | 94  | HIS  |
| 75  | R3    | 46  | ASN  |
| 76  | S3    | 9   | HIS  |
| 77  | T3    | 58  | ASN  |
| 79  | m     | 90  | GLN  |
| 79  | m     | 201 | ASN  |
| 79  | m     | 492 | ASN  |
| 79  | m     | 659 | ASN  |
| 79  | m     | 768 | HIS  |
| 80  | j     | 71  | ASN  |
| 80  | j     | 105 | ASN  |
| 81  | k     | 115 | GLN  |
| 81  | k     | 137 | GLN  |
| 83  | t     | 73  | GLN  |
| 83  | t     | 165 | ASN  |
| 84  | u     | 88  | ASN  |
| 84  | u     | 165 | GLN  |
| 85  | L1    | 19  | HIS  |
| 85  | L1    | 96  | ASN  |
| 85  | L1    | 182 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | B2    | 119/121 (98%)   | 16 (13%)          | 0               |
| 11  | C2    | 155/156 (99%)   | 28 (18%)          | 2 (1%)          |
| 46  | m2    | 1717/1871 (91%) | 385 (22%)         | 0               |
| 47  | n2    | 74/75 (98%)     | 24 (32%)          | 0               |
| 9   | A2    | 3691/4731 (78%) | 788 (21%)         | 13 (0%)         |
| All | All   | 5756/6954 (82%) | 1241 (21%)        | 15 (0%)         |

All (1241) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A2    | 2   | G    |
| 9   | A2    | 25  | A    |
| 9   | A2    | 39  | A    |
| 9   | A2    | 42  | A    |
| 9   | A2    | 48  | G    |
| 9   | A2    | 59  | A    |
| 9   | A2    | 64  | A    |
| 9   | A2    | 65  | A    |
| 9   | A2    | 66  | A    |
| 9   | A2    | 73  | A    |
| 9   | A2    | 76  | A    |
| 9   | A2    | 91  | G    |
| 9   | A2    | 95  | G    |
| 9   | A2    | 104 | G    |
| 9   | A2    | 106 | A    |
| 9   | A2    | 109 | G    |
| 9   | A2    | 116 | G    |
| 9   | A2    | 119 | G    |
| 9   | A2    | 120 | A    |
| 9   | A2    | 133 | C    |
| 9   | A2    | 134 | G    |
| 9   | A2    | 136 | C    |
| 9   | A2    | 137 | G    |
| 9   | A2    | 138 | C    |
| 9   | A2    | 143 | U    |
| 9   | A2    | 144 | G    |
| 9   | A2    | 158 | A    |
| 9   | A2    | 159 | C    |
| 9   | A2    | 164 | G    |
| 9   | A2    | 171 | U    |
| 9   | A2    | 172 | C    |
| 9   | A2    | 178 | C    |
| 9   | A2    | 179 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A2    | 183 | C    |
| 9   | A2    | 184 | U    |
| 9   | A2    | 185 | C    |
| 9   | A2    | 187 | U    |
| 9   | A2    | 188 | G    |
| 9   | A2    | 189 | G    |
| 9   | A2    | 197 | A    |
| 9   | A2    | 200 | U    |
| 9   | A2    | 201 | C    |
| 9   | A2    | 209 | U    |
| 9   | A2    | 216 | C    |
| 9   | A2    | 217 | C    |
| 9   | A2    | 218 | A    |
| 9   | A2    | 233 | U    |
| 9   | A2    | 234 | G    |
| 9   | A2    | 237 | B9B  |
| 9   | A2    | 238 | C    |
| 9   | A2    | 254 | G    |
| 9   | A2    | 258 | G    |
| 9   | A2    | 259 | C    |
| 9   | A2    | 265 | U    |
| 9   | A2    | 266 | C    |
| 9   | A2    | 267 | G    |
| 9   | A2    | 269 | G    |
| 9   | A2    | 274 | C    |
| 9   | A2    | 278 | G    |
| 9   | A2    | 280 | G    |
| 9   | A2    | 297 | U    |
| 9   | A2    | 315 | G    |
| 9   | A2    | 316 | U    |
| 9   | A2    | 328 | A    |
| 9   | A2    | 330 | G    |
| 9   | A2    | 340 | C    |
| 9   | A2    | 341 | G    |
| 9   | A2    | 345 | C    |
| 9   | A2    | 373 | OMG  |
| 9   | A2    | 387 | G    |
| 9   | A2    | 396 | A    |
| 9   | A2    | 398 | A2M  |
| 9   | A2    | 399 | G    |
| 9   | A2    | 407 | A    |
| 9   | A2    | 409 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A2    | 410 | A    |
| 9   | A2    | 412 | G    |
| 9   | A2    | 413 | G    |
| 9   | A2    | 418 | A    |
| 9   | A2    | 433 | A    |
| 9   | A2    | 439 | G    |
| 9   | A2    | 440 | U    |
| 9   | A2    | 450 | G    |
| 9   | A2    | 452 | A    |
| 9   | A2    | 453 | G    |
| 9   | A2    | 454 | U    |
| 9   | A2    | 456 | C    |
| 9   | A2    | 457 | G    |
| 9   | A2    | 467 | U    |
| 9   | A2    | 470 | A    |
| 9   | A2    | 486 | C    |
| 9   | A2    | 487 | C    |
| 9   | A2    | 489 | G    |
| 9   | A2    | 490 | C    |
| 9   | A2    | 491 | C    |
| 9   | A2    | 492 | G    |
| 9   | A2    | 498 | G    |
| 9   | A2    | 500 | G    |
| 9   | A2    | 501 | G    |
| 9   | A2    | 502 | U    |
| 9   | A2    | 504 | C    |
| 9   | A2    | 505 | G    |
| 9   | A2    | 510 | A    |
| 9   | A2    | 511 | U    |
| 9   | A2    | 513 | U    |
| 9   | A2    | 514 | U    |
| 9   | A2    | 515 | U    |
| 9   | A2    | 673 | G    |
| 9   | A2    | 674 | A    |
| 9   | A2    | 675 | C    |
| 9   | A2    | 681 | G    |
| 9   | A2    | 692 | C    |
| 9   | A2    | 693 | A    |
| 9   | A2    | 694 | C    |
| 9   | A2    | 703 | U    |
| 9   | A2    | 704 | G    |
| 9   | A2    | 711 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A2    | 715 | G    |
| 9   | A2    | 735 | C    |
| 9   | A2    | 736 | G    |
| 9   | A2    | 738 | G    |
| 9   | A2    | 740 | A    |
| 9   | A2    | 746 | G    |
| 9   | A2    | 747 | G    |
| 9   | A2    | 748 | U    |
| 9   | A2    | 749 | G    |
| 9   | A2    | 750 | G    |
| 9   | A2    | 751 | G    |
| 9   | A2    | 753 | A    |
| 9   | A2    | 756 | G    |
| 9   | A2    | 767 | G    |
| 9   | A2    | 770 | G    |
| 9   | A2    | 801 | C    |
| 9   | A2    | 802 | A    |
| 9   | A2    | 803 | C    |
| 9   | A2    | 809 | G    |
| 9   | A2    | 812 | U    |
| 9   | A2    | 814 | A    |
| 9   | A2    | 816 | A    |
| 9   | A2    | 822 | C    |
| 9   | A2    | 824 | G    |
| 9   | A2    | 831 | C    |
| 9   | A2    | 834 | U    |
| 9   | A2    | 839 | C    |
| 9   | A2    | 841 | A    |
| 9   | A2    | 842 | A    |
| 9   | A2    | 843 | U    |
| 9   | A2    | 844 | C    |
| 9   | A2    | 855 | G    |
| 9   | A2    | 857 | A    |
| 9   | A2    | 858 | A    |
| 9   | A2    | 859 | G    |
| 9   | A2    | 869 | C    |
| 9   | A2    | 877 | C    |
| 9   | A2    | 878 | 2MG  |
| 9   | A2    | 884 | C    |
| 9   | A2    | 886 | U    |
| 9   | A2    | 887 | C    |
| 9   | A2    | 888 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 921  | G    |
| 9   | A2    | 927  | C    |
| 9   | A2    | 934  | C    |
| 9   | A2    | 935  | C    |
| 9   | A2    | 936  | C    |
| 9   | A2    | 937  | C    |
| 9   | A2    | 938  | U    |
| 9   | A2    | 947  | G    |
| 9   | A2    | 1000 | G    |
| 9   | A2    | 1004 | C    |
| 9   | A2    | 1010 | G    |
| 9   | A2    | 1011 | U    |
| 9   | A2    | 1012 | C    |
| 9   | A2    | 1013 | C    |
| 9   | A2    | 1014 | C    |
| 9   | A2    | 1015 | C    |
| 9   | A2    | 1022 | C    |
| 9   | A2    | 1024 | C    |
| 9   | A2    | 1028 | G    |
| 9   | A2    | 1031 | U    |
| 9   | A2    | 1032 | C    |
| 9   | A2    | 1038 | G    |
| 9   | A2    | 1043 | C    |
| 9   | A2    | 1044 | G    |
| 9   | A2    | 1045 | G    |
| 9   | A2    | 1047 | U    |
| 9   | A2    | 1049 | C    |
| 9   | A2    | 1054 | G    |
| 9   | A2    | 1055 | G    |
| 9   | A2    | 1060 | G    |
| 9   | A2    | 1066 | C    |
| 9   | A2    | 1068 | C    |
| 9   | A2    | 1070 | C    |
| 9   | A2    | 1071 | G    |
| 9   | A2    | 1081 | G    |
| 9   | A2    | 1082 | A    |
| 9   | A2    | 1086 | C    |
| 9   | A2    | 1087 | G    |
| 9   | A2    | 1089 | G    |
| 9   | A2    | 1094 | C    |
| 9   | A2    | 1098 | G    |
| 9   | A2    | 1099 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 1101 | G    |
| 9   | A2    | 1108 | A    |
| 9   | A2    | 1110 | G    |
| 9   | A2    | 1116 | U    |
| 9   | A2    | 1117 | A    |
| 9   | A2    | 1118 | C    |
| 9   | A2    | 1136 | A    |
| 9   | A2    | 1137 | A    |
| 9   | A2    | 1140 | A2M  |
| 9   | A2    | 1158 | C    |
| 9   | A2    | 1168 | A    |
| 9   | A2    | 1172 | A    |
| 9   | A2    | 1173 | G    |
| 9   | A2    | 1178 | U    |
| 9   | A2    | 1184 | G    |
| 9   | A2    | 1191 | G    |
| 9   | A2    | 1193 | C    |
| 9   | A2    | 1201 | A    |
| 9   | A2    | 1207 | G    |
| 9   | A2    | 1208 | G    |
| 9   | A2    | 1211 | A    |
| 9   | A2    | 1212 | A    |
| 9   | A2    | 1217 | C    |
| 9   | A2    | 1224 | G    |
| 9   | A2    | 1229 | C    |
| 9   | A2    | 1232 | G    |
| 9   | A2    | 1233 | A    |
| 9   | A2    | 1252 | C    |
| 9   | A2    | 1259 | C    |
| 9   | A2    | 1278 | G    |
| 9   | A2    | 1298 | C    |
| 9   | A2    | 1310 | A    |
| 9   | A2    | 1311 | G    |
| 9   | A2    | 1315 | G    |
| 9   | A2    | 1329 | G    |
| 9   | A2    | 1338 | A    |
| 9   | A2    | 1347 | A2M  |
| 9   | A2    | 1360 | A    |
| 9   | A2    | 1377 | A    |
| 9   | A2    | 1379 | C    |
| 9   | A2    | 1387 | B9B  |
| 9   | A2    | 1391 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 1395 | PSU  |
| 9   | A2    | 1404 | U    |
| 9   | A2    | 1409 | U    |
| 9   | A2    | 1425 | G    |
| 9   | A2    | 1437 | G    |
| 9   | A2    | 1438 | OMG  |
| 9   | A2    | 1439 | G    |
| 9   | A2    | 1444 | A    |
| 9   | A2    | 1446 | G    |
| 9   | A2    | 1447 | A    |
| 9   | A2    | 1451 | A    |
| 9   | A2    | 1454 | G    |
| 9   | A2    | 1455 | A    |
| 9   | A2    | 1463 | A    |
| 9   | A2    | 1467 | G    |
| 9   | A2    | 1473 | U    |
| 9   | A2    | 1474 | C    |
| 9   | A2    | 1489 | C    |
| 9   | A2    | 1490 | PSU  |
| 9   | A2    | 1504 | G    |
| 9   | A2    | 1507 | C    |
| 9   | A2    | 1512 | U    |
| 9   | A2    | 1522 | C    |
| 9   | A2    | 1526 | G    |
| 9   | A2    | 1533 | C    |
| 9   | A2    | 1538 | A    |
| 9   | A2    | 1544 | A    |
| 9   | A2    | 1552 | G    |
| 9   | A2    | 1558 | U    |
| 9   | A2    | 1559 | U    |
| 9   | A2    | 1560 | G    |
| 9   | A2    | 1564 | C    |
| 9   | A2    | 1566 | G    |
| 9   | A2    | 1568 | A    |
| 9   | A2    | 1569 | A    |
| 9   | A2    | 1570 | C    |
| 9   | A2    | 1573 | U    |
| 9   | A2    | 1589 | A    |
| 9   | A2    | 1605 | G    |
| 9   | A2    | 1606 | A    |
| 9   | A2    | 1607 | A    |
| 9   | A2    | 1608 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 1617 | G    |
| 9   | A2    | 1621 | G    |
| 9   | A2    | 1623 | G    |
| 9   | A2    | 1624 | U    |
| 9   | A2    | 1625 | G    |
| 9   | A2    | 1635 | G    |
| 9   | A2    | 1638 | G    |
| 9   | A2    | 1639 | A    |
| 9   | A2    | 1644 | G    |
| 9   | A2    | 1657 | G    |
| 9   | A2    | 1665 | U    |
| 9   | A2    | 1668 | UR3  |
| 9   | A2    | 1671 | G    |
| 9   | A2    | 1685 | OMG  |
| 9   | A2    | 1690 | A    |
| 9   | A2    | 1699 | A    |
| 9   | A2    | 1700 | C    |
| 9   | A2    | 1717 | C    |
| 9   | A2    | 1721 | G    |
| 9   | A2    | 1722 | C    |
| 9   | A2    | 1723 | C    |
| 9   | A2    | 1724 | G    |
| 9   | A2    | 1733 | C    |
| 9   | A2    | 1734 | A    |
| 9   | A2    | 1737 | C    |
| 9   | A2    | 1740 | C    |
| 9   | A2    | 1742 | G    |
| 9   | A2    | 1750 | G    |
| 9   | A2    | 1761 | U    |
| 9   | A2    | 1763 | G    |
| 9   | A2    | 1766 | A    |
| 9   | A2    | 1768 | C    |
| 9   | A2    | 1775 | G    |
| 9   | A2    | 1776 | U    |
| 9   | A2    | 1777 | G    |
| 9   | A2    | 1778 | G    |
| 9   | A2    | 1779 | C    |
| 9   | A2    | 1781 | A    |
| 9   | A2    | 1782 | U    |
| 9   | A2    | 1783 | G    |
| 9   | A2    | 1784 | G    |
| 9   | A2    | 1785 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 1786 | A    |
| 9   | A2    | 1787 | G    |
| 9   | A2    | 1788 | U    |
| 9   | A2    | 1789 | C    |
| 9   | A2    | 1790 | G    |
| 9   | A2    | 1792 | A    |
| 9   | A2    | 1793 | A    |
| 9   | A2    | 1794 | U    |
| 9   | A2    | 1803 | G    |
| 9   | A2    | 1804 | A    |
| 9   | A2    | 1805 | G    |
| 9   | A2    | 1806 | U    |
| 9   | A2    | 1807 | G    |
| 9   | A2    | 1811 | A    |
| 9   | A2    | 1812 | A    |
| 9   | A2    | 1813 | C    |
| 9   | A2    | 1822 | U    |
| 9   | A2    | 1827 | A    |
| 9   | A2    | 1828 | A    |
| 9   | A2    | 1850 | U    |
| 9   | A2    | 1857 | G    |
| 9   | A2    | 1858 | G    |
| 9   | A2    | 1864 | C    |
| 9   | A2    | 1870 | C    |
| 9   | A2    | 1871 | A    |
| 9   | A2    | 1886 | C    |
| 9   | A2    | 1887 | G    |
| 9   | A2    | 1893 | C    |
| 9   | A2    | 1894 | G    |
| 9   | A2    | 1895 | G    |
| 9   | A2    | 1897 | A    |
| 9   | A2    | 1899 | G    |
| 9   | A2    | 1900 | G    |
| 9   | A2    | 1903 | C    |
| 9   | A2    | 1904 | G    |
| 9   | A2    | 1909 | G    |
| 9   | A2    | 1910 | G    |
| 9   | A2    | 1912 | A    |
| 9   | A2    | 2003 | C    |
| 9   | A2    | 2004 | G    |
| 9   | A2    | 2008 | G    |
| 9   | A2    | 2009 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 2012 | C    |
| 9   | A2    | 2013 | C    |
| 9   | A2    | 2014 | G    |
| 9   | A2    | 2015 | C    |
| 9   | A2    | 2044 | C    |
| 9   | A2    | 2055 | A    |
| 9   | A2    | 2056 | G    |
| 9   | A2    | 2061 | G    |
| 9   | A2    | 2068 | A    |
| 9   | A2    | 2071 | G    |
| 9   | A2    | 2077 | G    |
| 9   | A2    | 2086 | G    |
| 9   | A2    | 2088 | G    |
| 9   | A2    | 2094 | G    |
| 9   | A2    | 2103 | G    |
| 9   | A2    | 2106 | C    |
| 9   | A2    | 2115 | A    |
| 9   | A2    | 2119 | OMG  |
| 9   | A2    | 2137 | A    |
| 9   | A2    | 2150 | A    |
| 9   | A2    | 2152 | G    |
| 9   | A2    | 2156 | A2M  |
| 9   | A2    | 2165 | C    |
| 9   | A2    | 2172 | A    |
| 9   | A2    | 2176 | G    |
| 9   | A2    | 2177 | OMC  |
| 9   | A2    | 2179 | OMG  |
| 9   | A2    | 2180 | U    |
| 9   | A2    | 2181 | U    |
| 9   | A2    | 2183 | A    |
| 9   | A2    | 2196 | C    |
| 9   | A2    | 2229 | G    |
| 9   | A2    | 2230 | G    |
| 9   | A2    | 2233 | C    |
| 9   | A2    | 2239 | A    |
| 9   | A2    | 2245 | U    |
| 9   | A2    | 2257 | G    |
| 9   | A2    | 2258 | G    |
| 9   | A2    | 2259 | C    |
| 9   | A2    | 2260 | C    |
| 9   | A2    | 2262 | A    |
| 9   | A2    | 2268 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 2275 | C    |
| 9   | A2    | 2284 | A    |
| 9   | A2    | 2285 | U    |
| 9   | A2    | 2287 | C    |
| 9   | A2    | 2299 | G    |
| 9   | A2    | 2301 | G    |
| 9   | A2    | 2302 | G    |
| 9   | A2    | 2321 | G    |
| 9   | A2    | 2331 | G    |
| 9   | A2    | 2342 | A    |
| 9   | A2    | 2344 | C    |
| 9   | A2    | 2373 | G    |
| 9   | A2    | 2382 | C    |
| 9   | A2    | 2383 | U    |
| 9   | A2    | 2393 | G    |
| 9   | A2    | 2407 | G    |
| 9   | A2    | 2411 | U    |
| 9   | A2    | 2413 | G    |
| 9   | A2    | 2414 | A    |
| 9   | A2    | 2416 | U    |
| 9   | A2    | 2417 | G    |
| 9   | A2    | 2424 | C    |
| 9   | A2    | 2430 | G    |
| 9   | A2    | 2431 | A    |
| 9   | A2    | 2442 | U    |
| 9   | A2    | 2449 | G    |
| 9   | A2    | 2450 | A    |
| 9   | A2    | 2451 | A    |
| 9   | A2    | 2458 | G    |
| 9   | A2    | 2461 | G    |
| 9   | A2    | 2463 | U    |
| 9   | A2    | 2466 | G    |
| 9   | A2    | 2474 | C    |
| 9   | A2    | 2476 | G    |
| 9   | A2    | 2478 | U    |
| 9   | A2    | 2479 | G    |
| 9   | A2    | 2481 | G    |
| 9   | A2    | 2494 | C    |
| 9   | A2    | 2498 | A    |
| 9   | A2    | 2501 | A    |
| 9   | A2    | 2507 | G    |
| 9   | A2    | 2508 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 2515 | G    |
| 9   | A2    | 2516 | U    |
| 9   | A2    | 2518 | U    |
| 9   | A2    | 2519 | A    |
| 9   | A2    | 2524 | U    |
| 9   | A2    | 2525 | C    |
| 9   | A2    | 2527 | C    |
| 9   | A2    | 2528 | OMG  |
| 9   | A2    | 2542 | A    |
| 9   | A2    | 2543 | U    |
| 9   | A2    | 2545 | U    |
| 9   | A2    | 2549 | C    |
| 9   | A2    | 2554 | G    |
| 9   | A2    | 2581 | U    |
| 9   | A2    | 2582 | G    |
| 9   | A2    | 2590 | A    |
| 9   | A2    | 2603 | G    |
| 9   | A2    | 2610 | G    |
| 9   | A2    | 2611 | C    |
| 9   | A2    | 2632 | G    |
| 9   | A2    | 2652 | G    |
| 9   | A2    | 2659 | U    |
| 9   | A2    | 3243 | C    |
| 9   | A2    | 3246 | G    |
| 9   | A2    | 3250 | C    |
| 9   | A2    | 3253 | G    |
| 9   | A2    | 3254 | C    |
| 9   | A2    | 3271 | G    |
| 9   | A2    | 3272 | U    |
| 9   | A2    | 3273 | G    |
| 9   | A2    | 3282 | G    |
| 9   | A2    | 3286 | A    |
| 9   | A2    | 3291 | A    |
| 9   | A2    | 3302 | A    |
| 9   | A2    | 3318 | A    |
| 9   | A2    | 3320 | G    |
| 9   | A2    | 3329 | C    |
| 9   | A2    | 3330 | G    |
| 9   | A2    | 3347 | G    |
| 9   | A2    | 3348 | A    |
| 9   | A2    | 3364 | C    |
| 9   | A2    | 3367 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 3368 | A    |
| 9   | A2    | 3373 | A    |
| 9   | A2    | 3383 | A    |
| 9   | A2    | 3385 | PSU  |
| 9   | A2    | 3392 | A    |
| 9   | A2    | 3401 | U    |
| 9   | A2    | 3402 | A    |
| 9   | A2    | 3404 | A    |
| 9   | A2    | 3409 | G    |
| 9   | A2    | 3412 | A    |
| 9   | A2    | 3415 | A    |
| 9   | A2    | 3416 | A    |
| 9   | A2    | 3417 | C    |
| 9   | A2    | 3420 | PSU  |
| 9   | A2    | 3422 | A    |
| 9   | A2    | 3427 | C    |
| 9   | A2    | 3429 | U    |
| 9   | A2    | 3430 | A    |
| 9   | A2    | 3431 | A    |
| 9   | A2    | 3432 | G    |
| 9   | A2    | 3433 | G    |
| 9   | A2    | 3434 | U    |
| 9   | A2    | 3438 | 5MC  |
| 9   | A2    | 3441 | A2M  |
| 9   | A2    | 3442 | U    |
| 9   | A2    | 3458 | U    |
| 9   | A2    | 3466 | C    |
| 9   | A2    | 3467 | G    |
| 9   | A2    | 3470 | U    |
| 9   | A2    | 3473 | A    |
| 9   | A2    | 3474 | U    |
| 9   | A2    | 3475 | G    |
| 9   | A2    | 3480 | A    |
| 9   | A2    | 3496 | U    |
| 9   | A2    | 3499 | C    |
| 9   | A2    | 3507 | U    |
| 9   | A2    | 3523 | A2M  |
| 9   | A2    | 3524 | G    |
| 9   | A2    | 3533 | A    |
| 9   | A2    | 3534 | C    |
| 9   | A2    | 3535 | G    |
| 9   | A2    | 3536 | P7G  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 3543 | OMC  |
| 9   | A2    | 3546 | A    |
| 9   | A2    | 3548 | U    |
| 9   | A2    | 3553 | G    |
| 9   | A2    | 3554 | G    |
| 9   | A2    | 3557 | A    |
| 9   | A2    | 3562 | A    |
| 9   | A2    | 3563 | G    |
| 9   | A2    | 3564 | A    |
| 9   | A2    | 3571 | U    |
| 9   | A2    | 3582 | C    |
| 9   | A2    | 3585 | G    |
| 9   | A2    | 3587 | C    |
| 9   | A2    | 3594 | G    |
| 9   | A2    | 3599 | A    |
| 9   | A2    | 3610 | A    |
| 9   | A2    | 3612 | G    |
| 9   | A2    | 3613 | U    |
| 9   | A2    | 3614 | G    |
| 9   | A2    | 3615 | U    |
| 9   | A2    | 3617 | G    |
| 9   | A2    | 3618 | A    |
| 9   | A2    | 3619 | A    |
| 9   | A2    | 3620 | U    |
| 9   | A2    | 3621 | A    |
| 9   | A2    | 3622 | A    |
| 9   | A2    | 3625 | G    |
| 9   | A2    | 3627 | G    |
| 9   | A2    | 3630 | G    |
| 9   | A2    | 3631 | C    |
| 9   | A2    | 3688 | C    |
| 9   | A2    | 3689 | G    |
| 9   | A2    | 3690 | C    |
| 9   | A2    | 3693 | G    |
| 9   | A2    | 3694 | U    |
| 9   | A2    | 3695 | G    |
| 9   | A2    | 3696 | A    |
| 9   | A2    | 3697 | A    |
| 9   | A2    | 3698 | A    |
| 9   | A2    | 3699 | U    |
| 9   | A2    | 3701 | C    |
| 9   | A2    | 3702 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 3703 | A    |
| 9   | A2    | 3704 | C    |
| 9   | A2    | 3707 | C    |
| 9   | A2    | 3708 | U    |
| 9   | A2    | 3712 | A    |
| 9   | A2    | 3714 | C    |
| 9   | A2    | 3715 | G    |
| 9   | A2    | 3726 | G    |
| 9   | A2    | 3732 | G    |
| 9   | A2    | 3733 | U    |
| 9   | A2    | 3734 | G    |
| 9   | A2    | 3735 | A    |
| 9   | A2    | 3736 | G    |
| 9   | A2    | 3742 | G    |
| 9   | A2    | 3754 | G    |
| 9   | A2    | 3756 | G    |
| 9   | A2    | 3757 | G    |
| 9   | A2    | 3758 | G    |
| 9   | A2    | 3765 | G    |
| 9   | A2    | 3766 | C    |
| 9   | A2    | 3768 | U    |
| 9   | A2    | 3769 | C    |
| 9   | A2    | 3771 | G    |
| 9   | A2    | 3772 | G    |
| 9   | A2    | 3773 | C    |
| 9   | A2    | 3777 | A    |
| 9   | A2    | 3778 | A    |
| 9   | A2    | 3780 | C    |
| 9   | A2    | 3782 | U    |
| 9   | A2    | 3786 | U    |
| 9   | A2    | 3787 | C    |
| 9   | A2    | 3792 | G    |
| 9   | A2    | 3794 | G    |
| 9   | A2    | 3796 | G    |
| 9   | A2    | 3814 | C    |
| 9   | A2    | 3822 | A    |
| 9   | A2    | 3835 | G    |
| 9   | A2    | 3836 | G    |
| 9   | A2    | 3843 | G    |
| 9   | A2    | 3846 | I4U  |
| 9   | A2    | 3853 | G    |
| 9   | A2    | 3855 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 3864 | A    |
| 9   | A2    | 3872 | 6MZ  |
| 9   | A2    | 3873 | C    |
| 9   | A2    | 3874 | G    |
| 9   | A2    | 3877 | G    |
| 9   | A2    | 3881 | U    |
| 9   | A2    | 3884 | U    |
| 9   | A2    | 3885 | A    |
| 9   | A2    | 3886 | A    |
| 9   | A2    | 3893 | C    |
| 9   | A2    | 3894 | U    |
| 9   | A2    | 3895 | C    |
| 9   | A2    | 3903 | A    |
| 9   | A2    | 3906 | G    |
| 9   | A2    | 3907 | A    |
| 9   | A2    | 3909 | A    |
| 9   | A2    | 3910 | C    |
| 9   | A2    | 3917 | U    |
| 9   | A2    | 3920 | A    |
| 9   | A2    | 3923 | A    |
| 9   | A2    | 3925 | A    |
| 9   | A2    | 3932 | A    |
| 9   | A2    | 3933 | A    |
| 9   | A2    | 3941 | U    |
| 9   | A2    | 3943 | G    |
| 9   | A2    | 3945 | PSU  |
| 9   | A2    | 3947 | U    |
| 9   | A2    | 3956 | A    |
| 9   | A2    | 3957 | G    |
| 9   | A2    | 3958 | OMU  |
| 9   | A2    | 3965 | A    |
| 9   | A2    | 3966 | C    |
| 9   | A2    | 3971 | C    |
| 9   | A2    | 3982 | G    |
| 9   | A2    | 3984 | C    |
| 9   | A2    | 3987 | 5MC  |
| 9   | A2    | 4002 | C    |
| 9   | A2    | 4004 | U    |
| 9   | A2    | 4006 | U    |
| 9   | A2    | 4023 | MHG  |
| 9   | A2    | 4025 | G    |
| 9   | A2    | 4029 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 4030 | A    |
| 9   | A2    | 4032 | A    |
| 9   | A2    | 4033 | A    |
| 9   | A2    | 4039 | C    |
| 9   | A2    | 4045 | G    |
| 9   | A2    | 4046 | A    |
| 9   | A2    | 4050 | C    |
| 9   | A2    | 4073 | C    |
| 9   | A2    | 4096 | C    |
| 9   | A2    | 4100 | G    |
| 9   | A2    | 4101 | A    |
| 9   | A2    | 4102 | PSU  |
| 9   | A2    | 4104 | U    |
| 9   | A2    | 4105 | C    |
| 9   | A2    | 4116 | A    |
| 9   | A2    | 4118 | C    |
| 9   | A2    | 4127 | G    |
| 9   | A2    | 4164 | U    |
| 9   | A2    | 4165 | A    |
| 9   | A2    | 4170 | A    |
| 9   | A2    | 4171 | C    |
| 9   | A2    | 4174 | G    |
| 9   | A2    | 4176 | G    |
| 9   | A2    | 4180 | G    |
| 9   | A2    | 4183 | PSU  |
| 9   | A2    | 4184 | U    |
| 9   | A2    | 4200 | A    |
| 9   | A2    | 4201 | G    |
| 9   | A2    | 4212 | C    |
| 9   | A2    | 4219 | G    |
| 9   | A2    | 4225 | G    |
| 9   | A2    | 4227 | G    |
| 9   | A2    | 4241 | A    |
| 9   | A2    | 4242 | A    |
| 9   | A2    | 4252 | G    |
| 9   | A2    | 4262 | A    |
| 9   | A2    | 4272 | OMU  |
| 9   | A2    | 4279 | U    |
| 9   | A2    | 4287 | A    |
| 9   | A2    | 4288 | PSU  |
| 9   | A2    | 4304 | G    |
| 9   | A2    | 4308 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 4310 | G    |
| 9   | A2    | 4322 | C    |
| 9   | A2    | 4324 | A    |
| 9   | A2    | 4331 | G    |
| 9   | A2    | 4336 | A    |
| 9   | A2    | 4343 | A    |
| 9   | A2    | 4347 | C    |
| 9   | A2    | 4352 | A    |
| 9   | A2    | 4360 | A    |
| 9   | A2    | 4361 | U    |
| 9   | A2    | 4373 | G    |
| 9   | A2    | 4382 | C    |
| 9   | A2    | 4383 | G    |
| 9   | A2    | 4385 | C    |
| 9   | A2    | 4386 | A    |
| 9   | A2    | 4392 | G    |
| 9   | A2    | 4393 | A    |
| 9   | A2    | 4394 | G    |
| 9   | A2    | 4402 | G    |
| 9   | A2    | 4403 | G    |
| 9   | A2    | 4409 | C    |
| 9   | A2    | 4411 | C    |
| 9   | A2    | 4414 | A    |
| 9   | A2    | 4417 | G    |
| 9   | A2    | 4422 | G    |
| 9   | A2    | 4424 | U    |
| 9   | A2    | 4425 | C    |
| 9   | A2    | 4429 | G    |
| 9   | A2    | 4434 | U    |
| 9   | A2    | 4435 | C    |
| 9   | A2    | 4436 | C    |
| 9   | A2    | 4438 | C    |
| 9   | A2    | 4441 | U    |
| 9   | A2    | 4491 | C    |
| 9   | A2    | 4497 | U    |
| 9   | A2    | 4498 | C    |
| 9   | A2    | 4499 | G    |
| 9   | A2    | 4504 | C    |
| 9   | A2    | 4508 | G    |
| 9   | A2    | 4509 | U    |
| 9   | A2    | 4510 | C    |
| 9   | A2    | 4515 | OMG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 4516 | C    |
| 9   | A2    | 4519 | A    |
| 9   | A2    | 4520 | G    |
| 9   | A2    | 4527 | U    |
| 9   | A2    | 4528 | C    |
| 9   | A2    | 4540 | C    |
| 9   | A2    | 4545 | U    |
| 9   | A2    | 4546 | G    |
| 9   | A2    | 4548 | G    |
| 9   | A2    | 4552 | G    |
| 9   | A2    | 4553 | G    |
| 9   | A2    | 4554 | A    |
| 9   | A2    | 4555 | A    |
| 9   | A2    | 4557 | G    |
| 9   | A2    | 4560 | G    |
| 9   | A2    | 4566 | C    |
| 9   | A2    | 4569 | C    |
| 9   | A2    | 4570 | U    |
| 9   | A2    | 4571 | C    |
| 9   | A2    | 4573 | C    |
| 9   | A2    | 4582 | U    |
| 9   | A2    | 4583 | U    |
| 9   | A2    | 4587 | G    |
| 9   | A2    | 4589 | A    |
| 9   | A2    | 4596 | U    |
| 9   | A2    | 4609 | G    |
| 9   | A2    | 4612 | A    |
| 9   | A2    | 4622 | U    |
| 9   | A2    | 4634 | U    |
| 9   | A2    | 4636 | C    |
| 9   | A2    | 4637 | U    |
| 9   | A2    | 4652 | U    |
| 9   | A2    | 4663 | G    |
| 9   | A2    | 4672 | U    |
| 9   | A2    | 4680 | A    |
| 9   | A2    | 4687 | G    |
| 9   | A2    | 4696 | C    |
| 9   | A2    | 4701 | G    |
| 9   | A2    | 4702 | A    |
| 9   | A2    | 4707 | A    |
| 9   | A2    | 4715 | U    |
| 10  | B2    | 7    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | B2    | 11  | A    |
| 10  | B2    | 22  | A    |
| 10  | B2    | 24  | C    |
| 10  | B2    | 33  | U    |
| 10  | B2    | 47  | G    |
| 10  | B2    | 50  | A    |
| 10  | B2    | 53  | U    |
| 10  | B2    | 54  | A    |
| 10  | B2    | 63  | C    |
| 10  | B2    | 64  | G    |
| 10  | B2    | 89  | G    |
| 10  | B2    | 93  | G    |
| 10  | B2    | 100 | A    |
| 10  | B2    | 110 | G    |
| 10  | B2    | 120 | U    |
| 11  | C2    | 14  | OMU  |
| 11  | C2    | 15  | G    |
| 11  | C2    | 34  | U    |
| 11  | C2    | 35  | C    |
| 11  | C2    | 39  | G    |
| 11  | C2    | 49  | G    |
| 11  | C2    | 59  | A    |
| 11  | C2    | 60  | G    |
| 11  | C2    | 62  | A    |
| 11  | C2    | 63  | U    |
| 11  | C2    | 71  | A    |
| 11  | C2    | 82  | A    |
| 11  | C2    | 84  | A    |
| 11  | C2    | 85  | U    |
| 11  | C2    | 87  | G    |
| 11  | C2    | 88  | A    |
| 11  | C2    | 94  | G    |
| 11  | C2    | 103 | A    |
| 11  | C2    | 105 | C    |
| 11  | C2    | 110 | U    |
| 11  | C2    | 111 | U    |
| 11  | C2    | 114 | G    |
| 11  | C2    | 123 | U    |
| 11  | C2    | 125 | C    |
| 11  | C2    | 126 | C    |
| 11  | C2    | 147 | G    |
| 11  | C2    | 150 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | C2    | 156 | U    |
| 46  | m2    | 2   | A    |
| 46  | m2    | 4   | C    |
| 46  | m2    | 8   | U    |
| 46  | m2    | 14  | C    |
| 46  | m2    | 33  | G    |
| 46  | m2    | 41  | G    |
| 46  | m2    | 44  | U    |
| 46  | m2    | 45  | A    |
| 46  | m2    | 46  | A    |
| 46  | m2    | 56  | G    |
| 46  | m2    | 58  | C    |
| 46  | m2    | 62  | G    |
| 46  | m2    | 67  | C    |
| 46  | m2    | 68  | A    |
| 46  | m2    | 77  | A    |
| 46  | m2    | 78  | C    |
| 46  | m2    | 80  | G    |
| 46  | m2    | 103 | A    |
| 46  | m2    | 113 | G    |
| 46  | m2    | 115 | U    |
| 46  | m2    | 120 | U    |
| 46  | m2    | 126 | G    |
| 46  | m2    | 142 | C    |
| 46  | m2    | 143 | U    |
| 46  | m2    | 149 | A    |
| 46  | m2    | 151 | C    |
| 46  | m2    | 154 | U    |
| 46  | m2    | 157 | U    |
| 46  | m2    | 158 | A    |
| 46  | m2    | 160 | U    |
| 46  | m2    | 161 | U    |
| 46  | m2    | 162 | C    |
| 46  | m2    | 165 | G    |
| 46  | m2    | 166 | A2M  |
| 46  | m2    | 167 | G    |
| 46  | m2    | 169 | U    |
| 46  | m2    | 171 | A    |
| 46  | m2    | 172 | U    |
| 46  | m2    | 181 | A    |
| 46  | m2    | 182 | C    |
| 46  | m2    | 198 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | m2    | 202 | C    |
| 46  | m2    | 208 | G    |
| 46  | m2    | 209 | G    |
| 46  | m2    | 210 | G    |
| 46  | m2    | 215 | G    |
| 46  | m2    | 217 | G    |
| 46  | m2    | 222 | U    |
| 46  | m2    | 227 | G    |
| 46  | m2    | 228 | A    |
| 46  | m2    | 293 | G    |
| 46  | m2    | 294 | A    |
| 46  | m2    | 295 | C    |
| 46  | m2    | 296 | U    |
| 46  | m2    | 297 | C    |
| 46  | m2    | 299 | A    |
| 46  | m2    | 307 | U    |
| 46  | m2    | 309 | G    |
| 46  | m2    | 310 | G    |
| 46  | m2    | 311 | G    |
| 46  | m2    | 313 | C    |
| 46  | m2    | 314 | G    |
| 46  | m2    | 321 | C    |
| 46  | m2    | 324 | C    |
| 46  | m2    | 326 | C    |
| 46  | m2    | 327 | C    |
| 46  | m2    | 330 | U    |
| 46  | m2    | 331 | G    |
| 46  | m2    | 334 | G    |
| 46  | m2    | 337 | G    |
| 46  | m2    | 342 | C    |
| 46  | m2    | 349 | G    |
| 46  | m2    | 362 | A    |
| 46  | m2    | 364 | C    |
| 46  | m2    | 366 | A    |
| 46  | m2    | 372 | G    |
| 46  | m2    | 385 | G    |
| 46  | m2    | 386 | U    |
| 46  | m2    | 387 | G    |
| 46  | m2    | 394 | A    |
| 46  | m2    | 396 | G    |
| 46  | m2    | 400 | A    |
| 46  | m2    | 409 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | m2    | 410 | A    |
| 46  | m2    | 411 | C    |
| 46  | m2    | 423 | G    |
| 46  | m2    | 428 | A    |
| 46  | m2    | 429 | U    |
| 46  | m2    | 430 | U    |
| 46  | m2    | 440 | G    |
| 46  | m2    | 442 | G    |
| 46  | m2    | 443 | C    |
| 46  | m2    | 449 | A    |
| 46  | m2    | 450 | A    |
| 46  | m2    | 452 | C    |
| 46  | m2    | 453 | G    |
| 46  | m2    | 454 | G    |
| 46  | m2    | 466 | A    |
| 46  | m2    | 467 | A    |
| 46  | m2    | 473 | G    |
| 46  | m2    | 474 | C    |
| 46  | m2    | 476 | G    |
| 46  | m2    | 484 | G    |
| 46  | m2    | 489 | U    |
| 46  | m2    | 494 | C    |
| 46  | m2    | 495 | A    |
| 46  | m2    | 498 | C    |
| 46  | m2    | 503 | C    |
| 46  | m2    | 504 | C    |
| 46  | m2    | 519 | OMC  |
| 46  | m2    | 524 | A    |
| 46  | m2    | 531 | A    |
| 46  | m2    | 533 | A    |
| 46  | m2    | 536 | G    |
| 46  | m2    | 539 | C    |
| 46  | m2    | 544 | U    |
| 46  | m2    | 546 | G    |
| 46  | m2    | 551 | C    |
| 46  | m2    | 556 | A    |
| 46  | m2    | 557 | A    |
| 46  | m2    | 559 | U    |
| 46  | m2    | 562 | A    |
| 46  | m2    | 565 | G    |
| 46  | m2    | 566 | A    |
| 46  | m2    | 570 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | m2    | 585 | A    |
| 46  | m2    | 587 | C    |
| 46  | m2    | 589 | A    |
| 46  | m2    | 591 | G    |
| 46  | m2    | 593 | U    |
| 46  | m2    | 595 | C    |
| 46  | m2    | 598 | U    |
| 46  | m2    | 602 | G    |
| 46  | m2    | 606 | A    |
| 46  | m2    | 609 | U    |
| 46  | m2    | 619 | G    |
| 46  | m2    | 624 | C    |
| 46  | m2    | 625 | G    |
| 46  | m2    | 629 | U    |
| 46  | m2    | 630 | A    |
| 46  | m2    | 645 | A    |
| 46  | m2    | 657 | A    |
| 46  | m2    | 662 | C    |
| 46  | m2    | 670 | A2M  |
| 46  | m2    | 671 | A    |
| 46  | m2    | 673 | A    |
| 46  | m2    | 674 | A    |
| 46  | m2    | 675 | G    |
| 46  | m2    | 685 | OMG  |
| 46  | m2    | 686 | G    |
| 46  | m2    | 689 | C    |
| 46  | m2    | 690 | U    |
| 46  | m2    | 694 | G    |
| 46  | m2    | 695 | A    |
| 46  | m2    | 696 | G    |
| 46  | m2    | 697 | C    |
| 46  | m2    | 699 | G    |
| 46  | m2    | 700 | G    |
| 46  | m2    | 733 | G    |
| 46  | m2    | 734 | U    |
| 46  | m2    | 735 | C    |
| 46  | m2    | 737 | C    |
| 46  | m2    | 738 | C    |
| 46  | m2    | 739 | G    |
| 46  | m2    | 741 | C    |
| 46  | m2    | 752 | C    |
| 46  | m2    | 753 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | m2    | 754 | G    |
| 46  | m2    | 790 | G    |
| 46  | m2    | 791 | G    |
| 46  | m2    | 793 | C    |
| 46  | m2    | 794 | C    |
| 46  | m2    | 795 | G    |
| 46  | m2    | 797 | A    |
| 46  | m2    | 798 | G    |
| 46  | m2    | 801 | U    |
| 46  | m2    | 813 | A    |
| 46  | m2    | 823 | G    |
| 46  | m2    | 824 | PSU  |
| 46  | m2    | 832 | A    |
| 46  | m2    | 836 | C    |
| 46  | m2    | 838 | G    |
| 46  | m2    | 839 | A    |
| 46  | m2    | 841 | C    |
| 46  | m2    | 844 | C    |
| 46  | m2    | 849 | A    |
| 46  | m2    | 863 | A    |
| 46  | m2    | 864 | A    |
| 46  | m2    | 871 | A    |
| 46  | m2    | 872 | A    |
| 46  | m2    | 875 | G    |
| 46  | m2    | 876 | G    |
| 46  | m2    | 877 | A    |
| 46  | m2    | 878 | C    |
| 46  | m2    | 885 | U    |
| 46  | m2    | 886 | C    |
| 46  | m2    | 889 | U    |
| 46  | m2    | 890 | U    |
| 46  | m2    | 895 | U    |
| 46  | m2    | 896 | G    |
| 46  | m2    | 897 | G    |
| 46  | m2    | 898 | U    |
| 46  | m2    | 899 | U    |
| 46  | m2    | 901 | U    |
| 46  | m2    | 915 | A    |
| 46  | m2    | 919 | U    |
| 46  | m2    | 922 | A    |
| 46  | m2    | 924 | A    |
| 46  | m2    | 935 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | m2    | 936  | G    |
| 46  | m2    | 952  | C    |
| 46  | m2    | 971  | U    |
| 46  | m2    | 973  | G    |
| 46  | m2    | 980  | G    |
| 46  | m2    | 990  | C    |
| 46  | m2    | 992  | A    |
| 46  | m2    | 994  | A    |
| 46  | m2    | 999  | A    |
| 46  | m2    | 1001 | G    |
| 46  | m2    | 1003 | A    |
| 46  | m2    | 1019 | U    |
| 46  | m2    | 1025 | A    |
| 46  | m2    | 1029 | A    |
| 46  | m2    | 1047 | U    |
| 46  | m2    | 1063 | U    |
| 46  | m2    | 1064 | A    |
| 46  | m2    | 1085 | A    |
| 46  | m2    | 1087 | C    |
| 46  | m2    | 1117 | U    |
| 46  | m2    | 1118 | C    |
| 46  | m2    | 1120 | C    |
| 46  | m2    | 1123 | G    |
| 46  | m2    | 1133 | G    |
| 46  | m2    | 1135 | A    |
| 46  | m2    | 1140 | C    |
| 46  | m2    | 1152 | A    |
| 46  | m2    | 1155 | C    |
| 46  | m2    | 1156 | U    |
| 46  | m2    | 1172 | A    |
| 46  | m2    | 1197 | A    |
| 46  | m2    | 1217 | C    |
| 46  | m2    | 1218 | C    |
| 46  | m2    | 1219 | A    |
| 46  | m2    | 1226 | G    |
| 46  | m2    | 1229 | G    |
| 46  | m2    | 1230 | A    |
| 46  | m2    | 1242 | A    |
| 46  | m2    | 1243 | A    |
| 46  | m2    | 1244 | U    |
| 46  | m2    | 1245 | PSU  |
| 46  | m2    | 1253 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | m2    | 1255 | A    |
| 46  | m2    | 1258 | G    |
| 46  | m2    | 1259 | G    |
| 46  | m2    | 1274 | C    |
| 46  | m2    | 1275 | C    |
| 46  | m2    | 1276 | G    |
| 46  | m2    | 1277 | G    |
| 46  | m2    | 1285 | C    |
| 46  | m2    | 1288 | G    |
| 46  | m2    | 1299 | U    |
| 46  | m2    | 1300 | G    |
| 46  | m2    | 1302 | U    |
| 46  | m2    | 1304 | G    |
| 46  | m2    | 1305 | C    |
| 46  | m2    | 1310 | U    |
| 46  | m2    | 1315 | A    |
| 46  | m2    | 1335 | U    |
| 46  | m2    | 1343 | C    |
| 46  | m2    | 1344 | U    |
| 46  | m2    | 1345 | U    |
| 46  | m2    | 1346 | A    |
| 46  | m2    | 1356 | G    |
| 46  | m2    | 1373 | U    |
| 46  | m2    | 1374 | U    |
| 46  | m2    | 1377 | G    |
| 46  | m2    | 1380 | A    |
| 46  | m2    | 1384 | A    |
| 46  | m2    | 1398 | A    |
| 46  | m2    | 1399 | U    |
| 46  | m2    | 1400 | G    |
| 46  | m2    | 1404 | A    |
| 46  | m2    | 1414 | C    |
| 46  | m2    | 1417 | C    |
| 46  | m2    | 1419 | C    |
| 46  | m2    | 1420 | C    |
| 46  | m2    | 1421 | C    |
| 46  | m2    | 1422 | G    |
| 46  | m2    | 1424 | G    |
| 46  | m2    | 1426 | G    |
| 46  | m2    | 1431 | G    |
| 46  | m2    | 1435 | C    |
| 46  | m2    | 1436 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | m2    | 1437 | C    |
| 46  | m2    | 1438 | C    |
| 46  | m2    | 1439 | C    |
| 46  | m2    | 1440 | A    |
| 46  | m2    | 1444 | U    |
| 46  | m2    | 1446 | U    |
| 46  | m2    | 1448 | A    |
| 46  | m2    | 1452 | G    |
| 46  | m2    | 1454 | A    |
| 46  | m2    | 1455 | C    |
| 46  | m2    | 1456 | A    |
| 46  | m2    | 1465 | U    |
| 46  | m2    | 1473 | C    |
| 46  | m2    | 1475 | G    |
| 46  | m2    | 1490 | C    |
| 46  | m2    | 1491 | A    |
| 46  | m2    | 1492 | G    |
| 46  | m2    | 1496 | U    |
| 46  | m2    | 1499 | G    |
| 46  | m2    | 1500 | A    |
| 46  | m2    | 1507 | U    |
| 46  | m2    | 1509 | G    |
| 46  | m2    | 1510 | A    |
| 46  | m2    | 1520 | C    |
| 46  | m2    | 1522 | G    |
| 46  | m2    | 1523 | C    |
| 46  | m2    | 1533 | A    |
| 46  | m2    | 1535 | A    |
| 46  | m2    | 1554 | G    |
| 46  | m2    | 1555 | C    |
| 46  | m2    | 1557 | U    |
| 46  | m2    | 1558 | A    |
| 46  | m2    | 1560 | C    |
| 46  | m2    | 1562 | U    |
| 46  | m2    | 1570 | C    |
| 46  | m2    | 1577 | G    |
| 46  | m2    | 1582 | A    |
| 46  | m2    | 1587 | U    |
| 46  | m2    | 1589 | G    |
| 46  | m2    | 1590 | A    |
| 46  | m2    | 1594 | C    |
| 46  | m2    | 1603 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | m2    | 1606 | G    |
| 46  | m2    | 1608 | G    |
| 46  | m2    | 1619 | G    |
| 46  | m2    | 1623 | U    |
| 46  | m2    | 1625 | A    |
| 46  | m2    | 1626 | U    |
| 46  | m2    | 1632 | A    |
| 46  | m2    | 1636 | A    |
| 46  | m2    | 1638 | G    |
| 46  | m2    | 1639 | A    |
| 46  | m2    | 1640 | G    |
| 46  | m2    | 1650 | G    |
| 46  | m2    | 1656 | G    |
| 46  | m2    | 1662 | C    |
| 46  | m2    | 1665 | A    |
| 46  | m2    | 1667 | G    |
| 46  | m2    | 1680 | A    |
| 46  | m2    | 1682 | G    |
| 46  | m2    | 1685 | C    |
| 46  | m2    | 1703 | C    |
| 46  | m2    | 1711 | G    |
| 46  | m2    | 1714 | A    |
| 46  | m2    | 1717 | A    |
| 46  | m2    | 1723 | U    |
| 46  | m2    | 1724 | G    |
| 46  | m2    | 1731 | U    |
| 46  | m2    | 1747 | A    |
| 46  | m2    | 1753 | C    |
| 46  | m2    | 1756 | G    |
| 46  | m2    | 1759 | G    |
| 46  | m2    | 1777 | U    |
| 46  | m2    | 1784 | G    |
| 46  | m2    | 1785 | C    |
| 46  | m2    | 1786 | G    |
| 46  | m2    | 1815 | A    |
| 46  | m2    | 1827 | A    |
| 46  | m2    | 1832 | UR3  |
| 46  | m2    | 1833 | A    |
| 46  | m2    | 1837 | A    |
| 46  | m2    | 1840 | U    |
| 46  | m2    | 1844 | 4AC  |
| 46  | m2    | 1851 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | m2    | 1853 | A    |
| 46  | m2    | 1854 | C    |
| 46  | m2    | 1863 | G    |
| 46  | m2    | 1864 | G    |
| 46  | m2    | 1865 | A    |
| 46  | m2    | 1867 | C    |
| 46  | m2    | 1868 | A    |
| 46  | m2    | 1869 | U    |
| 47  | n2    | 9    | U    |
| 47  | n2    | 10   | G    |
| 47  | n2    | 11   | G    |
| 47  | n2    | 13   | G    |
| 47  | n2    | 15   | A    |
| 47  | n2    | 16   | G    |
| 47  | n2    | 17   | C    |
| 47  | n2    | 18   | G    |
| 47  | n2    | 19   | G    |
| 47  | n2    | 21   | A    |
| 47  | n2    | 26   | G    |
| 47  | n2    | 31   | G    |
| 47  | n2    | 34   | C    |
| 47  | n2    | 35   | A    |
| 47  | n2    | 37   | A    |
| 47  | n2    | 47   | U    |
| 47  | n2    | 48   | C    |
| 47  | n2    | 57   | G    |
| 47  | n2    | 58   | A    |
| 47  | n2    | 61   | C    |
| 47  | n2    | 63   | A    |
| 47  | n2    | 67   | U    |
| 47  | n2    | 75   | C    |
| 47  | n2    | 76   | A    |

All (15) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 143  | U    |
| 9   | A2    | 406  | C    |
| 9   | A2    | 1438 | OMG  |
| 9   | A2    | 1446 | G    |
| 9   | A2    | 1778 | G    |
| 9   | A2    | 1787 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A2    | 1792 | A    |
| 9   | A2    | 2382 | C    |
| 9   | A2    | 2430 | G    |
| 9   | A2    | 3772 | G    |
| 9   | A2    | 4330 | G    |
| 9   | A2    | 4351 | U    |
| 9   | A2    | 4582 | U    |
| 11  | C2    | 59   | A    |
| 11  | C2    | 83   | C    |

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

101 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 |
| 9   | 5MC  | A2    | 3987 | 9    | 19,22,23     | 3.90 | 8 (42%)  | 26,32,35    | 1.02 | 2 (7%)   |
| 9   | A2M  | A2    | 3374 | 9    | 22,25,26     | 2.64 | 11 (50%) | 30,36,39    | 2.36 | 8 (26%)  |
| 46  | 4AC  | m2    | 1844 | 46   | 21,24,25     | 3.67 | 9 (42%)  | 28,34,37    | 1.15 | 4 (14%)  |
| 9   | 5MC  | A2    | 3438 | 9    | 19,22,23     | 3.92 | 8 (42%)  | 26,32,35    | 0.97 | 1 (3%)   |
| 9   | OMC  | A2    | 2616 | 9    | 19,22,23     | 3.08 | 8 (42%)  | 25,31,34    | 0.92 | 1 (4%)   |
| 9   | PSU  | A2    | 4055 | 9    | 18,21,22     | 4.53 | 6 (33%)  | 21,30,33    | 3.00 | 7 (33%)  |
| 9   | PSU  | A2    | 1496 | 9    | 18,21,22     | 4.51 | 6 (33%)  | 21,30,33    | 3.04 | 6 (28%)  |
| 9   | P7G  | A2    | 1711 | 10,9 | 24,28,29     | 3.61 | 10 (41%) | 25,41,44    | 1.23 | 2 (8%)   |
| 9   | UR3  | A2    | 4249 | 9    | 19,22,23     | 3.20 | 8 (42%)  | 26,32,35    | 1.57 | 4 (15%)  |
| 11  | OMU  | C2    | 14   | 11   | 19,22,23     | 3.09 | 8 (42%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 9   | PSU  | A2    | 3420 | 9    | 18,21,22     | 4.52 | 6 (33%)  | 21,30,33    | 2.87 | 5 (23%)  |
| 9   | A2M  | A2    | 1337 | 9    | 22,25,26     | 2.64 | 11 (50%) | 30,36,39    | 2.35 | 9 (30%)  |
| 9   | B8T  | A2    | 4135 | 9    | 19,22,23     | 3.29 | 8 (42%)  | 25,31,34    | 0.86 | 1 (4%)   |
| 9   | OMG  | A2    | 1852 | 9    | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.07 | 10 (31%) |
| 9   | OMG  | A2    | 2528 | 9    | 23,26,27     | 2.49 | 8 (34%)  | 32,38,41    | 2.14 | 10 (31%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | OMC  | A2    | 3543 | 9    | 19,22,23     | 3.04 | 8 (42%)  | 25,31,34    | 0.85 | 0        |
| 9   | 2MG  | A2    | 1330 | 9    | 23,26,27     | 2.62 | 8 (34%)  | 33,38,41    | 2.30 | 12 (36%) |
| 9   | OMU  | A2    | 3958 | 9    | 19,22,23     | 3.02 | 8 (42%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 9   | A2M  | A2    | 1673 | 9    | 22,25,26     | 2.63 | 11 (50%) | 30,36,39    | 2.45 | 10 (33%) |
| 46  | A2M  | m2    | 166  | 46   | 22,25,26     | 2.66 | 11 (50%) | 30,36,39    | 2.34 | 9 (30%)  |
| 9   | E7G  | A2    | 1599 | 9    | 24,27,28     | 3.35 | 11 (45%) | 28,40,43    | 2.35 | 9 (32%)  |
| 9   | OMG  | A2    | 1685 | 9    | 23,26,27     | 2.47 | 9 (39%)  | 32,38,41    | 2.11 | 11 (34%) |
| 9   | A2M  | A2    | 1140 | 9    | 22,25,26     | 2.66 | 11 (50%) | 30,36,39    | 2.33 | 9 (30%)  |
| 9   | UR3  | A2    | 1668 | 9    | 19,22,23     | 3.25 | 8 (42%)  | 26,32,35    | 1.64 | 4 (15%)  |
| 9   | OMC  | A2    | 2120 | 9    | 19,22,23     | 3.04 | 7 (36%)  | 25,31,34    | 1.05 | 3 (12%)  |
| 9   | G7M  | A2    | 2277 | 9    | 23,26,27     | 3.52 | 11 (47%) | 34,39,42    | 1.74 | 6 (17%)  |
| 9   | OMU  | A2    | 4272 | 9    | 19,22,23     | 3.05 | 8 (42%)  | 25,31,34    | 1.76 | 5 (20%)  |
| 46  | PSU  | m2    | 614  | 46   | 18,21,22     | 4.50 | 6 (33%)  | 21,30,33    | 2.94 | 6 (28%)  |
| 46  | PSU  | m2    | 1083 | 46   | 18,21,22     | 4.52 | 6 (33%)  | 21,30,33    | 3.00 | 7 (33%)  |
| 9   | A2M  | A2    | 3481 | 9    | 22,25,26     | 2.63 | 11 (50%) | 30,36,39    | 2.33 | 10 (33%) |
| 9   | I4U  | A2    | 1472 | 9    | 20,24,25     | 4.77 | 15 (75%) | 27,34,37    | 1.84 | 3 (11%)  |
| 9   | I4U  | A2    | 3846 | 9    | 20,24,25     | 4.77 | 15 (75%) | 27,34,37    | 1.63 | 2 (7%)   |
| 9   | OMG  | A2    | 4022 | 9    | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.09 | 11 (34%) |
| 9   | OMG  | A2    | 3848 | 9    | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.08 | 11 (34%) |
| 9   | G7M  | A2    | 1418 | 9    | 23,26,27     | 3.53 | 11 (47%) | 34,39,42    | 1.74 | 6 (17%)  |
| 46  | OMC  | m2    | 519  | 46   | 19,22,23     | 3.07 | 8 (42%)  | 25,31,34    | 0.91 | 1 (4%)   |
| 9   | A2M  | A2    | 3379 | 9    | 22,25,26     | 2.65 | 11 (50%) | 30,36,39    | 2.31 | 10 (33%) |
| 9   | PSU  | A2    | 1395 | 9    | 18,21,22     | 4.54 | 7 (38%)  | 21,30,33    | 2.92 | 5 (23%)  |
| 9   | 2MG  | A2    | 878  | 9    | 23,26,27     | 2.64 | 7 (30%)  | 33,38,41    | 2.29 | 11 (33%) |
| 9   | B8W  | A2    | 3837 | 9    | 23,26,27     | 3.94 | 13 (56%) | 33,38,41    | 3.43 | 17 (51%) |
| 9   | OMC  | A2    | 4188 | 9    | 19,22,23     | 3.03 | 8 (42%)  | 25,31,34    | 0.79 | 0        |
| 46  | UR3  | m2    | 1832 | 46   | 19,22,23     | 3.21 | 8 (42%)  | 26,32,35    | 1.62 | 3 (11%)  |
| 9   | A2M  | A2    | 2156 | 9    | 22,25,26     | 2.65 | 11 (50%) | 30,36,39    | 2.33 | 9 (30%)  |
| 9   | OMG  | A2    | 3448 | 9    | 23,26,27     | 2.47 | 9 (39%)  | 32,38,41    | 2.16 | 11 (34%) |
| 9   | A2M  | A2    | 2118 | 9    | 22,25,26     | 2.64 | 11 (50%) | 30,36,39    | 2.32 | 9 (30%)  |
| 9   | OMG  | A2    | 1438 | 9    | 23,26,27     | 2.47 | 8 (34%)  | 32,38,41    | 2.15 | 10 (31%) |
| 9   | OMC  | A2    | 3565 | 9    | 19,22,23     | 3.06 | 8 (42%)  | 25,31,34    | 0.82 | 0        |
| 9   | G7M  | A2    | 4202 | 9    | 23,26,27     | 3.52 | 11 (47%) | 34,39,42    | 1.71 | 7 (20%)  |
| 9   | OMG  | A2    | 4275 | 9    | 23,26,27     | 2.47 | 9 (39%)  | 32,38,41    | 2.08 | 11 (34%) |
| 9   | PSU  | A2    | 2263 | 9    | 18,21,22     | 4.56 | 6 (33%)  | 21,30,33    | 2.90 | 6 (28%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | OMC  | A2    | 3525 | 9    | 19,22,23     | 3.03 | 8 (42%)  | 25,31,34    | 0.76 | 0        |
| 9   | PSU  | A2    | 4152 | 9    | 18,21,22     | 4.56 | 7 (38%)  | 21,30,33    | 3.06 | 6 (28%)  |
| 46  | PSU  | m2    | 1245 | 46   | 18,21,22     | 4.55 | 6 (33%)  | 21,30,33    | 2.95 | 6 (28%)  |
| 9   | PSU  | A2    | 3371 | 9    | 18,21,22     | 4.51 | 6 (33%)  | 21,30,33    | 2.93 | 6 (28%)  |
| 9   | 1MA  | A2    | 4067 | 9    | 21,25,26     | 2.47 | 5 (23%)  | 30,37,40    | 1.93 | 7 (23%)  |
| 46  | A2M  | m2    | 1033 | 46   | 22,25,26     | 2.64 | 11 (50%) | 30,36,39    | 2.29 | 9 (30%)  |
| 9   | OMC  | A2    | 2559 | 9    | 19,22,23     | 3.03 | 8 (42%)  | 25,31,34    | 0.73 | 0        |
| 9   | PSU  | A2    | 3945 | 9    | 18,21,22     | 4.49 | 6 (33%)  | 21,30,33    | 3.01 | 5 (23%)  |
| 9   | A2M  | A2    | 1347 | 9    | 22,25,26     | 2.67 | 11 (50%) | 30,36,39    | 2.32 | 8 (26%)  |
| 9   | B9B  | A2    | 237  | 9    | 25,28,29     | 3.46 | 11 (44%) | 35,40,43    | 2.47 | 13 (37%) |
| 46  | OMU  | m2    | 116  | 46   | 19,22,23     | 3.05 | 8 (42%)  | 25,31,34    | 1.71 | 4 (16%)  |
| 9   | OMG  | A2    | 4146 | 9    | 23,26,27     | 2.47 | 9 (39%)  | 32,38,41    | 2.09 | 11 (34%) |
| 9   | A2M  | A2    | 4223 | 9    | 22,25,26     | 2.65 | 11 (50%) | 30,36,39    | 2.34 | 10 (33%) |
| 9   | 6MZ  | A2    | 3872 | 9    | 22,25,26     | 2.46 | 4 (18%)  | 29,36,39    | 2.21 | 10 (34%) |
| 9   | P7G  | A2    | 3536 | 9    | 24,28,29     | 3.56 | 10 (41%) | 25,41,44    | 1.29 | 2 (8%)   |
| 46  | OMG  | m2    | 646  | 46   | 23,26,27     | 2.48 | 8 (34%)  | 32,38,41    | 2.12 | 11 (34%) |
| 9   | OMC  | A2    | 2177 | 9    | 19,22,23     | 3.05 | 8 (42%)  | 25,31,34    | 0.98 | 1 (4%)   |
| 46  | A2M  | m2    | 27   | 46   | 22,25,26     | 2.64 | 11 (50%) | 30,36,39    | 2.29 | 8 (26%)  |
| 46  | PSU  | m2    | 825  | 46   | 18,21,22     | 4.54 | 6 (33%)  | 21,30,33    | 3.02 | 6 (28%)  |
| 9   | PSU  | A2    | 4183 | 9    | 18,21,22     | 4.54 | 6 (33%)  | 21,30,33    | 3.09 | 6 (28%)  |
| 79  | DDE  | m     | 714  | 79   | 18,20,21     | 2.13 | 6 (33%)  | 17,28,30    | 1.07 | 1 (5%)   |
| 9   | B8Q  | A2    | 1269 | 9    | 18,22,23     | 3.02 | 4 (22%)  | 21,32,35    | 1.85 | 6 (28%)  |
| 9   | B9B  | A2    | 1387 | 9    | 25,28,29     | 3.47 | 10 (40%) | 35,40,43    | 2.39 | 14 (40%) |
| 9   | OMG  | A2    | 373  | 9    | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.04 | 11 (34%) |
| 9   | A2M  | A2    | 398  | 9    | 22,25,26     | 2.65 | 11 (50%) | 30,36,39    | 2.36 | 10 (33%) |
| 9   | OMC  | A2    | 3357 | 9    | 19,22,23     | 3.04 | 8 (42%)  | 25,31,34    | 0.72 | 0        |
| 46  | OMG  | m2    | 685  | 46   | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.08 | 11 (34%) |
| 9   | OMG  | A2    | 2119 | 9    | 23,26,27     | 2.45 | 9 (39%)  | 32,38,41    | 2.06 | 11 (34%) |
| 9   | OMG  | A2    | 4289 | 9    | 23,26,27     | 2.44 | 8 (34%)  | 32,38,41    | 2.11 | 11 (34%) |
| 9   | E7G  | A2    | 2052 | 9    | 24,27,28     | 3.34 | 11 (45%) | 28,40,43    | 2.33 | 8 (28%)  |
| 9   | B9H  | A2    | 2541 | 9    | 21,25,26     | 2.95 | 4 (19%)  | 22,35,38    | 1.82 | 5 (22%)  |
| 41  | MLZ  | g2    | 98   | 41   | 8,9,10       | 0.72 | 0        | 4,9,11      | 0.90 | 0        |
| 46  | A2M  | m2    | 670  | 46   | 22,25,26     | 2.68 | 11 (50%) | 30,36,39    | 2.30 | 10 (33%) |
| 9   | A2M  | A2    | 3523 | 9    | 22,25,26     | 2.65 | 11 (50%) | 30,36,39    | 2.27 | 9 (30%)  |
| 9   | PSU  | A2    | 4280 | 9    | 18,21,22     | 4.54 | 6 (33%)  | 21,30,33    | 2.99 | 6 (28%)  |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | MHG  | A2    | 4023 | 9    | 29,32,33     | 3.64 | 10 (34%) | 34,46,49    | 2.55 | 12 (35%) |
| 9   | 5MC  | A2    | 4099 | 9    | 19,22,23     | 3.83 | 8 (42%)  | 26,32,35    | 1.01 | 1 (3%)   |
| 9   | PSU  | A2    | 4102 | 9    | 18,21,22     | 4.51 | 6 (33%)  | 21,30,33    | 2.97 | 5 (23%)  |
| 9   | PSU  | A2    | 4288 | 9    | 18,21,22     | 4.53 | 7 (38%)  | 21,30,33    | 2.98 | 5 (23%)  |
| 46  | PSU  | m2    | 824  | 46   | 18,21,22     | 4.54 | 6 (33%)  | 21,30,33    | 2.96 | 5 (23%)  |
| 46  | B8N  | m2    | 1250 | 46   | 25,29,30     | 2.49 | 6 (24%)  | 28,42,45    | 2.13 | 7 (25%)  |
| 9   | E6G  | A2    | 4007 | 9    | 24,27,28     | 3.54 | 10 (41%) | 34,39,42    | 2.46 | 13 (38%) |
| 9   | OMG  | A2    | 1335 | 9    | 23,26,27     | 2.46 | 9 (39%)  | 32,38,41    | 2.09 | 11 (34%) |
| 14  | MLZ  | F2    | 333  | 14   | 8,9,10       | 0.73 | 0        | 4,9,11      | 0.91 | 0        |
| 9   | PSU  | A2    | 1490 | 9    | 18,21,22     | 4.53 | 6 (33%)  | 21,30,33    | 3.02 | 7 (33%)  |
| 9   | 2MG  | A2    | 4517 | 9    | 23,26,27     | 2.62 | 8 (34%)  | 33,38,41    | 2.27 | 12 (36%) |
| 9   | OMG  | A2    | 4515 | 9    | 23,26,27     | 2.46 | 8 (34%)  | 32,38,41    | 2.14 | 10 (31%) |
| 9   | PSU  | A2    | 3385 | 9    | 18,21,22     | 4.52 | 6 (33%)  | 21,30,33    | 3.00 | 5 (23%)  |
| 9   | A2M  | A2    | 3441 | 9    | 22,25,26     | 2.70 | 11 (50%) | 30,36,39    | 2.47 | 11 (36%) |
| 9   | OMG  | A2    | 2179 | 9    | 23,26,27     | 2.48 | 8 (34%)  | 32,38,41    | 2.04 | 10 (31%) |
| 9   | PSU  | A2    | 4094 | 9    | 18,21,22     | 4.58 | 7 (38%)  | 21,30,33    | 2.99 | 6 (28%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | 5MC  | A2    | 3987 | 9    | -       | 1/7/25/26  | 0/2/2/2 |
| 9   | A2M  | A2    | 3374 | 9    | -       | 1/9/27/28  | 0/3/3/3 |
| 46  | 4AC  | m2    | 1844 | 46   | -       | 0/11/29/30 | 0/2/2/2 |
| 9   | 5MC  | A2    | 3438 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 9   | OMC  | A2    | 2616 | 9    | -       | 0/9/27/28  | 0/2/2/2 |
| 9   | PSU  | A2    | 4055 | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | PSU  | A2    | 1496 | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | P7G  | A2    | 1711 | 10,9 | -       | 2/10/40/41 | 0/3/3/3 |
| 9   | UR3  | A2    | 4249 | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 11  | OMU  | C2    | 14   | 11   | -       | 1/9/27/28  | 0/2/2/2 |
| 9   | PSU  | A2    | 3420 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 9   | A2M  | A2    | 1337 | 9    | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | B8T  | A2    | 4135 | 9    | -       | 0/7/27/28  | 0/2/2/2 |
| 9   | OMG  | A2    | 1852 | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | OMG  | A2    | 2528 | 9    | -       | 2/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 9   | OMC  | A2    | 3543 | 9    | -       | 3/9/27/28 | 0/2/2/2 |
| 9   | 2MG  | A2    | 1330 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | OMU  | A2    | 3958 | 9    | -       | 3/9/27/28 | 0/2/2/2 |
| 9   | A2M  | A2    | 1673 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 46  | A2M  | m2    | 166  | 46   | -       | 3/9/27/28 | 0/3/3/3 |
| 9   | E7G  | A2    | 1599 | 9    | -       | 1/9/39/40 | 0/3/3/3 |
| 9   | OMG  | A2    | 1685 | 9    | -       | 2/9/27/28 | 0/3/3/3 |
| 9   | A2M  | A2    | 1140 | 9    | -       | 1/9/27/28 | 0/3/3/3 |
| 9   | UR3  | A2    | 1668 | 9    | -       | 2/7/25/26 | 0/2/2/2 |
| 9   | OMC  | A2    | 2120 | 9    | -       | 0/9/27/28 | 0/2/2/2 |
| 9   | G7M  | A2    | 2277 | 9    | -       | 0/7/25/26 | 0/3/3/3 |
| 9   | OMU  | A2    | 4272 | 9    | -       | 1/9/27/28 | 0/2/2/2 |
| 46  | PSU  | m2    | 614  | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | PSU  | m2    | 1083 | 46   | -       | 1/7/25/26 | 0/2/2/2 |
| 9   | A2M  | A2    | 3481 | 9    | -       | 1/9/27/28 | 0/3/3/3 |
| 9   | I4U  | A2    | 1472 | 9    | -       | 0/9/29/30 | 0/2/2/2 |
| 9   | I4U  | A2    | 3846 | 9    | -       | 2/9/29/30 | 0/2/2/2 |
| 9   | OMG  | A2    | 4022 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | OMG  | A2    | 3848 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | G7M  | A2    | 1418 | 9    | -       | 0/7/25/26 | 0/3/3/3 |
| 46  | OMC  | m2    | 519  | 46   | -       | 4/9/27/28 | 0/2/2/2 |
| 9   | A2M  | A2    | 3379 | 9    | -       | 1/9/27/28 | 0/3/3/3 |
| 9   | PSU  | A2    | 1395 | 9    | -       | 2/7/25/26 | 0/2/2/2 |
| 9   | 2MG  | A2    | 878  | 9    | -       | 2/9/27/28 | 0/3/3/3 |
| 9   | B8W  | A2    | 3837 | 9    | -       | 2/9/27/28 | 0/3/3/3 |
| 9   | OMC  | A2    | 4188 | 9    | -       | 0/9/27/28 | 0/2/2/2 |
| 46  | UR3  | m2    | 1832 | 46   | -       | 4/7/25/26 | 0/2/2/2 |
| 9   | A2M  | A2    | 2156 | 9    | -       | 2/9/27/28 | 0/3/3/3 |
| 9   | OMG  | A2    | 3448 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | A2M  | A2    | 2118 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | OMG  | A2    | 1438 | 9    | -       | 5/9/27/28 | 0/3/3/3 |
| 9   | OMC  | A2    | 3565 | 9    | -       | 0/9/27/28 | 0/2/2/2 |
| 9   | G7M  | A2    | 4202 | 9    | -       | 0/7/25/26 | 0/3/3/3 |
| 9   | OMG  | A2    | 4275 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | PSU  | A2    | 2263 | 9    | -       | 0/7/25/26 | 0/2/2/2 |
| 9   | OMC  | A2    | 3525 | 9    | -       | 0/9/27/28 | 0/2/2/2 |
| 9   | PSU  | A2    | 4152 | 9    | -       | 4/7/25/26 | 0/2/2/2 |
| 46  | PSU  | m2    | 1245 | 46   | -       | 3/7/25/26 | 0/2/2/2 |
| 9   | PSU  | A2    | 3371 | 9    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | 1MA  | A2    | 4067 | 9    | -       | 2/7/25/26  | 0/3/3/3 |
| 46  | A2M  | m2    | 1033 | 46   | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | OMC  | A2    | 2559 | 9    | -       | 0/9/27/28  | 0/2/2/2 |
| 9   | PSU  | A2    | 3945 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 9   | A2M  | A2    | 1347 | 9    | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | B9B  | A2    | 237  | 9    | -       | 6/11/29/30 | 0/3/3/3 |
| 46  | OMU  | m2    | 116  | 46   | -       | 1/9/27/28  | 0/2/2/2 |
| 9   | OMG  | A2    | 4146 | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | A2M  | A2    | 4223 | 9    | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | 6MZ  | A2    | 3872 | 9    | -       | 5/9/27/28  | 0/3/3/3 |
| 9   | P7G  | A2    | 3536 | 9    | -       | 3/10/40/41 | 0/3/3/3 |
| 46  | OMG  | m2    | 646  | 46   | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | OMC  | A2    | 2177 | 9    | -       | 3/9/27/28  | 0/2/2/2 |
| 46  | A2M  | m2    | 27   | 46   | -       | 1/9/27/28  | 0/3/3/3 |
| 46  | PSU  | m2    | 825  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | PSU  | A2    | 4183 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 79  | DDE  | m     | 714  | 79   | -       | 6/20/21/23 | 0/1/1/1 |
| 9   | B8Q  | A2    | 1269 | 9    | -       | 0/7/42/43  | 0/2/2/2 |
| 9   | B9B  | A2    | 1387 | 9    | -       | 3/11/29/30 | 0/3/3/3 |
| 9   | OMG  | A2    | 373  | 9    | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | A2M  | A2    | 398  | 9    | -       | 3/9/27/28  | 0/3/3/3 |
| 9   | OMC  | A2    | 3357 | 9    | -       | 5/9/27/28  | 0/2/2/2 |
| 46  | OMG  | m2    | 685  | 46   | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | OMG  | A2    | 2119 | 9    | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | OMG  | A2    | 4289 | 9    | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | E7G  | A2    | 2052 | 9    | -       | 4/9/39/40  | 0/3/3/3 |
| 9   | B9H  | A2    | 2541 | 9    | -       | 0/12/47/48 | 0/2/2/2 |
| 41  | MLZ  | g2    | 98   | 41   | -       | 1/7/8/10   | -       |
| 46  | A2M  | m2    | 670  | 46   | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | A2M  | A2    | 3523 | 9    | -       | 3/9/27/28  | 0/3/3/3 |
| 9   | PSU  | A2    | 4280 | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | MHG  | A2    | 4023 | 9    | -       | 4/16/46/47 | 0/3/3/3 |
| 9   | 5MC  | A2    | 4099 | 9    | -       | 4/7/25/26  | 0/2/2/2 |
| 9   | PSU  | A2    | 4102 | 9    | -       | 3/7/25/26  | 0/2/2/2 |
| 9   | PSU  | A2    | 4288 | 9    | -       | 5/7/25/26  | 0/2/2/2 |
| 46  | PSU  | m2    | 824  | 46   | -       | 3/7/25/26  | 0/2/2/2 |
| 46  | B8N  | m2    | 1250 | 46   | -       | 3/16/34/35 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | E6G  | A2    | 4007 | 9    | -       | 3/10/28/29 | 0/3/3/3 |
| 9   | OMG  | A2    | 1335 | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 14  | MLZ  | F2    | 333  | 14   | -       | 1/7/8/10   | -       |
| 9   | PSU  | A2    | 1490 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 9   | 2MG  | A2    | 4517 | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | OMG  | A2    | 4515 | 9    | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | PSU  | A2    | 3385 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 9   | A2M  | A2    | 3441 | 9    | -       | 3/9/27/28  | 0/3/3/3 |
| 9   | OMG  | A2    | 2179 | 9    | -       | 3/9/27/28  | 0/3/3/3 |
| 9   | PSU  | A2    | 4094 | 9    | -       | 0/7/25/26  | 0/2/2/2 |

All (845) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | m2    | 1245 | PSU  | C6-C5   | 12.72 | 1.49        | 1.35     |
| 9   | A2    | 4094 | PSU  | C6-C5   | 12.65 | 1.49        | 1.35     |
| 9   | A2    | 2263 | PSU  | C6-C5   | 12.63 | 1.49        | 1.35     |
| 9   | A2    | 4183 | PSU  | C6-C5   | 12.60 | 1.49        | 1.35     |
| 9   | A2    | 4152 | PSU  | C6-C5   | 12.59 | 1.49        | 1.35     |
| 9   | A2    | 4280 | PSU  | C6-C5   | 12.59 | 1.49        | 1.35     |
| 9   | A2    | 1395 | PSU  | C6-C5   | 12.54 | 1.49        | 1.35     |
| 9   | A2    | 3420 | PSU  | C6-C5   | 12.54 | 1.49        | 1.35     |
| 9   | A2    | 4055 | PSU  | C6-C5   | 12.52 | 1.49        | 1.35     |
| 46  | m2    | 825  | PSU  | C6-C5   | 12.51 | 1.49        | 1.35     |
| 46  | m2    | 1083 | PSU  | C6-C5   | 12.48 | 1.49        | 1.35     |
| 9   | A2    | 1496 | PSU  | C6-C5   | 12.48 | 1.49        | 1.35     |
| 46  | m2    | 824  | PSU  | C6-C5   | 12.47 | 1.49        | 1.35     |
| 9   | A2    | 4288 | PSU  | C6-C5   | 12.47 | 1.49        | 1.35     |
| 9   | A2    | 3371 | PSU  | C6-C5   | 12.46 | 1.49        | 1.35     |
| 9   | A2    | 3385 | PSU  | C6-C5   | 12.45 | 1.49        | 1.35     |
| 46  | m2    | 614  | PSU  | C6-C5   | 12.36 | 1.49        | 1.35     |
| 9   | A2    | 4102 | PSU  | C6-C5   | 12.36 | 1.49        | 1.35     |
| 9   | A2    | 3945 | PSU  | C6-C5   | 12.33 | 1.48        | 1.35     |
| 9   | A2    | 1490 | PSU  | C6-C5   | 12.32 | 1.48        | 1.35     |
| 9   | A2    | 3837 | B8W  | O4'-C1' | 11.10 | 1.67        | 1.42     |
| 9   | A2    | 4202 | G7M  | C8-N7   | 10.88 | 1.51        | 1.33     |
| 9   | A2    | 1418 | G7M  | C8-N7   | 10.84 | 1.51        | 1.33     |
| 9   | A2    | 2277 | G7M  | C8-N7   | 10.83 | 1.51        | 1.33     |
| 9   | A2    | 1472 | I4U  | C4-N3   | 10.82 | 1.45        | 1.31     |
| 9   | A2    | 3846 | I4U  | C4-N3   | 10.73 | 1.45        | 1.31     |
| 9   | A2    | 4023 | MHG  | C8-N9   | 10.24 | 1.52        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 9   | A2    | 1472 | I4U  | C3'-C2' | -10.04 | 1.26        | 1.53     |
| 9   | A2    | 1490 | PSU  | C2-N1   | 10.04  | 1.49        | 1.36     |
| 9   | A2    | 3872 | 6MZ  | C6-N6   | 10.03  | 1.45        | 1.34     |
| 9   | A2    | 2263 | PSU  | C2-N1   | 10.01  | 1.49        | 1.36     |
| 9   | A2    | 4152 | PSU  | C2-N1   | 10.00  | 1.49        | 1.36     |
| 9   | A2    | 4102 | PSU  | C2-N1   | 10.00  | 1.49        | 1.36     |
| 46  | m2    | 825  | PSU  | C2-N1   | 9.99   | 1.49        | 1.36     |
| 9   | A2    | 3846 | I4U  | C3'-C2' | -9.98  | 1.26        | 1.53     |
| 46  | m2    | 1083 | PSU  | C2-N1   | 9.95   | 1.49        | 1.36     |
| 9   | A2    | 3385 | PSU  | C2-N1   | 9.94   | 1.49        | 1.36     |
| 9   | A2    | 1395 | PSU  | C2-N1   | 9.94   | 1.49        | 1.36     |
| 9   | A2    | 4055 | PSU  | C2-N1   | 9.93   | 1.49        | 1.36     |
| 9   | A2    | 4288 | PSU  | C2-N1   | 9.93   | 1.49        | 1.36     |
| 9   | A2    | 4183 | PSU  | C2-N1   | 9.93   | 1.49        | 1.36     |
| 9   | A2    | 3945 | PSU  | C2-N1   | 9.91   | 1.49        | 1.36     |
| 9   | A2    | 4280 | PSU  | C2-N1   | 9.90   | 1.49        | 1.36     |
| 9   | A2    | 1496 | PSU  | C2-N1   | 9.89   | 1.49        | 1.36     |
| 46  | m2    | 1245 | PSU  | C2-N1   | 9.87   | 1.49        | 1.36     |
| 9   | A2    | 4094 | PSU  | C2-N1   | 9.85   | 1.49        | 1.36     |
| 46  | m2    | 824  | PSU  | C2-N1   | 9.82   | 1.49        | 1.36     |
| 9   | A2    | 3371 | PSU  | C2-N1   | 9.81   | 1.49        | 1.36     |
| 46  | m2    | 614  | PSU  | C2-N1   | 9.78   | 1.49        | 1.36     |
| 9   | A2    | 3420 | PSU  | C2-N1   | 9.75   | 1.49        | 1.36     |
| 9   | A2    | 1668 | UR3  | C2-N1   | 9.51   | 1.51        | 1.38     |
| 9   | A2    | 3438 | 5MC  | C6-C5   | 9.39   | 1.49        | 1.34     |
| 9   | A2    | 3987 | 5MC  | C6-C5   | 9.31   | 1.49        | 1.34     |
| 9   | A2    | 4249 | UR3  | C2-N1   | 9.21   | 1.51        | 1.38     |
| 9   | A2    | 1711 | P7G  | C8-N9   | 9.18   | 1.51        | 1.45     |
| 9   | A2    | 4099 | 5MC  | C6-C5   | 9.16   | 1.49        | 1.34     |
| 46  | m2    | 1832 | UR3  | C2-N1   | 9.16   | 1.51        | 1.38     |
| 9   | A2    | 4007 | E6G  | O4'-C1' | 9.15   | 1.63        | 1.42     |
| 9   | A2    | 237  | B9B  | O4'-C1' | 9.08   | 1.63        | 1.42     |
| 9   | A2    | 3536 | P7G  | C8-N9   | 9.05   | 1.51        | 1.45     |
| 9   | A2    | 4067 | 1MA  | C2-N3   | 9.02   | 1.47        | 1.30     |
| 9   | A2    | 1387 | B9B  | O4'-C1' | 8.98   | 1.62        | 1.42     |
| 9   | A2    | 4023 | MHG  | C2-N3   | 8.75   | 1.48        | 1.32     |
| 9   | A2    | 2052 | E7G  | C8-N9   | 8.53   | 1.51        | 1.45     |
| 9   | A2    | 1599 | E7G  | C8-N9   | 8.38   | 1.51        | 1.45     |
| 9   | A2    | 2541 | B9H  | C2-N3   | 8.38   | 1.48        | 1.37     |
| 46  | m2    | 1844 | 4AC  | C4-N3   | 8.23   | 1.46        | 1.32     |
| 9   | A2    | 1711 | P7G  | C5-N7   | 8.17   | 1.45        | 1.35     |
| 9   | A2    | 4023 | MHG  | C5-N7   | 8.06   | 1.45        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | m2    | 824  | PSU  | C2-N3   | 7.80  | 1.50        | 1.37     |
| 9   | A2    | 1269 | B8Q  | C2-N3   | 7.75  | 1.49        | 1.35     |
| 9   | A2    | 3536 | P7G  | C5-N7   | 7.68  | 1.45        | 1.35     |
| 9   | A2    | 4007 | E6G  | O4'-C4' | -7.68 | 1.27        | 1.45     |
| 9   | A2    | 1387 | B9B  | O4'-C4' | -7.67 | 1.27        | 1.45     |
| 9   | A2    | 878  | 2MG  | C2-N3   | 7.63  | 1.46        | 1.32     |
| 9   | A2    | 1387 | B9B  | C2'-C1' | -7.56 | 1.29        | 1.53     |
| 9   | A2    | 237  | B9B  | O4'-C4' | -7.56 | 1.28        | 1.45     |
| 9   | A2    | 4102 | PSU  | C2-N3   | 7.55  | 1.49        | 1.37     |
| 9   | A2    | 4094 | PSU  | C2-N3   | 7.54  | 1.49        | 1.37     |
| 9   | A2    | 4152 | PSU  | C2-N3   | 7.54  | 1.49        | 1.37     |
| 46  | m2    | 825  | PSU  | C2-N3   | 7.53  | 1.49        | 1.37     |
| 9   | A2    | 4280 | PSU  | C2-N3   | 7.53  | 1.49        | 1.37     |
| 9   | A2    | 4183 | PSU  | C2-N3   | 7.52  | 1.49        | 1.37     |
| 9   | A2    | 1395 | PSU  | C2-N3   | 7.52  | 1.49        | 1.37     |
| 9   | A2    | 4517 | 2MG  | C2-N3   | 7.51  | 1.46        | 1.32     |
| 9   | A2    | 4288 | PSU  | C2-N3   | 7.51  | 1.49        | 1.37     |
| 9   | A2    | 1490 | PSU  | C2-N3   | 7.50  | 1.49        | 1.37     |
| 46  | m2    | 614  | PSU  | C2-N3   | 7.49  | 1.49        | 1.37     |
| 9   | A2    | 3371 | PSU  | C2-N3   | 7.49  | 1.49        | 1.37     |
| 46  | m2    | 1245 | PSU  | C2-N3   | 7.47  | 1.49        | 1.37     |
| 9   | A2    | 1269 | B8Q  | C6-C5   | 7.47  | 1.48        | 1.33     |
| 9   | A2    | 4007 | E6G  | C2'-C1' | -7.47 | 1.30        | 1.53     |
| 9   | A2    | 1330 | 2MG  | C2-N3   | 7.46  | 1.46        | 1.32     |
| 9   | A2    | 1496 | PSU  | C2-N3   | 7.45  | 1.49        | 1.37     |
| 9   | A2    | 3385 | PSU  | C2-N3   | 7.45  | 1.49        | 1.37     |
| 9   | A2    | 3945 | PSU  | C2-N3   | 7.45  | 1.49        | 1.37     |
| 9   | A2    | 4135 | B8T  | C4-N3   | 7.42  | 1.45        | 1.32     |
| 9   | A2    | 237  | B9B  | C2'-C1' | -7.41 | 1.30        | 1.53     |
| 9   | A2    | 4055 | PSU  | C2-N3   | 7.40  | 1.49        | 1.37     |
| 9   | A2    | 3420 | PSU  | C2-N3   | 7.40  | 1.49        | 1.37     |
| 9   | A2    | 2541 | B9H  | C6-C5   | 7.40  | 1.48        | 1.33     |
| 46  | m2    | 1083 | PSU  | C2-N3   | 7.39  | 1.49        | 1.37     |
| 9   | A2    | 2263 | PSU  | C2-N3   | 7.36  | 1.49        | 1.37     |
| 46  | m2    | 1250 | B8N  | C4-N3   | -7.36 | 1.27        | 1.40     |
| 9   | A2    | 1599 | E7G  | C5-N7   | 7.31  | 1.44        | 1.35     |
| 46  | m2    | 1844 | 4AC  | C2-N3   | 7.27  | 1.50        | 1.36     |
| 11  | C2    | 14   | OMU  | C2-N1   | 7.17  | 1.49        | 1.38     |
| 9   | A2    | 2052 | E7G  | C5-N7   | 7.16  | 1.44        | 1.35     |
| 9   | A2    | 4272 | OMU  | C2-N3   | 7.09  | 1.50        | 1.38     |
| 46  | m2    | 116  | OMU  | C2-N3   | 7.06  | 1.50        | 1.38     |
| 46  | m2    | 116  | OMU  | C2-N1   | 7.03  | 1.49        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 4272 | OMU  | C2-N1   | 7.03  | 1.49        | 1.38     |
| 11  | C2    | 14   | OMU  | C2-N3   | 6.96  | 1.50        | 1.38     |
| 9   | A2    | 3958 | OMU  | C2-N3   | 6.96  | 1.50        | 1.38     |
| 9   | A2    | 3987 | 5MC  | C5-C4   | 6.95  | 1.49        | 1.44     |
| 9   | A2    | 3438 | 5MC  | C5-C4   | 6.95  | 1.49        | 1.44     |
| 9   | A2    | 3438 | 5MC  | C4-N3   | 6.92  | 1.45        | 1.34     |
| 46  | m2    | 1844 | 4AC  | C6-C5   | 6.90  | 1.51        | 1.35     |
| 9   | A2    | 3987 | 5MC  | C4-N3   | 6.89  | 1.45        | 1.34     |
| 9   | A2    | 3958 | OMU  | C2-N1   | 6.86  | 1.49        | 1.38     |
| 9   | A2    | 4099 | 5MC  | C4-N3   | 6.83  | 1.45        | 1.34     |
| 9   | A2    | 4023 | MHG  | C4-N9   | 6.78  | 1.46        | 1.37     |
| 9   | A2    | 3837 | B8W  | O4'-C4' | -6.74 | 1.30        | 1.45     |
| 9   | A2    | 878  | 2MG  | C4-N3   | 6.71  | 1.49        | 1.34     |
| 9   | A2    | 2528 | OMG  | C4-N3   | 6.70  | 1.49        | 1.34     |
| 9   | A2    | 3448 | OMG  | C4-N3   | 6.66  | 1.49        | 1.34     |
| 46  | m2    | 646  | OMG  | C4-N3   | 6.65  | 1.49        | 1.34     |
| 9   | A2    | 2179 | OMG  | C4-N3   | 6.64  | 1.49        | 1.34     |
| 9   | A2    | 3837 | B8W  | O6-C6   | 6.64  | 1.45        | 1.35     |
| 9   | A2    | 1685 | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 9   | A2    | 2616 | OMC  | C2-N3   | 6.63  | 1.49        | 1.36     |
| 9   | A2    | 4146 | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 9   | A2    | 1438 | OMG  | C4-N3   | 6.63  | 1.49        | 1.34     |
| 9   | A2    | 3565 | OMC  | C2-N3   | 6.61  | 1.49        | 1.36     |
| 9   | A2    | 4517 | 2MG  | C4-N3   | 6.61  | 1.49        | 1.34     |
| 46  | m2    | 685  | OMG  | C4-N3   | 6.61  | 1.49        | 1.34     |
| 9   | A2    | 2120 | OMC  | C2-N3   | 6.61  | 1.49        | 1.36     |
| 9   | A2    | 4515 | OMG  | C4-N3   | 6.60  | 1.49        | 1.34     |
| 9   | A2    | 3848 | OMG  | C4-N3   | 6.60  | 1.49        | 1.34     |
| 9   | A2    | 4022 | OMG  | C4-N3   | 6.60  | 1.49        | 1.34     |
| 9   | A2    | 4275 | OMG  | C4-N3   | 6.59  | 1.49        | 1.34     |
| 9   | A2    | 4289 | OMG  | C4-N3   | 6.59  | 1.49        | 1.34     |
| 9   | A2    | 1852 | OMG  | C4-N3   | 6.58  | 1.49        | 1.34     |
| 9   | A2    | 1330 | 2MG  | C4-N3   | 6.57  | 1.49        | 1.34     |
| 9   | A2    | 1335 | OMG  | C4-N3   | 6.57  | 1.49        | 1.34     |
| 9   | A2    | 3357 | OMC  | C2-N3   | 6.55  | 1.49        | 1.36     |
| 9   | A2    | 2177 | OMC  | C2-N3   | 6.54  | 1.49        | 1.36     |
| 9   | A2    | 2559 | OMC  | C2-N3   | 6.54  | 1.49        | 1.36     |
| 9   | A2    | 373  | OMG  | C4-N3   | 6.54  | 1.49        | 1.34     |
| 9   | A2    | 2119 | OMG  | C4-N3   | 6.51  | 1.49        | 1.34     |
| 46  | m2    | 519  | OMC  | C2-N3   | 6.51  | 1.49        | 1.36     |
| 9   | A2    | 4099 | 5MC  | C5-C4   | 6.51  | 1.49        | 1.44     |
| 9   | A2    | 4135 | B8T  | C2-N3   | 6.50  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 4188 | OMC  | C2-N3   | 6.46  | 1.49        | 1.36     |
| 9   | A2    | 2541 | B9H  | C2-N1   | 6.44  | 1.47        | 1.38     |
| 9   | A2    | 3525 | OMC  | C2-N3   | 6.43  | 1.49        | 1.36     |
| 9   | A2    | 4023 | MHG  | C2-N1   | 6.39  | 1.46        | 1.36     |
| 9   | A2    | 1472 | I4U  | C2-N3   | 6.33  | 1.48        | 1.36     |
| 9   | A2    | 3438 | 5MC  | C2-N3   | 6.32  | 1.48        | 1.36     |
| 9   | A2    | 3987 | 5MC  | C2-N3   | 6.26  | 1.48        | 1.36     |
| 9   | A2    | 3846 | I4U  | C6-C5   | 6.26  | 1.49        | 1.35     |
| 9   | A2    | 3846 | I4U  | C2-N3   | 6.24  | 1.48        | 1.36     |
| 9   | A2    | 4099 | 5MC  | C2-N3   | 6.23  | 1.48        | 1.36     |
| 9   | A2    | 3543 | OMC  | C6-C5   | 6.22  | 1.49        | 1.35     |
| 9   | A2    | 3837 | B8W  | C2'-C1' | -6.18 | 1.34        | 1.53     |
| 9   | A2    | 1472 | I4U  | C6-C5   | 6.18  | 1.49        | 1.35     |
| 9   | A2    | 1269 | B8Q  | C2-N1   | 6.17  | 1.47        | 1.38     |
| 9   | A2    | 3543 | OMC  | C2-N3   | 6.13  | 1.48        | 1.36     |
| 46  | m2    | 1844 | 4AC  | C4-N4   | 6.11  | 1.49        | 1.39     |
| 9   | A2    | 4135 | B8T  | C6-C5   | 6.10  | 1.49        | 1.35     |
| 9   | A2    | 3536 | P7G  | C4-N9   | 6.06  | 1.45        | 1.35     |
| 9   | A2    | 2177 | OMC  | C6-C5   | 6.05  | 1.49        | 1.35     |
| 46  | m2    | 1832 | UR3  | C6-C5   | 6.04  | 1.49        | 1.35     |
| 46  | m2    | 519  | OMC  | C6-C5   | 6.02  | 1.49        | 1.35     |
| 9   | A2    | 3357 | OMC  | C6-C5   | 6.00  | 1.49        | 1.35     |
| 9   | A2    | 1711 | P7G  | C4-N9   | 5.99  | 1.44        | 1.35     |
| 9   | A2    | 2616 | OMC  | C6-C5   | 5.99  | 1.49        | 1.35     |
| 9   | A2    | 4188 | OMC  | C6-C5   | 5.99  | 1.49        | 1.35     |
| 9   | A2    | 1668 | UR3  | C6-C5   | 5.97  | 1.48        | 1.35     |
| 9   | A2    | 3525 | OMC  | C6-C5   | 5.95  | 1.48        | 1.35     |
| 9   | A2    | 2559 | OMC  | C6-C5   | 5.94  | 1.48        | 1.35     |
| 9   | A2    | 1599 | E7G  | C2-N3   | 5.93  | 1.47        | 1.33     |
| 9   | A2    | 2052 | E7G  | C2-N3   | 5.91  | 1.47        | 1.33     |
| 9   | A2    | 3565 | OMC  | C6-C5   | 5.90  | 1.48        | 1.35     |
| 9   | A2    | 4249 | UR3  | C6-C5   | 5.90  | 1.48        | 1.35     |
| 9   | A2    | 1418 | G7M  | C2-N3   | 5.90  | 1.47        | 1.33     |
| 9   | A2    | 237  | B9B  | C2-N2   | 5.88  | 1.45        | 1.33     |
| 9   | A2    | 2277 | G7M  | C2-N3   | 5.84  | 1.47        | 1.33     |
| 9   | A2    | 2120 | OMC  | C6-C5   | 5.84  | 1.48        | 1.35     |
| 9   | A2    | 1387 | B9B  | C2-N2   | 5.83  | 1.45        | 1.33     |
| 9   | A2    | 4202 | G7M  | C2-N3   | 5.83  | 1.47        | 1.33     |
| 46  | m2    | 1250 | B8N  | C2-N1   | 5.82  | 1.56        | 1.39     |
| 9   | A2    | 4007 | E6G  | C2-N2   | 5.81  | 1.45        | 1.33     |
| 9   | A2    | 2277 | G7M  | C8-N9   | 5.79  | 1.51        | 1.35     |
| 9   | A2    | 1418 | G7M  | C8-N9   | 5.77  | 1.51        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 4202 | G7M  | C8-N9   | 5.76  | 1.51        | 1.35     |
| 46  | m2    | 1250 | B8N  | C6-C5   | 5.76  | 1.43        | 1.35     |
| 11  | C2    | 14   | OMU  | C6-C5   | 5.69  | 1.48        | 1.35     |
| 9   | A2    | 3958 | OMU  | C6-C5   | 5.67  | 1.48        | 1.35     |
| 9   | A2    | 4272 | OMU  | C6-C5   | 5.64  | 1.48        | 1.35     |
| 46  | m2    | 116  | OMU  | C6-C5   | 5.63  | 1.48        | 1.35     |
| 9   | A2    | 3536 | P7G  | C2-N1   | 5.58  | 1.46        | 1.33     |
| 9   | A2    | 3846 | I4U  | O4'-C1' | -5.57 | 1.29        | 1.42     |
| 9   | A2    | 2528 | OMG  | C2-N3   | 5.57  | 1.46        | 1.33     |
| 46  | m2    | 646  | OMG  | C2-N3   | 5.53  | 1.46        | 1.33     |
| 9   | A2    | 2179 | OMG  | C2-N3   | 5.52  | 1.46        | 1.33     |
| 9   | A2    | 4146 | OMG  | C2-N3   | 5.52  | 1.46        | 1.33     |
| 9   | A2    | 4515 | OMG  | C2-N3   | 5.51  | 1.46        | 1.33     |
| 9   | A2    | 1438 | OMG  | C2-N3   | 5.51  | 1.46        | 1.33     |
| 9   | A2    | 3448 | OMG  | C2-N3   | 5.50  | 1.46        | 1.33     |
| 9   | A2    | 4022 | OMG  | C2-N3   | 5.50  | 1.46        | 1.33     |
| 9   | A2    | 1711 | P7G  | C2-N1   | 5.48  | 1.46        | 1.33     |
| 9   | A2    | 4275 | OMG  | C2-N3   | 5.46  | 1.46        | 1.33     |
| 9   | A2    | 3848 | OMG  | C2-N3   | 5.46  | 1.46        | 1.33     |
| 9   | A2    | 4289 | OMG  | C2-N3   | 5.46  | 1.46        | 1.33     |
| 9   | A2    | 1685 | OMG  | C2-N3   | 5.46  | 1.46        | 1.33     |
| 46  | m2    | 685  | OMG  | C2-N3   | 5.45  | 1.46        | 1.33     |
| 9   | A2    | 3565 | OMC  | C4-N3   | 5.45  | 1.45        | 1.34     |
| 9   | A2    | 1852 | OMG  | C2-N3   | 5.44  | 1.46        | 1.33     |
| 9   | A2    | 1335 | OMG  | C2-N3   | 5.42  | 1.46        | 1.33     |
| 9   | A2    | 398  | A2M  | C6-N6   | 5.41  | 1.48        | 1.34     |
| 46  | m2    | 27   | A2M  | C6-N6   | 5.40  | 1.48        | 1.34     |
| 46  | m2    | 166  | A2M  | C6-N6   | 5.40  | 1.48        | 1.34     |
| 9   | A2    | 3357 | OMC  | C4-N3   | 5.39  | 1.45        | 1.34     |
| 9   | A2    | 3374 | A2M  | C6-N6   | 5.39  | 1.48        | 1.34     |
| 9   | A2    | 3481 | A2M  | C6-N6   | 5.39  | 1.48        | 1.34     |
| 9   | A2    | 2119 | OMG  | C2-N3   | 5.38  | 1.46        | 1.33     |
| 46  | m2    | 670  | A2M  | C6-N6   | 5.38  | 1.47        | 1.34     |
| 9   | A2    | 3379 | A2M  | C6-N6   | 5.37  | 1.47        | 1.34     |
| 79  | m     | 714  | DDE  | CBI-NAD | 5.37  | 1.45        | 1.32     |
| 9   | A2    | 3523 | A2M  | C6-N6   | 5.37  | 1.47        | 1.34     |
| 9   | A2    | 373  | OMG  | C2-N3   | 5.37  | 1.46        | 1.33     |
| 9   | A2    | 2118 | A2M  | C6-N6   | 5.36  | 1.47        | 1.34     |
| 9   | A2    | 4223 | A2M  | C6-N6   | 5.35  | 1.47        | 1.34     |
| 9   | A2    | 1673 | A2M  | C6-N6   | 5.35  | 1.47        | 1.34     |
| 9   | A2    | 1337 | A2M  | C6-N6   | 5.35  | 1.47        | 1.34     |
| 46  | m2    | 1033 | A2M  | C6-N6   | 5.35  | 1.47        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 2156 | A2M  | C6-N6   | 5.34  | 1.47        | 1.34     |
| 46  | m2    | 670  | A2M  | C2'-C1' | 5.34  | 1.66        | 1.53     |
| 9   | A2    | 1347 | A2M  | C6-N6   | 5.33  | 1.47        | 1.34     |
| 46  | m2    | 519  | OMC  | C4-N3   | 5.33  | 1.45        | 1.34     |
| 9   | A2    | 1140 | A2M  | C6-N6   | 5.33  | 1.47        | 1.34     |
| 9   | A2    | 2616 | OMC  | C4-N3   | 5.32  | 1.45        | 1.34     |
| 46  | m2    | 166  | A2M  | C2'-C1' | 5.31  | 1.66        | 1.53     |
| 9   | A2    | 2559 | OMC  | C4-N3   | 5.29  | 1.45        | 1.34     |
| 9   | A2    | 1337 | A2M  | C2'-C1' | 5.28  | 1.66        | 1.53     |
| 9   | A2    | 3525 | OMC  | C4-N3   | 5.27  | 1.45        | 1.34     |
| 9   | A2    | 3441 | A2M  | C6-N6   | 5.27  | 1.47        | 1.34     |
| 9   | A2    | 1472 | I4U  | O4'-C1' | -5.26 | 1.29        | 1.42     |
| 9   | A2    | 1599 | E7G  | C4-N9   | 5.26  | 1.44        | 1.37     |
| 9   | A2    | 3379 | A2M  | C2'-C1' | 5.25  | 1.66        | 1.53     |
| 9   | A2    | 3543 | OMC  | C4-N3   | 5.24  | 1.44        | 1.34     |
| 9   | A2    | 1490 | PSU  | C6-N1   | 5.22  | 1.44        | 1.36     |
| 9   | A2    | 2177 | OMC  | C4-N3   | 5.22  | 1.44        | 1.34     |
| 9   | A2    | 2120 | OMC  | C4-N3   | 5.21  | 1.44        | 1.34     |
| 9   | A2    | 4188 | OMC  | C4-N3   | 5.21  | 1.44        | 1.34     |
| 9   | A2    | 4288 | PSU  | C6-N1   | 5.20  | 1.44        | 1.36     |
| 46  | m2    | 825  | PSU  | C6-N1   | 5.19  | 1.44        | 1.36     |
| 9   | A2    | 4223 | A2M  | C2'-C1' | 5.19  | 1.65        | 1.53     |
| 9   | A2    | 2263 | PSU  | C6-N1   | 5.18  | 1.44        | 1.36     |
| 9   | A2    | 4249 | UR3  | C2-N3   | 5.18  | 1.49        | 1.39     |
| 9   | A2    | 3385 | PSU  | C6-N1   | 5.18  | 1.44        | 1.36     |
| 46  | m2    | 1832 | UR3  | C2-N3   | 5.18  | 1.49        | 1.39     |
| 9   | A2    | 1711 | P7G  | C2-N2   | 5.18  | 1.46        | 1.34     |
| 9   | A2    | 3536 | P7G  | C2-N2   | 5.18  | 1.46        | 1.34     |
| 9   | A2    | 2120 | OMC  | C2-N1   | 5.17  | 1.50        | 1.40     |
| 9   | A2    | 398  | A2M  | C2'-C1' | 5.15  | 1.65        | 1.53     |
| 9   | A2    | 4055 | PSU  | C6-N1   | 5.14  | 1.44        | 1.36     |
| 9   | A2    | 4102 | PSU  | C6-N1   | 5.14  | 1.44        | 1.36     |
| 9   | A2    | 3420 | PSU  | C6-N1   | 5.14  | 1.44        | 1.36     |
| 9   | A2    | 3374 | A2M  | C2'-C1' | 5.14  | 1.65        | 1.53     |
| 9   | A2    | 4152 | PSU  | C6-N1   | 5.13  | 1.44        | 1.36     |
| 46  | m2    | 1245 | PSU  | C6-N1   | 5.12  | 1.44        | 1.36     |
| 46  | m2    | 614  | PSU  | C6-N1   | 5.12  | 1.44        | 1.36     |
| 9   | A2    | 1496 | PSU  | C6-N1   | 5.11  | 1.44        | 1.36     |
| 9   | A2    | 4094 | PSU  | C6-N1   | 5.11  | 1.44        | 1.36     |
| 9   | A2    | 1668 | UR3  | C2-N3   | 5.11  | 1.49        | 1.39     |
| 46  | m2    | 1083 | PSU  | C6-N1   | 5.11  | 1.44        | 1.36     |
| 9   | A2    | 1140 | A2M  | C2'-C1' | 5.11  | 1.65        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 9   | A2    | 4280 | PSU  | C6-N1   | 5.10 | 1.44        | 1.36     |
| 9   | A2    | 3371 | PSU  | C6-N1   | 5.09 | 1.44        | 1.36     |
| 9   | A2    | 4183 | PSU  | C6-N1   | 5.08 | 1.44        | 1.36     |
| 9   | A2    | 3945 | PSU  | C6-N1   | 5.08 | 1.44        | 1.36     |
| 9   | A2    | 1395 | PSU  | C6-N1   | 5.07 | 1.44        | 1.36     |
| 46  | m2    | 1033 | A2M  | C2'-C1' | 5.07 | 1.65        | 1.53     |
| 9   | A2    | 2118 | A2M  | C2'-C1' | 5.04 | 1.65        | 1.53     |
| 9   | A2    | 1673 | A2M  | C2'-C1' | 5.03 | 1.65        | 1.53     |
| 9   | A2    | 2156 | A2M  | C2'-C1' | 5.03 | 1.65        | 1.53     |
| 9   | A2    | 3441 | A2M  | C2'-C1' | 5.02 | 1.65        | 1.53     |
| 9   | A2    | 3543 | OMC  | C4-N4   | 5.01 | 1.46        | 1.33     |
| 9   | A2    | 2052 | E7G  | C4-N9   | 5.00 | 1.44        | 1.37     |
| 46  | m2    | 27   | A2M  | C2'-C1' | 5.00 | 1.65        | 1.53     |
| 9   | A2    | 1347 | A2M  | C2'-C1' | 4.99 | 1.65        | 1.53     |
| 9   | A2    | 2616 | OMC  | C2-N1   | 4.98 | 1.50        | 1.40     |
| 9   | A2    | 1330 | 2MG  | C2-N1   | 4.96 | 1.44        | 1.36     |
| 46  | m2    | 519  | OMC  | C2-N1   | 4.96 | 1.50        | 1.40     |
| 46  | m2    | 646  | OMG  | C2-N2   | 4.96 | 1.45        | 1.34     |
| 9   | A2    | 4515 | OMG  | C2-N2   | 4.93 | 1.45        | 1.34     |
| 9   | A2    | 3481 | A2M  | C2'-C1' | 4.91 | 1.65        | 1.53     |
| 9   | A2    | 2528 | OMG  | C2-N2   | 4.91 | 1.45        | 1.34     |
| 9   | A2    | 878  | 2MG  | C2-N1   | 4.90 | 1.44        | 1.36     |
| 46  | m2    | 685  | OMG  | C2-N2   | 4.90 | 1.45        | 1.34     |
| 9   | A2    | 3523 | A2M  | C2'-C1' | 4.90 | 1.65        | 1.53     |
| 9   | A2    | 2179 | OMG  | C2-N2   | 4.90 | 1.45        | 1.34     |
| 9   | A2    | 1685 | OMG  | C2-N2   | 4.89 | 1.45        | 1.34     |
| 9   | A2    | 1335 | OMG  | C2-N2   | 4.89 | 1.45        | 1.34     |
| 9   | A2    | 373  | OMG  | C2-N2   | 4.89 | 1.45        | 1.34     |
| 9   | A2    | 1438 | OMG  | C2-N2   | 4.89 | 1.45        | 1.34     |
| 46  | m2    | 1844 | 4AC  | C2-N1   | 4.89 | 1.50        | 1.40     |
| 9   | A2    | 4146 | OMG  | C2-N2   | 4.88 | 1.45        | 1.34     |
| 9   | A2    | 3848 | OMG  | C2-N2   | 4.88 | 1.45        | 1.34     |
| 9   | A2    | 4022 | OMG  | C2-N2   | 4.87 | 1.45        | 1.34     |
| 9   | A2    | 3448 | OMG  | C2-N2   | 4.87 | 1.45        | 1.34     |
| 46  | m2    | 824  | PSU  | C6-N1   | 4.87 | 1.44        | 1.36     |
| 9   | A2    | 2052 | E7G  | C2-N2   | 4.87 | 1.45        | 1.34     |
| 9   | A2    | 4517 | 2MG  | C2-N1   | 4.86 | 1.44        | 1.36     |
| 9   | A2    | 4275 | OMG  | C2-N2   | 4.85 | 1.45        | 1.34     |
| 9   | A2    | 1418 | G7M  | C5-N7   | 4.85 | 1.44        | 1.39     |
| 9   | A2    | 1852 | OMG  | C2-N2   | 4.85 | 1.45        | 1.34     |
| 9   | A2    | 2119 | OMG  | C2-N2   | 4.83 | 1.45        | 1.34     |
| 9   | A2    | 4289 | OMG  | C2-N2   | 4.82 | 1.45        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 1599 | E7G  | C2-N2   | 4.81  | 1.45        | 1.34     |
| 9   | A2    | 4202 | G7M  | C5-N7   | 4.80  | 1.44        | 1.39     |
| 9   | A2    | 3441 | A2M  | O4'-C1' | -4.79 | 1.30        | 1.42     |
| 9   | A2    | 2277 | G7M  | C2-N2   | 4.77  | 1.45        | 1.34     |
| 9   | A2    | 3565 | OMC  | C4-N4   | 4.76  | 1.45        | 1.33     |
| 9   | A2    | 2277 | G7M  | C5-N7   | 4.76  | 1.44        | 1.39     |
| 9   | A2    | 3525 | OMC  | C4-N4   | 4.75  | 1.45        | 1.33     |
| 9   | A2    | 2177 | OMC  | C4-N4   | 4.74  | 1.45        | 1.33     |
| 9   | A2    | 4188 | OMC  | C4-N4   | 4.73  | 1.45        | 1.33     |
| 9   | A2    | 1418 | G7M  | C2-N2   | 4.73  | 1.45        | 1.34     |
| 9   | A2    | 4202 | G7M  | C2-N2   | 4.73  | 1.45        | 1.34     |
| 9   | A2    | 2616 | OMC  | C4-N4   | 4.73  | 1.45        | 1.33     |
| 46  | m2    | 519  | OMC  | C4-N4   | 4.72  | 1.45        | 1.33     |
| 9   | A2    | 2120 | OMC  | C4-N4   | 4.72  | 1.45        | 1.33     |
| 9   | A2    | 3357 | OMC  | C4-N4   | 4.69  | 1.45        | 1.33     |
| 9   | A2    | 2559 | OMC  | C4-N4   | 4.69  | 1.45        | 1.33     |
| 9   | A2    | 1472 | I4U  | C2'-C1' | 4.68  | 1.68        | 1.53     |
| 9   | A2    | 3565 | OMC  | C2-N1   | 4.68  | 1.49        | 1.40     |
| 9   | A2    | 4188 | OMC  | C2-N1   | 4.67  | 1.49        | 1.40     |
| 9   | A2    | 3438 | 5MC  | C6-N1   | 4.67  | 1.45        | 1.38     |
| 9   | A2    | 3525 | OMC  | C2-N1   | 4.65  | 1.49        | 1.40     |
| 9   | A2    | 2559 | OMC  | C2-N1   | 4.64  | 1.49        | 1.40     |
| 9   | A2    | 1347 | A2M  | O4'-C1' | -4.63 | 1.31        | 1.42     |
| 9   | A2    | 4099 | 5MC  | C6-N1   | 4.60  | 1.45        | 1.38     |
| 9   | A2    | 4135 | B8T  | C4-N4   | 4.59  | 1.45        | 1.36     |
| 9   | A2    | 3357 | OMC  | C2-N1   | 4.58  | 1.49        | 1.40     |
| 9   | A2    | 3536 | P7G  | C2-N3   | 4.57  | 1.48        | 1.37     |
| 9   | A2    | 3846 | I4U  | C2'-C1' | 4.52  | 1.67        | 1.53     |
| 46  | m2    | 824  | PSU  | C4-N3   | 4.51  | 1.47        | 1.38     |
| 46  | m2    | 670  | A2M  | O4'-C1' | -4.51 | 1.31        | 1.42     |
| 9   | A2    | 3543 | OMC  | C2-N1   | 4.50  | 1.49        | 1.40     |
| 9   | A2    | 1711 | P7G  | C2-N3   | 4.46  | 1.48        | 1.37     |
| 9   | A2    | 3438 | 5MC  | C4-N4   | 4.45  | 1.45        | 1.34     |
| 9   | A2    | 3987 | 5MC  | C6-N1   | 4.45  | 1.45        | 1.38     |
| 9   | A2    | 3846 | I4U  | O4'-C4' | 4.45  | 1.54        | 1.45     |
| 9   | A2    | 1472 | I4U  | C5'-C4' | -4.44 | 1.38        | 1.51     |
| 9   | A2    | 3846 | I4U  | C5'-C4' | -4.43 | 1.38        | 1.51     |
| 9   | A2    | 3837 | B8W  | C2-N2   | 4.43  | 1.42        | 1.33     |
| 9   | A2    | 1472 | I4U  | O4'-C4' | 4.42  | 1.54        | 1.45     |
| 9   | A2    | 3987 | 5MC  | C4-N4   | 4.41  | 1.45        | 1.34     |
| 9   | A2    | 4099 | 5MC  | C4-N4   | 4.41  | 1.45        | 1.34     |
| 9   | A2    | 1140 | A2M  | O4'-C1' | -4.40 | 1.31        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | m2    | 1844 | 4AC  | C5-C4   | 4.39  | 1.50        | 1.41     |
| 9   | A2    | 4135 | B8T  | C2-N1   | 4.38  | 1.49        | 1.40     |
| 9   | A2    | 2177 | OMC  | C2-N1   | 4.37  | 1.49        | 1.40     |
| 9   | A2    | 3523 | A2M  | O4'-C1' | -4.36 | 1.31        | 1.42     |
| 9   | A2    | 2156 | A2M  | O4'-C1' | -4.33 | 1.32        | 1.42     |
| 9   | A2    | 4099 | 5MC  | C2-N1   | 4.31  | 1.49        | 1.40     |
| 9   | A2    | 1337 | A2M  | O4'-C1' | -4.31 | 1.32        | 1.42     |
| 46  | m2    | 27   | A2M  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 9   | A2    | 3481 | A2M  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 9   | A2    | 2118 | A2M  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 9   | A2    | 4223 | A2M  | O4'-C1' | -4.28 | 1.32        | 1.42     |
| 46  | m2    | 166  | A2M  | O4'-C1' | -4.27 | 1.32        | 1.42     |
| 9   | A2    | 3987 | 5MC  | C2-N1   | 4.27  | 1.49        | 1.40     |
| 9   | A2    | 3379 | A2M  | O4'-C1' | -4.25 | 1.32        | 1.42     |
| 46  | m2    | 1033 | A2M  | O4'-C1' | -4.25 | 1.32        | 1.42     |
| 46  | m2    | 116  | OMU  | C4-N3   | 4.25  | 1.45        | 1.38     |
| 11  | C2    | 14   | OMU  | C4-N3   | 4.25  | 1.45        | 1.38     |
| 9   | A2    | 398  | A2M  | O4'-C1' | -4.24 | 1.32        | 1.42     |
| 9   | A2    | 1673 | A2M  | O4'-C1' | -4.24 | 1.32        | 1.42     |
| 9   | A2    | 1472 | I4U  | C2-N1   | 4.24  | 1.49        | 1.40     |
| 9   | A2    | 3374 | A2M  | O4'-C1' | -4.22 | 1.32        | 1.42     |
| 9   | A2    | 3846 | I4U  | C2-N1   | 4.18  | 1.48        | 1.40     |
| 9   | A2    | 3958 | OMU  | C4-N3   | 4.17  | 1.45        | 1.38     |
| 46  | m2    | 614  | PSU  | C4-N3   | 4.14  | 1.46        | 1.38     |
| 9   | A2    | 4272 | OMU  | C4-N3   | 4.13  | 1.45        | 1.38     |
| 9   | A2    | 1668 | UR3  | O4-C4   | -4.11 | 1.14        | 1.23     |
| 9   | A2    | 3837 | B8W  | O3'-C3' | -4.11 | 1.32        | 1.43     |
| 9   | A2    | 3438 | 5MC  | C2-N1   | 4.10  | 1.48        | 1.40     |
| 9   | A2    | 3385 | PSU  | C4-N3   | 4.07  | 1.46        | 1.38     |
| 9   | A2    | 4094 | PSU  | C4-N3   | 4.07  | 1.46        | 1.38     |
| 9   | A2    | 4249 | UR3  | O4-C4   | -4.06 | 1.15        | 1.23     |
| 9   | A2    | 3420 | PSU  | C4-N3   | 4.05  | 1.46        | 1.38     |
| 9   | A2    | 3945 | PSU  | C4-N3   | 4.04  | 1.46        | 1.38     |
| 9   | A2    | 4152 | PSU  | C4-N3   | 4.04  | 1.46        | 1.38     |
| 9   | A2    | 4288 | PSU  | C4-N3   | 4.04  | 1.46        | 1.38     |
| 9   | A2    | 1490 | PSU  | C4-N3   | 4.03  | 1.46        | 1.38     |
| 9   | A2    | 2263 | PSU  | C4-N3   | 4.02  | 1.46        | 1.38     |
| 46  | m2    | 1832 | UR3  | O4-C4   | -4.02 | 1.15        | 1.23     |
| 9   | A2    | 3371 | PSU  | C4-N3   | 4.02  | 1.46        | 1.38     |
| 9   | A2    | 4280 | PSU  | C4-N3   | 4.01  | 1.46        | 1.38     |
| 46  | m2    | 825  | PSU  | C4-N3   | 4.01  | 1.46        | 1.38     |
| 9   | A2    | 4102 | PSU  | C4-N3   | 4.00  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 4055 | PSU  | C4-N3   | 4.00  | 1.46        | 1.38     |
| 46  | m2    | 1083 | PSU  | C4-N3   | 4.00  | 1.46        | 1.38     |
| 9   | A2    | 1395 | PSU  | C4-N3   | 4.00  | 1.46        | 1.38     |
| 9   | A2    | 4183 | PSU  | C4-N3   | 3.99  | 1.46        | 1.38     |
| 9   | A2    | 1496 | PSU  | C4-N3   | 3.97  | 1.46        | 1.38     |
| 46  | m2    | 1245 | PSU  | C4-N3   | 3.92  | 1.46        | 1.38     |
| 46  | m2    | 1844 | 4AC  | C7-N4   | 3.89  | 1.45        | 1.37     |
| 9   | A2    | 2277 | G7M  | C2-N1   | 3.80  | 1.46        | 1.37     |
| 9   | A2    | 4202 | G7M  | C2-N1   | 3.80  | 1.46        | 1.37     |
| 9   | A2    | 4067 | 1MA  | C5-C6   | 3.80  | 1.53        | 1.43     |
| 9   | A2    | 1418 | G7M  | C2-N1   | 3.78  | 1.46        | 1.37     |
| 9   | A2    | 4067 | 1MA  | C2-N1   | 3.77  | 1.43        | 1.35     |
| 9   | A2    | 237  | B9B  | O6-C6   | 3.73  | 1.40        | 1.34     |
| 9   | A2    | 1599 | E7G  | C2-N1   | 3.72  | 1.46        | 1.37     |
| 9   | A2    | 4023 | MHG  | C5-C6   | 3.71  | 1.52        | 1.43     |
| 9   | A2    | 2052 | E7G  | C2-N1   | 3.70  | 1.46        | 1.37     |
| 79  | m     | 714  | DDE  | CG-ND1  | -3.70 | 1.31        | 1.38     |
| 9   | A2    | 3536 | P7G  | C6-N1   | 3.68  | 1.44        | 1.38     |
| 9   | A2    | 1711 | P7G  | C6-N1   | 3.67  | 1.44        | 1.38     |
| 9   | A2    | 4135 | B8T  | C5-C4   | 3.66  | 1.49        | 1.41     |
| 9   | A2    | 4023 | MHG  | C8-N7   | 3.64  | 1.52        | 1.45     |
| 9   | A2    | 1599 | E7G  | C5-C6   | 3.62  | 1.52        | 1.43     |
| 9   | A2    | 3837 | B8W  | C5-C4   | -3.61 | 1.32        | 1.39     |
| 9   | A2    | 2177 | OMC  | C6-N1   | 3.61  | 1.46        | 1.38     |
| 9   | A2    | 1711 | P7G  | C8-N7   | 3.58  | 1.52        | 1.45     |
| 9   | A2    | 2052 | E7G  | C5-C6   | 3.57  | 1.52        | 1.43     |
| 9   | A2    | 1337 | A2M  | C5'-C4' | -3.56 | 1.40        | 1.51     |
| 9   | A2    | 3374 | A2M  | C5'-C4' | -3.55 | 1.40        | 1.51     |
| 9   | A2    | 1387 | B9B  | O6-C6   | 3.54  | 1.40        | 1.34     |
| 9   | A2    | 237  | B9B  | O2'-C2' | 3.54  | 1.51        | 1.43     |
| 9   | A2    | 3523 | A2M  | C5'-C4' | -3.53 | 1.40        | 1.51     |
| 9   | A2    | 4007 | E6G  | O2'-C2' | 3.52  | 1.51        | 1.43     |
| 46  | m2    | 670  | A2M  | C5'-C4' | -3.51 | 1.41        | 1.51     |
| 9   | A2    | 1140 | A2M  | C5'-C4' | -3.51 | 1.41        | 1.51     |
| 9   | A2    | 1387 | B9B  | O2'-C2' | 3.50  | 1.51        | 1.43     |
| 9   | A2    | 3481 | A2M  | C5'-C4' | -3.50 | 1.41        | 1.51     |
| 46  | m2    | 1033 | A2M  | C5'-C4' | -3.49 | 1.41        | 1.51     |
| 9   | A2    | 4007 | E6G  | O6-C6   | 3.49  | 1.40        | 1.34     |
| 9   | A2    | 2120 | OMC  | C6-N1   | 3.49  | 1.46        | 1.38     |
| 9   | A2    | 3441 | A2M  | C4-N9   | -3.48 | 1.30        | 1.37     |
| 9   | A2    | 2156 | A2M  | C5'-C4' | -3.48 | 1.41        | 1.51     |
| 9   | A2    | 3543 | OMC  | C6-N1   | 3.47  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 4223 | A2M  | C5'-C4' | -3.47 | 1.41        | 1.51     |
| 9   | A2    | 398  | A2M  | C5'-C4' | -3.45 | 1.41        | 1.51     |
| 9   | A2    | 3441 | A2M  | C5'-C4' | -3.45 | 1.41        | 1.51     |
| 79  | m     | 714  | DDE  | CBW-NCB | -3.44 | 1.47        | 1.54     |
| 9   | A2    | 1140 | A2M  | C4-N9   | -3.44 | 1.30        | 1.37     |
| 9   | A2    | 3481 | A2M  | C4-N9   | -3.43 | 1.30        | 1.37     |
| 9   | A2    | 3379 | A2M  | C5'-C4' | -3.42 | 1.41        | 1.51     |
| 9   | A2    | 3523 | A2M  | C4-N9   | -3.42 | 1.30        | 1.37     |
| 9   | A2    | 4223 | A2M  | C4-N9   | -3.42 | 1.30        | 1.37     |
| 9   | A2    | 1347 | A2M  | C5'-C4' | -3.41 | 1.41        | 1.51     |
| 46  | m2    | 166  | A2M  | C5'-C4' | -3.41 | 1.41        | 1.51     |
| 9   | A2    | 1673 | A2M  | C4-N9   | -3.40 | 1.30        | 1.37     |
| 46  | m2    | 27   | A2M  | C5'-C4' | -3.40 | 1.41        | 1.51     |
| 9   | A2    | 1673 | A2M  | C5'-C4' | -3.40 | 1.41        | 1.51     |
| 9   | A2    | 398  | A2M  | C4-N9   | -3.40 | 1.30        | 1.37     |
| 46  | m2    | 27   | A2M  | C4-N9   | -3.39 | 1.30        | 1.37     |
| 9   | A2    | 2118 | A2M  | C4-N9   | -3.38 | 1.30        | 1.37     |
| 9   | A2    | 1347 | A2M  | C4-N9   | -3.37 | 1.30        | 1.37     |
| 9   | A2    | 2118 | A2M  | C5'-C4' | -3.35 | 1.41        | 1.51     |
| 9   | A2    | 2156 | A2M  | C4-N9   | -3.35 | 1.30        | 1.37     |
| 9   | A2    | 3525 | OMC  | C6-N1   | 3.35  | 1.46        | 1.38     |
| 46  | m2    | 670  | A2M  | C4-N9   | -3.34 | 1.30        | 1.37     |
| 9   | A2    | 3379 | A2M  | C4-N9   | -3.32 | 1.30        | 1.37     |
| 9   | A2    | 4188 | OMC  | C6-N1   | 3.31  | 1.46        | 1.38     |
| 9   | A2    | 3441 | A2M  | C3'-C4' | 3.30  | 1.61        | 1.53     |
| 46  | m2    | 519  | OMC  | C6-N1   | 3.30  | 1.46        | 1.38     |
| 9   | A2    | 2616 | OMC  | C6-N1   | 3.30  | 1.46        | 1.38     |
| 9   | A2    | 3536 | P7G  | C8-N7   | 3.30  | 1.51        | 1.45     |
| 9   | A2    | 2559 | OMC  | C6-N1   | 3.28  | 1.45        | 1.38     |
| 9   | A2    | 4202 | G7M  | C5-C6   | 3.28  | 1.52        | 1.43     |
| 46  | m2    | 1033 | A2M  | C4-N9   | -3.27 | 1.30        | 1.37     |
| 9   | A2    | 3565 | OMC  | C6-N1   | 3.27  | 1.45        | 1.38     |
| 9   | A2    | 1418 | G7M  | C5-C6   | 3.27  | 1.52        | 1.43     |
| 9   | A2    | 3357 | OMC  | C6-N1   | 3.26  | 1.45        | 1.38     |
| 9   | A2    | 2277 | G7M  | C5-C6   | 3.24  | 1.52        | 1.43     |
| 9   | A2    | 3374 | A2M  | C4-N9   | -3.24 | 1.30        | 1.37     |
| 9   | A2    | 1337 | A2M  | C4-N9   | -3.23 | 1.31        | 1.37     |
| 46  | m2    | 166  | A2M  | C4-N9   | -3.23 | 1.31        | 1.37     |
| 9   | A2    | 2052 | E7G  | C8-N7   | 3.22  | 1.51        | 1.45     |
| 9   | A2    | 1599 | E7G  | C8-N7   | 3.22  | 1.51        | 1.45     |
| 46  | m2    | 1832 | UR3  | C5-C4   | 3.19  | 1.51        | 1.43     |
| 9   | A2    | 3846 | I4U  | O4-C41  | -3.19 | 1.40        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 2277 | G7M  | C6-N1   | 3.19  | 1.44        | 1.38     |
| 9   | A2    | 1418 | G7M  | C6-N1   | 3.19  | 1.44        | 1.38     |
| 9   | A2    | 4202 | G7M  | C6-N1   | 3.18  | 1.44        | 1.38     |
| 9   | A2    | 1347 | A2M  | C3'-C4' | 3.17  | 1.61        | 1.53     |
| 9   | A2    | 3837 | B8W  | C8-N9   | -3.16 | 1.32        | 1.37     |
| 9   | A2    | 3846 | I4U  | C6-N1   | 3.15  | 1.45        | 1.38     |
| 9   | A2    | 3523 | A2M  | C3'-C4' | 3.12  | 1.60        | 1.53     |
| 9   | A2    | 3536 | P7G  | C5-C4   | 3.12  | 1.44        | 1.36     |
| 9   | A2    | 1668 | UR3  | C5-C4   | 3.12  | 1.51        | 1.43     |
| 46  | m2    | 166  | A2M  | C3'-C4' | 3.12  | 1.60        | 1.53     |
| 9   | A2    | 4135 | B8T  | C6-N1   | 3.12  | 1.45        | 1.38     |
| 9   | A2    | 1472 | I4U  | O4-C41  | -3.12 | 1.40        | 1.47     |
| 46  | m2    | 1844 | 4AC  | C6-N1   | 3.12  | 1.45        | 1.38     |
| 9   | A2    | 1472 | I4U  | C6-N1   | 3.11  | 1.45        | 1.38     |
| 9   | A2    | 4249 | UR3  | C5-C4   | 3.10  | 1.51        | 1.43     |
| 9   | A2    | 1711 | P7G  | C5-C4   | 3.09  | 1.44        | 1.36     |
| 9   | A2    | 1599 | E7G  | C6-N1   | 3.06  | 1.44        | 1.38     |
| 9   | A2    | 3379 | A2M  | O2'-C2' | 3.06  | 1.50        | 1.42     |
| 9   | A2    | 2156 | A2M  | C3'-C4' | 3.04  | 1.60        | 1.53     |
| 9   | A2    | 2118 | A2M  | C3'-C4' | 3.03  | 1.60        | 1.53     |
| 9   | A2    | 1140 | A2M  | O2'-C2' | 3.02  | 1.50        | 1.42     |
| 46  | m2    | 27   | A2M  | O2'-C2' | 3.02  | 1.50        | 1.42     |
| 9   | A2    | 1140 | A2M  | C3'-C4' | 3.02  | 1.60        | 1.53     |
| 46  | m2    | 1033 | A2M  | O2'-C2' | 3.02  | 1.50        | 1.42     |
| 9   | A2    | 398  | A2M  | O2'-C2' | 3.01  | 1.50        | 1.42     |
| 46  | m2    | 166  | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 46  | m2    | 27   | A2M  | C3'-C4' | 3.00  | 1.60        | 1.53     |
| 9   | A2    | 1387 | B9B  | C5-C4   | -3.00 | 1.33        | 1.39     |
| 46  | m2    | 1033 | A2M  | C3'-C4' | 2.99  | 1.60        | 1.53     |
| 9   | A2    | 4517 | 2MG  | C5-N7   | -2.99 | 1.33        | 1.39     |
| 9   | A2    | 1337 | A2M  | O2'-C2' | 2.99  | 1.50        | 1.42     |
| 9   | A2    | 398  | A2M  | C3'-C4' | 2.98  | 1.60        | 1.53     |
| 9   | A2    | 878  | 2MG  | C5-N7   | -2.98 | 1.33        | 1.39     |
| 9   | A2    | 4223 | A2M  | O2'-C2' | 2.98  | 1.50        | 1.42     |
| 46  | m2    | 670  | A2M  | C3'-C4' | 2.98  | 1.60        | 1.53     |
| 9   | A2    | 1347 | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 9   | A2    | 3481 | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 9   | A2    | 3374 | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 9   | A2    | 3523 | A2M  | O2'-C2' | 2.97  | 1.49        | 1.42     |
| 9   | A2    | 3837 | B8W  | C3'-C4' | 2.97  | 1.60        | 1.53     |
| 46  | m2    | 670  | A2M  | O2'-C2' | 2.97  | 1.49        | 1.42     |
| 11  | C2    | 14   | OMU  | O4-C4   | -2.96 | 1.18        | 1.24     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 3379 | A2M  | C3'-C4' | 2.96  | 1.60        | 1.53     |
| 9   | A2    | 2156 | A2M  | O2'-C2' | 2.96  | 1.49        | 1.42     |
| 9   | A2    | 3481 | A2M  | C3'-C4' | 2.96  | 1.60        | 1.53     |
| 9   | A2    | 1673 | A2M  | O2'-C2' | 2.95  | 1.49        | 1.42     |
| 9   | A2    | 3872 | 6MZ  | C5-C4   | -2.95 | 1.33        | 1.39     |
| 9   | A2    | 2118 | A2M  | O2'-C2' | 2.95  | 1.49        | 1.42     |
| 9   | A2    | 4223 | A2M  | C3'-C4' | 2.94  | 1.60        | 1.53     |
| 9   | A2    | 3441 | A2M  | O2'-C2' | 2.94  | 1.49        | 1.42     |
| 9   | A2    | 3958 | OMU  | O4-C4   | -2.94 | 1.18        | 1.24     |
| 9   | A2    | 2118 | A2M  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 9   | A2    | 4007 | E6G  | C5-C4   | -2.93 | 1.33        | 1.39     |
| 9   | A2    | 1330 | 2MG  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 9   | A2    | 2052 | E7G  | C6-N1   | 2.93  | 1.44        | 1.38     |
| 9   | A2    | 1347 | A2M  | C5-N7   | -2.93 | 1.33        | 1.39     |
| 9   | A2    | 4272 | OMU  | O4-C4   | -2.93 | 1.18        | 1.24     |
| 46  | m2    | 116  | OMU  | O4-C4   | -2.92 | 1.18        | 1.24     |
| 9   | A2    | 1140 | A2M  | C5-N7   | -2.89 | 1.33        | 1.39     |
| 9   | A2    | 2156 | A2M  | C5-N7   | -2.89 | 1.33        | 1.39     |
| 9   | A2    | 3374 | A2M  | C3'-C4' | 2.89  | 1.60        | 1.53     |
| 9   | A2    | 3374 | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 46  | m2    | 670  | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 9   | A2    | 3523 | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 46  | m2    | 670  | A2M  | O3'-C3' | 2.87  | 1.50        | 1.43     |
| 9   | A2    | 2528 | OMG  | C2-N1   | 2.87  | 1.44        | 1.37     |
| 9   | A2    | 2119 | OMG  | C2-N1   | 2.86  | 1.44        | 1.37     |
| 9   | A2    | 1711 | P7G  | O6-C6   | -2.86 | 1.18        | 1.23     |
| 46  | m2    | 646  | OMG  | C2-N1   | 2.86  | 1.44        | 1.37     |
| 9   | A2    | 1438 | OMG  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 46  | m2    | 27   | A2M  | C5-N7   | -2.86 | 1.33        | 1.39     |
| 9   | A2    | 1673 | A2M  | C3'-C4' | 2.85  | 1.60        | 1.53     |
| 9   | A2    | 373  | OMG  | C2-N1   | 2.85  | 1.44        | 1.37     |
| 9   | A2    | 2179 | OMG  | C2-N1   | 2.85  | 1.44        | 1.37     |
| 9   | A2    | 4515 | OMG  | C2-N1   | 2.84  | 1.44        | 1.37     |
| 11  | C2    | 14   | OMU  | C6-N1   | 2.84  | 1.44        | 1.38     |
| 46  | m2    | 1033 | A2M  | C5-N7   | -2.84 | 1.33        | 1.39     |
| 9   | A2    | 1337 | A2M  | C3'-C4' | 2.84  | 1.60        | 1.53     |
| 46  | m2    | 685  | OMG  | C2-N1   | 2.84  | 1.44        | 1.37     |
| 9   | A2    | 3536 | P7G  | O6-C6   | -2.84 | 1.18        | 1.23     |
| 9   | A2    | 1337 | A2M  | C5-N7   | -2.84 | 1.33        | 1.39     |
| 9   | A2    | 1673 | A2M  | C5-N7   | -2.84 | 1.33        | 1.39     |
| 9   | A2    | 3848 | OMG  | C2-N1   | 2.83  | 1.44        | 1.37     |
| 9   | A2    | 4023 | MHG  | C6-N1   | 2.83  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 398  | A2M  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 9   | A2    | 3441 | A2M  | C5-N7   | -2.83 | 1.33        | 1.39     |
| 9   | A2    | 4223 | A2M  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 9   | A2    | 1472 | I4U  | O3'-C3' | 2.82  | 1.49        | 1.43     |
| 46  | m2    | 166  | A2M  | O3'-C3' | 2.82  | 1.49        | 1.43     |
| 9   | A2    | 4275 | OMG  | C2-N1   | 2.82  | 1.44        | 1.37     |
| 9   | A2    | 1685 | OMG  | C2-N1   | 2.82  | 1.44        | 1.37     |
| 46  | m2    | 166  | A2M  | O4'-C4' | 2.82  | 1.51        | 1.45     |
| 9   | A2    | 2528 | OMG  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 46  | m2    | 166  | A2M  | C5-N7   | -2.81 | 1.33        | 1.39     |
| 46  | m2    | 116  | OMU  | C6-N1   | 2.81  | 1.44        | 1.38     |
| 9   | A2    | 3448 | OMG  | C5-N7   | -2.81 | 1.33        | 1.39     |
| 9   | A2    | 3374 | A2M  | O4'-C4' | 2.81  | 1.51        | 1.45     |
| 9   | A2    | 1335 | OMG  | C2-N1   | 2.81  | 1.44        | 1.37     |
| 9   | A2    | 3481 | A2M  | C5-N7   | -2.81 | 1.34        | 1.39     |
| 46  | m2    | 1832 | UR3  | C6-N1   | 2.81  | 1.44        | 1.38     |
| 9   | A2    | 1438 | OMG  | C2-N1   | 2.81  | 1.44        | 1.37     |
| 9   | A2    | 3958 | OMU  | C6-N1   | 2.81  | 1.44        | 1.38     |
| 9   | A2    | 2156 | A2M  | O4'-C4' | 2.81  | 1.51        | 1.45     |
| 9   | A2    | 4146 | OMG  | C5-N7   | -2.80 | 1.33        | 1.39     |
| 9   | A2    | 237  | B9B  | C5-C4   | -2.80 | 1.34        | 1.39     |
| 9   | A2    | 1673 | A2M  | O4'-C4' | 2.80  | 1.51        | 1.45     |
| 9   | A2    | 4146 | OMG  | C2-N1   | 2.79  | 1.44        | 1.37     |
| 9   | A2    | 3448 | OMG  | C2-N1   | 2.79  | 1.44        | 1.37     |
| 9   | A2    | 2156 | A2M  | O3'-C3' | 2.79  | 1.49        | 1.43     |
| 9   | A2    | 1668 | UR3  | C6-N1   | 2.79  | 1.44        | 1.38     |
| 9   | A2    | 3379 | A2M  | C5-N7   | -2.78 | 1.34        | 1.39     |
| 9   | A2    | 2179 | OMG  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 9   | A2    | 1852 | OMG  | C2-N1   | 2.78  | 1.44        | 1.37     |
| 9   | A2    | 1852 | OMG  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 46  | m2    | 646  | OMG  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 9   | A2    | 3441 | A2M  | O3'-C3' | 2.77  | 1.49        | 1.43     |
| 46  | m2    | 1844 | 4AC  | O7-C7   | -2.77 | 1.17        | 1.23     |
| 9   | A2    | 4022 | OMG  | C2-N1   | 2.77  | 1.44        | 1.37     |
| 9   | A2    | 4275 | OMG  | C5-N7   | -2.77 | 1.33        | 1.39     |
| 9   | A2    | 1387 | B9B  | O3'-C3' | -2.77 | 1.36        | 1.43     |
| 9   | A2    | 1685 | OMG  | C5-N7   | -2.76 | 1.33        | 1.39     |
| 9   | A2    | 3846 | I4U  | O3'-C3' | 2.76  | 1.49        | 1.43     |
| 9   | A2    | 4007 | E6G  | O3'-C3' | -2.76 | 1.36        | 1.43     |
| 9   | A2    | 2177 | OMC  | O2-C2   | -2.76 | 1.18        | 1.23     |
| 9   | A2    | 3837 | B8W  | C4-N3   | 2.75  | 1.37        | 1.34     |
| 9   | A2    | 398  | A2M  | O4'-C4' | 2.74  | 1.51        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 2118 | A2M  | O3'-C3' | 2.74  | 1.49        | 1.43     |
| 9   | A2    | 3523 | A2M  | O4'-C4' | 2.74  | 1.51        | 1.45     |
| 46  | m2    | 1033 | A2M  | O3'-C3' | 2.74  | 1.49        | 1.43     |
| 9   | A2    | 3379 | A2M  | O3'-C3' | 2.74  | 1.49        | 1.43     |
| 9   | A2    | 3523 | A2M  | O3'-C3' | 2.74  | 1.49        | 1.43     |
| 9   | A2    | 398  | A2M  | O3'-C3' | 2.74  | 1.49        | 1.43     |
| 9   | A2    | 4022 | OMG  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 9   | A2    | 4289 | OMG  | C2-N1   | 2.74  | 1.44        | 1.37     |
| 46  | m2    | 27   | A2M  | O3'-C3' | 2.73  | 1.49        | 1.43     |
| 9   | A2    | 2118 | A2M  | O4'-C4' | 2.73  | 1.51        | 1.45     |
| 9   | A2    | 1140 | A2M  | O3'-C3' | 2.73  | 1.49        | 1.43     |
| 9   | A2    | 1335 | OMG  | C5-N7   | -2.73 | 1.33        | 1.39     |
| 46  | m2    | 1033 | A2M  | O4'-C4' | 2.73  | 1.51        | 1.45     |
| 9   | A2    | 237  | B9B  | C5-N7   | -2.73 | 1.34        | 1.39     |
| 9   | A2    | 4272 | OMU  | C6-N1   | 2.72  | 1.44        | 1.38     |
| 9   | A2    | 4223 | A2M  | O3'-C3' | 2.72  | 1.49        | 1.43     |
| 9   | A2    | 4223 | A2M  | O4'-C4' | 2.72  | 1.51        | 1.45     |
| 9   | A2    | 3481 | A2M  | O3'-C3' | 2.71  | 1.49        | 1.43     |
| 9   | A2    | 2616 | OMC  | O2-C2   | -2.71 | 1.18        | 1.23     |
| 9   | A2    | 4289 | OMG  | C5-C6   | 2.71  | 1.54        | 1.44     |
| 9   | A2    | 3846 | I4U  | O2-C2   | -2.70 | 1.18        | 1.23     |
| 9   | A2    | 1337 | A2M  | O3'-C3' | 2.70  | 1.49        | 1.43     |
| 9   | A2    | 1472 | I4U  | O2-C2   | -2.69 | 1.18        | 1.23     |
| 9   | A2    | 1347 | A2M  | O3'-C3' | 2.69  | 1.49        | 1.43     |
| 9   | A2    | 2119 | OMG  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 46  | m2    | 685  | OMG  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 9   | A2    | 3848 | OMG  | C5-N7   | -2.69 | 1.33        | 1.39     |
| 9   | A2    | 3374 | A2M  | O3'-C3' | 2.69  | 1.49        | 1.43     |
| 9   | A2    | 3837 | B8W  | C5-N7   | -2.68 | 1.34        | 1.39     |
| 9   | A2    | 2559 | OMC  | O2-C2   | -2.68 | 1.18        | 1.23     |
| 9   | A2    | 4135 | B8T  | O2-C2   | -2.68 | 1.18        | 1.23     |
| 9   | A2    | 4249 | UR3  | C6-N1   | 2.68  | 1.44        | 1.38     |
| 9   | A2    | 3525 | OMC  | O2-C2   | -2.68 | 1.18        | 1.23     |
| 9   | A2    | 373  | OMG  | C5-N7   | -2.67 | 1.33        | 1.39     |
| 9   | A2    | 3379 | A2M  | O4'-C4' | 2.67  | 1.50        | 1.45     |
| 9   | A2    | 4202 | G7M  | O6-C6   | -2.67 | 1.18        | 1.23     |
| 9   | A2    | 1269 | B8Q  | C6-N1   | 2.67  | 1.44        | 1.38     |
| 46  | m2    | 27   | A2M  | O4'-C4' | 2.67  | 1.50        | 1.45     |
| 9   | A2    | 2277 | G7M  | O6-C6   | -2.66 | 1.18        | 1.23     |
| 9   | A2    | 3481 | A2M  | O4'-C4' | 2.66  | 1.50        | 1.45     |
| 9   | A2    | 237  | B9B  | O3'-C3' | -2.66 | 1.36        | 1.43     |
| 9   | A2    | 1347 | A2M  | O4'-C4' | 2.66  | 1.50        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 4515 | OMG  | C5-N7   | -2.65 | 1.33        | 1.39     |
| 9   | A2    | 3438 | 5MC  | O2-C2   | -2.65 | 1.18        | 1.23     |
| 9   | A2    | 4188 | OMC  | O2-C2   | -2.64 | 1.18        | 1.23     |
| 9   | A2    | 3565 | OMC  | O2-C2   | -2.64 | 1.18        | 1.23     |
| 9   | A2    | 1673 | A2M  | O3'-C3' | 2.64  | 1.49        | 1.43     |
| 79  | m     | 714  | DDE  | OAG-CBI | -2.64 | 1.19        | 1.23     |
| 9   | A2    | 3987 | 5MC  | O2-C2   | -2.64 | 1.18        | 1.23     |
| 9   | A2    | 4289 | OMG  | C5-N7   | -2.63 | 1.33        | 1.39     |
| 9   | A2    | 3357 | OMC  | O2-C2   | -2.63 | 1.18        | 1.23     |
| 9   | A2    | 3543 | OMC  | O2-C2   | -2.63 | 1.18        | 1.23     |
| 9   | A2    | 3837 | B8W  | O2'-C2' | 2.62  | 1.49        | 1.43     |
| 9   | A2    | 1140 | A2M  | O4'-C4' | 2.61  | 1.50        | 1.45     |
| 9   | A2    | 1418 | G7M  | O6-C6   | -2.61 | 1.18        | 1.23     |
| 46  | m2    | 519  | OMC  | O2-C2   | -2.61 | 1.18        | 1.23     |
| 9   | A2    | 1685 | OMG  | O6-C6   | -2.60 | 1.18        | 1.23     |
| 9   | A2    | 3441 | A2M  | O4'-C4' | 2.60  | 1.50        | 1.45     |
| 9   | A2    | 1387 | B9B  | C5-N7   | -2.60 | 1.34        | 1.39     |
| 9   | A2    | 4007 | E6G  | C5-N7   | -2.59 | 1.34        | 1.39     |
| 9   | A2    | 2052 | E7G  | O6-C6   | -2.58 | 1.18        | 1.23     |
| 9   | A2    | 4146 | OMG  | O6-C6   | -2.57 | 1.18        | 1.23     |
| 9   | A2    | 1852 | OMG  | O6-C6   | -2.57 | 1.18        | 1.23     |
| 9   | A2    | 3872 | 6MZ  | C5-N7   | -2.57 | 1.34        | 1.39     |
| 9   | A2    | 4099 | 5MC  | O2-C2   | -2.56 | 1.18        | 1.23     |
| 9   | A2    | 1599 | E7G  | O6-C6   | -2.56 | 1.18        | 1.23     |
| 9   | A2    | 3565 | OMC  | C5-C4   | 2.56  | 1.48        | 1.42     |
| 9   | A2    | 3543 | OMC  | C5-C4   | 2.55  | 1.48        | 1.42     |
| 9   | A2    | 4094 | PSU  | O4'-C1' | -2.55 | 1.40        | 1.43     |
| 9   | A2    | 4515 | OMG  | O6-C6   | -2.54 | 1.18        | 1.23     |
| 9   | A2    | 4275 | OMG  | O6-C6   | -2.53 | 1.18        | 1.23     |
| 9   | A2    | 4067 | 1MA  | C5-N7   | -2.53 | 1.34        | 1.39     |
| 46  | m2    | 670  | A2M  | O4'-C4' | 2.53  | 1.50        | 1.45     |
| 9   | A2    | 2179 | OMG  | O6-C6   | -2.52 | 1.18        | 1.23     |
| 9   | A2    | 2119 | OMG  | O6-C6   | -2.52 | 1.18        | 1.23     |
| 9   | A2    | 373  | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 9   | A2    | 878  | 2MG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 9   | A2    | 1335 | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 9   | A2    | 2528 | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 9   | A2    | 3448 | OMG  | O6-C6   | -2.51 | 1.18        | 1.23     |
| 9   | A2    | 373  | OMG  | C6-N1   | 2.50  | 1.43        | 1.38     |
| 9   | A2    | 3848 | OMG  | C6-N1   | 2.49  | 1.43        | 1.38     |
| 9   | A2    | 2119 | OMG  | C6-N1   | 2.49  | 1.43        | 1.38     |
| 9   | A2    | 1335 | OMG  | C5-C6   | 2.49  | 1.53        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 2179 | OMG  | C5-C6   | 2.49  | 1.53        | 1.44     |
| 46  | m2    | 646  | OMG  | C5-C6   | 2.49  | 1.53        | 1.44     |
| 9   | A2    | 1438 | OMG  | O6-C6   | -2.49 | 1.18        | 1.23     |
| 9   | A2    | 4022 | OMG  | O6-C6   | -2.49 | 1.18        | 1.23     |
| 9   | A2    | 1337 | A2M  | O4'-C4' | 2.49  | 1.50        | 1.45     |
| 11  | C2    | 14   | OMU  | C5-C4   | 2.49  | 1.49        | 1.43     |
| 9   | A2    | 3420 | PSU  | C1'-C5  | 2.48  | 1.55        | 1.50     |
| 9   | A2    | 1330 | 2MG  | C5-C6   | 2.48  | 1.53        | 1.44     |
| 46  | m2    | 646  | OMG  | O6-C6   | -2.48 | 1.18        | 1.23     |
| 9   | A2    | 2541 | B9H  | C6-N1   | 2.47  | 1.44        | 1.38     |
| 9   | A2    | 4275 | OMG  | C5-C6   | 2.47  | 1.53        | 1.44     |
| 46  | m2    | 685  | OMG  | C5-C6   | 2.47  | 1.53        | 1.44     |
| 9   | A2    | 1335 | OMG  | C6-N1   | 2.47  | 1.43        | 1.38     |
| 46  | m2    | 685  | OMG  | C6-N1   | 2.47  | 1.43        | 1.38     |
| 9   | A2    | 2179 | OMG  | C6-N1   | 2.46  | 1.43        | 1.38     |
| 9   | A2    | 1330 | 2MG  | O6-C6   | -2.46 | 1.18        | 1.23     |
| 9   | A2    | 3848 | OMG  | C5-C6   | 2.46  | 1.53        | 1.44     |
| 46  | m2    | 519  | OMC  | C5-C4   | 2.46  | 1.48        | 1.42     |
| 9   | A2    | 2119 | OMG  | C5-C6   | 2.46  | 1.53        | 1.44     |
| 9   | A2    | 3357 | OMC  | C5-C4   | 2.46  | 1.48        | 1.42     |
| 9   | A2    | 3848 | OMG  | O6-C6   | -2.46 | 1.18        | 1.23     |
| 9   | A2    | 4515 | OMG  | C6-N1   | 2.46  | 1.43        | 1.38     |
| 9   | A2    | 1418 | G7M  | C4-N9   | 2.45  | 1.44        | 1.38     |
| 9   | A2    | 4275 | OMG  | C6-N1   | 2.45  | 1.43        | 1.38     |
| 9   | A2    | 2277 | G7M  | C4-N9   | 2.45  | 1.44        | 1.38     |
| 9   | A2    | 1852 | OMG  | C6-N1   | 2.45  | 1.43        | 1.38     |
| 9   | A2    | 4022 | OMG  | C5-C6   | 2.44  | 1.53        | 1.44     |
| 9   | A2    | 1852 | OMG  | C5-C6   | 2.44  | 1.53        | 1.44     |
| 9   | A2    | 373  | OMG  | C5-C6   | 2.44  | 1.53        | 1.44     |
| 46  | m2    | 824  | PSU  | C1'-C5  | 2.44  | 1.55        | 1.50     |
| 9   | A2    | 1685 | OMG  | C6-N1   | 2.43  | 1.43        | 1.38     |
| 9   | A2    | 4517 | 2MG  | C5-C6   | 2.43  | 1.53        | 1.44     |
| 9   | A2    | 4517 | 2MG  | O6-C6   | -2.43 | 1.18        | 1.23     |
| 9   | A2    | 4188 | OMC  | C5-C4   | 2.43  | 1.48        | 1.42     |
| 9   | A2    | 2528 | OMG  | C6-N1   | 2.43  | 1.43        | 1.38     |
| 9   | A2    | 4022 | OMG  | C6-N1   | 2.43  | 1.43        | 1.38     |
| 9   | A2    | 878  | 2MG  | C5-C6   | 2.43  | 1.53        | 1.44     |
| 9   | A2    | 1438 | OMG  | C5-C6   | 2.43  | 1.53        | 1.44     |
| 9   | A2    | 4272 | OMU  | O2-C2   | -2.43 | 1.18        | 1.23     |
| 9   | A2    | 4146 | OMG  | C5-C6   | 2.42  | 1.53        | 1.44     |
| 46  | m2    | 685  | OMG  | O6-C6   | -2.42 | 1.19        | 1.23     |
| 46  | m2    | 1832 | UR3  | O2-C2   | -2.42 | 1.18        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 3525 | OMC  | C5-C4   | 2.42  | 1.48        | 1.42     |
| 9   | A2    | 3846 | I4U  | C3'-C4' | 2.42  | 1.59        | 1.53     |
| 9   | A2    | 1418 | G7M  | C5-C4   | 2.42  | 1.44        | 1.38     |
| 9   | A2    | 2559 | OMC  | C5-C4   | 2.42  | 1.48        | 1.42     |
| 9   | A2    | 2528 | OMG  | C5-C6   | 2.41  | 1.53        | 1.44     |
| 9   | A2    | 3448 | OMG  | C5-C6   | 2.41  | 1.53        | 1.44     |
| 9   | A2    | 2177 | OMC  | C5-C4   | 2.41  | 1.48        | 1.42     |
| 9   | A2    | 2616 | OMC  | C5-C4   | 2.41  | 1.48        | 1.42     |
| 9   | A2    | 4023 | MHG  | C5-C4   | 2.41  | 1.45        | 1.37     |
| 9   | A2    | 3371 | PSU  | C1'-C5  | 2.41  | 1.55        | 1.50     |
| 9   | A2    | 4094 | PSU  | C1'-C5  | 2.41  | 1.55        | 1.50     |
| 9   | A2    | 3958 | OMU  | O2-C2   | -2.40 | 1.18        | 1.23     |
| 46  | m2    | 646  | OMG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 9   | A2    | 4289 | OMG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 9   | A2    | 4146 | OMG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 9   | A2    | 1685 | OMG  | C5-C6   | 2.39  | 1.53        | 1.44     |
| 9   | A2    | 3448 | OMG  | C6-N1   | 2.39  | 1.43        | 1.38     |
| 11  | C2    | 14   | OMU  | O2-C2   | -2.39 | 1.18        | 1.23     |
| 9   | A2    | 2277 | G7M  | C5-C4   | 2.39  | 1.44        | 1.38     |
| 46  | m2    | 1250 | B8N  | C4-C5   | -2.39 | 1.42        | 1.47     |
| 9   | A2    | 2263 | PSU  | C1'-C5  | 2.38  | 1.55        | 1.50     |
| 9   | A2    | 1438 | OMG  | C6-N1   | 2.38  | 1.43        | 1.38     |
| 9   | A2    | 1330 | 2MG  | C6-N1   | 2.38  | 1.43        | 1.38     |
| 9   | A2    | 1668 | UR3  | O2-C2   | -2.37 | 1.18        | 1.22     |
| 9   | A2    | 4515 | OMG  | C5-C6   | 2.37  | 1.53        | 1.44     |
| 9   | A2    | 4202 | G7M  | C5-C4   | 2.36  | 1.44        | 1.38     |
| 9   | A2    | 3441 | A2M  | C5-C4   | -2.36 | 1.34        | 1.39     |
| 9   | A2    | 4249 | UR3  | O2-C2   | -2.35 | 1.18        | 1.22     |
| 46  | m2    | 116  | OMU  | O2-C2   | -2.35 | 1.18        | 1.23     |
| 9   | A2    | 1472 | I4U  | C5-C4   | 2.35  | 1.49        | 1.43     |
| 9   | A2    | 3846 | I4U  | C5-C4   | 2.34  | 1.49        | 1.43     |
| 46  | m2    | 1245 | PSU  | C1'-C5  | 2.34  | 1.55        | 1.50     |
| 9   | A2    | 4202 | G7M  | C4-N9   | 2.33  | 1.44        | 1.38     |
| 9   | A2    | 3872 | 6MZ  | C8-N9   | -2.32 | 1.33        | 1.37     |
| 9   | A2    | 4517 | 2MG  | C6-N1   | 2.31  | 1.43        | 1.38     |
| 9   | A2    | 3958 | OMU  | C5-C4   | 2.30  | 1.48        | 1.43     |
| 46  | m2    | 116  | OMU  | C5-C4   | 2.29  | 1.48        | 1.43     |
| 9   | A2    | 4280 | PSU  | C1'-C5  | 2.29  | 1.55        | 1.50     |
| 46  | m2    | 614  | PSU  | C1'-C5  | 2.29  | 1.55        | 1.50     |
| 9   | A2    | 4023 | MHG  | O6-C6   | -2.29 | 1.19        | 1.23     |
| 9   | A2    | 1395 | PSU  | C1'-C5  | 2.28  | 1.55        | 1.50     |
| 9   | A2    | 3385 | PSU  | C1'-C5  | 2.26  | 1.55        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 1673 | A2M  | C5-C4   | -2.26 | 1.35        | 1.39     |
| 9   | A2    | 4055 | PSU  | C1'-C5  | 2.26  | 1.55        | 1.50     |
| 9   | A2    | 878  | 2MG  | C6-N1   | 2.26  | 1.43        | 1.38     |
| 9   | A2    | 1387 | B9B  | C8-N9   | -2.25 | 1.33        | 1.37     |
| 9   | A2    | 373  | OMG  | C4-N9   | -2.25 | 1.32        | 1.38     |
| 9   | A2    | 4288 | PSU  | C1'-C5  | 2.24  | 1.55        | 1.50     |
| 9   | A2    | 237  | B9B  | C8-N9   | -2.24 | 1.33        | 1.37     |
| 9   | A2    | 3837 | B8W  | C1'-N9  | -2.23 | 1.40        | 1.46     |
| 46  | m2    | 1083 | PSU  | C1'-C5  | 2.22  | 1.55        | 1.50     |
| 9   | A2    | 2119 | OMG  | C4-N9   | -2.22 | 1.32        | 1.38     |
| 9   | A2    | 1347 | A2M  | C5-C4   | -2.21 | 1.35        | 1.39     |
| 9   | A2    | 1490 | PSU  | C1'-C5  | 2.21  | 1.55        | 1.50     |
| 9   | A2    | 1472 | I4U  | C3'-C4' | 2.21  | 1.58        | 1.53     |
| 9   | A2    | 3523 | A2M  | C5-C4   | -2.20 | 1.35        | 1.39     |
| 46  | m2    | 825  | PSU  | C1'-C5  | 2.20  | 1.55        | 1.50     |
| 9   | A2    | 1496 | PSU  | C1'-C5  | 2.20  | 1.55        | 1.50     |
| 9   | A2    | 1337 | A2M  | C5-C4   | -2.19 | 1.35        | 1.39     |
| 9   | A2    | 2156 | A2M  | C5-C4   | -2.19 | 1.35        | 1.39     |
| 79  | m     | 714  | DDE  | CD2-NE2 | -2.19 | 1.31        | 1.36     |
| 9   | A2    | 4152 | PSU  | C1'-C5  | 2.19  | 1.55        | 1.50     |
| 9   | A2    | 4183 | PSU  | C1'-C5  | 2.19  | 1.55        | 1.50     |
| 9   | A2    | 2118 | A2M  | C5-C4   | -2.19 | 1.35        | 1.39     |
| 9   | A2    | 2120 | OMC  | C5-C4   | 2.18  | 1.48        | 1.42     |
| 9   | A2    | 4272 | OMU  | C5-C4   | 2.18  | 1.48        | 1.43     |
| 9   | A2    | 3481 | A2M  | C5-C4   | -2.18 | 1.35        | 1.39     |
| 9   | A2    | 4223 | A2M  | C5-C4   | -2.18 | 1.35        | 1.39     |
| 9   | A2    | 1140 | A2M  | C5-C4   | -2.18 | 1.35        | 1.39     |
| 46  | m2    | 685  | OMG  | C4-N9   | -2.16 | 1.32        | 1.38     |
| 46  | m2    | 670  | A2M  | C5-C4   | -2.14 | 1.35        | 1.39     |
| 9   | A2    | 4289 | OMG  | O6-C6   | -2.14 | 1.19        | 1.23     |
| 9   | A2    | 3945 | PSU  | C1'-C5  | 2.14  | 1.55        | 1.50     |
| 46  | m2    | 1832 | UR3  | C4-N3   | 2.14  | 1.44        | 1.40     |
| 9   | A2    | 398  | A2M  | C5-C4   | -2.14 | 1.35        | 1.39     |
| 46  | m2    | 1033 | A2M  | C5-C4   | -2.14 | 1.35        | 1.39     |
| 46  | m2    | 1250 | B8N  | C1'-C5  | 2.13  | 1.55        | 1.50     |
| 46  | m2    | 27   | A2M  | C5-C4   | -2.13 | 1.35        | 1.39     |
| 46  | m2    | 1250 | B8N  | O4'-C1' | -2.12 | 1.40        | 1.43     |
| 9   | A2    | 4007 | E6G  | C8-N9   | -2.12 | 1.33        | 1.37     |
| 46  | m2    | 166  | A2M  | C5-C4   | -2.12 | 1.35        | 1.39     |
| 9   | A2    | 2052 | E7G  | C5-C4   | 2.11  | 1.44        | 1.37     |
| 9   | A2    | 1685 | OMG  | C4-N9   | -2.11 | 1.32        | 1.38     |
| 9   | A2    | 3379 | A2M  | C5-C4   | -2.11 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A2    | 1335 | OMG  | C4-N9   | -2.11 | 1.32        | 1.38     |
| 9   | A2    | 4022 | OMG  | C4-N9   | -2.10 | 1.32        | 1.38     |
| 9   | A2    | 1599 | E7G  | C5-C4   | 2.10  | 1.44        | 1.37     |
| 9   | A2    | 4275 | OMG  | C4-N9   | -2.10 | 1.32        | 1.38     |
| 9   | A2    | 4249 | UR3  | C4-N3   | 2.09  | 1.44        | 1.40     |
| 9   | A2    | 1852 | OMG  | C4-N9   | -2.09 | 1.32        | 1.38     |
| 9   | A2    | 3374 | A2M  | C5-C4   | -2.08 | 1.35        | 1.39     |
| 9   | A2    | 3848 | OMG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 9   | A2    | 3448 | OMG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 9   | A2    | 1668 | UR3  | C4-N3   | 2.06  | 1.44        | 1.40     |
| 9   | A2    | 237  | B9B  | C5-C6   | -2.05 | 1.37        | 1.41     |
| 9   | A2    | 4102 | PSU  | C1'-C5  | 2.04  | 1.54        | 1.50     |
| 9   | A2    | 1330 | 2MG  | C4-N9   | -2.03 | 1.32        | 1.38     |
| 9   | A2    | 4146 | OMG  | C4-N9   | -2.03 | 1.32        | 1.38     |
| 79  | m     | 714  | DDE  | CAT-CE1 | 2.03  | 1.53        | 1.49     |
| 9   | A2    | 4152 | PSU  | O4-C4   | -2.02 | 1.19        | 1.23     |
| 9   | A2    | 4288 | PSU  | O4-C4   | -2.01 | 1.19        | 1.23     |
| 9   | A2    | 1395 | PSU  | O4-C4   | -2.01 | 1.19        | 1.23     |
| 9   | A2    | 4517 | 2MG  | C4-N9   | -2.01 | 1.32        | 1.38     |
| 9   | A2    | 4067 | 1MA  | C6-N6   | -2.01 | 1.23        | 1.28     |

All (686) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 9   | A2    | 3837 | B8W  | N2-C2-N3 | 8.58 | 130.08      | 117.22   |
| 9   | A2    | 3837 | B8W  | O6-C6-N1 | 8.28 | 129.96      | 118.96   |
| 9   | A2    | 4183 | PSU  | N1-C2-N3 | 8.07 | 123.68      | 115.17   |
| 9   | A2    | 4152 | PSU  | N1-C2-N3 | 7.93 | 123.53      | 115.17   |
| 9   | A2    | 4023 | MHG  | C2-N3-C4 | 7.92 | 121.90      | 112.00   |
| 9   | A2    | 1496 | PSU  | N1-C2-N3 | 7.90 | 123.50      | 115.17   |
| 9   | A2    | 4055 | PSU  | N1-C2-N3 | 7.85 | 123.45      | 115.17   |
| 46  | m2    | 825  | PSU  | N1-C2-N3 | 7.83 | 123.43      | 115.17   |
| 9   | A2    | 3385 | PSU  | N1-C2-N3 | 7.82 | 123.42      | 115.17   |
| 9   | A2    | 4094 | PSU  | N1-C2-N3 | 7.82 | 123.42      | 115.17   |
| 46  | m2    | 1083 | PSU  | N1-C2-N3 | 7.80 | 123.39      | 115.17   |
| 9   | A2    | 3945 | PSU  | N1-C2-N3 | 7.79 | 123.39      | 115.17   |
| 9   | A2    | 4280 | PSU  | N1-C2-N3 | 7.77 | 123.36      | 115.17   |
| 9   | A2    | 1490 | PSU  | N1-C2-N3 | 7.77 | 123.36      | 115.17   |
| 9   | A2    | 4102 | PSU  | N1-C2-N3 | 7.73 | 123.32      | 115.17   |
| 9   | A2    | 4288 | PSU  | N1-C2-N3 | 7.72 | 123.31      | 115.17   |
| 9   | A2    | 2263 | PSU  | N1-C2-N3 | 7.70 | 123.29      | 115.17   |
| 46  | m2    | 614  | PSU  | N1-C2-N3 | 7.70 | 123.29      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 46  | m2    | 1245 | PSU  | N1-C2-N3 | 7.68  | 123.27      | 115.17   |
| 9   | A2    | 3371 | PSU  | N1-C2-N3 | 7.66  | 123.25      | 115.17   |
| 9   | A2    | 1395 | PSU  | N1-C2-N3 | 7.64  | 123.23      | 115.17   |
| 9   | A2    | 3420 | PSU  | N1-C2-N3 | 7.63  | 123.21      | 115.17   |
| 9   | A2    | 237  | B9B  | C5-C4-N3 | -7.38 | 119.40      | 127.18   |
| 9   | A2    | 1472 | I4U  | O4-C4-C5 | 7.37  | 120.68      | 115.45   |
| 9   | A2    | 3837 | B8W  | C5-C4-N3 | -7.18 | 119.61      | 127.18   |
| 46  | m2    | 824  | PSU  | N1-C2-N3 | 7.13  | 122.69      | 115.17   |
| 9   | A2    | 4007 | E6G  | C5-C4-N3 | -6.91 | 119.90      | 127.18   |
| 9   | A2    | 1387 | B9B  | C5-C4-N3 | -6.89 | 119.92      | 127.18   |
| 9   | A2    | 4023 | MHG  | C4-C5-N7 | 6.89  | 110.52      | 104.94   |
| 9   | A2    | 1496 | PSU  | C4-N3-C2 | -6.60 | 117.28      | 126.37   |
| 9   | A2    | 4152 | PSU  | C4-N3-C2 | -6.56 | 117.33      | 126.37   |
| 9   | A2    | 1490 | PSU  | C4-N3-C2 | -6.55 | 117.34      | 126.37   |
| 46  | m2    | 825  | PSU  | C4-N3-C2 | -6.52 | 117.39      | 126.37   |
| 9   | A2    | 4055 | PSU  | C4-N3-C2 | -6.51 | 117.40      | 126.37   |
| 46  | m2    | 824  | PSU  | O2-C2-N1 | -6.51 | 116.08      | 122.79   |
| 9   | A2    | 3945 | PSU  | C4-N3-C2 | -6.49 | 117.43      | 126.37   |
| 9   | A2    | 4183 | PSU  | C4-N3-C2 | -6.47 | 117.46      | 126.37   |
| 9   | A2    | 4288 | PSU  | C4-N3-C2 | -6.47 | 117.46      | 126.37   |
| 9   | A2    | 4102 | PSU  | C4-N3-C2 | -6.46 | 117.47      | 126.37   |
| 9   | A2    | 878  | 2MG  | C2-N3-C4 | 6.46  | 120.08      | 112.00   |
| 46  | m2    | 1083 | PSU  | C4-N3-C2 | -6.45 | 117.49      | 126.37   |
| 9   | A2    | 1330 | 2MG  | C2-N3-C4 | 6.41  | 120.01      | 112.00   |
| 9   | A2    | 3385 | PSU  | C4-N3-C2 | -6.40 | 117.56      | 126.37   |
| 9   | A2    | 4280 | PSU  | C4-N3-C2 | -6.39 | 117.58      | 126.37   |
| 9   | A2    | 2052 | E7G  | C4-C5-N7 | 6.36  | 110.10      | 104.94   |
| 9   | A2    | 1395 | PSU  | C4-N3-C2 | -6.32 | 117.67      | 126.37   |
| 9   | A2    | 2263 | PSU  | C4-N3-C2 | -6.32 | 117.67      | 126.37   |
| 9   | A2    | 4094 | PSU  | C4-N3-C2 | -6.29 | 117.70      | 126.37   |
| 9   | A2    | 1599 | E7G  | C4-C5-N7 | 6.28  | 110.03      | 104.94   |
| 9   | A2    | 3846 | I4U  | O4-C4-C5 | 6.25  | 119.89      | 115.45   |
| 9   | A2    | 4517 | 2MG  | C2-N3-C4 | 6.20  | 119.76      | 112.00   |
| 46  | m2    | 1245 | PSU  | C4-N3-C2 | -6.17 | 117.87      | 126.37   |
| 9   | A2    | 3371 | PSU  | C4-N3-C2 | -6.16 | 117.88      | 126.37   |
| 46  | m2    | 824  | PSU  | C4-N3-C2 | -6.16 | 117.88      | 126.37   |
| 46  | m2    | 614  | PSU  | C4-N3-C2 | -6.16 | 117.89      | 126.37   |
| 9   | A2    | 3420 | PSU  | C4-N3-C2 | -6.01 | 118.10      | 126.37   |
| 9   | A2    | 4183 | PSU  | C6-N1-C2 | -5.88 | 117.23      | 122.69   |
| 46  | m2    | 1250 | B8N  | C4-N3-C2 | -5.88 | 118.39      | 125.62   |
| 9   | A2    | 3420 | PSU  | C6-N1-C2 | -5.84 | 117.27      | 122.69   |
| 9   | A2    | 3837 | B8W  | O6-C6-C5 | -5.84 | 110.13      | 117.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | A2    | 3371 | PSU  | C6-N1-C2 | -5.83 | 117.28      | 122.69   |
| 9   | A2    | 4094 | PSU  | C6-N1-C2 | -5.82 | 117.29      | 122.69   |
| 46  | m2    | 614  | PSU  | C6-N1-C2 | -5.77 | 117.33      | 122.69   |
| 46  | m2    | 1245 | PSU  | C6-N1-C2 | -5.76 | 117.34      | 122.69   |
| 46  | m2    | 166  | A2M  | N3-C2-N1 | -5.70 | 119.95      | 128.58   |
| 11  | C2    | 14   | OMU  | C4-N3-C2 | -5.70 | 119.54      | 126.61   |
| 9   | A2    | 3441 | A2M  | N3-C2-N1 | -5.69 | 119.97      | 128.58   |
| 9   | A2    | 1140 | A2M  | N3-C2-N1 | -5.67 | 120.00      | 128.58   |
| 9   | A2    | 4223 | A2M  | N3-C2-N1 | -5.67 | 120.00      | 128.58   |
| 9   | A2    | 4280 | PSU  | C6-N1-C2 | -5.66 | 117.43      | 122.69   |
| 9   | A2    | 1673 | A2M  | N3-C2-N1 | -5.66 | 120.01      | 128.58   |
| 9   | A2    | 2156 | A2M  | N3-C2-N1 | -5.66 | 120.01      | 128.58   |
| 9   | A2    | 398  | A2M  | N3-C2-N1 | -5.66 | 120.01      | 128.58   |
| 46  | m2    | 1832 | UR3  | C4-N3-C2 | -5.66 | 120.02      | 124.58   |
| 9   | A2    | 1599 | E7G  | C2-N3-C4 | 5.66  | 122.05      | 112.30   |
| 9   | A2    | 3374 | A2M  | N3-C2-N1 | -5.65 | 120.03      | 128.58   |
| 9   | A2    | 3481 | A2M  | N3-C2-N1 | -5.64 | 120.05      | 128.58   |
| 9   | A2    | 3872 | 6MZ  | N1-C2-N3 | -5.63 | 120.06      | 128.58   |
| 9   | A2    | 1418 | G7M  | C2-N3-C4 | 5.63  | 121.99      | 112.30   |
| 46  | m2    | 27   | A2M  | N3-C2-N1 | -5.62 | 120.08      | 128.58   |
| 9   | A2    | 3385 | PSU  | C6-N1-C2 | -5.61 | 117.48      | 122.69   |
| 9   | A2    | 1337 | A2M  | N3-C2-N1 | -5.61 | 120.10      | 128.58   |
| 9   | A2    | 2277 | G7M  | C2-N3-C4 | 5.60  | 121.95      | 112.30   |
| 9   | A2    | 3958 | OMU  | C4-N3-C2 | -5.59 | 119.68      | 126.61   |
| 46  | m2    | 1033 | A2M  | N3-C2-N1 | -5.58 | 120.14      | 128.58   |
| 9   | A2    | 3379 | A2M  | N3-C2-N1 | -5.57 | 120.16      | 128.58   |
| 9   | A2    | 3945 | PSU  | C6-N1-C2 | -5.56 | 117.53      | 122.69   |
| 9   | A2    | 1347 | A2M  | N3-C2-N1 | -5.56 | 120.16      | 128.58   |
| 9   | A2    | 4202 | G7M  | C2-N3-C4 | 5.56  | 121.88      | 112.30   |
| 9   | A2    | 4152 | PSU  | C6-N1-C2 | -5.55 | 117.54      | 122.69   |
| 9   | A2    | 3441 | A2M  | N9-C8-N7 | -5.54 | 106.08      | 113.94   |
| 46  | m2    | 825  | PSU  | C6-N1-C2 | -5.52 | 117.57      | 122.69   |
| 9   | A2    | 4055 | PSU  | C6-N1-C2 | -5.52 | 117.57      | 122.69   |
| 9   | A2    | 2263 | PSU  | C6-N1-C2 | -5.52 | 117.57      | 122.69   |
| 9   | A2    | 1395 | PSU  | C6-N1-C2 | -5.51 | 117.58      | 122.69   |
| 9   | A2    | 1496 | PSU  | C6-N1-C2 | -5.49 | 117.59      | 122.69   |
| 9   | A2    | 2052 | E7G  | C2-N3-C4 | 5.48  | 121.74      | 112.30   |
| 9   | A2    | 4102 | PSU  | C6-N1-C2 | -5.48 | 117.61      | 122.69   |
| 9   | A2    | 4288 | PSU  | C6-N1-C2 | -5.47 | 117.61      | 122.69   |
| 46  | m2    | 670  | A2M  | N3-C2-N1 | -5.46 | 120.32      | 128.58   |
| 46  | m2    | 1083 | PSU  | C6-N1-C2 | -5.46 | 117.62      | 122.69   |
| 9   | A2    | 2118 | A2M  | N3-C2-N1 | -5.41 | 120.39      | 128.58   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | A2    | 1490 | PSU  | C6-N1-C2 | -5.40 | 117.68      | 122.69   |
| 9   | A2    | 3481 | A2M  | N9-C8-N7 | -5.38 | 106.30      | 113.94   |
| 9   | A2    | 1140 | A2M  | N9-C8-N7 | -5.37 | 106.32      | 113.94   |
| 9   | A2    | 1673 | A2M  | N9-C8-N7 | -5.35 | 106.34      | 113.94   |
| 9   | A2    | 398  | A2M  | N9-C8-N7 | -5.33 | 106.38      | 113.94   |
| 9   | A2    | 3523 | A2M  | N3-C2-N1 | -5.33 | 120.52      | 128.58   |
| 9   | A2    | 1668 | UR3  | C4-N3-C2 | -5.31 | 120.30      | 124.58   |
| 9   | A2    | 4223 | A2M  | N9-C8-N7 | -5.31 | 106.40      | 113.94   |
| 9   | A2    | 878  | 2MG  | C5-C4-N3 | -5.30 | 119.95      | 128.39   |
| 9   | A2    | 4067 | 1MA  | N1-C2-N3 | -5.29 | 119.71      | 126.00   |
| 9   | A2    | 3523 | A2M  | N9-C8-N7 | -5.27 | 106.46      | 113.94   |
| 9   | A2    | 2156 | A2M  | N9-C8-N7 | -5.26 | 106.47      | 113.94   |
| 46  | m2    | 27   | A2M  | N9-C8-N7 | -5.25 | 106.48      | 113.94   |
| 9   | A2    | 2118 | A2M  | N9-C8-N7 | -5.24 | 106.50      | 113.94   |
| 46  | m2    | 670  | A2M  | N9-C8-N7 | -5.23 | 106.51      | 113.94   |
| 9   | A2    | 4249 | UR3  | C4-N3-C2 | -5.23 | 120.37      | 124.58   |
| 9   | A2    | 1337 | A2M  | N9-C8-N7 | -5.21 | 106.55      | 113.94   |
| 46  | m2    | 824  | PSU  | C6-N1-C2 | -5.20 | 117.86      | 122.69   |
| 9   | A2    | 3379 | A2M  | N9-C8-N7 | -5.20 | 106.56      | 113.94   |
| 9   | A2    | 1347 | A2M  | N9-C8-N7 | -5.20 | 106.56      | 113.94   |
| 46  | m2    | 116  | OMU  | C4-N3-C2 | -5.17 | 120.20      | 126.61   |
| 9   | A2    | 1438 | OMG  | C5-C4-N3 | -5.16 | 120.18      | 128.39   |
| 46  | m2    | 1033 | A2M  | N9-C8-N7 | -5.14 | 106.64      | 113.94   |
| 46  | m2    | 166  | A2M  | N9-C8-N7 | -5.14 | 106.64      | 113.94   |
| 9   | A2    | 3374 | A2M  | N9-C8-N7 | -5.14 | 106.64      | 113.94   |
| 9   | A2    | 4517 | 2MG  | C5-C4-N3 | -5.13 | 120.23      | 128.39   |
| 9   | A2    | 3448 | OMG  | C5-C4-N3 | -5.10 | 120.27      | 128.39   |
| 9   | A2    | 237  | B9B  | C4-C5-C6 | 5.09  | 120.22      | 115.22   |
| 46  | m2    | 1250 | B8N  | C5-C4-N3 | 5.09  | 125.39      | 116.15   |
| 9   | A2    | 4272 | OMU  | C4-N3-C2 | -5.08 | 120.31      | 126.61   |
| 9   | A2    | 2528 | OMG  | C5-C4-N3 | -5.06 | 120.33      | 128.39   |
| 9   | A2    | 1330 | 2MG  | C5-C4-N3 | -5.05 | 120.35      | 128.39   |
| 9   | A2    | 3837 | B8W  | N2-C2-N1 | -5.05 | 109.65      | 117.22   |
| 9   | A2    | 4515 | OMG  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 9   | A2    | 4289 | OMG  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 46  | m2    | 646  | OMG  | C5-C4-N3 | -4.98 | 120.46      | 128.39   |
| 9   | A2    | 4146 | OMG  | C5-C4-N3 | -4.90 | 120.59      | 128.39   |
| 9   | A2    | 3536 | P7G  | C4-C5-N7 | 4.90  | 110.01      | 106.71   |
| 9   | A2    | 1852 | OMG  | C5-C4-N3 | -4.90 | 120.59      | 128.39   |
| 9   | A2    | 2179 | OMG  | C5-C4-N3 | -4.88 | 120.62      | 128.39   |
| 9   | A2    | 4275 | OMG  | C5-C4-N3 | -4.86 | 120.66      | 128.39   |
| 9   | A2    | 3837 | B8W  | C4-C5-C6 | 4.86  | 119.99      | 115.22   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | A2    | 1685 | OMG  | C5-C4-N3  | -4.85 | 120.67      | 128.39   |
| 9   | A2    | 4022 | OMG  | C5-C4-N3  | -4.84 | 120.68      | 128.39   |
| 9   | A2    | 1335 | OMG  | C5-C4-N3  | -4.84 | 120.69      | 128.39   |
| 9   | A2    | 3872 | 6MZ  | C5-C4-N3  | -4.83 | 120.07      | 126.72   |
| 46  | m2    | 1250 | B8N  | C1'-C5-C4 | 4.82  | 124.92      | 117.61   |
| 9   | A2    | 4067 | 1MA  | C2-N3-C4  | 4.82  | 121.98      | 112.53   |
| 9   | A2    | 3848 | OMG  | C5-C4-N3  | -4.81 | 120.73      | 128.39   |
| 9   | A2    | 1337 | A2M  | C5-C4-N3  | -4.81 | 120.09      | 126.72   |
| 9   | A2    | 4023 | MHG  | C2-N1-C6  | -4.80 | 118.75      | 124.55   |
| 46  | m2    | 685  | OMG  | C5-C4-N3  | -4.77 | 120.80      | 128.39   |
| 9   | A2    | 3374 | A2M  | C5-C4-N3  | -4.76 | 120.16      | 126.72   |
| 9   | A2    | 4102 | PSU  | C6-C5-C4  | 4.74  | 121.37      | 118.17   |
| 9   | A2    | 2118 | A2M  | C5-C4-N3  | -4.72 | 120.21      | 126.72   |
| 46  | m2    | 166  | A2M  | C5-C4-N3  | -4.71 | 120.23      | 126.72   |
| 9   | A2    | 3441 | A2M  | C4-N9-C8  | 4.70  | 110.67      | 105.74   |
| 9   | A2    | 2119 | OMG  | C5-C4-N3  | -4.69 | 120.93      | 128.39   |
| 46  | m2    | 1033 | A2M  | C5-C4-N3  | -4.68 | 120.27      | 126.72   |
| 9   | A2    | 4152 | PSU  | C6-C5-C4  | 4.67  | 121.32      | 118.17   |
| 46  | m2    | 670  | A2M  | C5-C4-N3  | -4.65 | 120.31      | 126.72   |
| 9   | A2    | 2156 | A2M  | C5-C4-N3  | -4.64 | 120.32      | 126.72   |
| 9   | A2    | 1347 | A2M  | C5-C4-N3  | -4.64 | 120.33      | 126.72   |
| 9   | A2    | 4007 | E6G  | C4-C5-C6  | 4.63  | 119.77      | 115.22   |
| 9   | A2    | 1673 | A2M  | C5-C4-N3  | -4.62 | 120.35      | 126.72   |
| 9   | A2    | 1490 | PSU  | C6-C5-C4  | 4.62  | 121.29      | 118.17   |
| 9   | A2    | 3379 | A2M  | C5-C4-N3  | -4.60 | 120.39      | 126.72   |
| 9   | A2    | 4183 | PSU  | C6-C5-C4  | 4.60  | 121.28      | 118.17   |
| 9   | A2    | 2541 | B9H  | C31-N3-C2 | 4.58  | 122.92      | 117.29   |
| 9   | A2    | 1387 | B9B  | C4-C5-C6  | 4.58  | 119.72      | 115.22   |
| 9   | A2    | 3523 | A2M  | C5-C4-N3  | -4.58 | 120.41      | 126.72   |
| 9   | A2    | 3448 | OMG  | C1'-N9-C8 | -4.58 | 113.73      | 126.73   |
| 9   | A2    | 4183 | PSU  | O2-C2-N1  | -4.55 | 118.09      | 122.79   |
| 9   | A2    | 373  | OMG  | C5-C4-N3  | -4.55 | 121.15      | 128.39   |
| 46  | m2    | 614  | PSU  | O2-C2-N1  | -4.55 | 118.10      | 122.79   |
| 9   | A2    | 237  | B9B  | N3-C4-N9  | 4.55  | 132.76      | 126.99   |
| 9   | A2    | 1140 | A2M  | C5-C4-N3  | -4.54 | 120.46      | 126.72   |
| 9   | A2    | 3441 | A2M  | C5-C4-N3  | -4.54 | 120.47      | 126.72   |
| 46  | m2    | 27   | A2M  | C5-C4-N3  | -4.53 | 120.47      | 126.72   |
| 9   | A2    | 398  | A2M  | C5-C4-N3  | -4.53 | 120.48      | 126.72   |
| 46  | m2    | 825  | PSU  | C6-C5-C4  | 4.53  | 121.23      | 118.17   |
| 9   | A2    | 4515 | OMG  | C1'-N9-C8 | -4.53 | 113.87      | 126.73   |
| 9   | A2    | 1496 | PSU  | C6-C5-C4  | 4.52  | 121.23      | 118.17   |
| 9   | A2    | 3385 | PSU  | O2-C2-N1  | -4.52 | 118.13      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | A2    | 3945 | PSU  | C6-C5-C4  | 4.50  | 121.21      | 118.17   |
| 9   | A2    | 4223 | A2M  | C5-C4-N3  | -4.49 | 120.54      | 126.72   |
| 46  | m2    | 1083 | PSU  | C6-C5-C4  | 4.49  | 121.20      | 118.17   |
| 9   | A2    | 4152 | PSU  | O2-C2-N1  | -4.47 | 118.18      | 122.79   |
| 9   | A2    | 4094 | PSU  | O2-C2-N1  | -4.47 | 118.18      | 122.79   |
| 9   | A2    | 2528 | OMG  | C1'-N9-C8 | -4.47 | 114.04      | 126.73   |
| 9   | A2    | 4280 | PSU  | O2-C2-N1  | -4.46 | 118.19      | 122.79   |
| 9   | A2    | 1335 | OMG  | C2-N3-C4  | 4.44  | 119.95      | 112.30   |
| 9   | A2    | 3481 | A2M  | C5-C4-N3  | -4.44 | 120.60      | 126.72   |
| 9   | A2    | 3481 | A2M  | C4-N9-C8  | 4.43  | 110.39      | 105.74   |
| 9   | A2    | 3448 | OMG  | C2-N3-C4  | 4.43  | 119.93      | 112.30   |
| 9   | A2    | 1496 | PSU  | O2-C2-N1  | -4.43 | 118.22      | 122.79   |
| 9   | A2    | 3371 | PSU  | O2-C2-N1  | -4.43 | 118.22      | 122.79   |
| 9   | A2    | 1599 | E7G  | C5-C6-N1  | 4.42  | 118.73      | 110.94   |
| 9   | A2    | 2528 | OMG  | C2-N3-C4  | 4.42  | 119.92      | 112.30   |
| 9   | A2    | 3385 | PSU  | C6-C5-C4  | 4.42  | 121.16      | 118.17   |
| 9   | A2    | 1438 | OMG  | C2-N3-C4  | 4.42  | 119.91      | 112.30   |
| 46  | m2    | 646  | OMG  | C1'-N9-C8 | -4.41 | 114.20      | 126.73   |
| 9   | A2    | 4288 | PSU  | O2-C2-N1  | -4.39 | 118.26      | 122.79   |
| 9   | A2    | 1685 | OMG  | C2-N3-C4  | 4.39  | 119.86      | 112.30   |
| 9   | A2    | 2179 | OMG  | C2-N3-C4  | 4.39  | 119.85      | 112.30   |
| 9   | A2    | 4275 | OMG  | C2-N3-C4  | 4.39  | 119.85      | 112.30   |
| 9   | A2    | 4289 | OMG  | C2-N3-C4  | 4.38  | 119.85      | 112.30   |
| 46  | m2    | 646  | OMG  | C2-N3-C4  | 4.38  | 119.84      | 112.30   |
| 9   | A2    | 1673 | A2M  | C4-N9-C8  | 4.37  | 110.33      | 105.74   |
| 46  | m2    | 825  | PSU  | O2-C2-N1  | -4.37 | 118.29      | 122.79   |
| 9   | A2    | 398  | A2M  | C4-N9-C8  | 4.36  | 110.32      | 105.74   |
| 9   | A2    | 4055 | PSU  | O2-C2-N1  | -4.36 | 118.29      | 122.79   |
| 46  | m2    | 27   | A2M  | C4-N9-C8  | 4.36  | 110.31      | 105.74   |
| 9   | A2    | 3420 | PSU  | O2-C2-N1  | -4.36 | 118.29      | 122.79   |
| 9   | A2    | 4022 | OMG  | C2-N3-C4  | 4.36  | 119.80      | 112.30   |
| 9   | A2    | 3945 | PSU  | O2-C2-N1  | -4.35 | 118.30      | 122.79   |
| 9   | A2    | 3848 | OMG  | C2-N3-C4  | 4.35  | 119.79      | 112.30   |
| 9   | A2    | 1438 | OMG  | C1'-N9-C8 | -4.35 | 114.39      | 126.73   |
| 9   | A2    | 4146 | OMG  | C2-N3-C4  | 4.34  | 119.78      | 112.30   |
| 9   | A2    | 1395 | PSU  | O2-C2-N1  | -4.34 | 118.31      | 122.79   |
| 9   | A2    | 1852 | OMG  | C2-N3-C4  | 4.34  | 119.77      | 112.30   |
| 9   | A2    | 1711 | P7G  | C4-C5-N7  | 4.34  | 109.63      | 106.71   |
| 9   | A2    | 4023 | MHG  | C5-C6-N1  | 4.34  | 118.57      | 110.94   |
| 9   | A2    | 4515 | OMG  | C2-N3-C4  | 4.33  | 119.76      | 112.30   |
| 9   | A2    | 2119 | OMG  | C2-N3-C4  | 4.33  | 119.76      | 112.30   |
| 46  | m2    | 1083 | PSU  | O2-C2-N1  | -4.33 | 118.32      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 9   | A2    | 1140 | A2M  | C4-N9-C8   | 4.31  | 110.27      | 105.74   |
| 9   | A2    | 1490 | PSU  | O2-C2-N1   | -4.31 | 118.34      | 122.79   |
| 9   | A2    | 4223 | A2M  | C4-N9-C8   | 4.30  | 110.26      | 105.74   |
| 46  | m2    | 685  | OMG  | C2-N3-C4   | 4.29  | 119.69      | 112.30   |
| 9   | A2    | 4102 | PSU  | O2-C2-N1   | -4.29 | 118.37      | 122.79   |
| 9   | A2    | 1347 | A2M  | C4-N9-C8   | 4.27  | 110.22      | 105.74   |
| 46  | m2    | 1245 | PSU  | C6-C5-C4   | 4.26  | 121.05      | 118.17   |
| 9   | A2    | 1269 | B8Q  | C31-N3-C4  | 4.26  | 122.13      | 114.76   |
| 9   | A2    | 4288 | PSU  | C6-C5-C4   | 4.25  | 121.04      | 118.17   |
| 9   | A2    | 2263 | PSU  | O2-C2-N1   | -4.25 | 118.41      | 122.79   |
| 9   | A2    | 2052 | E7G  | C5-C6-N1   | 4.25  | 118.42      | 110.94   |
| 9   | A2    | 3837 | B8W  | N3-C4-N9   | 4.24  | 132.38      | 126.99   |
| 9   | A2    | 373  | OMG  | C2-N3-C4   | 4.24  | 119.60      | 112.30   |
| 9   | A2    | 4289 | OMG  | C1'-N9-C8  | -4.24 | 114.70      | 126.73   |
| 9   | A2    | 4055 | PSU  | C6-C5-C4   | 4.23  | 121.03      | 118.17   |
| 9   | A2    | 2118 | A2M  | C4-N9-C8   | 4.22  | 110.17      | 105.74   |
| 46  | m2    | 1245 | PSU  | O2-C2-N1   | -4.22 | 118.44      | 122.79   |
| 9   | A2    | 4007 | E6G  | N9-C8-N7   | -4.21 | 107.96      | 113.94   |
| 9   | A2    | 3872 | 6MZ  | N9-C8-N7   | -4.21 | 107.96      | 113.94   |
| 9   | A2    | 4022 | OMG  | C1'-N9-C8  | -4.21 | 114.78      | 126.73   |
| 9   | A2    | 1387 | B9B  | N9-C8-N7   | -4.21 | 107.97      | 113.94   |
| 9   | A2    | 2156 | A2M  | C4-N9-C8   | 4.21  | 110.15      | 105.74   |
| 9   | A2    | 4280 | PSU  | C6-C5-C4   | 4.21  | 121.01      | 118.17   |
| 46  | m2    | 685  | OMG  | C1'-N9-C8  | -4.20 | 114.81      | 126.73   |
| 46  | m2    | 670  | A2M  | C4-N9-C8   | 4.18  | 110.12      | 105.74   |
| 9   | A2    | 4146 | OMG  | C1'-N9-C8  | -4.17 | 114.88      | 126.73   |
| 9   | A2    | 3374 | A2M  | C4-N9-C8   | 4.17  | 110.12      | 105.74   |
| 9   | A2    | 1852 | OMG  | C1'-N9-C8  | -4.17 | 114.88      | 126.73   |
| 9   | A2    | 1337 | A2M  | C4-N9-C8   | 4.16  | 110.11      | 105.74   |
| 9   | A2    | 3379 | A2M  | C4-N9-C8   | 4.16  | 110.11      | 105.74   |
| 9   | A2    | 3848 | OMG  | C1'-N9-C8  | -4.15 | 114.94      | 126.73   |
| 9   | A2    | 1673 | A2M  | C2'-C1'-N9 | -4.15 | 106.93      | 113.75   |
| 9   | A2    | 1395 | PSU  | C6-C5-C4   | 4.14  | 120.97      | 118.17   |
| 9   | A2    | 3837 | B8W  | N9-C8-N7   | -4.14 | 108.06      | 113.94   |
| 9   | A2    | 1330 | 2MG  | C2-N1-C6   | -4.13 | 119.56      | 124.55   |
| 9   | A2    | 4517 | 2MG  | C1'-N9-C8  | -4.12 | 115.03      | 126.73   |
| 9   | A2    | 878  | 2MG  | C2-N1-C6   | -4.12 | 119.57      | 124.55   |
| 9   | A2    | 3523 | A2M  | C4-N9-C8   | 4.11  | 110.05      | 105.74   |
| 46  | m2    | 1033 | A2M  | C4-N9-C8   | 4.10  | 110.05      | 105.74   |
| 9   | A2    | 4517 | 2MG  | C2-N1-C6   | -4.10 | 119.60      | 124.55   |
| 9   | A2    | 4007 | E6G  | N3-C4-N9   | 4.09  | 132.18      | 126.99   |
| 9   | A2    | 878  | 2MG  | C1'-N9-C8  | -4.08 | 115.13      | 126.73   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | A2    | 4067 | 1MA  | C5-C4-N3  | -4.07 | 121.28      | 127.27   |
| 9   | A2    | 1387 | B9B  | N3-C4-N9  | 4.03  | 132.11      | 126.99   |
| 46  | m2    | 614  | PSU  | C6-C5-C4  | 4.03  | 120.89      | 118.17   |
| 9   | A2    | 1685 | OMG  | C1'-N9-C8 | -4.03 | 115.28      | 126.73   |
| 9   | A2    | 2119 | OMG  | C1'-N9-C8 | -4.03 | 115.30      | 126.73   |
| 9   | A2    | 4094 | PSU  | C6-C5-C4  | 3.97  | 120.85      | 118.17   |
| 46  | m2    | 166  | A2M  | C4-N9-C8  | 3.97  | 109.91      | 105.74   |
| 9   | A2    | 4272 | OMU  | N3-C2-N1  | 3.97  | 120.06      | 114.89   |
| 9   | A2    | 4275 | OMG  | C1'-N9-C8 | -3.96 | 115.48      | 126.73   |
| 9   | A2    | 4007 | E6G  | C61-O6-C6 | -3.96 | 113.64      | 117.57   |
| 9   | A2    | 4023 | MHG  | C5-C4-N3  | -3.92 | 120.78      | 128.13   |
| 9   | A2    | 1269 | B8Q  | N3-C2-N1  | 3.91  | 122.61      | 117.16   |
| 9   | A2    | 373  | OMG  | C1'-N9-C8 | -3.86 | 115.77      | 126.73   |
| 9   | A2    | 373  | OMG  | N9-C8-N7  | -3.83 | 106.29      | 113.40   |
| 9   | A2    | 1330 | 2MG  | C1'-N9-C8 | -3.82 | 115.87      | 126.73   |
| 9   | A2    | 3371 | PSU  | C6-C5-C4  | 3.82  | 120.75      | 118.17   |
| 11  | C2    | 14   | OMU  | N3-C2-N1  | 3.82  | 119.87      | 114.89   |
| 9   | A2    | 2179 | OMG  | C1'-N9-C8 | -3.81 | 115.90      | 126.73   |
| 9   | A2    | 1335 | OMG  | C1'-N9-C8 | -3.80 | 115.94      | 126.73   |
| 9   | A2    | 1335 | OMG  | N9-C8-N7  | -3.78 | 106.39      | 113.40   |
| 46  | m2    | 685  | OMG  | N9-C8-N7  | -3.77 | 106.40      | 113.40   |
| 9   | A2    | 4007 | E6G  | N2-C2-N3  | 3.76  | 122.86      | 117.22   |
| 9   | A2    | 3958 | OMU  | N3-C2-N1  | 3.76  | 119.78      | 114.89   |
| 9   | A2    | 1418 | G7M  | C2-N1-C6  | -3.74 | 118.32      | 125.11   |
| 9   | A2    | 2277 | G7M  | C2-N1-C6  | -3.73 | 118.34      | 125.11   |
| 9   | A2    | 2263 | PSU  | C6-C5-C4  | 3.72  | 120.69      | 118.17   |
| 9   | A2    | 3848 | OMG  | N9-C8-N7  | -3.72 | 106.50      | 113.40   |
| 9   | A2    | 2119 | OMG  | N9-C8-N7  | -3.71 | 106.52      | 113.40   |
| 9   | A2    | 4022 | OMG  | N9-C8-N7  | -3.71 | 106.52      | 113.40   |
| 9   | A2    | 4275 | OMG  | N9-C8-N7  | -3.71 | 106.52      | 113.40   |
| 9   | A2    | 1685 | OMG  | N9-C8-N7  | -3.70 | 106.54      | 113.40   |
| 9   | A2    | 3448 | OMG  | N9-C8-N7  | -3.69 | 106.55      | 113.40   |
| 9   | A2    | 237  | B9B  | N9-C8-N7  | -3.69 | 108.70      | 113.94   |
| 9   | A2    | 4289 | OMG  | N9-C8-N7  | -3.69 | 106.56      | 113.40   |
| 11  | C2    | 14   | OMU  | C5-C4-N3  | 3.68  | 119.95      | 114.80   |
| 9   | A2    | 1599 | E7G  | C5-C4-N3  | -3.66 | 121.26      | 128.13   |
| 46  | m2    | 824  | PSU  | C6-C5-C4  | 3.66  | 120.64      | 118.17   |
| 9   | A2    | 4146 | OMG  | N9-C8-N7  | -3.65 | 106.62      | 113.40   |
| 9   | A2    | 1418 | G7M  | C5-C4-N3  | -3.65 | 121.24      | 128.15   |
| 9   | A2    | 1330 | 2MG  | N1-C2-N2  | 3.65  | 120.29      | 116.56   |
| 46  | m2    | 1832 | UR3  | C5-C4-N3  | 3.65  | 119.84      | 115.04   |
| 46  | m2    | 116  | OMU  | N3-C2-N1  | 3.65  | 119.64      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | A2    | 4202 | G7M  | C2-N1-C6  | -3.65 | 118.50      | 125.11   |
| 9   | A2    | 1599 | E7G  | C2-N1-C6  | -3.64 | 118.50      | 125.11   |
| 9   | A2    | 3958 | OMU  | C5-C4-N3  | 3.64  | 119.90      | 114.80   |
| 46  | m2    | 646  | OMG  | N9-C8-N7  | -3.63 | 106.67      | 113.40   |
| 9   | A2    | 1387 | B9B  | O6-C6-C5  | 3.62  | 121.51      | 116.73   |
| 9   | A2    | 3374 | A2M  | N3-C4-N9  | 3.62  | 133.32      | 127.17   |
| 9   | A2    | 1337 | A2M  | N3-C4-N9  | 3.59  | 133.27      | 127.17   |
| 9   | A2    | 1668 | UR3  | C5-C4-N3  | 3.58  | 119.76      | 115.04   |
| 9   | A2    | 2277 | G7M  | C5-C4-N3  | -3.58 | 121.38      | 128.15   |
| 9   | A2    | 237  | B9B  | O6-C6-C5  | 3.58  | 121.46      | 116.73   |
| 9   | A2    | 2528 | OMG  | N9-C4-N3  | 3.56  | 133.08      | 125.95   |
| 9   | A2    | 1472 | I4U  | C5-C4-N3  | -3.56 | 119.64      | 124.86   |
| 9   | A2    | 1852 | OMG  | N9-C8-N7  | -3.56 | 106.81      | 113.40   |
| 9   | A2    | 4249 | UR3  | C5-C4-N3  | 3.55  | 119.72      | 115.04   |
| 9   | A2    | 878  | 2MG  | C1'-N9-C4 | 3.54  | 136.93      | 126.49   |
| 9   | A2    | 1438 | OMG  | N9-C4-N3  | 3.53  | 133.02      | 125.95   |
| 9   | A2    | 4007 | E6G  | N3-C2-N1  | -3.53 | 120.07      | 125.48   |
| 9   | A2    | 3448 | OMG  | N9-C4-N3  | 3.53  | 133.01      | 125.95   |
| 9   | A2    | 2052 | E7G  | C5-C4-N3  | -3.53 | 121.51      | 128.13   |
| 9   | A2    | 4202 | G7M  | C5-C4-N3  | -3.52 | 121.50      | 128.15   |
| 9   | A2    | 3420 | PSU  | C6-C5-C4  | 3.52  | 120.55      | 118.17   |
| 9   | A2    | 2118 | A2M  | N3-C4-N9  | 3.50  | 133.12      | 127.17   |
| 9   | A2    | 3441 | A2M  | N3-C4-N9  | 3.50  | 133.12      | 127.17   |
| 9   | A2    | 2541 | B9H  | C4-N3-C2  | -3.49 | 115.70      | 122.00   |
| 9   | A2    | 2179 | OMG  | N9-C8-N7  | -3.49 | 106.92      | 113.40   |
| 9   | A2    | 1438 | OMG  | N9-C8-N7  | -3.48 | 106.94      | 113.40   |
| 9   | A2    | 4515 | OMG  | N9-C8-N7  | -3.48 | 106.94      | 113.40   |
| 9   | A2    | 2528 | OMG  | N9-C8-N7  | -3.47 | 106.96      | 113.40   |
| 9   | A2    | 3846 | I4U  | C5-C4-N3  | -3.46 | 119.78      | 124.86   |
| 9   | A2    | 1347 | A2M  | N3-C4-N9  | 3.46  | 133.05      | 127.17   |
| 9   | A2    | 4517 | 2MG  | C1'-N9-C4 | 3.45  | 136.69      | 126.49   |
| 9   | A2    | 2156 | A2M  | N3-C4-N9  | 3.45  | 133.04      | 127.17   |
| 46  | m2    | 27   | A2M  | N3-C4-N9  | 3.45  | 133.04      | 127.17   |
| 9   | A2    | 1387 | B9B  | N3-C2-N1  | -3.45 | 120.20      | 125.48   |
| 9   | A2    | 2052 | E7G  | C2-N1-C6  | -3.45 | 118.86      | 125.11   |
| 46  | m2    | 646  | OMG  | N9-C4-N3  | 3.44  | 132.83      | 125.95   |
| 46  | m2    | 1033 | A2M  | N3-C4-N9  | 3.44  | 133.01      | 127.17   |
| 9   | A2    | 1673 | A2M  | N3-C4-N9  | 3.43  | 133.00      | 127.17   |
| 9   | A2    | 1685 | OMG  | N9-C4-N3  | 3.41  | 132.77      | 125.95   |
| 9   | A2    | 3872 | 6MZ  | C4-C5-C6  | 3.41  | 119.61      | 116.78   |
| 46  | m2    | 670  | A2M  | N3-C4-N9  | 3.41  | 132.96      | 127.17   |
| 9   | A2    | 237  | B9B  | N3-C2-N1  | -3.40 | 120.26      | 125.48   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | A2    | 3837 | B8W  | N1-C2-N3  | -3.40 | 120.27      | 125.48   |
| 46  | m2    | 166  | A2M  | N3-C4-N9  | 3.40  | 132.94      | 127.17   |
| 9   | A2    | 3872 | 6MZ  | C2-N3-C4  | 3.39  | 120.12      | 111.83   |
| 46  | m2    | 1250 | B8N  | O4-C4-N3  | -3.39 | 114.48      | 119.99   |
| 46  | m2    | 116  | OMU  | C5-C4-N3  | 3.39  | 119.55      | 114.80   |
| 9   | A2    | 1337 | A2M  | C2-N3-C4  | 3.38  | 120.08      | 111.83   |
| 9   | A2    | 4022 | OMG  | N9-C4-N3  | 3.38  | 132.70      | 125.95   |
| 46  | m2    | 166  | A2M  | C2-N3-C4  | 3.37  | 120.07      | 111.83   |
| 9   | A2    | 4146 | OMG  | N9-C4-N3  | 3.37  | 132.69      | 125.95   |
| 9   | A2    | 398  | A2M  | N3-C4-N9  | 3.36  | 132.89      | 127.17   |
| 9   | A2    | 3374 | A2M  | C2-N3-C4  | 3.36  | 120.03      | 111.83   |
| 9   | A2    | 3379 | A2M  | N3-C4-N9  | 3.34  | 132.85      | 127.17   |
| 9   | A2    | 2156 | A2M  | C2-N3-C4  | 3.34  | 119.99      | 111.83   |
| 9   | A2    | 1140 | A2M  | C2-N3-C4  | 3.32  | 119.93      | 111.83   |
| 9   | A2    | 1673 | A2M  | C2-N3-C4  | 3.31  | 119.92      | 111.83   |
| 9   | A2    | 3441 | A2M  | C2-N3-C4  | 3.31  | 119.92      | 111.83   |
| 46  | m2    | 1033 | A2M  | C2-N3-C4  | 3.31  | 119.91      | 111.83   |
| 9   | A2    | 1140 | A2M  | N3-C4-N9  | 3.31  | 132.79      | 127.17   |
| 9   | A2    | 1269 | B8Q  | C6-N1-C2  | -3.31 | 119.10      | 121.80   |
| 9   | A2    | 4223 | A2M  | N3-C4-N9  | 3.31  | 132.79      | 127.17   |
| 9   | A2    | 3481 | A2M  | N3-C4-N9  | 3.30  | 132.78      | 127.17   |
| 9   | A2    | 2528 | OMG  | C1'-N9-C4 | 3.30  | 136.23      | 126.49   |
| 9   | A2    | 3448 | OMG  | C1'-N9-C4 | 3.30  | 136.22      | 126.49   |
| 9   | A2    | 398  | A2M  | C2-N3-C4  | 3.30  | 119.88      | 111.83   |
| 9   | A2    | 3379 | A2M  | C2-N3-C4  | 3.29  | 119.87      | 111.83   |
| 9   | A2    | 2277 | G7M  | C5-C6-N1  | 3.29  | 118.64      | 111.84   |
| 9   | A2    | 1418 | G7M  | C5-C6-N1  | 3.28  | 118.62      | 111.84   |
| 9   | A2    | 4223 | A2M  | C2-N3-C4  | 3.28  | 119.84      | 111.83   |
| 9   | A2    | 1347 | A2M  | C2-N3-C4  | 3.27  | 119.82      | 111.83   |
| 9   | A2    | 1852 | OMG  | N9-C4-N3  | 3.27  | 132.50      | 125.95   |
| 46  | m2    | 685  | OMG  | N9-C4-N3  | 3.27  | 132.49      | 125.95   |
| 9   | A2    | 3848 | OMG  | N9-C4-N3  | 3.26  | 132.48      | 125.95   |
| 9   | A2    | 2179 | OMG  | N9-C4-N3  | 3.26  | 132.47      | 125.95   |
| 46  | m2    | 27   | A2M  | C2-N3-C4  | 3.26  | 119.79      | 111.83   |
| 9   | A2    | 3481 | A2M  | C2-N3-C4  | 3.26  | 119.79      | 111.83   |
| 46  | m2    | 670  | A2M  | C2-N3-C4  | 3.26  | 119.78      | 111.83   |
| 9   | A2    | 2118 | A2M  | C2-N3-C4  | 3.26  | 119.78      | 111.83   |
| 9   | A2    | 1140 | A2M  | C5-N7-C8  | 3.25  | 108.56      | 103.45   |
| 9   | A2    | 237  | B9B  | N2-C2-N3  | 3.25  | 122.09      | 117.22   |
| 9   | A2    | 4272 | OMU  | C5-C4-N3  | 3.24  | 119.33      | 114.80   |
| 9   | A2    | 4275 | OMG  | N9-C4-N3  | 3.23  | 132.42      | 125.95   |
| 9   | A2    | 4289 | OMG  | N9-C4-N3  | 3.23  | 132.41      | 125.95   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | A2    | 3523 | A2M  | N3-C4-N9  | 3.23  | 132.66      | 127.17   |
| 9   | A2    | 1335 | OMG  | N9-C4-N3  | 3.23  | 132.41      | 125.95   |
| 9   | A2    | 1330 | 2MG  | C1'-N9-C4 | 3.22  | 136.01      | 126.49   |
| 9   | A2    | 1438 | OMG  | C1'-N9-C4 | 3.22  | 135.99      | 126.49   |
| 9   | A2    | 3441 | A2M  | C5-N7-C8  | 3.21  | 108.50      | 103.45   |
| 9   | A2    | 2118 | A2M  | C5-N7-C8  | 3.21  | 108.50      | 103.45   |
| 9   | A2    | 3481 | A2M  | C5-N7-C8  | 3.21  | 108.50      | 103.45   |
| 9   | A2    | 3523 | A2M  | C5-N7-C8  | 3.21  | 108.50      | 103.45   |
| 9   | A2    | 398  | A2M  | C5-N7-C8  | 3.21  | 108.50      | 103.45   |
| 9   | A2    | 1673 | A2M  | C5-N7-C8  | 3.20  | 108.48      | 103.45   |
| 9   | A2    | 4515 | OMG  | N9-C4-N3  | 3.20  | 132.34      | 125.95   |
| 9   | A2    | 4202 | G7M  | C5-C6-N1  | 3.19  | 118.44      | 111.84   |
| 9   | A2    | 4223 | A2M  | C5-N7-C8  | 3.19  | 108.47      | 103.45   |
| 46  | m2    | 670  | A2M  | C5-N7-C8  | 3.19  | 108.47      | 103.45   |
| 46  | m2    | 646  | OMG  | C1'-N9-C4 | 3.19  | 135.91      | 126.49   |
| 9   | A2    | 3523 | A2M  | C2-N3-C4  | 3.18  | 119.60      | 111.83   |
| 9   | A2    | 4515 | OMG  | C1'-N9-C4 | 3.18  | 135.87      | 126.49   |
| 46  | m2    | 166  | A2M  | C5-N7-C8  | 3.17  | 108.44      | 103.45   |
| 9   | A2    | 3987 | 5MC  | C5-C6-N1  | -3.17 | 119.87      | 123.31   |
| 9   | A2    | 878  | 2MG  | N9-C4-N3  | 3.17  | 132.29      | 125.95   |
| 9   | A2    | 1387 | B9B  | N2-C2-N3  | 3.16  | 121.97      | 117.22   |
| 9   | A2    | 2156 | A2M  | C5-N7-C8  | 3.16  | 108.42      | 103.45   |
| 9   | A2    | 1337 | A2M  | C5-N7-C8  | 3.16  | 108.42      | 103.45   |
| 46  | m2    | 1033 | A2M  | C5-N7-C8  | 3.15  | 108.40      | 103.45   |
| 9   | A2    | 1269 | B8Q  | O2-C2-N3  | -3.15 | 118.53      | 122.95   |
| 9   | A2    | 3374 | A2M  | C5-N7-C8  | 3.14  | 108.39      | 103.45   |
| 46  | m2    | 27   | A2M  | C5-N7-C8  | 3.14  | 108.39      | 103.45   |
| 9   | A2    | 3379 | A2M  | C5-N7-C8  | 3.13  | 108.38      | 103.45   |
| 9   | A2    | 1347 | A2M  | C5-N7-C8  | 3.13  | 108.38      | 103.45   |
| 9   | A2    | 2119 | OMG  | N9-C4-N3  | 3.10  | 132.16      | 125.95   |
| 9   | A2    | 4067 | 1MA  | C1'-N9-C4 | -3.10 | 117.33      | 126.49   |
| 9   | A2    | 1438 | OMG  | C2-N1-C6  | -3.10 | 119.49      | 125.11   |
| 9   | A2    | 373  | OMG  | N9-C4-N3  | 3.08  | 132.11      | 125.95   |
| 9   | A2    | 4289 | OMG  | C1'-N9-C4 | 3.06  | 135.52      | 126.49   |
| 9   | A2    | 4099 | 5MC  | C5-C6-N1  | -3.05 | 120.00      | 123.31   |
| 9   | A2    | 4517 | 2MG  | N9-C4-N3  | 3.05  | 132.05      | 125.95   |
| 9   | A2    | 4289 | OMG  | C2-N1-C6  | -3.05 | 119.58      | 125.11   |
| 9   | A2    | 3872 | 6MZ  | C5-N7-C8  | 3.05  | 108.24      | 103.45   |
| 46  | m2    | 1844 | 4AC  | C6-C5-C4  | 3.04  | 120.67      | 117.00   |
| 9   | A2    | 4067 | 1MA  | N9-C8-N7  | -3.04 | 107.76      | 113.40   |
| 9   | A2    | 3448 | OMG  | C2-N1-C6  | -3.03 | 119.61      | 125.11   |
| 9   | A2    | 1852 | OMG  | C2-N1-C6  | -3.03 | 119.62      | 125.11   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 9   | A2    | 2528 | OMG  | C2-N1-C6   | -3.03 | 119.62      | 125.11   |
| 9   | A2    | 4275 | OMG  | C2-N1-C6   | -3.03 | 119.62      | 125.11   |
| 9   | A2    | 3438 | 5MC  | C5-C6-N1   | -3.02 | 120.03      | 123.31   |
| 9   | A2    | 1335 | OMG  | C2-N1-C6   | -3.02 | 119.63      | 125.11   |
| 9   | A2    | 1852 | OMG  | C1'-N9-C4  | 3.01  | 135.38      | 126.49   |
| 9   | A2    | 1685 | OMG  | C2-N1-C6   | -3.00 | 119.67      | 125.11   |
| 9   | A2    | 2119 | OMG  | C2-N1-C6   | -2.99 | 119.68      | 125.11   |
| 9   | A2    | 4146 | OMG  | C2-N1-C6   | -2.99 | 119.69      | 125.11   |
| 9   | A2    | 4022 | OMG  | C2-N1-C6   | -2.99 | 119.69      | 125.11   |
| 9   | A2    | 2541 | B9H  | C6-N1-C2   | -2.98 | 119.36      | 121.80   |
| 46  | m2    | 646  | OMG  | C2-N1-C6   | -2.98 | 119.70      | 125.11   |
| 9   | A2    | 2052 | E7G  | C5-C4-N9   | 2.98  | 110.14      | 106.33   |
| 9   | A2    | 4515 | OMG  | C2-N1-C6   | -2.96 | 119.74      | 125.11   |
| 9   | A2    | 4146 | OMG  | C1'-N9-C4  | 2.96  | 135.23      | 126.49   |
| 9   | A2    | 3958 | OMU  | O4-C4-C5   | -2.96 | 120.06      | 125.16   |
| 9   | A2    | 2277 | G7M  | O6-C6-C5   | -2.95 | 121.42      | 128.01   |
| 9   | A2    | 4517 | 2MG  | N9-C8-N7   | -2.94 | 107.94      | 113.40   |
| 9   | A2    | 2179 | OMG  | C2-N1-C6   | -2.94 | 119.78      | 125.11   |
| 9   | A2    | 4007 | E6G  | C5-N7-C8   | 2.93  | 108.06      | 103.45   |
| 9   | A2    | 3848 | OMG  | C2-N1-C6   | -2.93 | 119.79      | 125.11   |
| 9   | A2    | 1330 | 2MG  | N9-C8-N7   | -2.93 | 107.97      | 113.40   |
| 9   | A2    | 3374 | A2M  | C2'-C1'-N9 | -2.93 | 108.93      | 113.75   |
| 46  | m2    | 685  | OMG  | C2-N1-C6   | -2.93 | 119.80      | 125.11   |
| 9   | A2    | 4023 | MHG  | N9-C4-N3   | 2.93  | 129.75      | 125.46   |
| 9   | A2    | 3837 | B8W  | C5-N7-C8   | 2.92  | 108.04      | 103.45   |
| 9   | A2    | 4022 | OMG  | C1'-N9-C4  | 2.91  | 135.07      | 126.49   |
| 9   | A2    | 1387 | B9B  | C5-N7-C8   | 2.91  | 108.02      | 103.45   |
| 9   | A2    | 398  | A2M  | C2'-C1'-N9 | -2.90 | 108.98      | 113.75   |
| 9   | A2    | 3848 | OMG  | C1'-N9-C4  | 2.89  | 135.02      | 126.49   |
| 9   | A2    | 1418 | G7M  | O6-C6-C5   | -2.89 | 121.57      | 128.01   |
| 46  | m2    | 685  | OMG  | C1'-N9-C4  | 2.88  | 134.98      | 126.49   |
| 9   | A2    | 1599 | E7G  | C5-C4-N9   | 2.87  | 110.01      | 106.33   |
| 9   | A2    | 3837 | B8W  | C2-N1-C6   | 2.87  | 119.95      | 115.96   |
| 46  | m2    | 116  | OMU  | O4-C4-C5   | -2.87 | 120.22      | 125.16   |
| 9   | A2    | 373  | OMG  | C2-N1-C6   | -2.86 | 119.92      | 125.11   |
| 9   | A2    | 1668 | UR3  | C6-N1-C2   | -2.86 | 119.46      | 121.80   |
| 9   | A2    | 4007 | E6G  | C2-N1-C6   | 2.86  | 119.94      | 115.96   |
| 9   | A2    | 878  | 2MG  | N1-C2-N2   | 2.84  | 119.47      | 116.56   |
| 9   | A2    | 1330 | 2MG  | N9-C4-N3   | 2.84  | 131.64      | 125.95   |
| 9   | A2    | 1269 | B8Q  | C31-N3-C2  | 2.83  | 122.15      | 117.70   |
| 9   | A2    | 4272 | OMU  | O4-C4-C5   | -2.81 | 120.31      | 125.16   |
| 9   | A2    | 237  | B9B  | C2-N1-C6   | 2.80  | 119.85      | 115.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | C2    | 14   | OMU  | O4-C4-C5    | -2.79 | 120.35      | 125.16   |
| 9   | A2    | 4202 | G7M  | O6-C6-C5    | -2.79 | 121.79      | 128.01   |
| 9   | A2    | 1668 | UR3  | C1'-N1-C2   | 2.78  | 121.59      | 117.04   |
| 9   | A2    | 2119 | OMG  | C1'-N9-C4   | 2.77  | 134.68      | 126.49   |
| 9   | A2    | 4223 | A2M  | C2'-C1'-N9  | -2.77 | 109.20      | 113.75   |
| 9   | A2    | 237  | B9B  | C5-N7-C8    | 2.76  | 107.79      | 103.45   |
| 9   | A2    | 878  | 2MG  | N9-C8-N7    | -2.76 | 108.28      | 113.40   |
| 9   | A2    | 2541 | B9H  | O3'-C3'-C2' | 2.75  | 118.87      | 111.19   |
| 9   | A2    | 4275 | OMG  | C1'-N9-C4   | 2.74  | 134.58      | 126.49   |
| 9   | A2    | 3441 | A2M  | C4'-O4'-C1' | -2.74 | 103.42      | 109.47   |
| 9   | A2    | 2179 | OMG  | C1'-N9-C4   | 2.72  | 134.52      | 126.49   |
| 9   | A2    | 2177 | OMC  | C1'-N1-C6   | 2.72  | 126.58      | 120.78   |
| 9   | A2    | 1685 | OMG  | C5-C6-N1    | 2.71  | 120.15      | 113.25   |
| 9   | A2    | 1387 | B9B  | C2-N1-C6    | 2.70  | 119.72      | 115.96   |
| 9   | A2    | 1685 | OMG  | C1'-N9-C4   | 2.70  | 134.47      | 126.49   |
| 9   | A2    | 3872 | 6MZ  | N3-C4-N9    | 2.70  | 131.76      | 127.17   |
| 9   | A2    | 237  | B9B  | C3'-C2'-C1' | 2.70  | 106.56      | 101.46   |
| 9   | A2    | 2528 | OMG  | C5-C6-N1    | 2.69  | 120.10      | 113.25   |
| 9   | A2    | 1335 | OMG  | C5-C6-N1    | 2.69  | 120.10      | 113.25   |
| 9   | A2    | 4022 | OMG  | C5-C6-N1    | 2.68  | 120.08      | 113.25   |
| 9   | A2    | 4275 | OMG  | C5-C6-N1    | 2.68  | 120.08      | 113.25   |
| 9   | A2    | 878  | 2MG  | C5-C6-N1    | 2.68  | 120.07      | 113.25   |
| 9   | A2    | 3837 | B8W  | C5-C6-N1    | -2.68 | 119.91      | 123.49   |
| 9   | A2    | 4146 | OMG  | C5-C6-N1    | 2.68  | 120.06      | 113.25   |
| 9   | A2    | 4517 | 2MG  | N1-C2-N2    | 2.68  | 119.29      | 116.56   |
| 9   | A2    | 2528 | OMG  | O6-C6-C5    | -2.67 | 119.50      | 126.53   |
| 9   | A2    | 3448 | OMG  | C5-C6-N1    | 2.66  | 120.03      | 113.25   |
| 9   | A2    | 1438 | OMG  | C5-C6-N1    | 2.66  | 120.02      | 113.25   |
| 9   | A2    | 2119 | OMG  | C5-C6-N1    | 2.65  | 120.01      | 113.25   |
| 46  | m2    | 1250 | B8N  | C31-N3-C4   | 2.65  | 120.93      | 117.18   |
| 9   | A2    | 1330 | 2MG  | C5-C6-N1    | 2.64  | 119.98      | 113.25   |
| 9   | A2    | 2179 | OMG  | C5-C6-N1    | 2.64  | 119.97      | 113.25   |
| 9   | A2    | 1852 | OMG  | C5-C6-N1    | 2.64  | 119.96      | 113.25   |
| 9   | A2    | 4249 | UR3  | C6-N1-C2    | -2.63 | 119.65      | 121.80   |
| 46  | m2    | 646  | OMG  | C5-C6-N1    | 2.63  | 119.95      | 113.25   |
| 9   | A2    | 1685 | OMG  | O6-C6-C5    | -2.63 | 119.59      | 126.53   |
| 9   | A2    | 4067 | 1MA  | C1'-N9-C8   | 2.62  | 134.17      | 126.73   |
| 9   | A2    | 3848 | OMG  | C5-C6-N1    | 2.61  | 119.91      | 113.25   |
| 9   | A2    | 3441 | A2M  | C2'-C1'-N9  | -2.61 | 109.45      | 113.75   |
| 9   | A2    | 3872 | 6MZ  | C4-C5-N7    | -2.60 | 107.61      | 110.58   |
| 46  | m2    | 685  | OMG  | C5-C6-N1    | 2.60  | 119.88      | 113.25   |
| 9   | A2    | 4515 | OMG  | O6-C6-C5    | -2.60 | 119.67      | 126.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | A2    | 4515 | OMG  | C5-C6-N1    | 2.60  | 119.86      | 113.25   |
| 9   | A2    | 1599 | E7G  | O6-C6-C5    | -2.59 | 121.25      | 127.62   |
| 9   | A2    | 1472 | I4U  | C3'-C2'-C1' | 2.59  | 106.37      | 101.46   |
| 9   | A2    | 4289 | OMG  | C5-C6-N1    | 2.59  | 119.85      | 113.25   |
| 9   | A2    | 2156 | A2M  | C2'-C1'-N9  | -2.58 | 109.50      | 113.75   |
| 9   | A2    | 373  | OMG  | C5-C6-N1    | 2.58  | 119.82      | 113.25   |
| 9   | A2    | 4517 | 2MG  | C5-C6-N1    | 2.58  | 119.81      | 113.25   |
| 9   | A2    | 2118 | A2M  | C2'-C1'-N9  | -2.57 | 109.52      | 113.75   |
| 9   | A2    | 237  | B9B  | C5-C6-N1    | -2.57 | 120.05      | 123.49   |
| 9   | A2    | 4289 | OMG  | C8-N7-C5    | 2.56  | 108.82      | 104.26   |
| 9   | A2    | 3379 | A2M  | C2'-C1'-N9  | -2.55 | 109.55      | 113.75   |
| 9   | A2    | 1335 | OMG  | C1'-N9-C4   | 2.55  | 134.01      | 126.49   |
| 9   | A2    | 2179 | OMG  | O6-C6-C5    | -2.53 | 119.84      | 126.53   |
| 9   | A2    | 2119 | OMG  | O6-C6-C5    | -2.53 | 119.86      | 126.53   |
| 9   | A2    | 3837 | B8W  | C2-N3-C4    | 2.52  | 120.27      | 113.51   |
| 9   | A2    | 878  | 2MG  | O6-C6-C5    | -2.52 | 119.87      | 126.53   |
| 46  | m2    | 670  | A2M  | C2'-C1'-N9  | -2.52 | 109.61      | 113.75   |
| 9   | A2    | 373  | OMG  | C1'-N9-C4   | 2.51  | 133.90      | 126.49   |
| 9   | A2    | 237  | B9B  | C2-N3-C4    | 2.50  | 120.21      | 113.51   |
| 9   | A2    | 4275 | OMG  | O6-C6-C5    | -2.50 | 119.93      | 126.53   |
| 9   | A2    | 1335 | OMG  | O6-C6-C5    | -2.50 | 119.94      | 126.53   |
| 9   | A2    | 373  | OMG  | O6-C6-C5    | -2.49 | 119.95      | 126.53   |
| 9   | A2    | 1330 | 2MG  | O6-C6-C5    | -2.49 | 119.95      | 126.53   |
| 46  | m2    | 685  | OMG  | O6-C6-C5    | -2.49 | 119.96      | 126.53   |
| 46  | m2    | 646  | OMG  | O6-C6-C5    | -2.49 | 119.97      | 126.53   |
| 9   | A2    | 3848 | OMG  | O6-C6-C5    | -2.49 | 119.97      | 126.53   |
| 9   | A2    | 3448 | OMG  | O6-C6-C5    | -2.49 | 119.97      | 126.53   |
| 9   | A2    | 2052 | E7G  | N9-C8-N7    | 2.49  | 106.89      | 103.37   |
| 9   | A2    | 4007 | E6G  | C2-N3-C4    | 2.48  | 120.14      | 113.51   |
| 9   | A2    | 1438 | OMG  | O6-C6-C5    | -2.48 | 120.00      | 126.53   |
| 9   | A2    | 4007 | E6G  | C5-C6-N1    | -2.47 | 120.18      | 123.49   |
| 9   | A2    | 4022 | OMG  | O6-C6-C5    | -2.46 | 120.03      | 126.53   |
| 9   | A2    | 4146 | OMG  | O6-C6-C5    | -2.45 | 120.05      | 126.53   |
| 9   | A2    | 1387 | B9B  | C2-N3-C4    | 2.45  | 120.09      | 113.51   |
| 9   | A2    | 4023 | MHG  | C5-C4-N9    | 2.45  | 109.48      | 106.33   |
| 9   | A2    | 4517 | 2MG  | O6-C6-C5    | -2.45 | 120.06      | 126.53   |
| 9   | A2    | 1335 | OMG  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 9   | A2    | 4023 | MHG  | N9-C8-N7    | 2.44  | 106.83      | 103.37   |
| 9   | A2    | 3441 | A2M  | C4-N9-C1'   | -2.44 | 120.93      | 126.63   |
| 9   | A2    | 1852 | OMG  | O6-C6-C5    | -2.44 | 120.10      | 126.53   |
| 9   | A2    | 2052 | E7G  | O6-C6-C5    | -2.43 | 121.65      | 127.62   |
| 9   | A2    | 3441 | A2M  | O4'-C1'-N9  | 2.43  | 112.75      | 108.09   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 46  | m2    | 646  | OMG  | C8-N7-C5   | 2.42  | 108.57      | 104.26   |
| 9   | A2    | 4275 | OMG  | C8-N7-C5   | 2.42  | 108.57      | 104.26   |
| 46  | m2    | 1844 | 4AC  | C5-C4-N3   | -2.42 | 118.82      | 122.60   |
| 9   | A2    | 3448 | OMG  | C8-N7-C5   | 2.42  | 108.56      | 104.26   |
| 46  | m2    | 685  | OMG  | C8-N7-C5   | 2.41  | 108.55      | 104.26   |
| 9   | A2    | 1337 | A2M  | C2'-C1'-N9 | -2.41 | 109.79      | 113.75   |
| 9   | A2    | 3481 | A2M  | C2'-C1'-N9 | -2.40 | 109.80      | 113.75   |
| 9   | A2    | 4202 | G7M  | N9-C8-N7   | -2.40 | 106.65      | 112.48   |
| 46  | m2    | 1844 | 4AC  | N4-C4-N3   | 2.40  | 117.76      | 113.87   |
| 9   | A2    | 2541 | B9H  | O2-C2-N3   | -2.39 | 119.04      | 122.10   |
| 9   | A2    | 3523 | A2M  | C4-N9-C1'  | -2.38 | 121.06      | 126.63   |
| 9   | A2    | 3848 | OMG  | C8-N7-C5   | 2.38  | 108.50      | 104.26   |
| 9   | A2    | 4135 | B8T  | C6-C5-C4   | 2.38  | 119.86      | 117.00   |
| 9   | A2    | 1599 | E7G  | N9-C8-N7   | 2.38  | 106.74      | 103.37   |
| 9   | A2    | 4146 | OMG  | C8-N7-C5   | 2.37  | 108.48      | 104.26   |
| 9   | A2    | 4515 | OMG  | C8-N7-C5   | 2.36  | 108.46      | 104.26   |
| 9   | A2    | 3837 | B8W  | C4-C5-N7   | -2.36 | 107.89      | 110.58   |
| 9   | A2    | 4023 | MHG  | C21-N2-C2  | -2.36 | 118.59      | 123.65   |
| 9   | A2    | 4023 | MHG  | O6-C6-C5   | -2.35 | 121.84      | 127.62   |
| 9   | A2    | 373  | OMG  | C8-N7-C5   | 2.35  | 108.45      | 104.26   |
| 9   | A2    | 1387 | B9B  | C5-C6-N1   | -2.34 | 120.35      | 123.49   |
| 9   | A2    | 2119 | OMG  | C8-N7-C5   | 2.34  | 108.43      | 104.26   |
| 9   | A2    | 4022 | OMG  | C8-N7-C5   | 2.34  | 108.42      | 104.26   |
| 9   | A2    | 3536 | P7G  | N9-C8-N7   | 2.34  | 106.68      | 103.37   |
| 9   | A2    | 2120 | OMC  | O2-C2-N1   | 2.34  | 123.47      | 118.90   |
| 9   | A2    | 3481 | A2M  | C4-N9-C1'  | -2.33 | 121.19      | 126.63   |
| 9   | A2    | 1387 | B9B  | C4-C5-N7   | -2.32 | 107.93      | 110.58   |
| 9   | A2    | 1438 | OMG  | C8-N7-C5   | 2.32  | 108.40      | 104.26   |
| 9   | A2    | 1685 | OMG  | C8-N7-C5   | 2.32  | 108.39      | 104.26   |
| 9   | A2    | 2120 | OMC  | O2-C2-N3   | -2.32 | 118.67      | 122.33   |
| 9   | A2    | 4249 | UR3  | C1'-N1-C2  | 2.32  | 120.83      | 117.04   |
| 9   | A2    | 1711 | P7G  | N9-C8-N7   | 2.31  | 106.64      | 103.37   |
| 9   | A2    | 4223 | A2M  | C4-N9-C1'  | -2.30 | 121.25      | 126.63   |
| 9   | A2    | 373  | OMG  | C8-N9-C4   | 2.29  | 110.32      | 106.03   |
| 9   | A2    | 1852 | OMG  | C8-N7-C5   | 2.29  | 108.34      | 104.26   |
| 9   | A2    | 1418 | G7M  | N9-C8-N7   | -2.28 | 106.94      | 112.48   |
| 9   | A2    | 4007 | E6G  | C4-C5-N7   | -2.28 | 107.98      | 110.58   |
| 9   | A2    | 2179 | OMG  | C8-N7-C5   | 2.28  | 108.32      | 104.26   |
| 46  | m2    | 1832 | UR3  | C6-N1-C2   | -2.28 | 119.94      | 121.80   |
| 9   | A2    | 1387 | B9B  | C4-N9-C8   | 2.27  | 108.12      | 105.74   |
| 9   | A2    | 2277 | G7M  | N9-C8-N7   | -2.27 | 106.97      | 112.48   |
| 9   | A2    | 2616 | OMC  | O2-C2-N3   | -2.26 | 118.76      | 122.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | A2    | 1140 | A2M  | C4-N9-C1'   | -2.26 | 121.35      | 126.63   |
| 9   | A2    | 398  | A2M  | C4-N9-C1'   | -2.25 | 121.37      | 126.63   |
| 9   | A2    | 4023 | MHG  | N1-C2-N2    | 2.24  | 118.85      | 116.56   |
| 9   | A2    | 2528 | OMG  | C8-N7-C5    | 2.24  | 108.25      | 104.26   |
| 9   | A2    | 3958 | OMU  | O2-C2-N1    | -2.24 | 119.88      | 122.80   |
| 9   | A2    | 4517 | 2MG  | CM2-N2-C2   | -2.24 | 118.84      | 123.65   |
| 9   | A2    | 4007 | E6G  | C4-N9-C8    | 2.24  | 108.08      | 105.74   |
| 9   | A2    | 1685 | OMG  | C8-N9-C4    | 2.23  | 110.21      | 106.03   |
| 46  | m2    | 685  | OMG  | C8-N9-C4    | 2.23  | 110.21      | 106.03   |
| 9   | A2    | 1599 | E7G  | N9-C4-N3    | 2.23  | 128.73      | 125.46   |
| 9   | A2    | 3837 | B8W  | C61-O6-C6   | -2.22 | 115.13      | 117.20   |
| 9   | A2    | 3523 | A2M  | C4-C5-N7    | -2.21 | 108.06      | 110.58   |
| 46  | m2    | 1033 | A2M  | C2'-C1'-N9  | -2.21 | 110.12      | 113.75   |
| 9   | A2    | 4289 | OMG  | O6-C6-C5    | -2.20 | 120.72      | 126.53   |
| 9   | A2    | 1673 | A2M  | C4-N9-C1'   | -2.20 | 121.49      | 126.63   |
| 9   | A2    | 4022 | OMG  | C8-N9-C4    | 2.20  | 110.14      | 106.03   |
| 9   | A2    | 2156 | A2M  | C4-N9-C1'   | -2.19 | 121.51      | 126.63   |
| 9   | A2    | 3379 | A2M  | C4-N9-C1'   | -2.18 | 121.53      | 126.63   |
| 9   | A2    | 3872 | 6MZ  | C4-N9-C8    | 2.18  | 108.03      | 105.74   |
| 79  | m     | 714  | DDE  | OAG-CBI-NAD | -2.18 | 119.19      | 123.04   |
| 9   | A2    | 3872 | 6MZ  | C5-C4-N9    | 2.16  | 108.17      | 105.81   |
| 9   | A2    | 237  | B9B  | C4-C5-N7    | -2.16 | 108.11      | 110.58   |
| 9   | A2    | 1140 | A2M  | C4-C5-N7    | -2.16 | 108.11      | 110.58   |
| 9   | A2    | 3837 | B8W  | C4-N9-C8    | 2.16  | 108.01      | 105.74   |
| 9   | A2    | 4067 | 1MA  | C8-N7-C5    | 2.16  | 108.11      | 104.26   |
| 9   | A2    | 3371 | PSU  | O4'-C1'-C2' | 2.15  | 108.12      | 105.15   |
| 9   | A2    | 3448 | OMG  | C8-N9-C4    | 2.14  | 110.04      | 106.03   |
| 9   | A2    | 3848 | OMG  | C8-N9-C4    | 2.14  | 110.04      | 106.03   |
| 46  | m2    | 166  | A2M  | C4-N9-C1'   | -2.14 | 121.63      | 126.63   |
| 9   | A2    | 1335 | OMG  | C8-N9-C4    | 2.14  | 110.03      | 106.03   |
| 9   | A2    | 2119 | OMG  | C8-N9-C4    | 2.13  | 110.03      | 106.03   |
| 46  | m2    | 27   | A2M  | C4-N9-C1'   | -2.13 | 121.64      | 126.63   |
| 9   | A2    | 878  | 2MG  | N1-C2-N3    | -2.12 | 120.10      | 123.68   |
| 46  | m2    | 1250 | B8N  | O4'-C1'-C2' | 2.12  | 108.08      | 105.15   |
| 9   | A2    | 4023 | MHG  | N1-C2-N3    | -2.11 | 120.12      | 123.68   |
| 9   | A2    | 2118 | A2M  | C4-C5-N7    | -2.11 | 108.17      | 110.58   |
| 46  | m2    | 670  | A2M  | C4-C5-N7    | -2.11 | 108.17      | 110.58   |
| 9   | A2    | 398  | A2M  | C4-C5-N7    | -2.11 | 108.17      | 110.58   |
| 9   | A2    | 1330 | 2MG  | N1-C2-N3    | -2.11 | 120.13      | 123.68   |
| 9   | A2    | 4272 | OMU  | C6-N1-C2    | -2.10 | 118.44      | 121.00   |
| 9   | A2    | 3987 | 5MC  | CM5-C5-C6   | -2.10 | 120.01      | 122.85   |
| 46  | m2    | 614  | PSU  | O4'-C1'-C2' | 2.10  | 108.05      | 105.15   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | m2    | 519  | OMC  | O2-C2-N3    | -2.09 | 119.03      | 122.33   |
| 9   | A2    | 3481 | A2M  | C4-C5-N7    | -2.09 | 108.19      | 110.58   |
| 46  | m2    | 166  | A2M  | C4-C5-N7    | -2.09 | 108.19      | 110.58   |
| 9   | A2    | 2120 | OMC  | C1'-N1-C2   | 2.09  | 123.06      | 118.44   |
| 9   | A2    | 4275 | OMG  | C8-N9-C4    | 2.09  | 109.94      | 106.03   |
| 9   | A2    | 1673 | A2M  | C4-C5-N7    | -2.09 | 108.19      | 110.58   |
| 9   | A2    | 3379 | A2M  | C4-C5-N7    | -2.09 | 108.19      | 110.58   |
| 9   | A2    | 4223 | A2M  | C4-C5-N7    | -2.08 | 108.20      | 110.58   |
| 46  | m2    | 1033 | A2M  | C4-C5-N7    | -2.08 | 108.20      | 110.58   |
| 9   | A2    | 4055 | PSU  | O4'-C1'-C2' | 2.07  | 108.02      | 105.15   |
| 46  | m2    | 1844 | 4AC  | CM7-C7-N4   | 2.07  | 118.61      | 115.27   |
| 9   | A2    | 1269 | B8Q  | C1'-N1-C2   | 2.07  | 120.42      | 117.04   |
| 46  | m2    | 1250 | B8N  | C31-N3-C2   | 2.06  | 120.69      | 117.64   |
| 9   | A2    | 4517 | 2MG  | C8-N7-C5    | 2.06  | 107.94      | 104.26   |
| 9   | A2    | 4146 | OMG  | C8-N9-C4    | 2.06  | 109.89      | 106.03   |
| 9   | A2    | 1330 | 2MG  | C8-N7-C5    | 2.06  | 107.93      | 104.26   |
| 9   | A2    | 1347 | A2M  | C4-C5-N7    | -2.06 | 108.23      | 110.58   |
| 46  | m2    | 646  | OMG  | C8-N9-C4    | 2.05  | 109.87      | 106.03   |
| 9   | A2    | 4183 | PSU  | O2-C2-N3    | -2.05 | 118.22      | 121.86   |
| 9   | A2    | 1490 | PSU  | O4'-C1'-C2' | 2.05  | 107.98      | 105.15   |
| 11  | C2    | 14   | OMU  | O2-C2-N1    | -2.05 | 120.13      | 122.80   |
| 9   | A2    | 4094 | PSU  | O4'-C1'-C2' | 2.04  | 107.97      | 105.15   |
| 9   | A2    | 4055 | PSU  | O2-C2-N3    | -2.03 | 118.25      | 121.86   |
| 46  | m2    | 1083 | PSU  | O4'-C1'-C2' | 2.03  | 107.96      | 105.15   |
| 9   | A2    | 4280 | PSU  | O4'-C1'-C2' | 2.03  | 107.96      | 105.15   |
| 9   | A2    | 3837 | B8W  | C5-C4-N9    | 2.02  | 108.01      | 105.81   |
| 9   | A2    | 1387 | B9B  | C61-O6-C6   | -2.02 | 114.14      | 117.66   |
| 9   | A2    | 1496 | PSU  | O2-C2-N3    | -2.02 | 118.28      | 121.86   |
| 46  | m2    | 1083 | PSU  | O2-C2-N3    | -2.02 | 118.28      | 121.86   |
| 46  | m2    | 1245 | PSU  | O2-C2-N3    | -2.01 | 118.29      | 121.86   |
| 46  | m2    | 825  | PSU  | O2-C2-N3    | -2.01 | 118.29      | 121.86   |
| 9   | A2    | 4152 | PSU  | O2-C2-N3    | -2.01 | 118.29      | 121.86   |
| 9   | A2    | 1337 | A2M  | C4-C5-N7    | -2.01 | 108.28      | 110.58   |
| 46  | m2    | 670  | A2M  | C4-N9-C1'   | -2.01 | 121.93      | 126.63   |
| 9   | A2    | 1490 | PSU  | O2-C2-N3    | -2.01 | 118.29      | 121.86   |
| 9   | A2    | 2263 | PSU  | O2-C2-N3    | -2.01 | 118.30      | 121.86   |
| 9   | A2    | 4202 | G7M  | C5-C4-N9    | 2.00  | 110.15      | 105.88   |
| 9   | A2    | 4289 | OMG  | C8-N9-C4    | 2.00  | 109.78      | 106.03   |

There are no chirality outliers.

All (162) torsion outliers are listed below:



| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | F2    | 333  | MLZ  | CD-CE-NZ-CM     |
| 41  | g2    | 98   | MLZ  | C-CA-CB-CG      |
| 79  | m     | 714  | DDE  | O-C-CA-CB       |
| 79  | m     | 714  | DDE  | NAD-CBI-CBW-NCB |
| 79  | m     | 714  | DDE  | CAT-CAU-CBW-CBI |
| 79  | m     | 714  | DDE  | CAT-CAU-CBW-NCB |
| 9   | A2    | 237  | B9B  | C5-C6-O6-C61    |
| 9   | A2    | 237  | B9B  | N1-C6-O6-C61    |
| 9   | A2    | 237  | B9B  | C3'-C4'-C5'-O5' |
| 9   | A2    | 237  | B9B  | C4'-C5'-O5'-P   |
| 9   | A2    | 237  | B9B  | C62-C61-O6-C6   |
| 9   | A2    | 398  | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 878  | 2MG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 878  | 2MG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 1140 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 1387 | B9B  | C5-C6-O6-C61    |
| 9   | A2    | 1387 | B9B  | N1-C6-O6-C61    |
| 9   | A2    | 1395 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 1490 | PSU  | C2'-C1'-C5-C4   |
| 9   | A2    | 1668 | UR3  | O4'-C4'-C5'-O5' |
| 9   | A2    | 1685 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 2052 | E7G  | C72-C71-N7-C5   |
| 9   | A2    | 2119 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 2156 | A2M  | O4'-C4'-C5'-O5' |
| 9   | A2    | 2156 | A2M  | C3'-C4'-C5'-O5' |
| 9   | A2    | 2177 | OMC  | C1'-C2'-O2'-CM2 |
| 9   | A2    | 2528 | OMG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3374 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 3379 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 3385 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3420 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3438 | 5MC  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3481 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 3523 | A2M  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3523 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 3536 | P7G  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3837 | B8W  | C5-C6-O6-C61    |
| 9   | A2    | 3837 | B8W  | N1-C6-O6-C61    |
| 9   | A2    | 3846 | I4U  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3872 | 6MZ  | C5-C6-N6-C9     |
| 9   | A2    | 3872 | 6MZ  | N1-C6-N6-C9     |
| 9   | A2    | 3958 | OMU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3958 | OMU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | A2    | 4007 | E6G  | C5-C6-O6-C61    |
| 9   | A2    | 4007 | E6G  | N1-C6-O6-C61    |
| 9   | A2    | 4023 | MHG  | C2'-C1'-N9-C8   |
| 9   | A2    | 4099 | 5MC  | C2'-C1'-N1-C2   |
| 9   | A2    | 4099 | 5MC  | C2'-C1'-N1-C6   |
| 9   | A2    | 4183 | PSU  | O4'-C1'-C5-C6   |
| 9   | A2    | 4223 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 4272 | OMU  | C1'-C2'-O2'-CM2 |
| 9   | A2    | 4288 | PSU  | C2'-C1'-C5-C4   |
| 9   | A2    | 4288 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 4515 | OMG  | C4'-C5'-O5'-P   |
| 46  | m2    | 27   | A2M  | C1'-C2'-O2'-CM' |
| 46  | m2    | 116  | OMU  | C1'-C2'-O2'-CM2 |
| 46  | m2    | 519  | OMC  | O4'-C4'-C5'-O5' |
| 46  | m2    | 646  | OMG  | C1'-C2'-O2'-CM2 |
| 46  | m2    | 685  | OMG  | O4'-C4'-C5'-O5' |
| 46  | m2    | 824  | PSU  | C2'-C1'-C5-C6   |
| 46  | m2    | 824  | PSU  | C3'-C4'-C5'-O5' |
| 46  | m2    | 824  | PSU  | O4'-C4'-C5'-O5' |
| 46  | m2    | 1250 | B8N  | O4'-C1'-C5-C6   |
| 46  | m2    | 1250 | B8N  | O4'-C1'-C5-C4   |
| 9   | A2    | 237  | B9B  | O4'-C4'-C5'-O5' |
| 9   | A2    | 398  | A2M  | O4'-C4'-C5'-O5' |
| 9   | A2    | 1395 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 1668 | UR3  | C3'-C4'-C5'-O5' |
| 9   | A2    | 1685 | OMG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 2119 | OMG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3420 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3523 | A2M  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3536 | P7G  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3543 | OMC  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3945 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 4288 | PSU  | C3'-C4'-C5'-O5' |
| 46  | m2    | 166  | A2M  | O4'-C4'-C5'-O5' |
| 46  | m2    | 166  | A2M  | C3'-C4'-C5'-O5' |
| 46  | m2    | 685  | OMG  | C3'-C4'-C5'-O5' |
| 11  | C2    | 14   | OMU  | C4'-C5'-O5'-P   |
| 9   | A2    | 1347 | A2M  | O4'-C4'-C5'-O5' |
| 9   | A2    | 1438 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 2528 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3945 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 4023 | MHG  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | A2    | 4102 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 4102 | PSU  | O4'-C4'-C5'-O5' |
| 46  | m2    | 1245 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3385 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 4152 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3357 | OMC  | C2'-C1'-N1-C6   |
| 46  | m2    | 1832 | UR3  | C2'-C1'-N1-C6   |
| 9   | A2    | 1347 | A2M  | C3'-C4'-C5'-O5' |
| 9   | A2    | 1438 | OMG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3438 | 5MC  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3846 | I4U  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3872 | 6MZ  | C3'-C4'-C5'-O5' |
| 46  | m2    | 519  | OMC  | C3'-C4'-C5'-O5' |
| 9   | A2    | 398  | A2M  | C3'-C4'-C5'-O5' |
| 9   | A2    | 2179 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 2179 | OMG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3543 | OMC  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3872 | 6MZ  | O4'-C4'-C5'-O5' |
| 9   | A2    | 4067 | 1MA  | O4'-C4'-C5'-O5' |
| 9   | A2    | 4152 | PSU  | O4'-C4'-C5'-O5' |
| 9   | A2    | 2052 | E7G  | C72-C71-N7-C8   |
| 9   | A2    | 3543 | OMC  | C4'-C5'-O5'-P   |
| 9   | A2    | 4023 | MHG  | C3'-C4'-C5'-O5' |
| 9   | A2    | 4067 | 1MA  | C3'-C4'-C5'-O5' |
| 9   | A2    | 1711 | P7G  | C72-C71-N7-C8   |
| 9   | A2    | 3441 | A2M  | O4'-C4'-C5'-O5' |
| 46  | m2    | 1245 | PSU  | C3'-C4'-C5'-O5' |
| 9   | A2    | 3441 | A2M  | C3'-C4'-C5'-O5' |
| 9   | A2    | 4007 | E6G  | O4'-C4'-C5'-O5' |
| 9   | A2    | 4099 | 5MC  | O4'-C1'-N1-C6   |
| 46  | m2    | 1033 | A2M  | C1'-C2'-O2'-CM' |
| 9   | A2    | 4099 | 5MC  | O4'-C1'-N1-C2   |
| 9   | A2    | 1438 | OMG  | C4'-C5'-O5'-P   |
| 46  | m2    | 670  | A2M  | C4'-C5'-O5'-P   |
| 9   | A2    | 4289 | OMG  | C3'-C4'-C5'-O5' |
| 46  | m2    | 1832 | UR3  | O4'-C1'-N1-C6   |
| 46  | m2    | 1832 | UR3  | C2'-C1'-N1-C2   |
| 9   | A2    | 3357 | OMC  | O4'-C1'-N1-C6   |
| 9   | A2    | 2052 | E7G  | C3'-C4'-C5'-O5' |
| 46  | m2    | 1250 | B8N  | N3-C31-C32-C33  |
| 46  | m2    | 166  | A2M  | C4'-C5'-O5'-P   |
| 9   | A2    | 3357 | OMC  | C2'-C1'-N1-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 46  | m2    | 1832 | UR3  | O4'-C1'-N1-C2   |
| 9   | A2    | 2179 | OMG  | C4'-C5'-O5'-P   |
| 9   | A2    | 3958 | OMU  | C4'-C5'-O5'-P   |
| 9   | A2    | 3987 | 5MC  | C4'-C5'-O5'-P   |
| 9   | A2    | 4152 | PSU  | C4'-C5'-O5'-P   |
| 9   | A2    | 4288 | PSU  | C4'-C5'-O5'-P   |
| 9   | A2    | 1490 | PSU  | O4'-C1'-C5-C4   |
| 9   | A2    | 4102 | PSU  | O4'-C1'-C5-C4   |
| 9   | A2    | 4152 | PSU  | O4'-C1'-C5-C4   |
| 9   | A2    | 4288 | PSU  | O4'-C1'-C5-C4   |
| 46  | m2    | 1245 | PSU  | O4'-C1'-C5-C4   |
| 46  | m2    | 519  | OMC  | C4'-C5'-O5'-P   |
| 9   | A2    | 3357 | OMC  | O4'-C1'-N1-C2   |
| 9   | A2    | 3357 | OMC  | C3'-C2'-O2'-CM2 |
| 46  | m2    | 519  | OMC  | C3'-C2'-O2'-CM2 |
| 9   | A2    | 1599 | E7G  | O4'-C4'-C5'-O5' |
| 9   | A2    | 373  | OMG  | C4'-C5'-O5'-P   |
| 9   | A2    | 1387 | B9B  | C4'-C5'-O5'-P   |
| 46  | m2    | 1083 | PSU  | C4'-C5'-O5'-P   |
| 9   | A2    | 2052 | E7G  | O4'-C4'-C5'-O5' |
| 9   | A2    | 4289 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A2    | 3536 | P7G  | N7-C71-C72-C73  |
| 79  | m     | 714  | DDE  | CA-CB-CG-CD2    |
| 9   | A2    | 1438 | OMG  | C2'-C1'-N9-C8   |
| 9   | A2    | 1711 | P7G  | C72-C71-N7-C5   |
| 46  | m2    | 646  | OMG  | C4'-C5'-O5'-P   |
| 79  | m     | 714  | DDE  | CA-CB-CG-ND1    |
| 9   | A2    | 4023 | MHG  | C2'-C1'-N9-C4   |
| 9   | A2    | 1438 | OMG  | C2'-C1'-N9-C4   |
| 9   | A2    | 4183 | PSU  | C2'-C1'-C5-C6   |
| 9   | A2    | 3872 | 6MZ  | C4'-C5'-O5'-P   |
| 9   | A2    | 3441 | A2M  | C2'-C1'-N9-C8   |
| 9   | A2    | 2177 | OMC  | O4'-C1'-N1-C6   |
| 9   | A2    | 2177 | OMC  | O4'-C1'-N1-C2   |
| 9   | A2    | 1337 | A2M  | O4'-C1'-N9-C8   |

There are no ring outliers.

48 monomers are involved in 81 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | A2    | 1496 | PSU  | 2       | 0            |
| 9   | A2    | 3420 | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | A2    | 1852 | OMG  | 3       | 0            |
| 9   | A2    | 3543 | OMC  | 1       | 0            |
| 9   | A2    | 1673 | A2M  | 1       | 0            |
| 9   | A2    | 1599 | E7G  | 1       | 0            |
| 9   | A2    | 1140 | A2M  | 5       | 0            |
| 9   | A2    | 1668 | UR3  | 1       | 0            |
| 9   | A2    | 2277 | G7M  | 1       | 0            |
| 9   | A2    | 4272 | OMU  | 2       | 0            |
| 46  | m2    | 614  | PSU  | 2       | 0            |
| 9   | A2    | 3481 | A2M  | 2       | 0            |
| 9   | A2    | 3846 | I4U  | 1       | 0            |
| 46  | m2    | 519  | OMC  | 1       | 0            |
| 9   | A2    | 3379 | A2M  | 5       | 0            |
| 9   | A2    | 878  | 2MG  | 1       | 0            |
| 9   | A2    | 3837 | B8W  | 1       | 0            |
| 9   | A2    | 4188 | OMC  | 2       | 0            |
| 46  | m2    | 1832 | UR3  | 1       | 0            |
| 9   | A2    | 2118 | A2M  | 1       | 0            |
| 9   | A2    | 3565 | OMC  | 2       | 0            |
| 9   | A2    | 4275 | OMG  | 2       | 0            |
| 9   | A2    | 4152 | PSU  | 1       | 0            |
| 46  | m2    | 1245 | PSU  | 2       | 0            |
| 46  | m2    | 1033 | A2M  | 1       | 0            |
| 9   | A2    | 2559 | OMC  | 1       | 0            |
| 9   | A2    | 3945 | PSU  | 1       | 0            |
| 9   | A2    | 1347 | A2M  | 1       | 0            |
| 46  | m2    | 116  | OMU  | 3       | 0            |
| 9   | A2    | 4223 | A2M  | 2       | 0            |
| 9   | A2    | 3872 | 6MZ  | 2       | 0            |
| 9   | A2    | 2177 | OMC  | 3       | 0            |
| 46  | m2    | 27   | A2M  | 3       | 0            |
| 46  | m2    | 825  | PSU  | 1       | 0            |
| 9   | A2    | 4183 | PSU  | 1       | 0            |
| 79  | m     | 714  | DDE  | 2       | 0            |
| 9   | A2    | 1269 | B8Q  | 1       | 0            |
| 9   | A2    | 1387 | B9B  | 2       | 0            |
| 9   | A2    | 373  | OMG  | 1       | 0            |
| 46  | m2    | 685  | OMG  | 1       | 0            |
| 9   | A2    | 2052 | E7G  | 1       | 0            |
| 9   | A2    | 3523 | A2M  | 2       | 0            |
| 9   | A2    | 4099 | 5MC  | 1       | 0            |
| 9   | A2    | 4288 | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 46  | m2    | 824  | PSU  | 1       | 0            |
| 9   | A2    | 4517 | 2MG  | 1       | 0            |
| 9   | A2    | 4515 | OMG  | 5       | 0            |
| 9   | A2    | 3385 | PSU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 88  | GDP  | m     | 900 | -    | 29,30,30     | 3.23 | 17 (58%)    | 45,47,47    | 2.11 | 12 (26%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 88  | GDP  | m     | 900 | -    | -       | 4/16/32/32 | 0/3/3/3 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 88  | m     | 900 | GDP  | C4-N3   | 6.54  | 1.49        | 1.34     |
| 88  | m     | 900 | GDP  | O4'-C4' | -6.03 | 1.31        | 1.45     |
| 88  | m     | 900 | GDP  | C2-N3   | 5.58  | 1.46        | 1.33     |
| 88  | m     | 900 | GDP  | C3'-C4' | 5.48  | 1.66        | 1.53     |
| 88  | m     | 900 | GDP  | PA-O3A  | 5.28  | 1.65        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 88  | m     | 900 | GDP  | C1'-N9  | -5.21 | 1.32        | 1.47     |
| 88  | m     | 900 | GDP  | C2-N2   | 4.70  | 1.45        | 1.34     |
| 88  | m     | 900 | GDP  | O4'-C1' | 4.27  | 1.51        | 1.42     |
| 88  | m     | 900 | GDP  | O2'-C2' | 3.15  | 1.50        | 1.43     |
| 88  | m     | 900 | GDP  | C2-N1   | 2.86  | 1.44        | 1.37     |
| 88  | m     | 900 | GDP  | O6-C6   | -2.54 | 1.18        | 1.23     |
| 88  | m     | 900 | GDP  | C5-C6   | 2.53  | 1.53        | 1.44     |
| 88  | m     | 900 | GDP  | C6-N1   | 2.50  | 1.43        | 1.38     |
| 88  | m     | 900 | GDP  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 88  | m     | 900 | GDP  | C4-N9   | -2.26 | 1.32        | 1.38     |
| 88  | m     | 900 | GDP  | C2'-C1' | 2.17  | 1.60        | 1.53     |
| 88  | m     | 900 | GDP  | O3'-C3' | 2.14  | 1.48        | 1.43     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 88  | m     | 900 | GDP  | C1'-N9-C8   | -6.41 | 108.53      | 126.73   |
| 88  | m     | 900 | GDP  | N9-C8-N7    | -4.82 | 104.46      | 113.40   |
| 88  | m     | 900 | GDP  | C5-C4-N3    | -4.49 | 121.25      | 128.39   |
| 88  | m     | 900 | GDP  | C2-N3-C4    | 4.12  | 119.39      | 112.30   |
| 88  | m     | 900 | GDP  | C1'-N9-C4   | 4.11  | 138.62      | 126.49   |
| 88  | m     | 900 | GDP  | N9-C4-N3    | 3.89  | 133.72      | 125.95   |
| 88  | m     | 900 | GDP  | C8-N9-C4    | 3.64  | 112.85      | 106.03   |
| 88  | m     | 900 | GDP  | C2-N1-C6    | -2.90 | 119.85      | 125.11   |
| 88  | m     | 900 | GDP  | C8-N7-C5    | 2.74  | 109.14      | 104.26   |
| 88  | m     | 900 | GDP  | C5-C6-N1    | 2.61  | 119.90      | 113.25   |
| 88  | m     | 900 | GDP  | O6-C6-C5    | -2.47 | 120.00      | 126.53   |
| 88  | m     | 900 | GDP  | O4'-C4'-C3' | 2.16  | 109.45      | 105.15   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

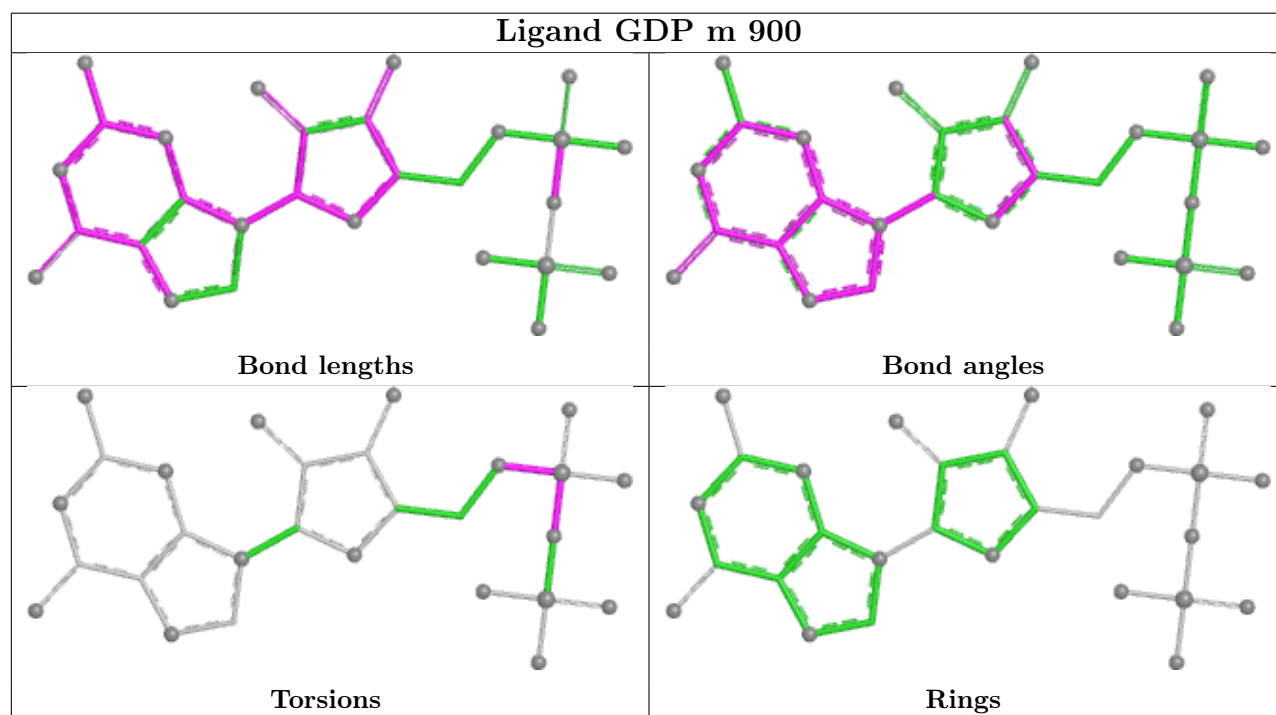
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 88  | m     | 900 | GDP  | C5'-O5'-PA-O3A |
| 88  | m     | 900 | GDP  | C5'-O5'-PA-O1A |
| 88  | m     | 900 | GDP  | C5'-O5'-PA-O2A |
| 88  | m     | 900 | GDP  | PB-O3A-PA-O2A  |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 88  | m     | 900 | GDP  | 1       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



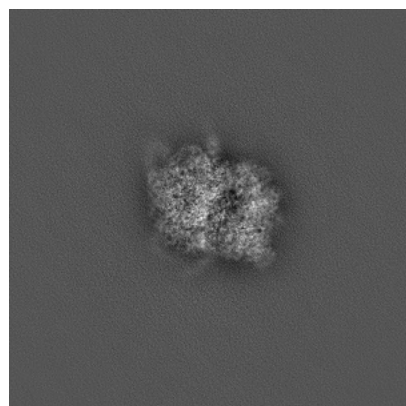
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23501. These allow visual inspection of the internal detail of the map and identification of artifacts.

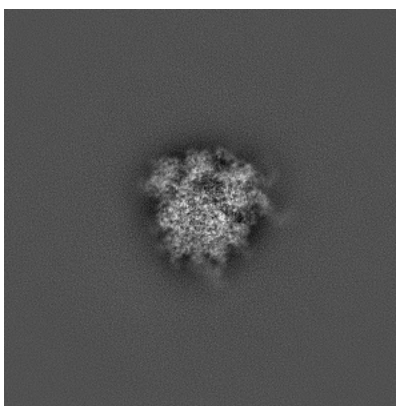
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

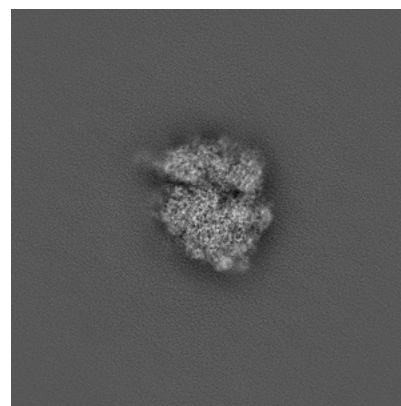
#### 6.1.1 Primary map



X

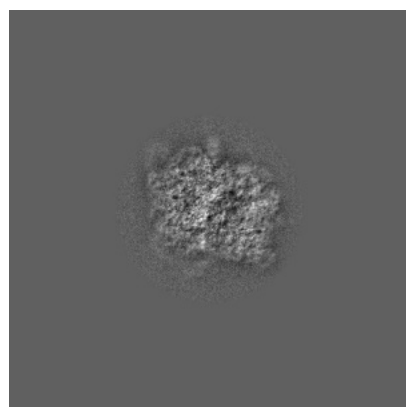


Y

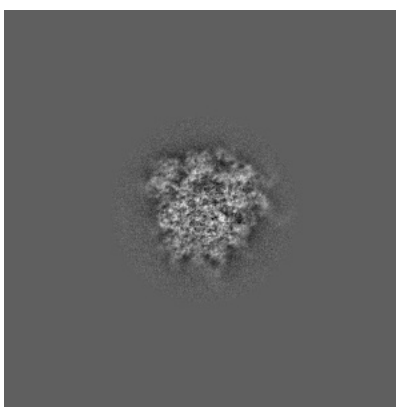


Z

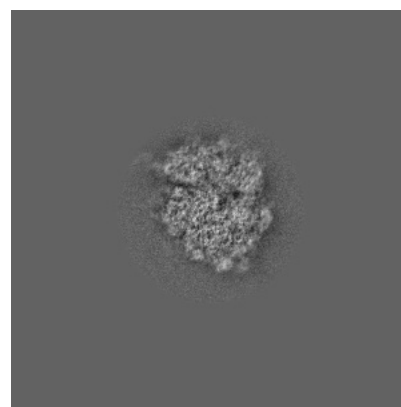
#### 6.1.2 Raw map



X



Y

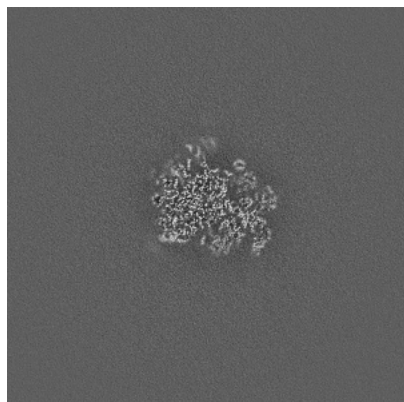


Z

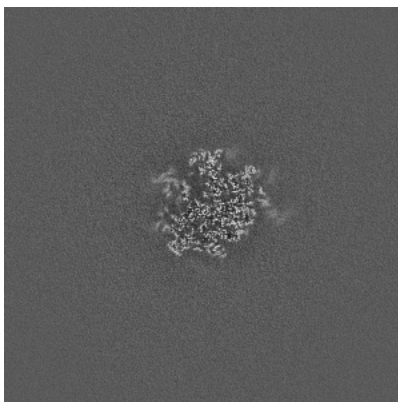
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

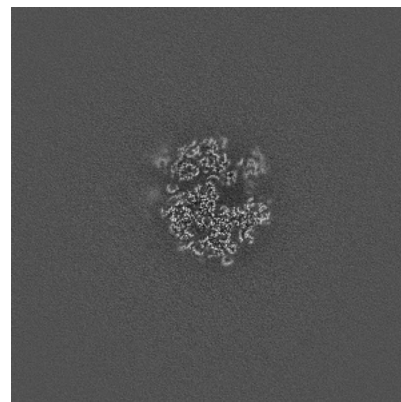
### 6.2.1 Primary map



X Index: 384

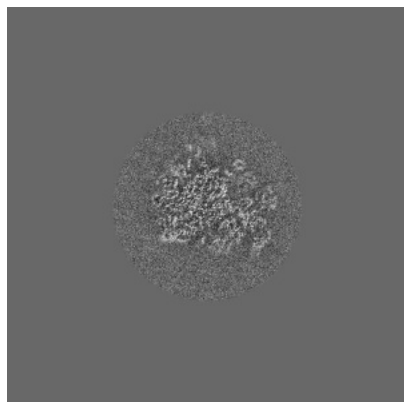


Y Index: 384

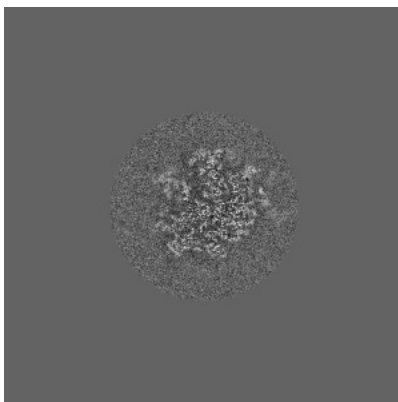


Z Index: 384

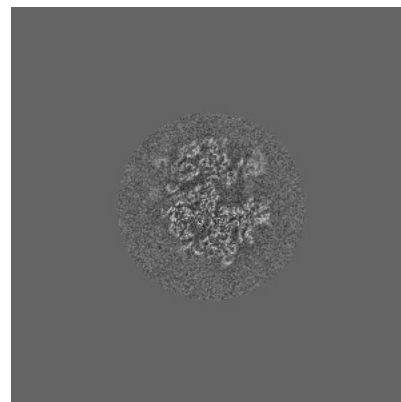
### 6.2.2 Raw map



X Index: 384



Y Index: 384

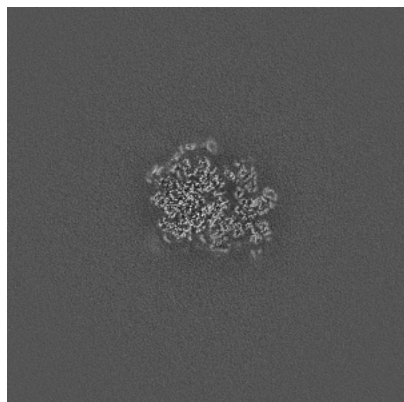


Z Index: 384

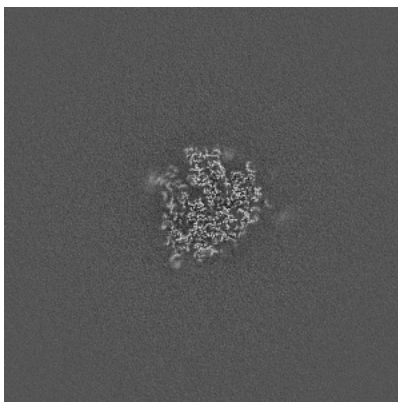
The images above show central slices of the map in three orthogonal directions.

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

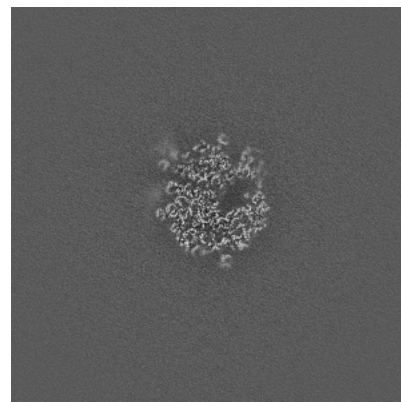
### 6.3.1 Primary map



X Index: 390

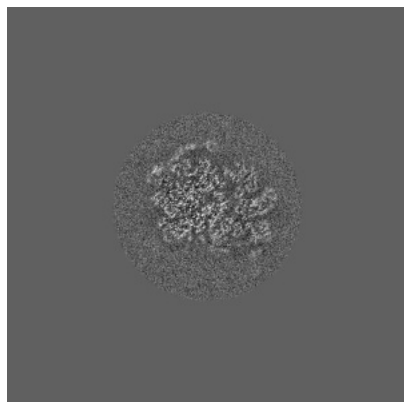


Y Index: 376

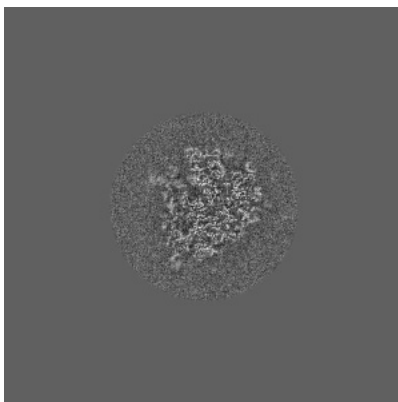


Z Index: 375

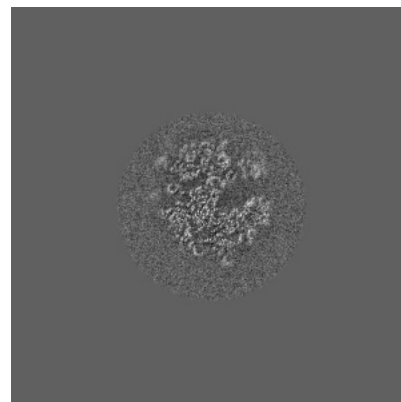
### 6.3.2 Raw map



X Index: 390



Y Index: 376

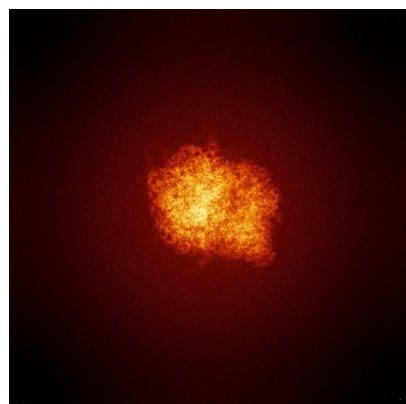


Z Index: 381

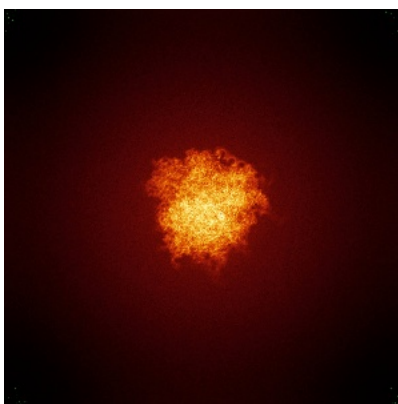
The images above show the largest variance slices of the map in three orthogonal directions.

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

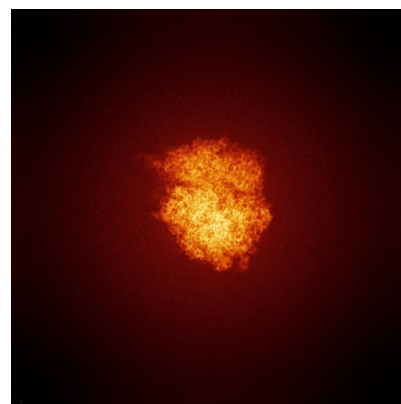
### 6.4.1 Primary map



X

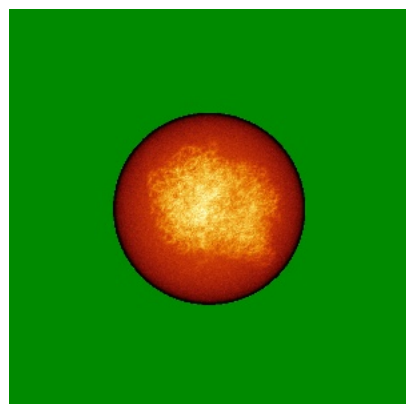


Y

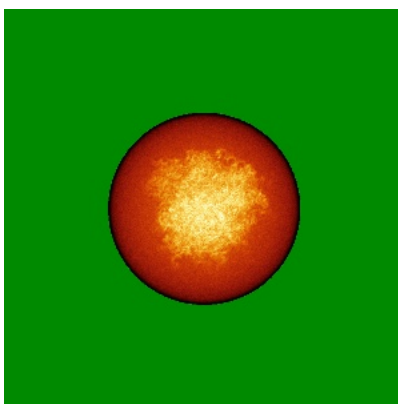


Z

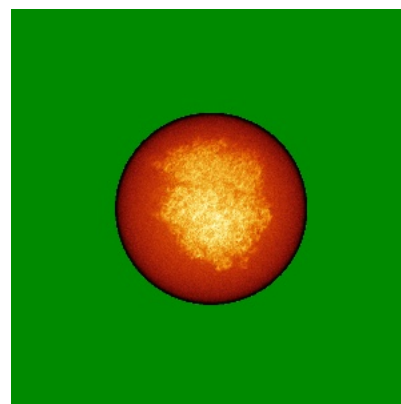
### 6.4.2 Raw map



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



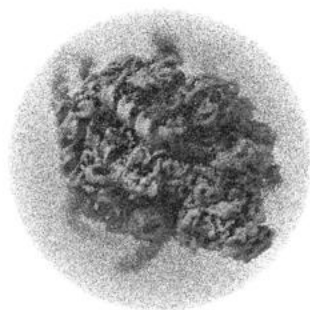
Y



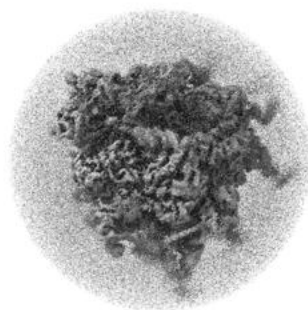
Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

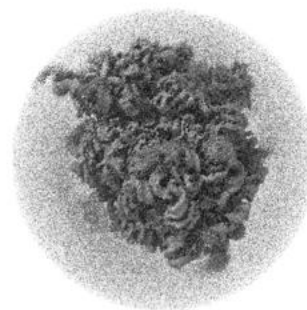
### 6.5.2 Raw map



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.

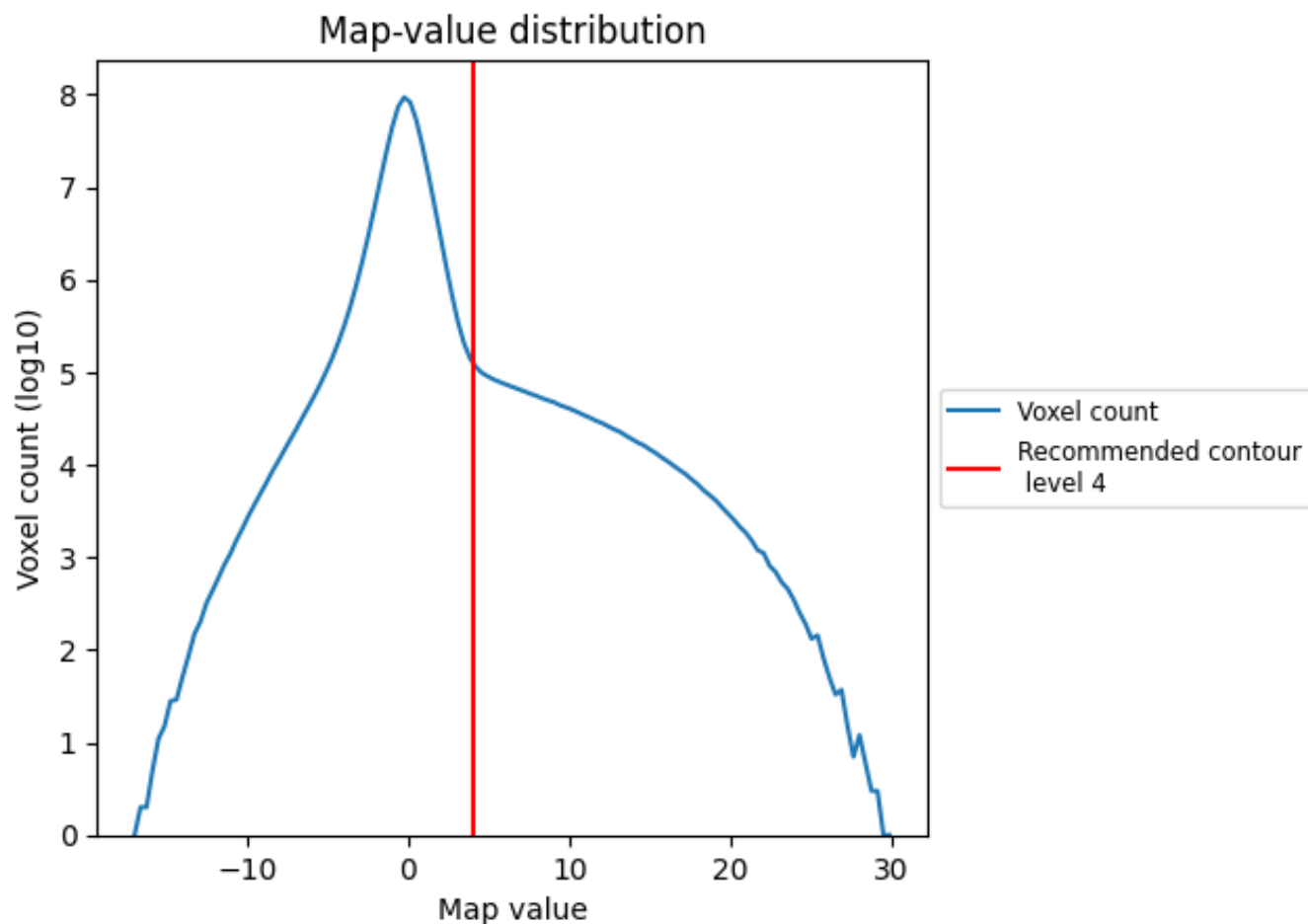
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

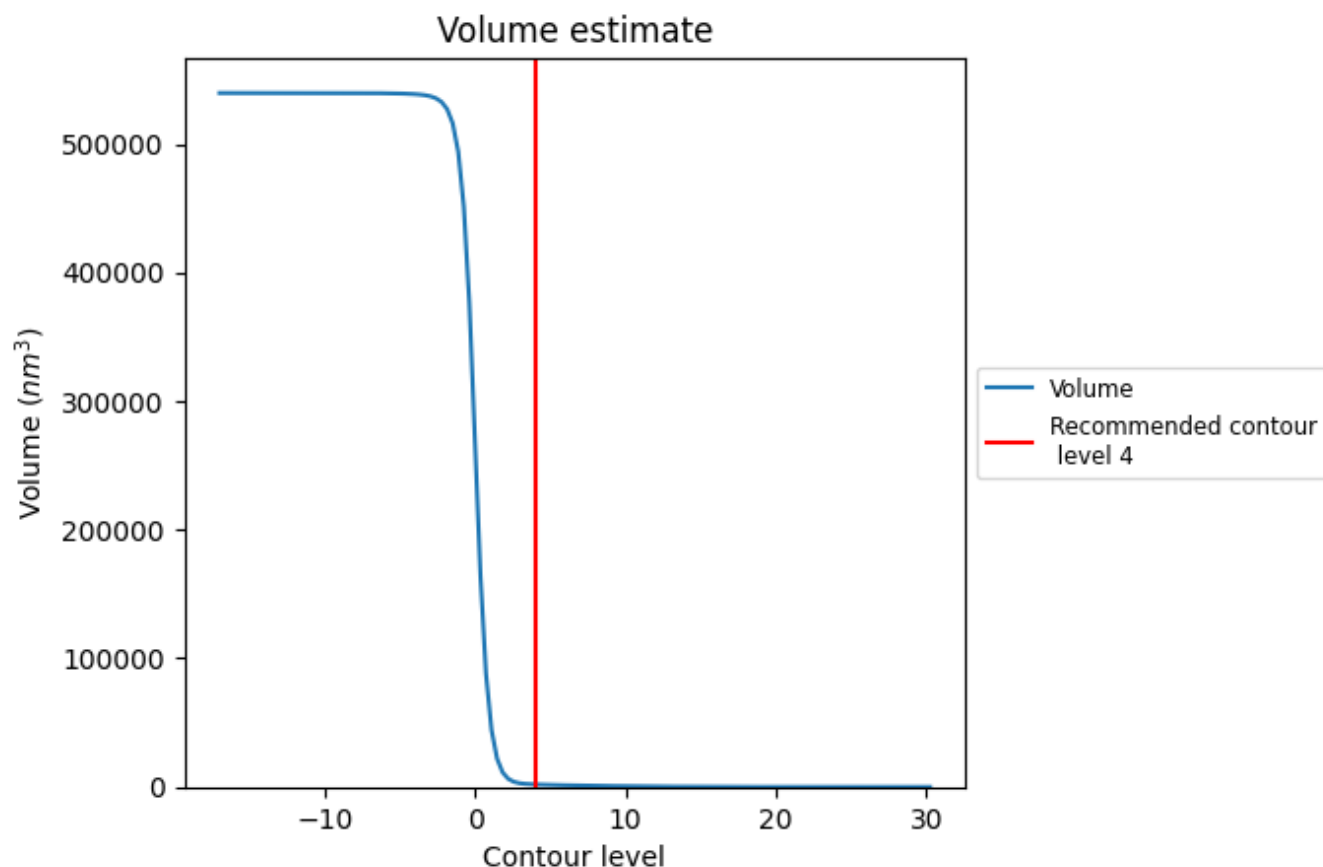
This section contains the results of statistical analysis of the map.

### 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](#)

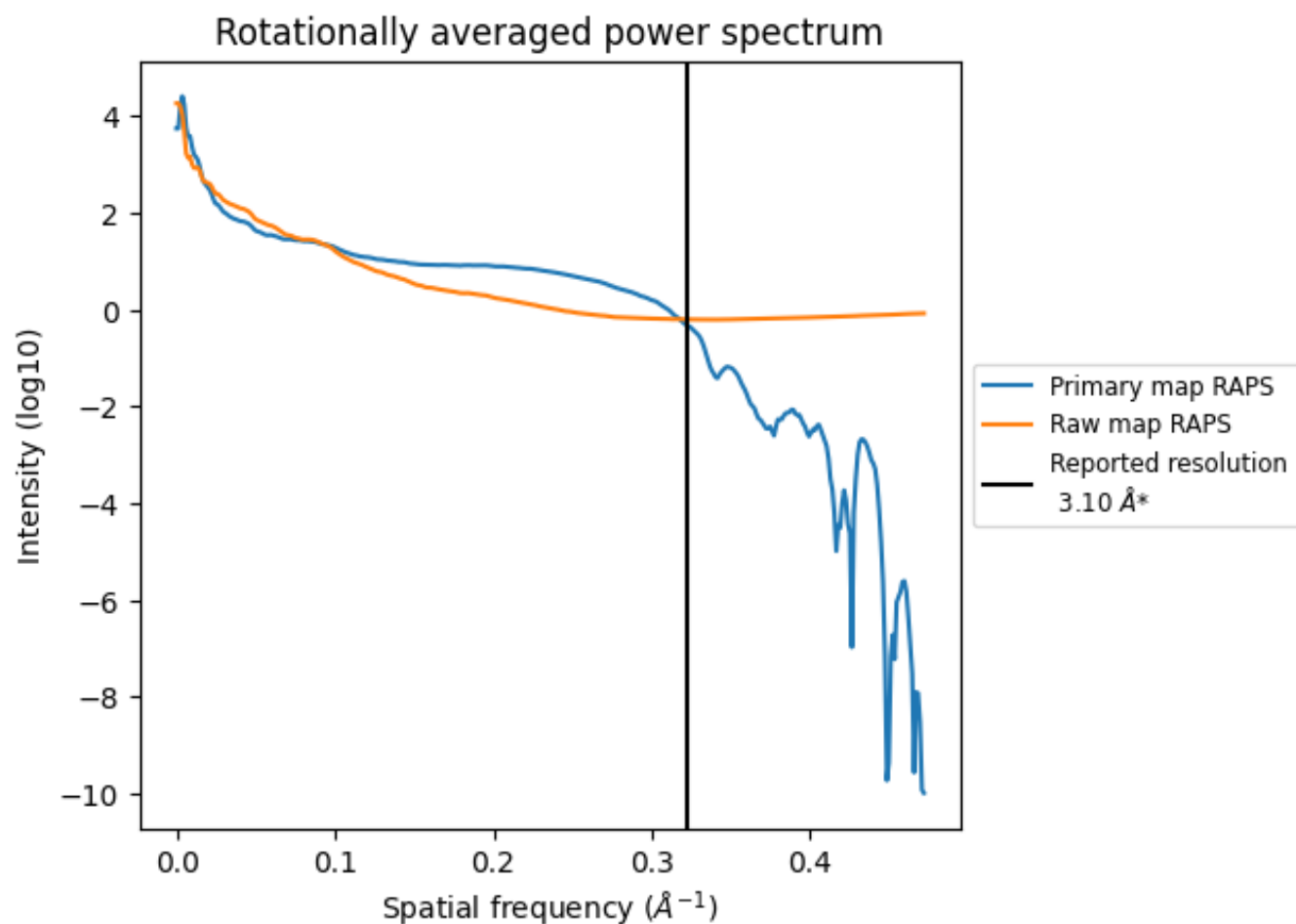


The volume at the recommended contour level is 1947  $\text{nm}^3$ ; this corresponds to an approximate mass of 1759 kDa.

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 ⓘ



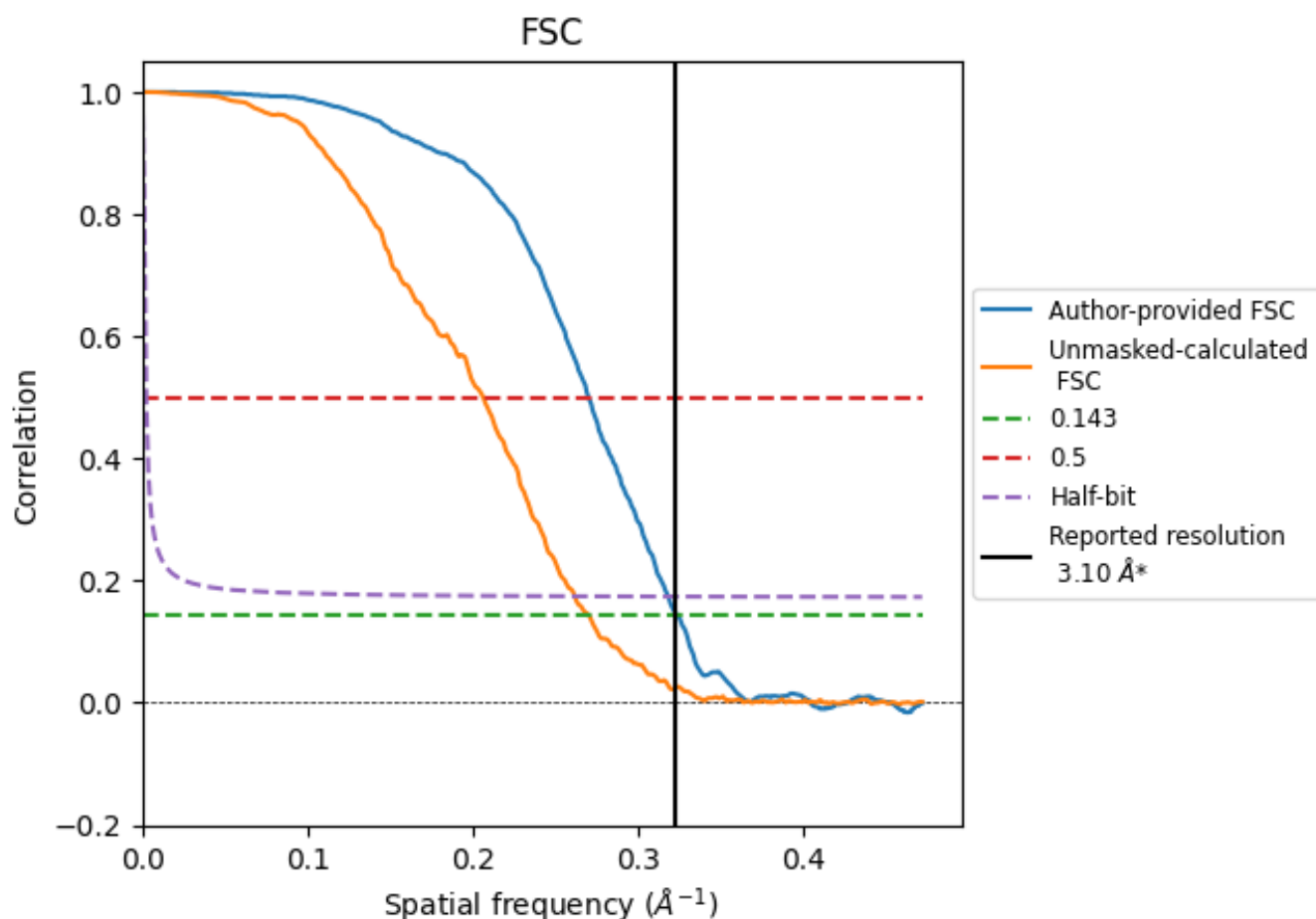
\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>



## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

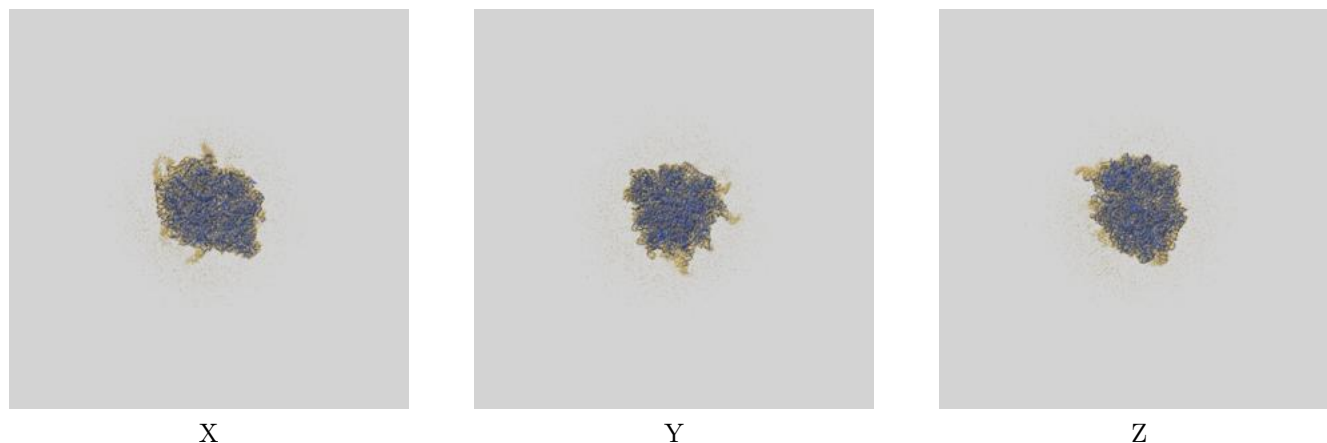
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.10                               | -    | -        |
| Author-provided FSC curve | 3.08                               | 3.71 | 3.14     |
| Unmasked-calculated*      | 3.70                               | 4.85 | 3.82     |

\*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 3.70 differs from the reported value 3.1 by more than 10 %

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

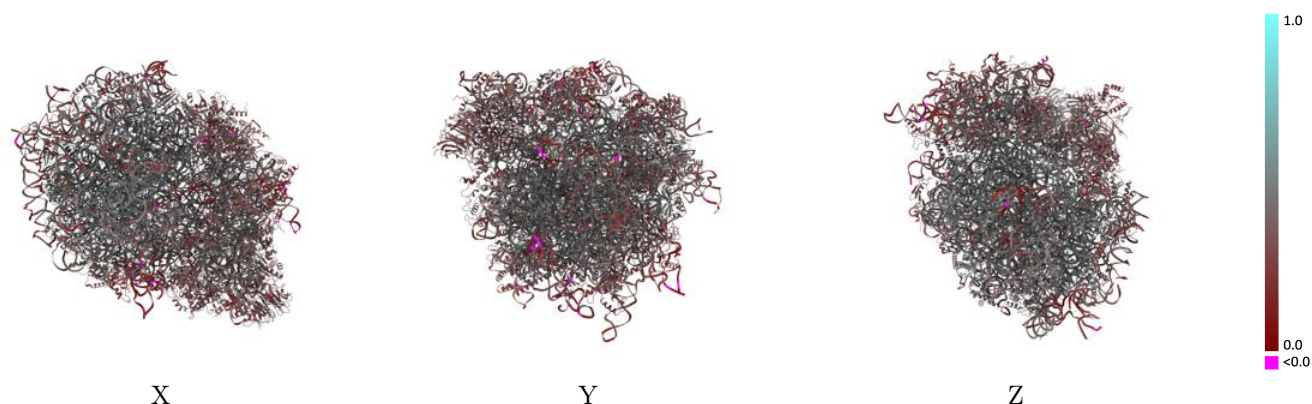
This section contains information regarding the fit between EMDB map EMD-23501 and PDB model 7LS2. Per-residue inclusion information can be found in section 3 on page 21.

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



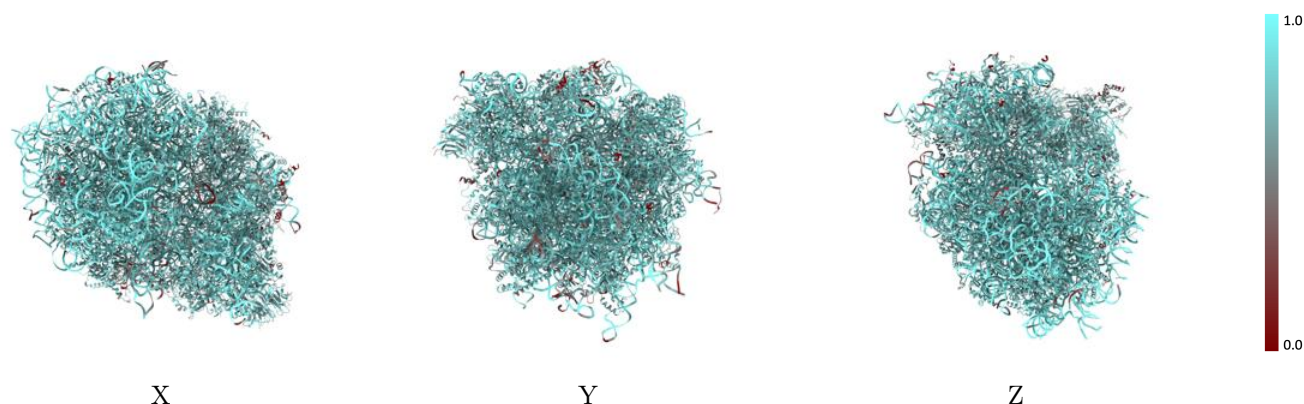
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



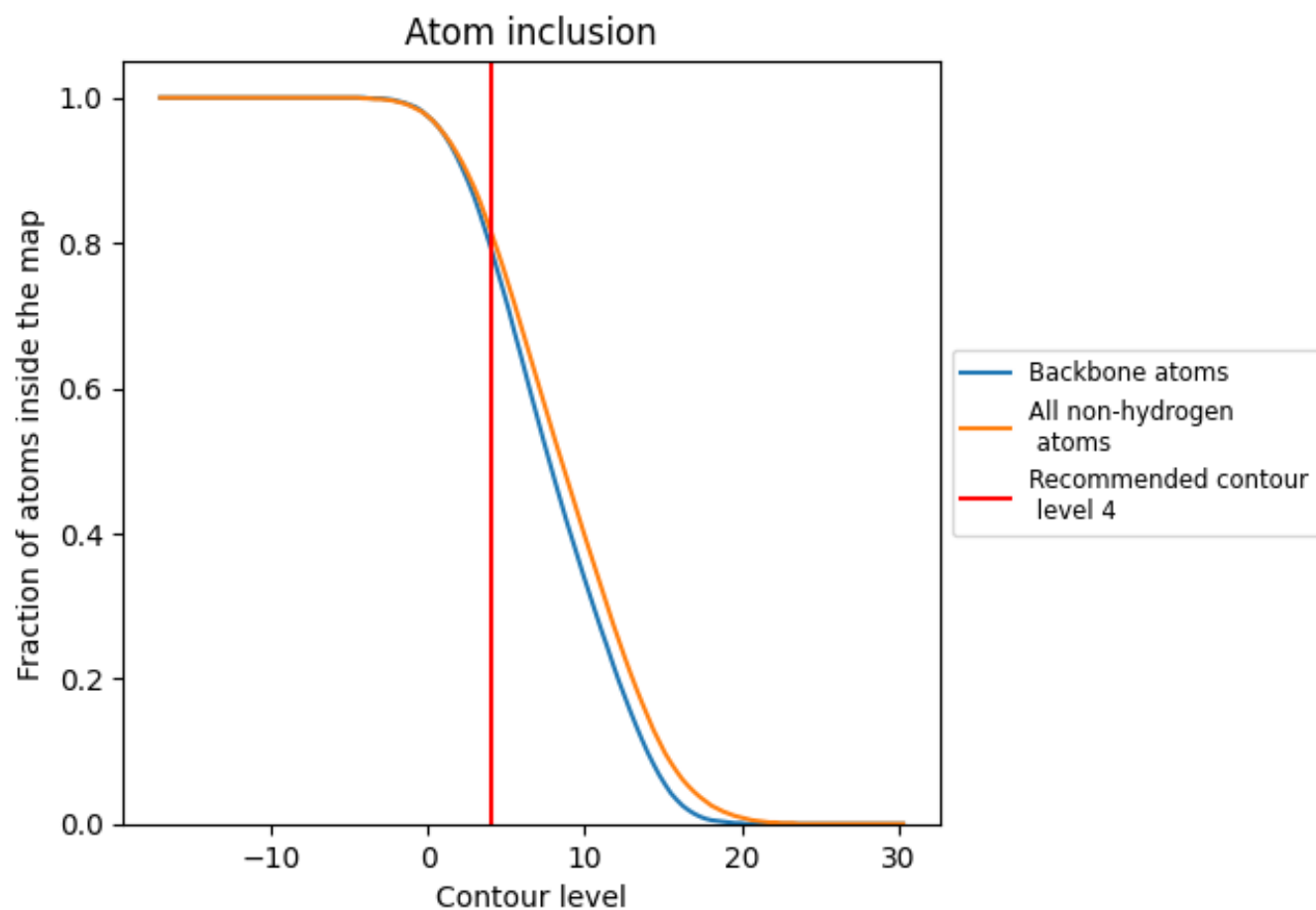
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 82% 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 (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8180   |  0.4180   |
| A     |  0.4700   |  0.3630   |
| A1    |  0.7780   |  0.4580   |
| A2    |  0.8970   |  0.4300   |
| A3    |  0.7120   |  0.3420   |
| B1    |  0.7880   |  0.4240   |
| B2    |  0.9540   |  0.4720   |
| B3    |  0.7440   |  0.3570   |
| C1    |  0.7800   |  0.4590   |
| C2    |  0.9040   |  0.4380   |
| C3    |  0.7140   |  0.3830   |
| D1    |  0.7730   |  0.4580   |
| D2    |  0.7590   |  0.4860   |
| D3    |  0.7780   |  0.4410   |
| E1    |  0.7680  |  0.4040  |
| E2    |  0.7830 |  0.4710 |
| E3    |  0.6950 |  0.4540 |
| F1    |  0.8060 |  0.4500 |
| F2    |  0.7790 |  0.4700 |
| F3    |  0.7430 |  0.4340 |
| G1    |  0.8210 |  0.4530 |
| G2    |  0.8280 |  0.4350 |
| G3    |  0.5950 |  0.3320 |
| H1    |  0.8020 |  0.4830 |
| H2    |  0.8040 |  0.4460 |
| H3    |  0.7470 |  0.4140 |
| I2    |  0.7930 |  0.4640 |
| I3    |  0.7380 |  0.3410 |
| J2    |  0.8090 |  0.4840 |
| J3    |  0.7490 |  0.4370 |
| K2    |  0.7850 |  0.4790 |
| K3    |  0.6940 |  0.3330 |
| L1    |  0.5420 |  0.2240 |
| L2    |  0.7780 |  0.4350 |
| L3    |  0.7300 |  0.3840 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| M2    |  0.8200   |  0.4820   |
| M3    |  0.5300   |  0.2310   |
| N2    |  0.7910   |  0.4700   |
| N3    |  0.7250   |  0.4080   |
| O2    |  0.7560   |  0.3970   |
| O3    |  0.7060   |  0.3950   |
| P2    |  0.7270   |  0.4840   |
| P3    |  0.7230   |  0.4420   |
| Q2    |  0.7210   |  0.3850   |
| Q3    |  0.6740   |  0.3340   |
| R2    |  0.7830   |  0.4460   |
| R3    |  0.6790   |  0.3080   |
| S2    |  0.8010   |  0.4570   |
| S3    |  0.7300   |  0.4000   |
| T2    |  0.8160   |  0.4530   |
| T3    |  0.6970   |  0.4040   |
| U2    |  0.8140   |  0.4920   |
| U3    |  0.6830  |  0.2920  |
| V2    |  0.7270 |  0.4210 |
| W2    |  0.7940 |  0.4470 |
| X2    |  0.7890 |  0.4580 |
| Y2    |  0.7800 |  0.4850 |
| Z2    |  0.8150 |  0.4950 |
| a2    |  0.7790 |  0.4630 |
| b2    |  0.7760 |  0.4260 |
| c2    |  0.8060 |  0.4400 |
| d2    |  0.7870 |  0.4870 |
| e2    |  0.7230 |  0.4070 |
| f2    |  0.7610 |  0.4530 |
| g2    |  0.7890 |  0.4750 |
| h2    |  0.7030 |  0.4520 |
| i2    |  0.7770 |  0.4710 |
| j     |  0.7270 |  0.3390 |
| j2    |  0.7560 |  0.4500 |
| k     |  0.6280 |  0.2890 |
| k2    |  0.8350 |  0.4750 |
| m     |  0.7040 |  0.3900 |
| m2    |  0.8860 |  0.3980 |
| n2    |  0.8430 |  0.3610 |
| o2    |  0.7720 |  0.4090 |
| p2    |  0.7020 |  0.3900 |
| q2    |  0.7120 |  0.3860 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| r2    |  0.7160 |  0.4040 |
| s2    |  0.6480 |  0.3140 |
| t     |  0.7170 |  0.3620 |
| u     |  0.6780 |  0.3720 |
| v2    |  0.7150 |  0.3530 |
| w2    |  0.6800 |  0.4210 |
| x2    |  0.7060 |  0.3510 |
| y2    |  0.7120 |  0.3540 |
| z2    |  0.7150 |  0.3830 |