



## Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 05:43 AM EDT

PDB ID : 6XA1 / pdb\_00006xa1  
EMDB ID : EMD-22085  
Title : Structure of a drug-like compound stalled human translation termination complex  
Authors : Li, W.; Cate, J.  
Deposited on : 2020-06-03  
Resolution : 2.80 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:

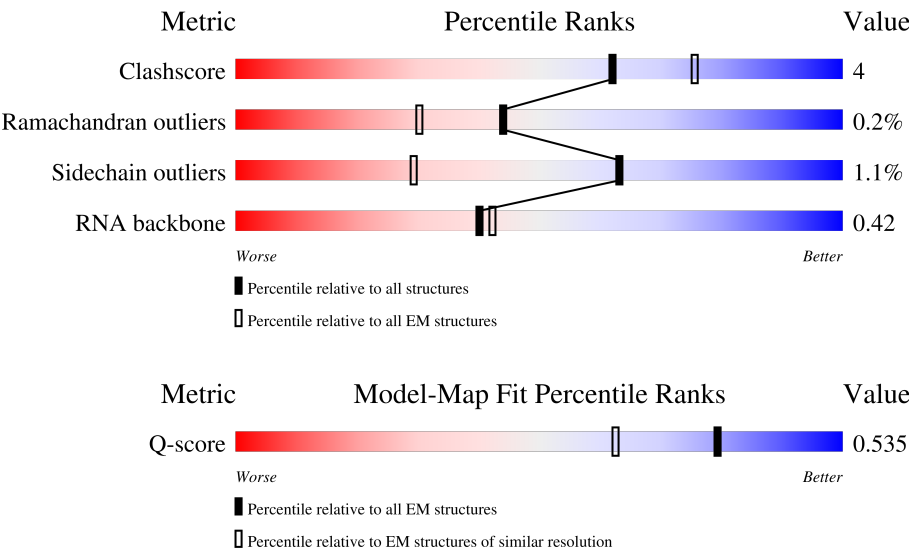
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.80 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.



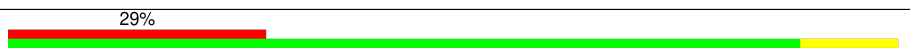
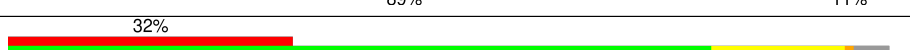
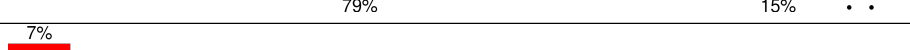
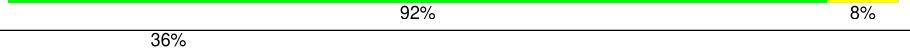
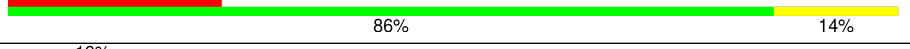
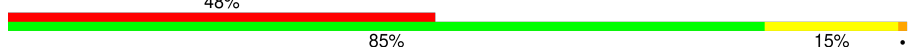
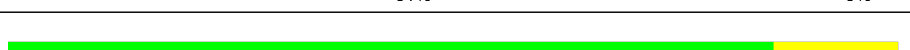
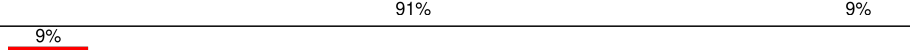
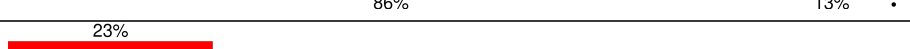
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11806 ( 2.30 - 3.30 )                                    |

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   | LA    | 248    | <div> <div>14%</div> <div>86%</div> <div>14%</div> </div>              |
| 2   | LB    | 396    | <div> <div>14%</div> <div>90%</div> <div>10%</div> </div>              |
| 3   | L5    | 3510   | <div> <div>17%</div> <div>68%</div> <div>28%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | L7    | 120    |    |
| 5   | L8    | 155    |    |
| 6   | LC    | 358    |    |
| 7   | LD    | 290    |    |
| 8   | LE    | 247    |    |
| 9   | LF    | 225    |    |
| 10  | LG    | 241    |    |
| 11  | LH    | 190    |    |
| 12  | LI    | 213    |    |
| 13  | LJ    | 176    |    |
| 14  | LL    | 204    |    |
| 15  | LM    | 139    |    |
| 16  | LN    | 203    |   |
| 17  | LO    | 201    |  |
| 18  | LP    | 153    |  |
| 19  | LQ    | 187    |  |
| 20  | LR    | 187    |  |
| 21  | LS    | 175    |  |
| 22  | LT    | 159    |  |
| 23  | LU    | 101    |  |
| 24  | LV    | 131    |  |
| 25  | LW    | 124    |  |
| 26  | LX    | 120    |  |
| 27  | LY    | 134    |  |
| 28  | LZ    | 135    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | La    | 147    |                  |
| 30  | Lb    | 121    |                  |
| 31  | Lc    | 98     |                  |
| 32  | Ld    | 107    |                  |
| 33  | Le    | 128    |                  |
| 34  | Lf    | 109    |                  |
| 35  | Lg    | 114    |                  |
| 36  | Lh    | 122    |                  |
| 37  | Li    | 102    |                  |
| 38  | Lj    | 86     |                  |
| 39  | Lk    | 69     |                  |
| 40  | Ll    | 50     |                  |
| 41  | Lm    | 52     |                  |
| 42  | Ln    | 24     |                  |
| 43  | Lo    | 105    |                  |
| 44  | Lp    | 91     |                  |
| 45  | Lr    | 125    |                  |
| 46  | S2    | 1590   |                  |
| 47  | SA    | 216    |                  |
| 48  | SB    | 211    |                  |
| 49  | SD    | 224    |                  |
| 50  | SE    | 258    |                  |
| 51  | SF    | 189    |                  |
| 52  | SH    | 189    |                  |
| 53  | SI    | 205    |                  |

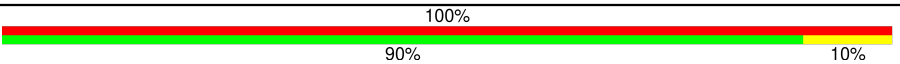
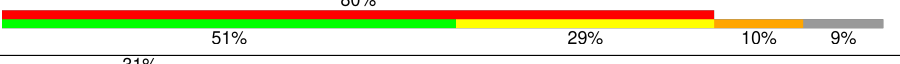
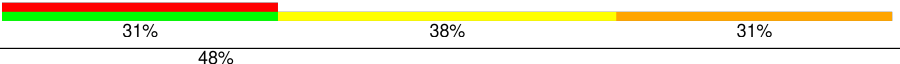
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | SK    | 95     |                  |
| 55  | SL    | 150    |                  |
| 56  | SP    | 131    |                  |
| 57  | SQ    | 140    |                  |
| 58  | SR    | 131    |                  |
| 59  | SS    | 143    |                  |
| 60  | ST    | 141    |                  |
| 61  | SU    | 100    |                  |
| 62  | SV    | 84     |                  |
| 63  | SX    | 139    |                  |
| 64  | Sa    | 99     |                  |
| 65  | Sc    | 61     |                  |
| 66  | Sd    | 55     |                  |
| 67  | Sg    | 313    |                  |
| 68  | SC    | 220    |                  |
| 69  | SG    | 228    |                  |
| 70  | SJ    | 180    |                  |
| 71  | SM    | 120    |                  |
| 72  | SN    | 150    |                  |
| 73  | SO    | 135    |                  |
| 74  | SW    | 129    |                  |
| 75  | SY    | 122    |                  |
| 76  | SZ    | 70     |                  |
| 77  | Sb    | 82     |                  |
| 78  | Se    | 54     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 79  | Sf    | 63     |  |
| 80  | Bv    | 76     |  |
| 81  | j     | 411    |  |
| 82  | k     | 13     |  |
| 83  | NC    | 25     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 46  | B8N  | S2    | 1248 | X         | -        | -       | -                |
| 81  | MEQ  | j     | 185  | -         | -        | X       | -                |

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 211887 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 L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | LA    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

- Molecule 2 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | LB    | 396      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3197  | 2036 | 601 | 546 | 14 |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | L5    | 3510     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 75317 | 33580 | 13769 | 24459 | 3509 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | L7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2562  | 1141 | 456 | 845 | 120 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5   | L8    | 155      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3298  | 1472 | 582 | 1089 | 155 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | LC    | 358      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2855  | 1797 | 570 | 473 | 15 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | LD    | 290      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2357  | 1493 | 428 | 422 | 14 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | LE    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1904  | 1222 | 361 | 317 | 4 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | LF    | 225      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1878  | 1207 | 361 | 301 | 9 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | LG    | 241      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1935  | 1233 | 374 | 324 | 4 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | LI    | 207      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1677  | 1064 | 323 | 276 | 14 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | LJ    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 888 | 263 | 253 | 6 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | LL    | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 1032 | 343 | 270 | 4 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | LM    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 730 | 218 | 183 | 7 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | LO    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LP    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | LR    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 971 | 336 | 250 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | LS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | LT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 23 is a protein called Heparin-binding protein HBp15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | LU    | 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  | LV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LW    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 634 | 207 | 170 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 630 | 185 | 169 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LY    | 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  | LZ    | 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  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Lb    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 882   | 549 | 192 | 137 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Lb    | 89      | ALA      | VAL    | conflict | UNP P47914 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Lc    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Ld    | 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  | Le    | 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  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Lg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Lj    | 86       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 713   | 439 | 158 | 111 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 39  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | Lm    | 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  | Ln    | 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  | Lo    | 105      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 870   | 547 | 178 | 139 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 46  | S2    | 1590     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 34012 | 15211 | 6116 | 11096 | 1589 |         |       |

- Molecule 47 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | SA    | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1083 | 299 | 315 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | SB    | 211      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1718  | 1091 | 307 | 306 | 14 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | SD    | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1745  | 1112 | 314 | 312 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | SE    | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2050  | 1311 | 381 | 350 | 8 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | SF    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1471  | 921 | 277 | 266 | 7 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | SH    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1490  | 953 | 272 | 264 | 1 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | SI    | 197      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1019 | 321 | 279 | 5 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | SK    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 524 | 139 | 130 | 6 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | SL    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1144  | 729 | 214 | 195 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | SP    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 682 | 204 | 182 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SQ    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1117  | 710 | 211 | 193 | 3 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | SR    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 668 | 198 | 194 | 4 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | SS    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 743 | 240 | 200 | 1 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | ST    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1094  | 685 | 210 | 196 | 3 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SU    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 798   | 501 | 152 | 141 | 4 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | SV    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 639   | 395 | 117 | 122 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| SV    | 0       | ACE      | -      | acetylation | UNP P63220 |

- Molecule 63 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | SX    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 682 | 214 | 181 | 3 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | Sa    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 65  | Sc    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 479   | 292 | 95 | 90 | 2 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 66  | Sd    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 67 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 67  | Sg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 68  | SC    | 220      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1715  | 1109 | 296 | 300 | 10 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 69  | SG    | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1848  | 1155 | 368 | 318 | 7 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SJ    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1499  | 955 | 300 | 242 | 2 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | SM    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 860   | 540 | 149 | 163 | 8 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | SO    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1010  | 618 | 198 | 188 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| SO    | 138     | IAS      | ASP    | conflict | UNP P62263 |

- Molecule 74 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | SY    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 635 | 196 | 166 | 5 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 76  | SZ    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 559   | 360 | 102 | 96 | 1 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Sb    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 640   | 402 | 118 | 113 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78  | Se    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 407   | 251 | 90 | 65 | 1 |         |       |

- Molecule 79 is a protein called 40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 79  | Sf    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 515   | 324 | 98 | 86 | 7 |         |       |

- Molecule 80 is a RNA chain called P-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 80  | Bv    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1621  | 725 | 289 | 532 | 75 |         |       |

- Molecule 81 is a protein called Eukaryotic peptide chain release factor subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 81  | j     | 373      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2930  | 1874 | 500 | 547 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| j     | 63      | UXY      | LYS    | conflict | UNP P62495 |

- Molecule 82 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 82  | k     | 13       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 270   | 122 | 44 | 91 | 13 |         |       |

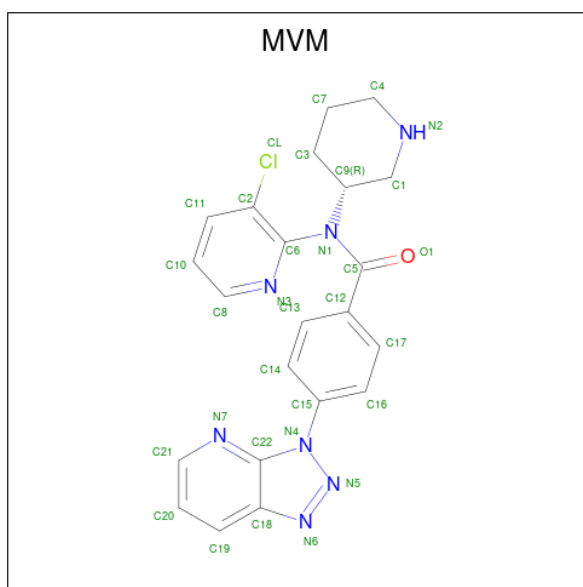
- Molecule 83 is a protein called Stalled Nascent chain.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 83  | NC    | 25       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 177   | 121 | 28 | 28 |         |       |

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 84  | L5    | 145      | Total | Mg  | 0       |
|     |       |          | 145   | 145 |         |
| 84  | L7    | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 84  | L8    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 84  | S2    | 35       | Total | Mg  | 0       |
|     |       |          | 35    | 35  |         |
| 84  | Bv    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 84  | k     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 85 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (CCD ID: MVM) (formula: C<sub>22</sub>H<sub>20</sub>ClN<sub>7</sub>O) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 85  | L5    | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 31    | 22 | 1  | 7 | 1 |         |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 86  | Lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Lm    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Lo    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Lp    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Sa    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Sd    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 86  | Sf    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

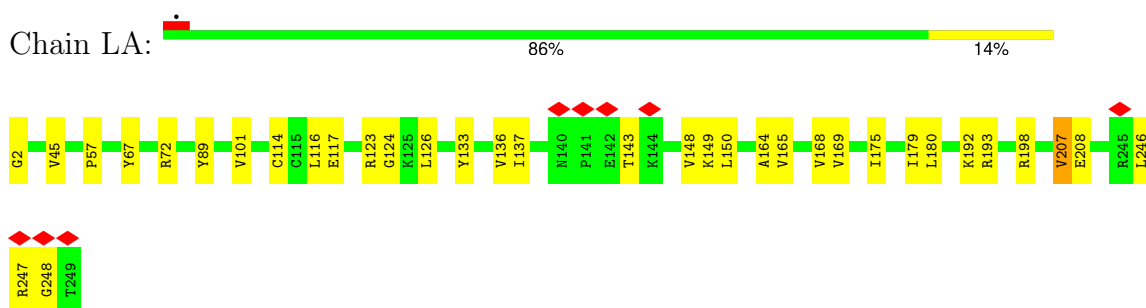
- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 87  | Bv    | 2        | Total | K | 0       |
|     |       |          | 2     | 2 |         |

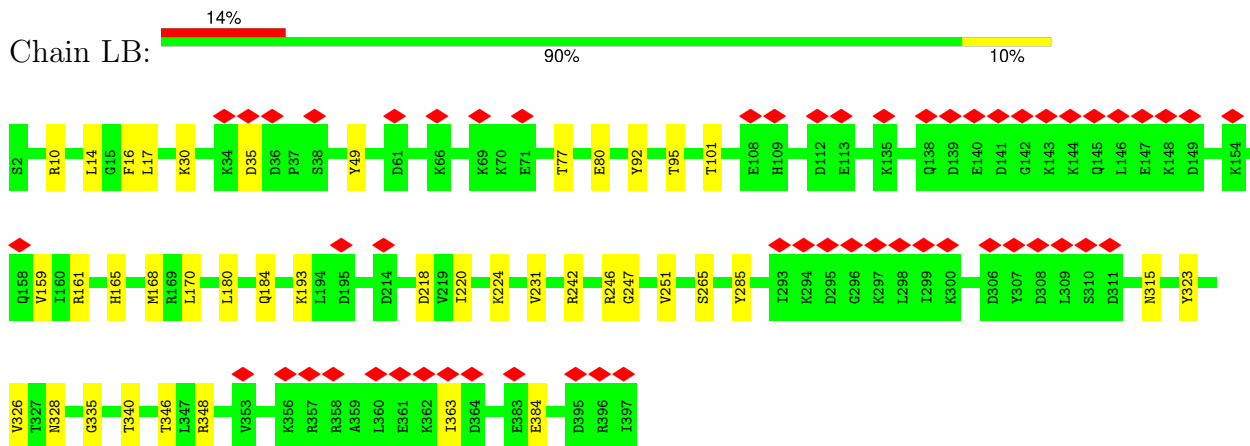
### 3 Residue-property plots

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.

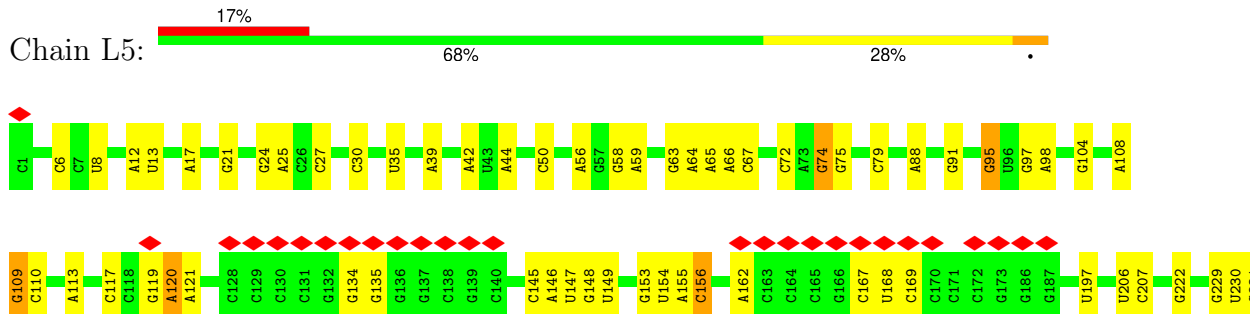
- Molecule 1: 60S ribosomal protein L8

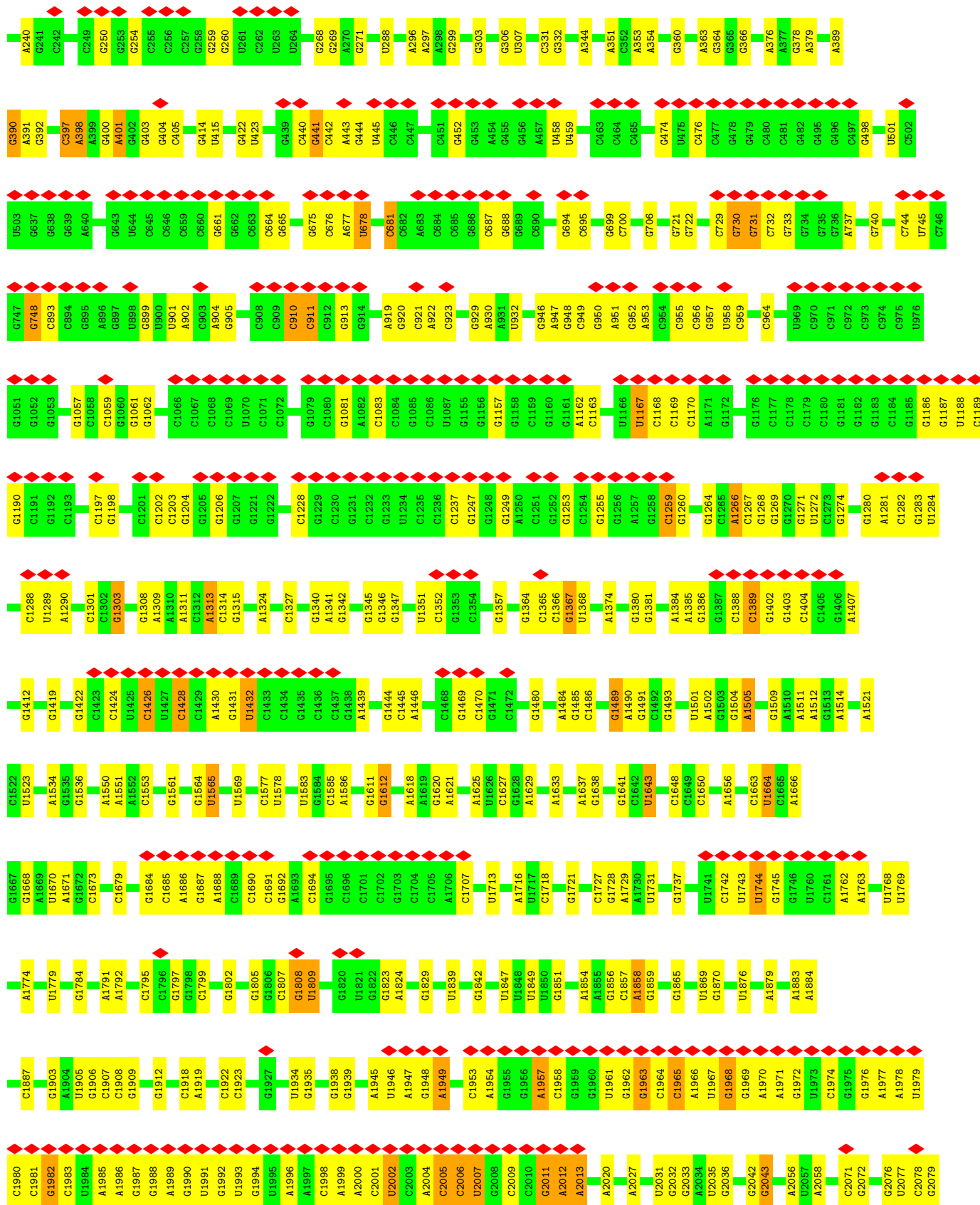


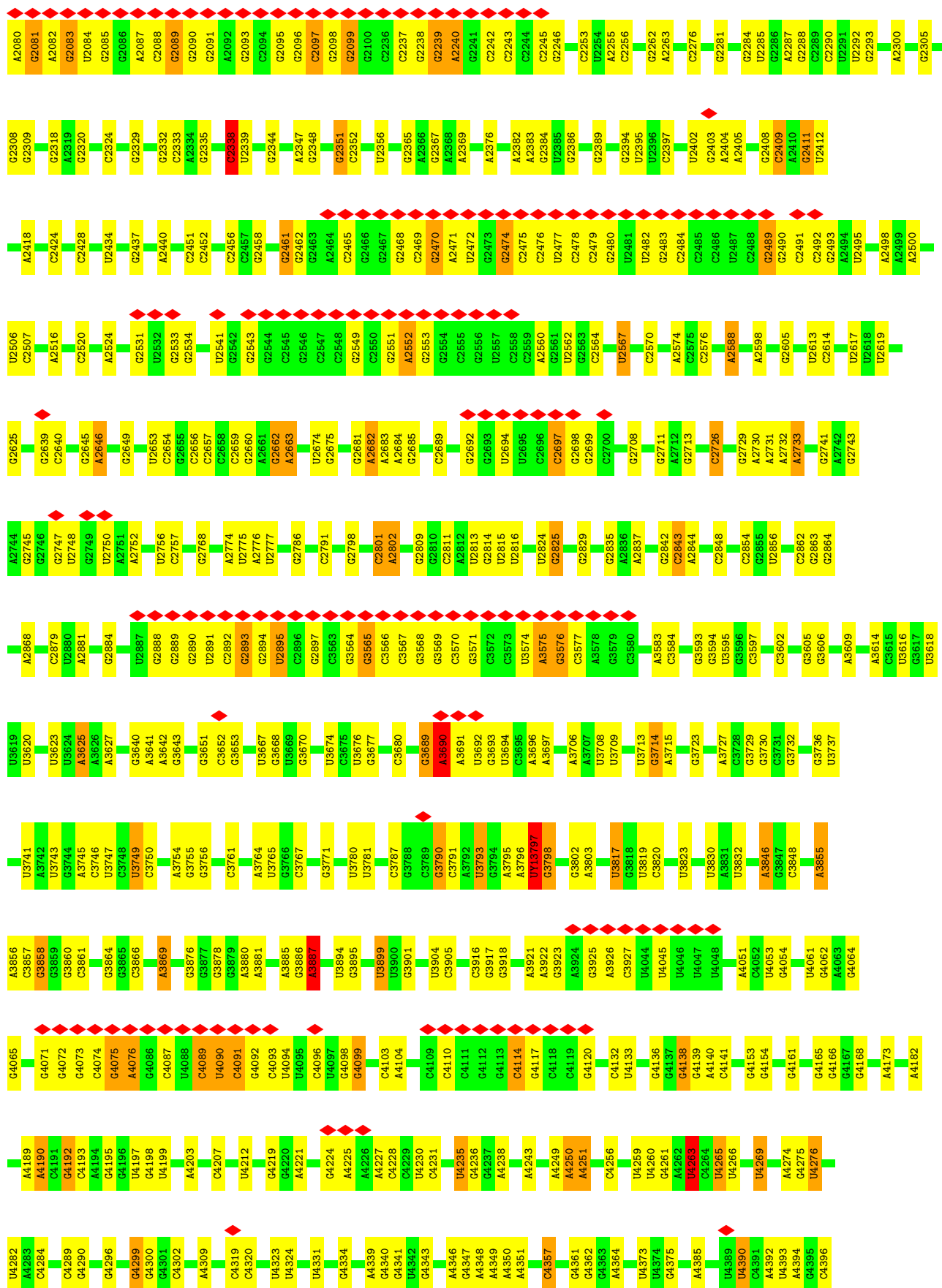
- Molecule 2: 60S ribosomal protein L3

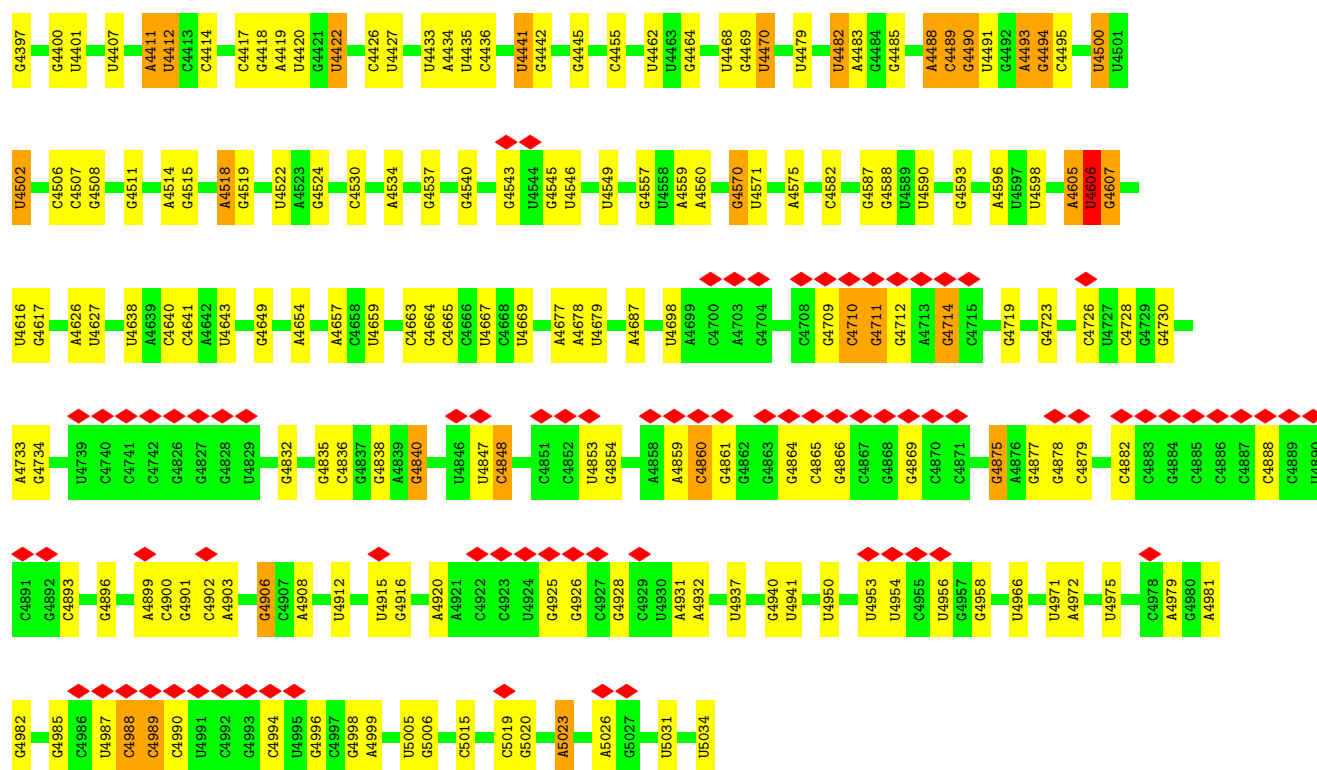


- Molecule 3: 28S rRNA

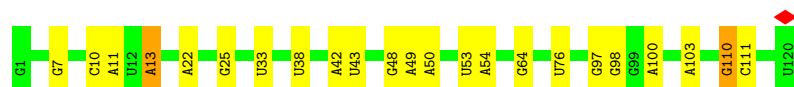
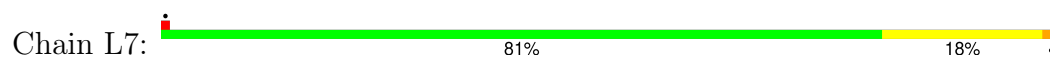




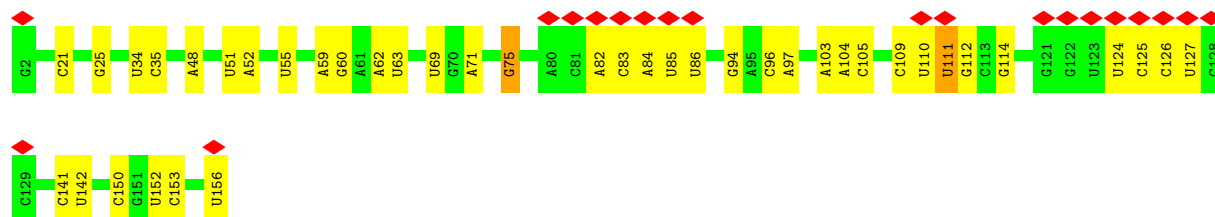
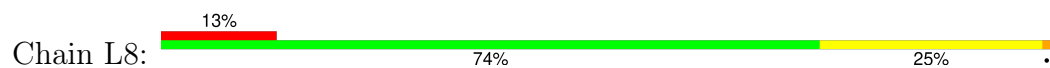




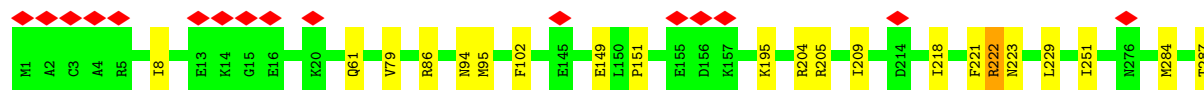
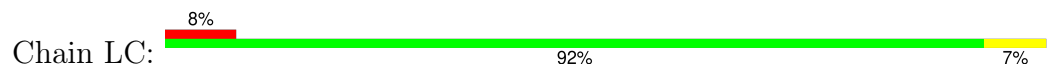
• Molecule 4: 5S rRNA

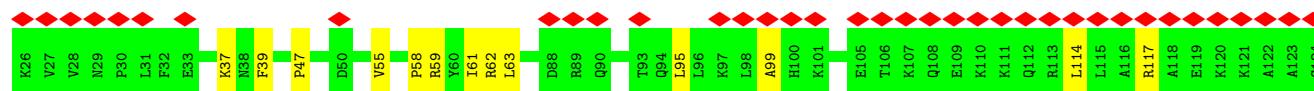


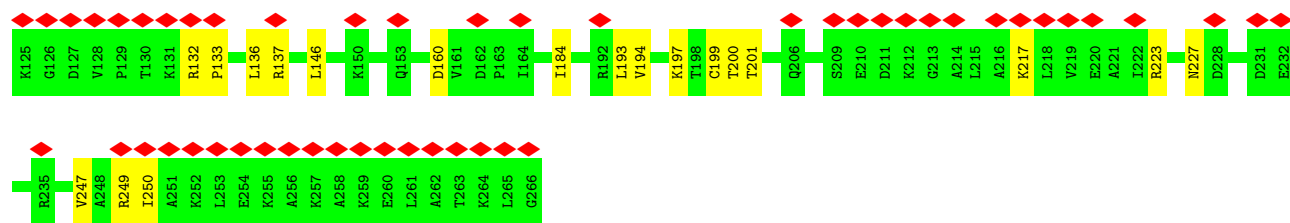
• Molecule 5: 5.8S rRNA



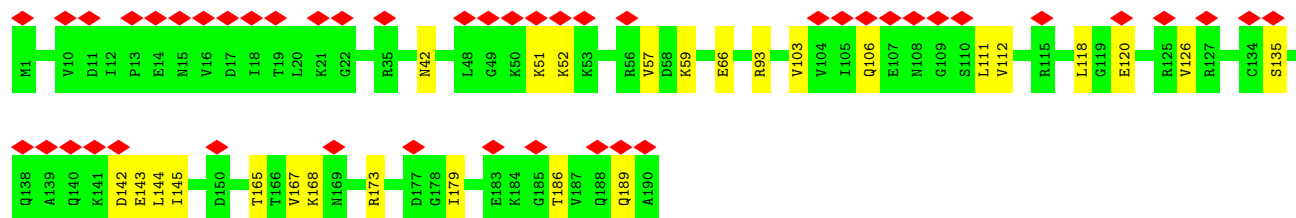
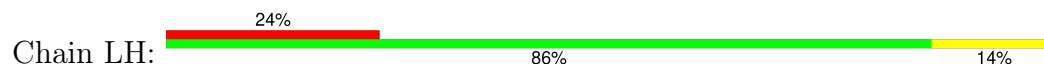
• Molecule 6: 60S ribosomal protein L4



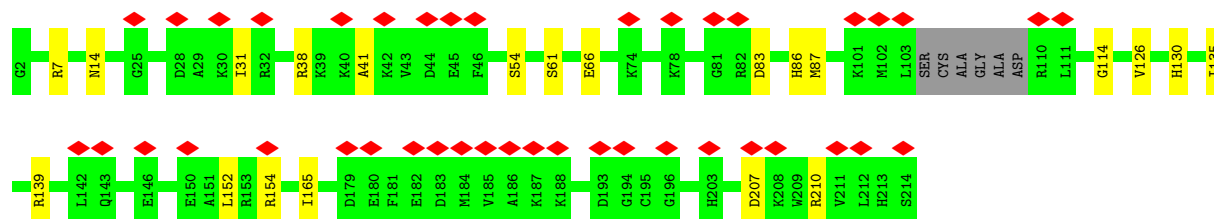
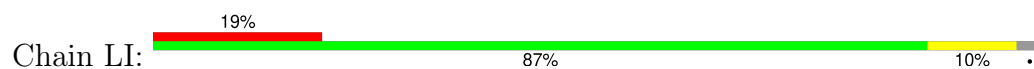




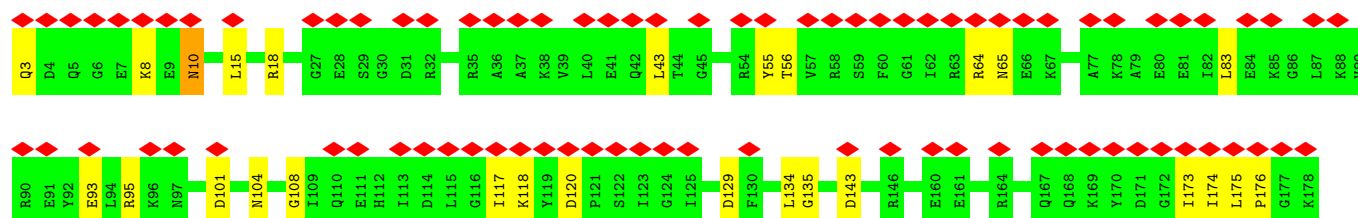
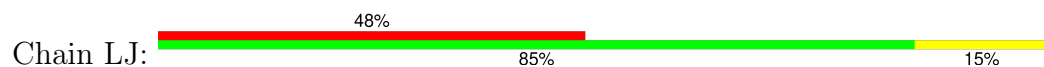
• Molecule 11: 60S ribosomal protein L9



• Molecule 12: 60S ribosomal protein L10-like

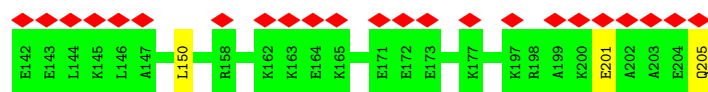


• Molecule 13: 60S ribosomal protein L11

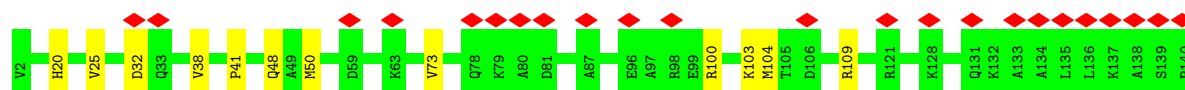


• Molecule 14: 60S ribosomal protein L13

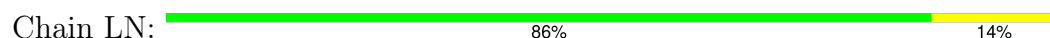




- Molecule 15: 60S ribosomal protein L14



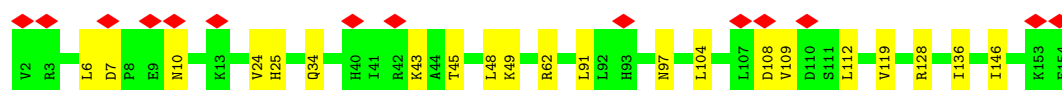
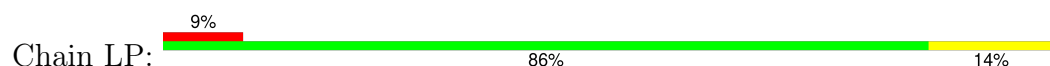
- Molecule 16: 60S ribosomal protein L15



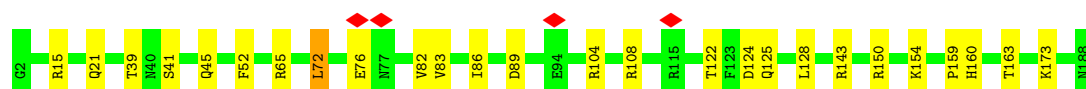
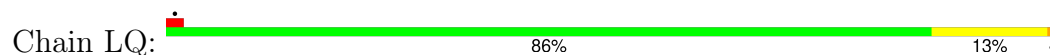
- Molecule 17: 60S ribosomal protein L13a



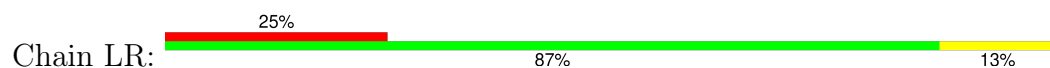
- Molecule 18: 60S ribosomal protein L17

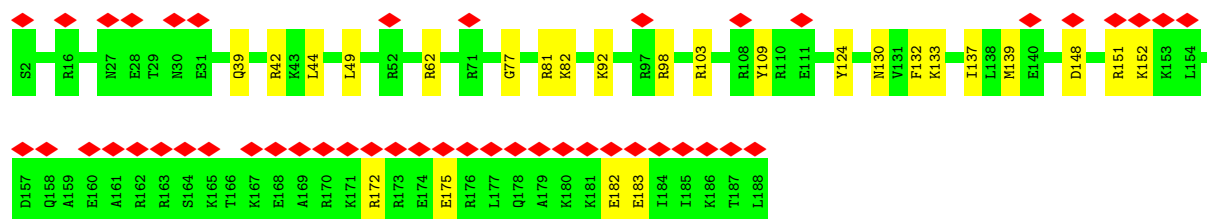


- Molecule 19: 60S ribosomal protein L18

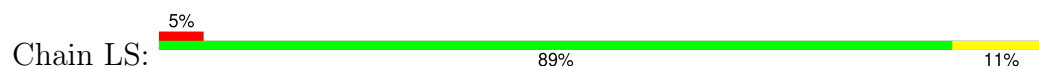


- Molecule 20: 60S ribosomal protein L19

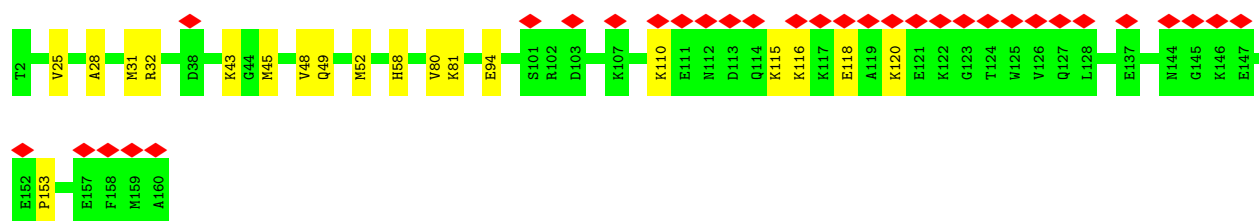
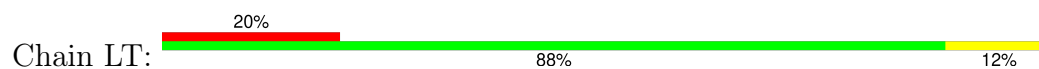




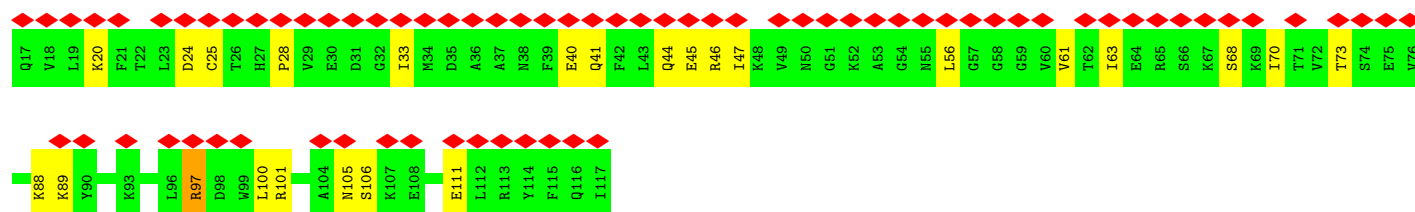
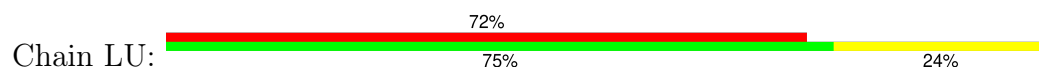
- Molecule 21: 60S ribosomal protein L18a



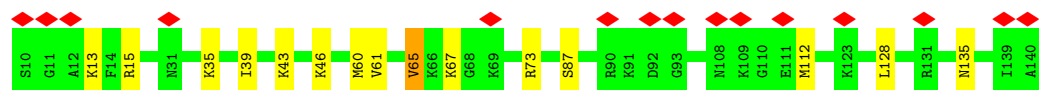
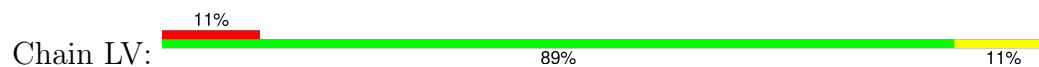
- Molecule 22: 60S ribosomal protein L21



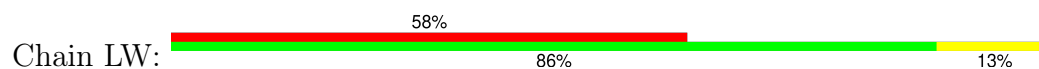
- Molecule 23: Heparin-binding protein HBp15

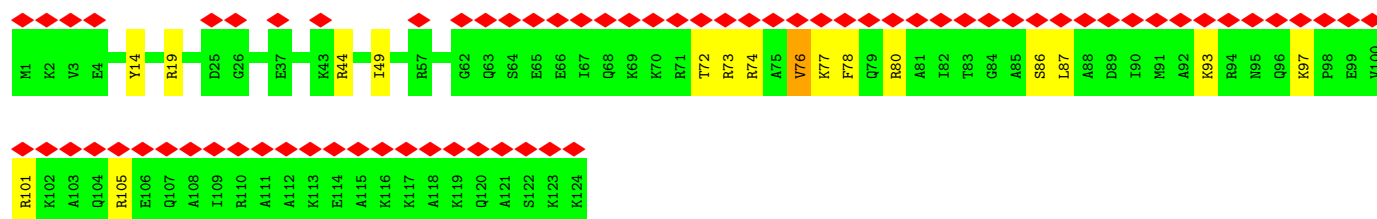


- Molecule 24: 60S ribosomal protein L23

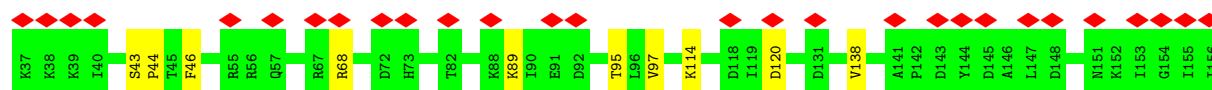


- Molecule 25: 60S ribosomal protein L24

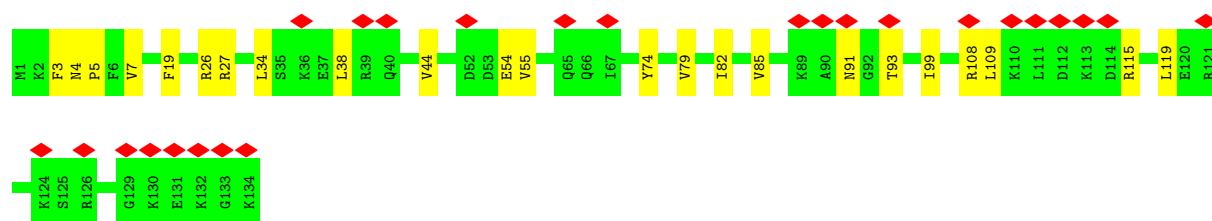
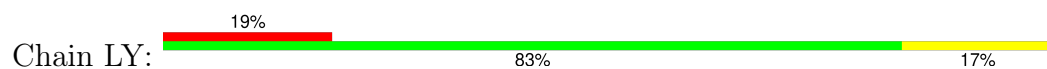




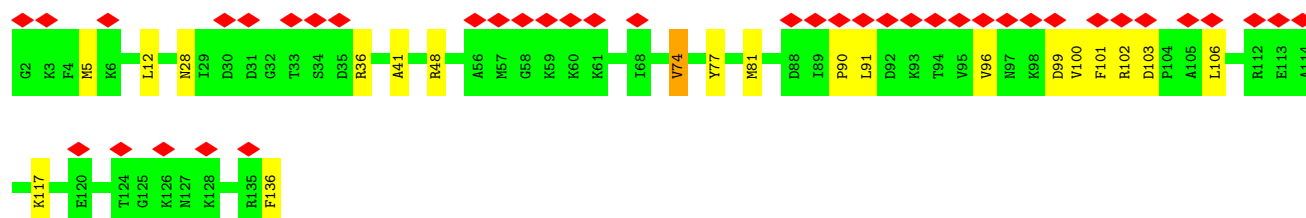
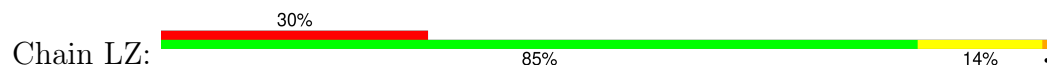
- Molecule 26: 60S ribosomal protein L23a



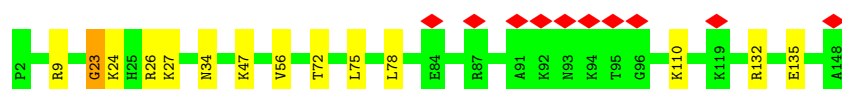
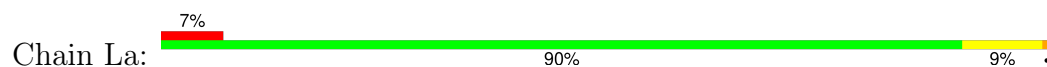
- Molecule 27: 60S ribosomal protein L26



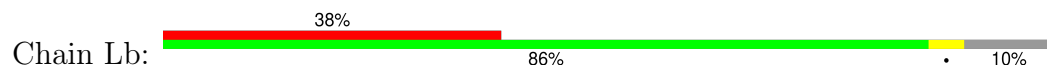
- Molecule 28: 60S ribosomal protein L27

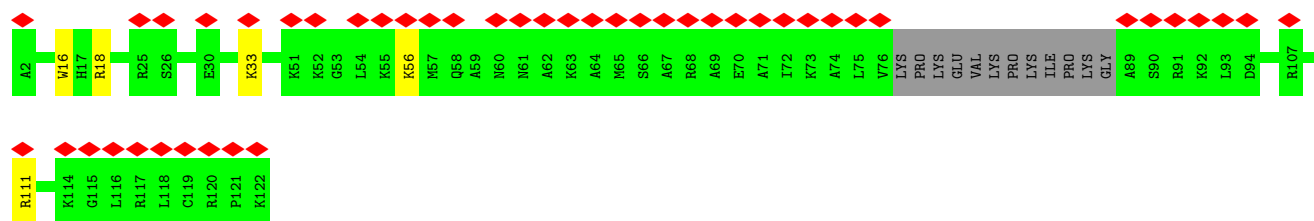


- Molecule 29: 60S ribosomal protein L27a

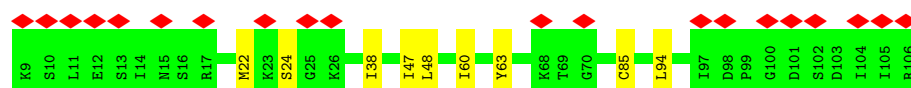
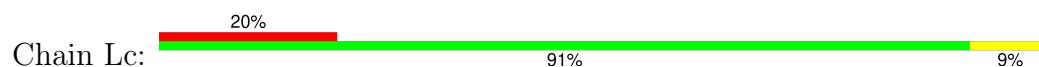


- Molecule 30: 60S ribosomal protein L29

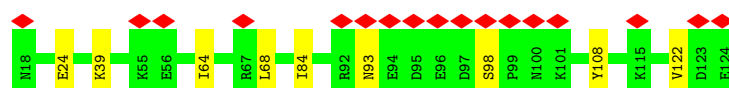




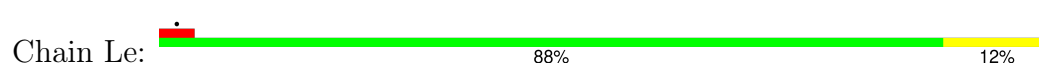
- Molecule 31: 60S ribosomal protein L30



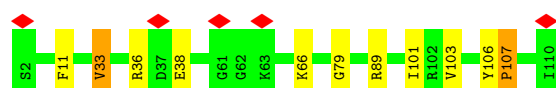
- Molecule 32: 60S ribosomal protein L31



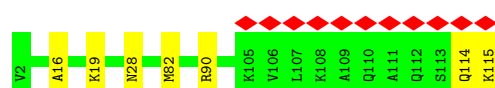
- Molecule 33: 60S ribosomal protein L32



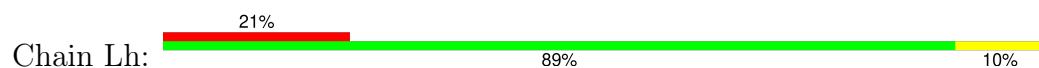
- Molecule 34: 60S ribosomal protein L35a

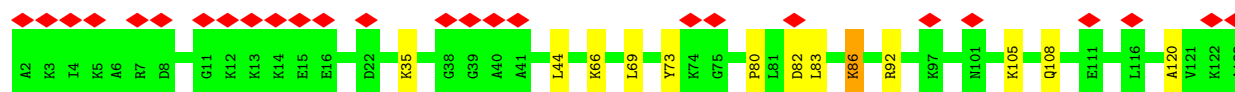


- Molecule 35: 60S ribosomal protein L34

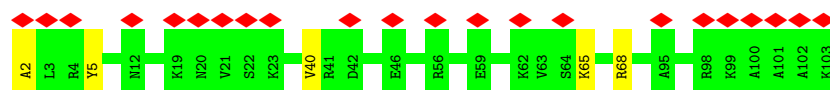


- Molecule 36: 60S ribosomal protein L35

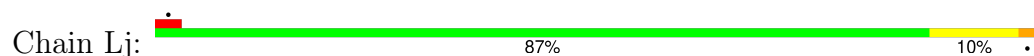




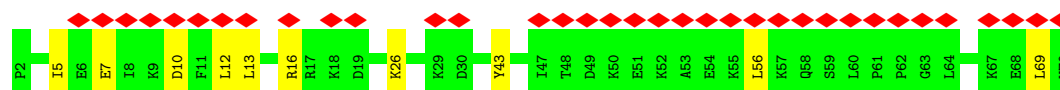
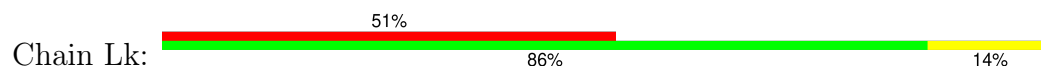
- Molecule 37: 60S ribosomal protein L36



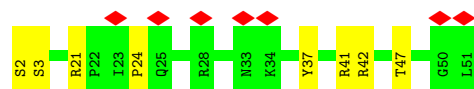
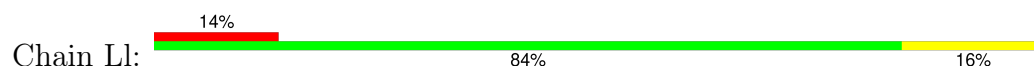
- Molecule 38: 60S ribosomal protein L37



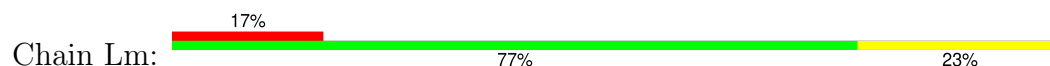
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



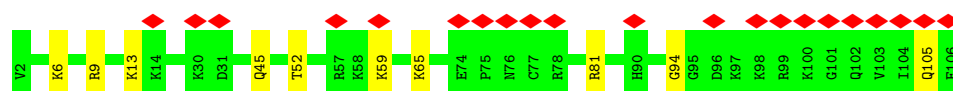
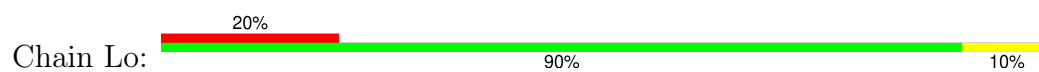
- Molecule 41: 60S ribosomal protein L40



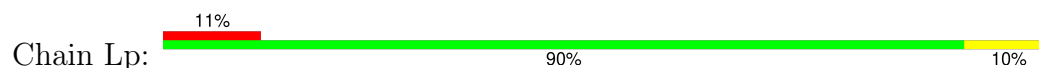
- Molecule 42: 60S ribosomal protein L41



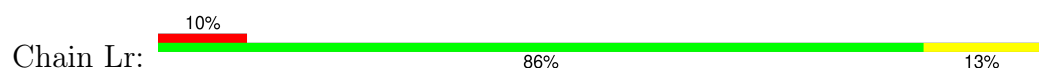
- Molecule 43: 60S ribosomal protein L36a



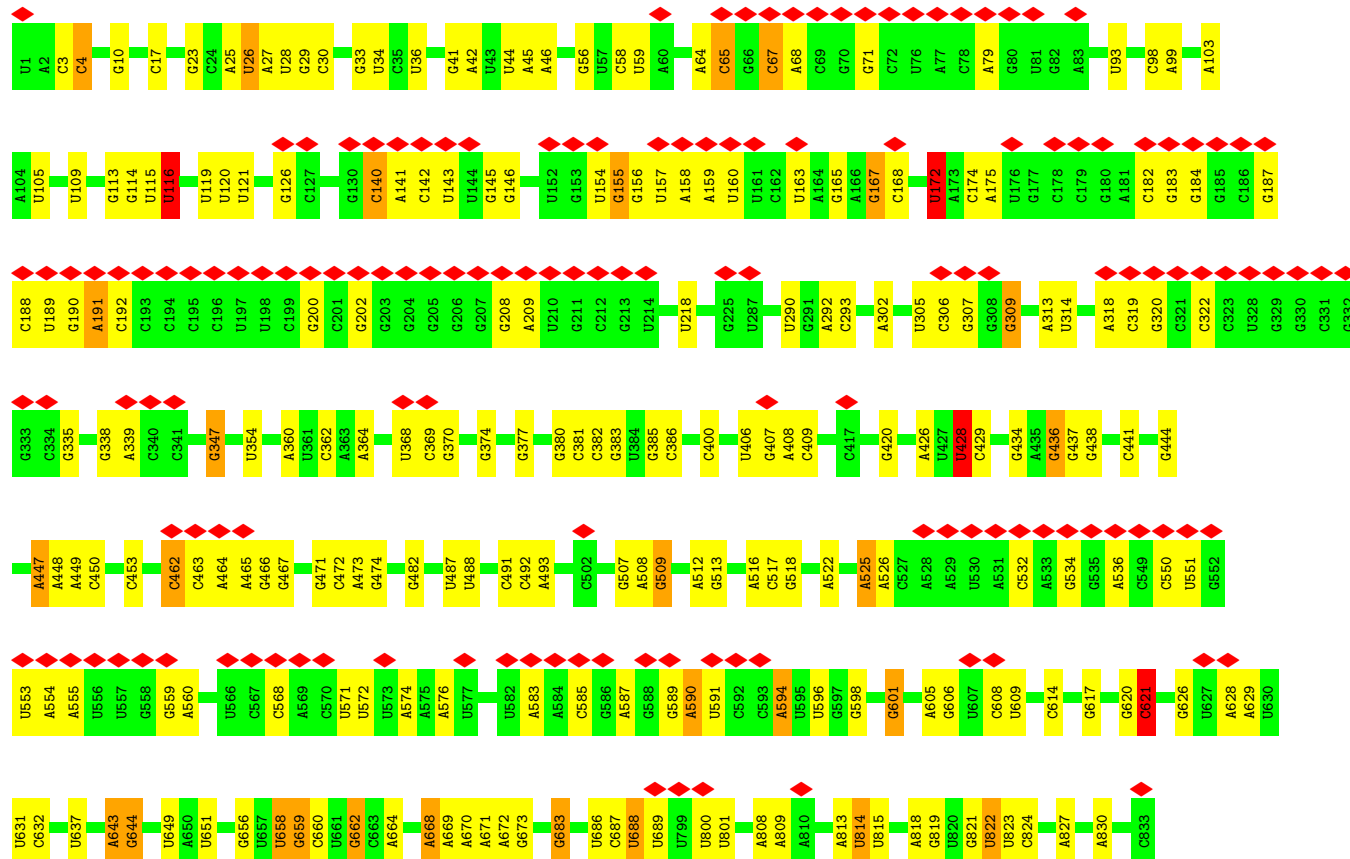
- Molecule 44: 60S ribosomal protein L37a

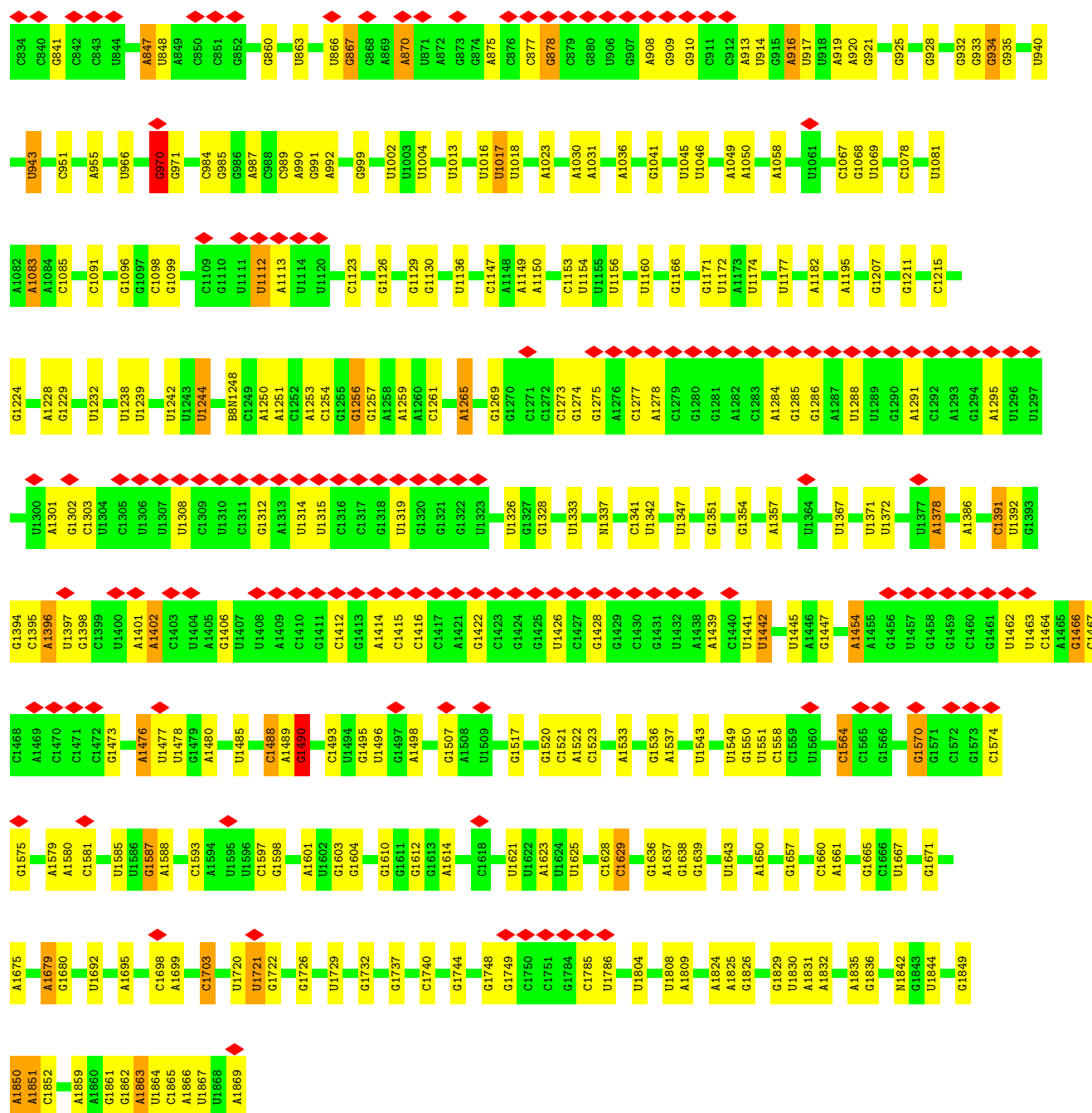


- Molecule 45: 60S ribosomal protein L28

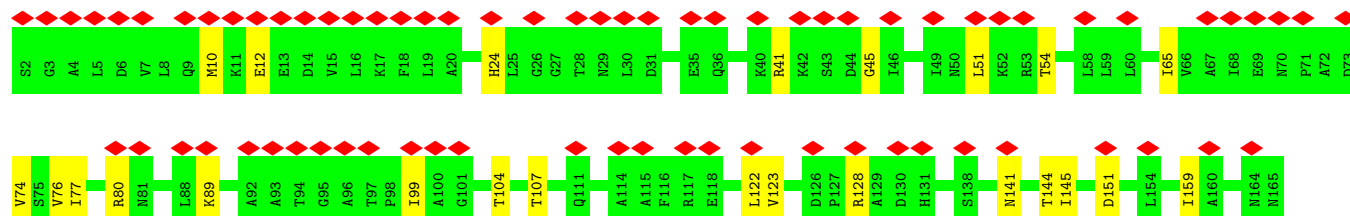


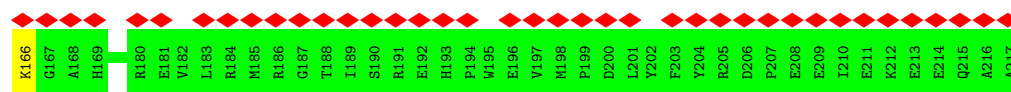
- Molecule 46: 18S rRNA



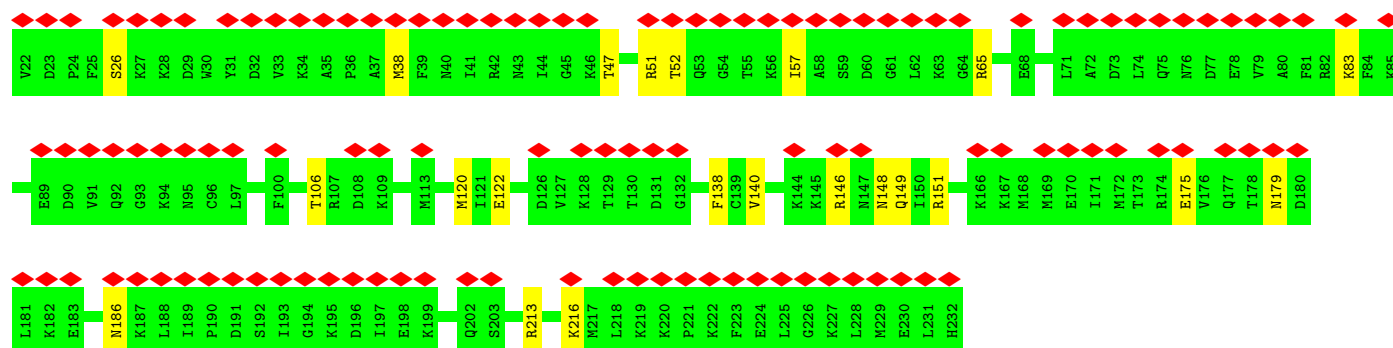
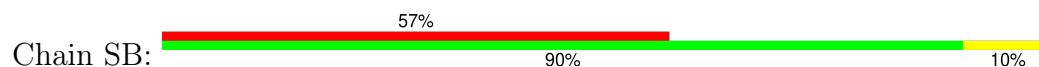


• Molecule 47: 40S ribosomal protein SA

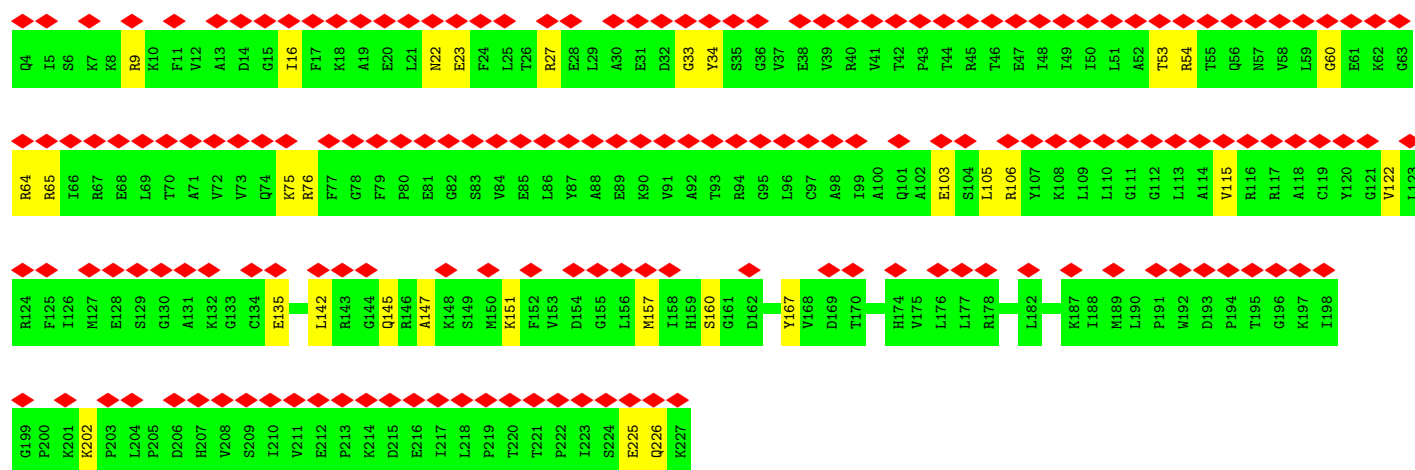
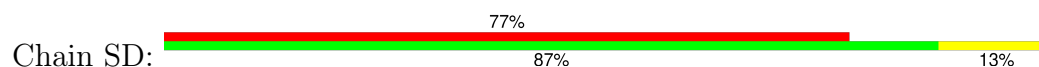




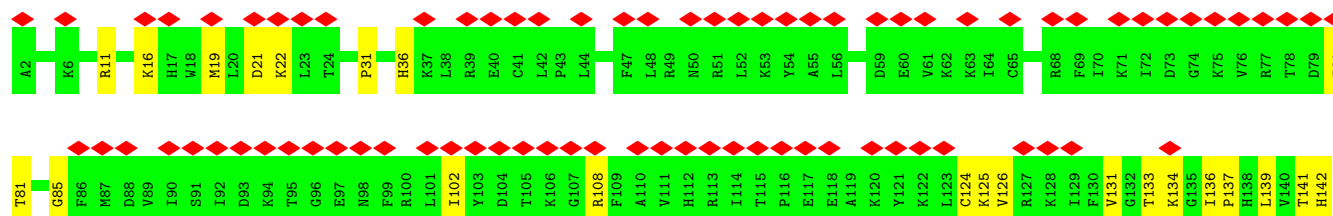
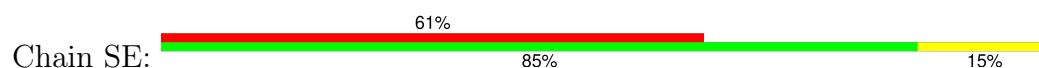
• Molecule 48: 40S ribosomal protein S3a

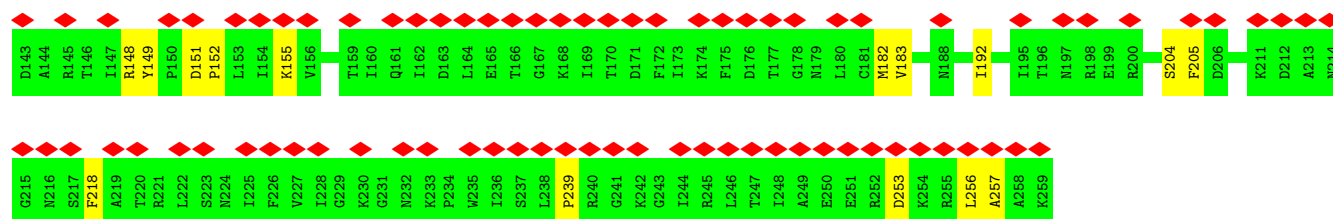


• Molecule 49: 40S ribosomal protein S3



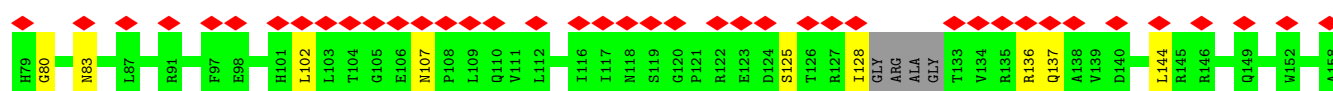
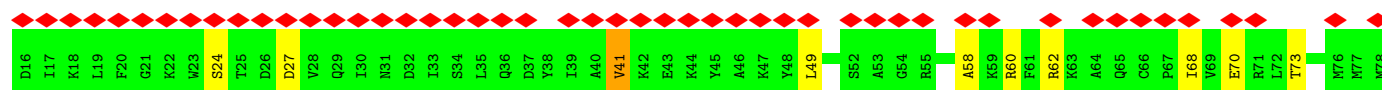
• Molecule 50: 40S ribosomal protein S4, X isoform





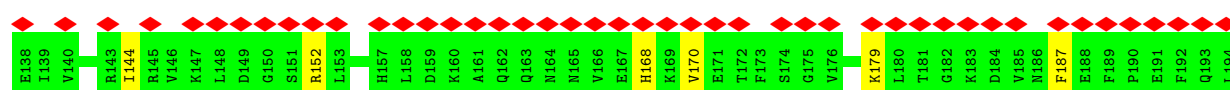
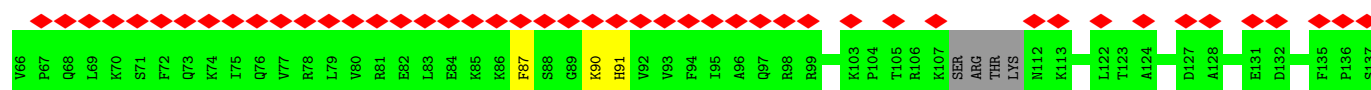
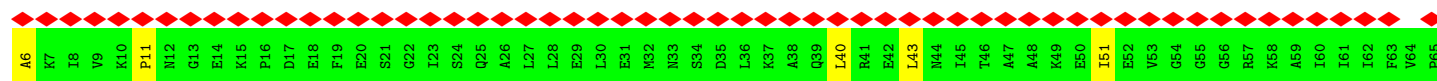
• Molecule 51: 40S ribosomal protein S5

Chain SF: 66% 86% 11% ..



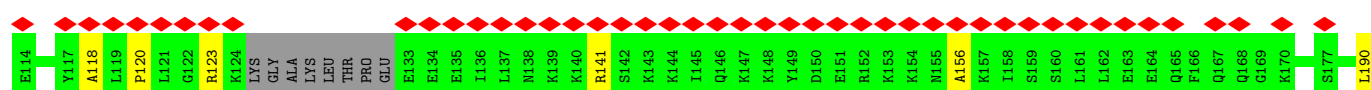
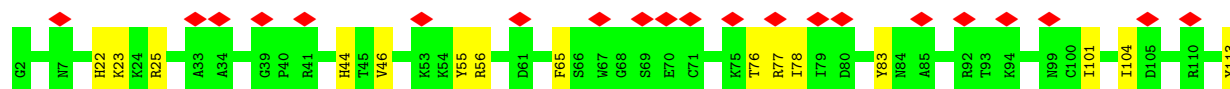
• Molecule 52: 40S ribosomal protein S7

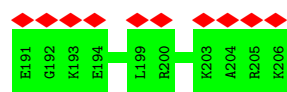
Chain SH: 80% 90% 7% .



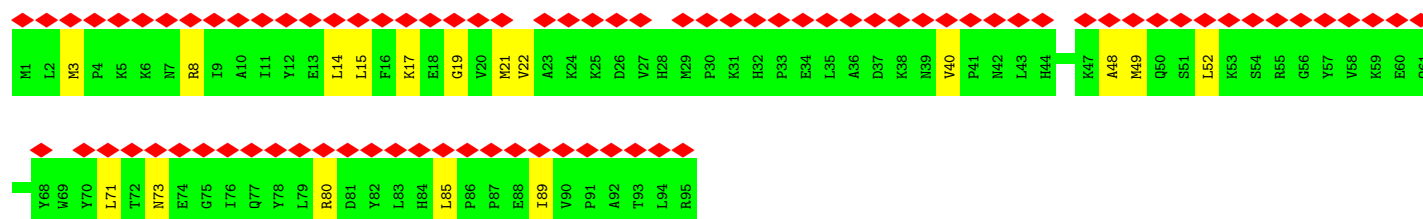
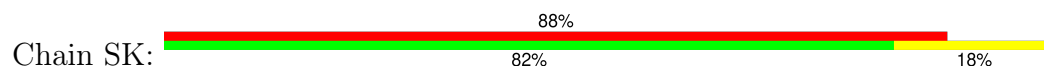
• Molecule 53: 40S ribosomal protein S8

Chain SI: 38% 86% 10% .

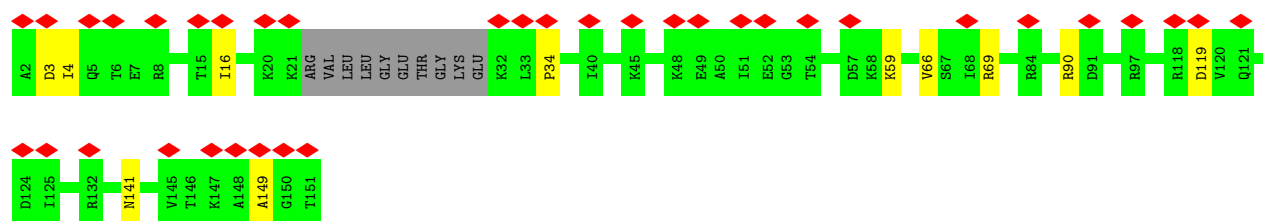
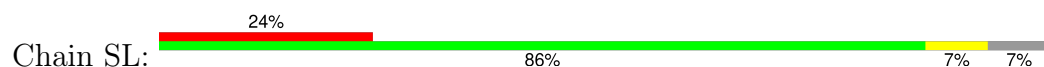




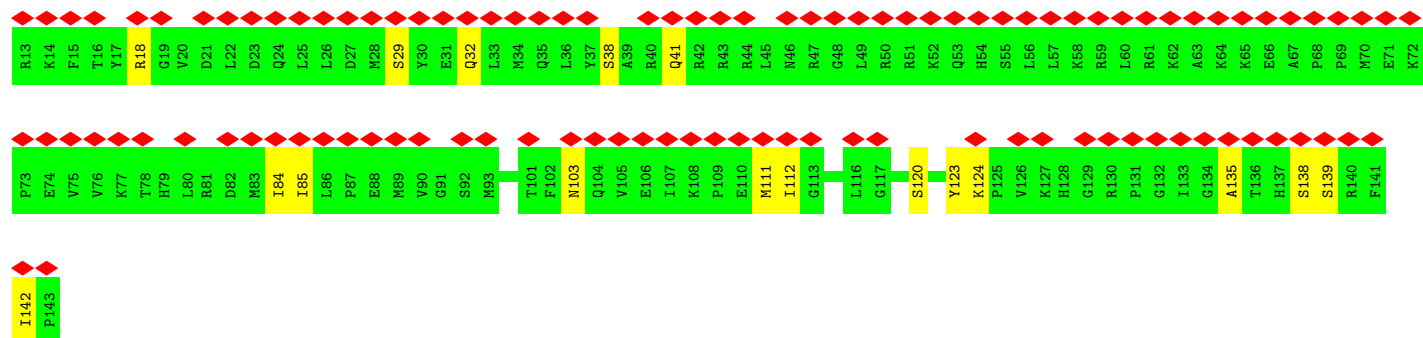
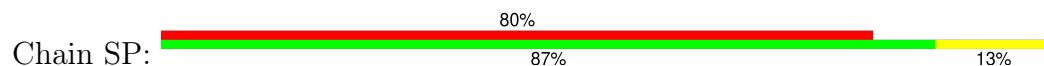
- Molecule 54: 40S ribosomal protein S10



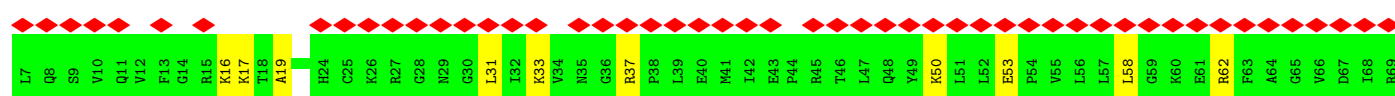
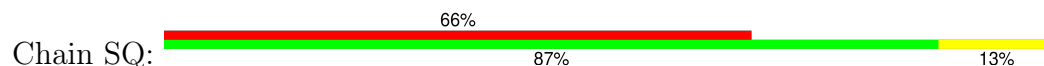
- Molecule 55: 40S ribosomal protein S11

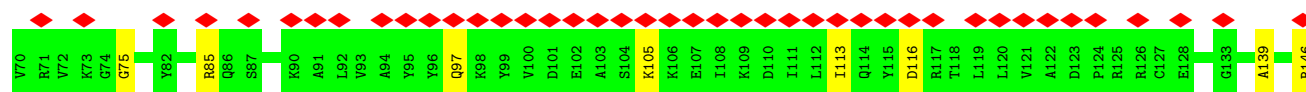


- Molecule 56: 40S ribosomal protein S15

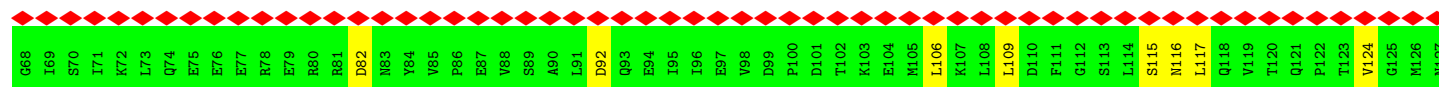
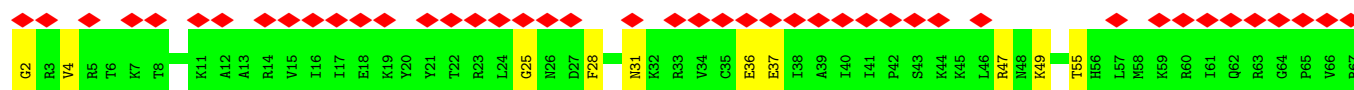
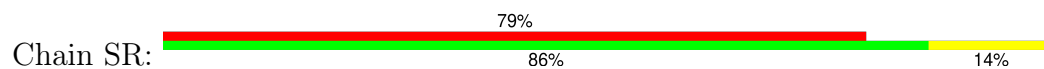


- Molecule 57: 40S ribosomal protein S16

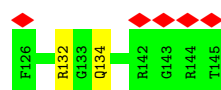
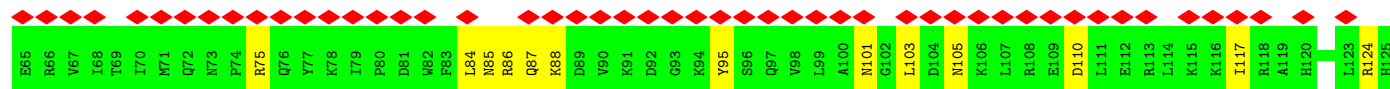
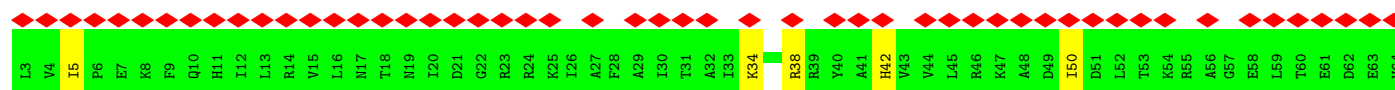
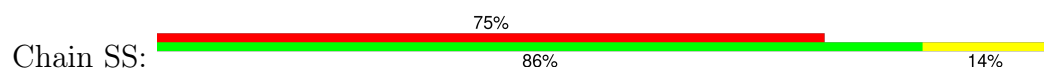




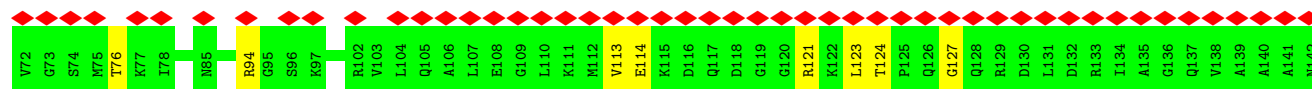
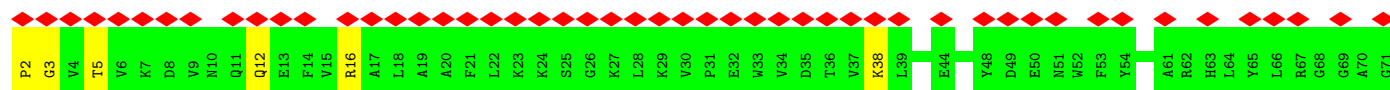
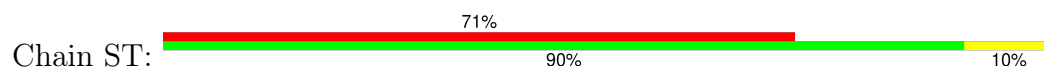
- Molecule 58: 40S ribosomal protein S17



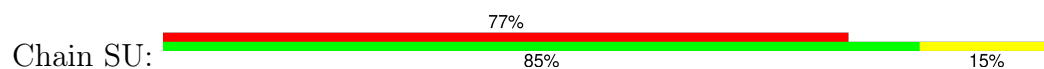
- Molecule 59: 40S ribosomal protein S18

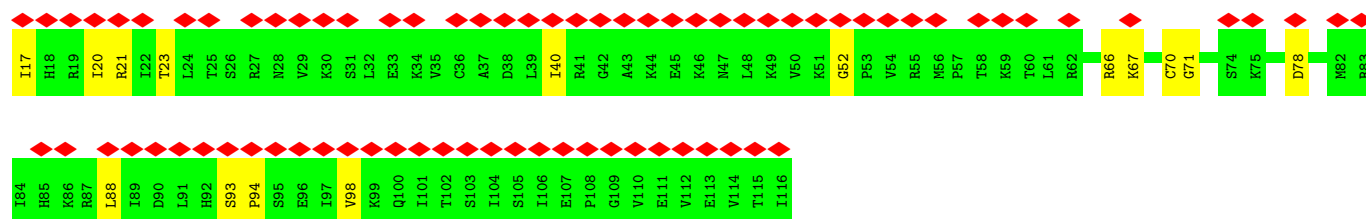


- Molecule 60: 40S ribosomal protein S19

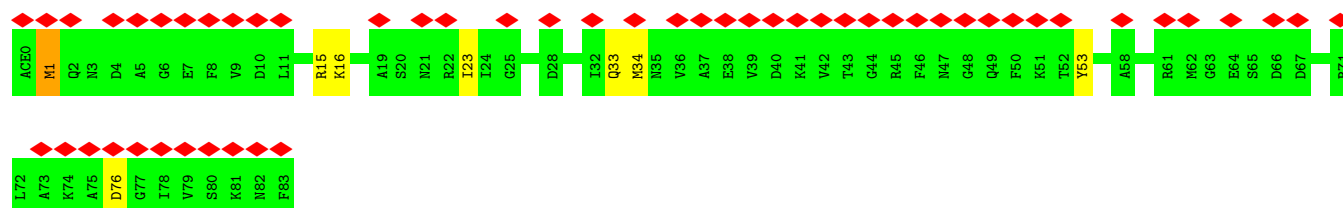
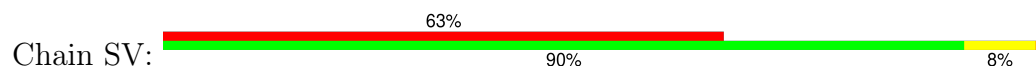


- Molecule 61: 40S ribosomal protein S20

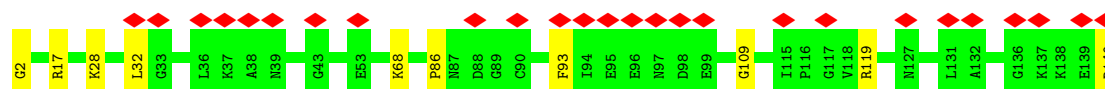




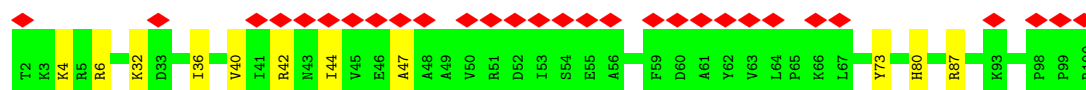
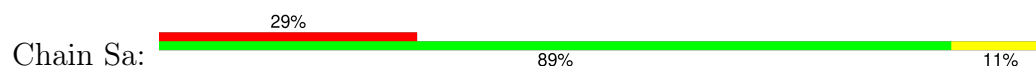
- Molecule 62: 40S ribosomal protein S21



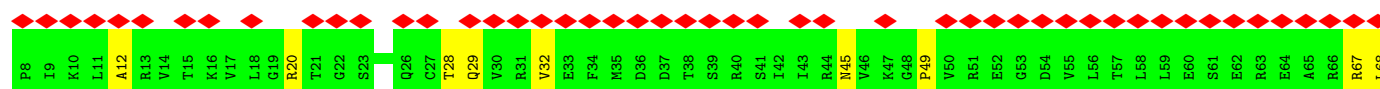
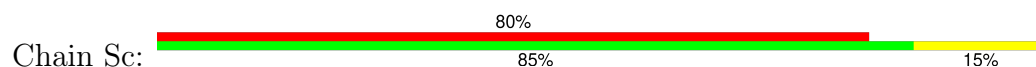
- Molecule 63: 40S ribosomal protein S23



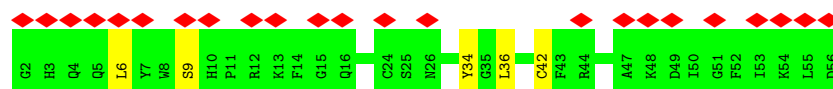
- Molecule 64: 40S ribosomal protein S26



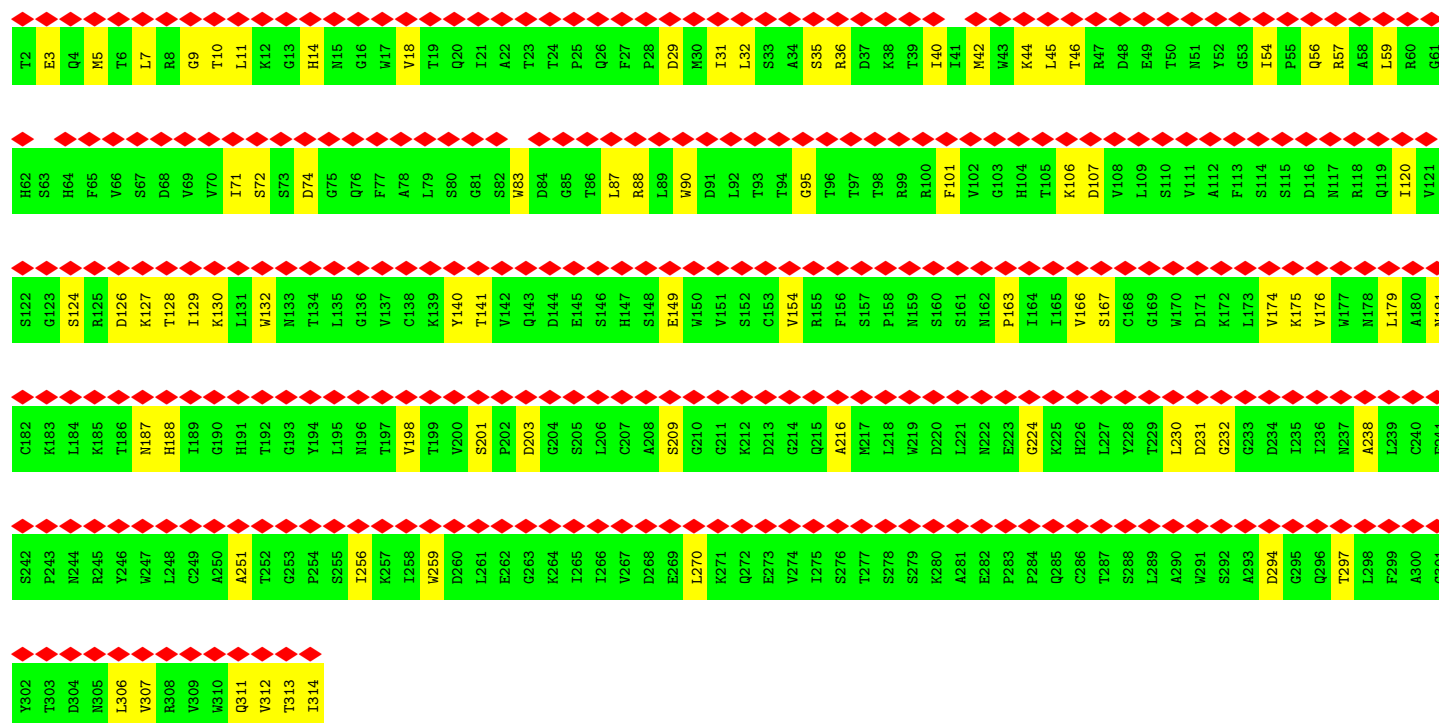
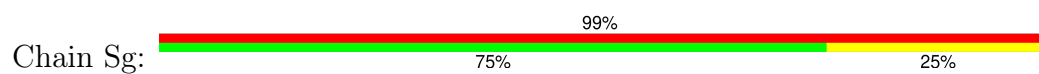
- Molecule 65: 40S ribosomal protein S28



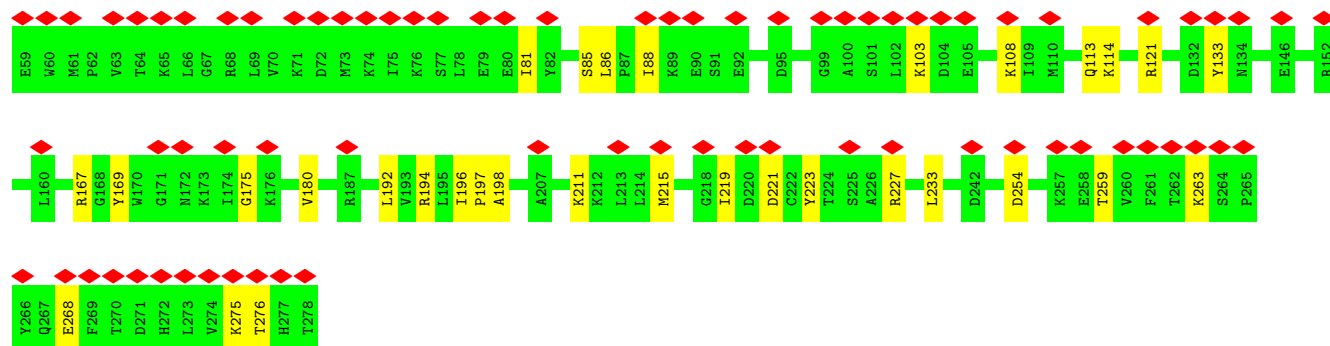
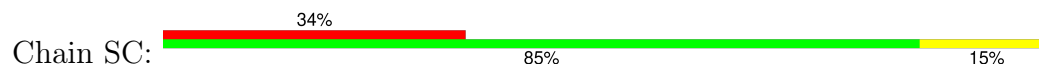
- Molecule 66: 40S ribosomal protein S29



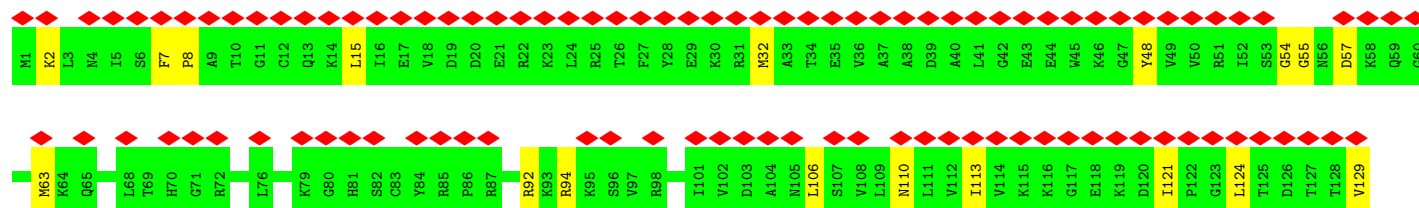
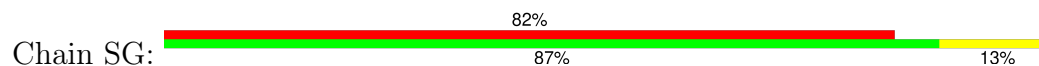
- Molecule 67: Receptor of activated protein C kinase 1



• Molecule 68: 40S ribosomal protein S2

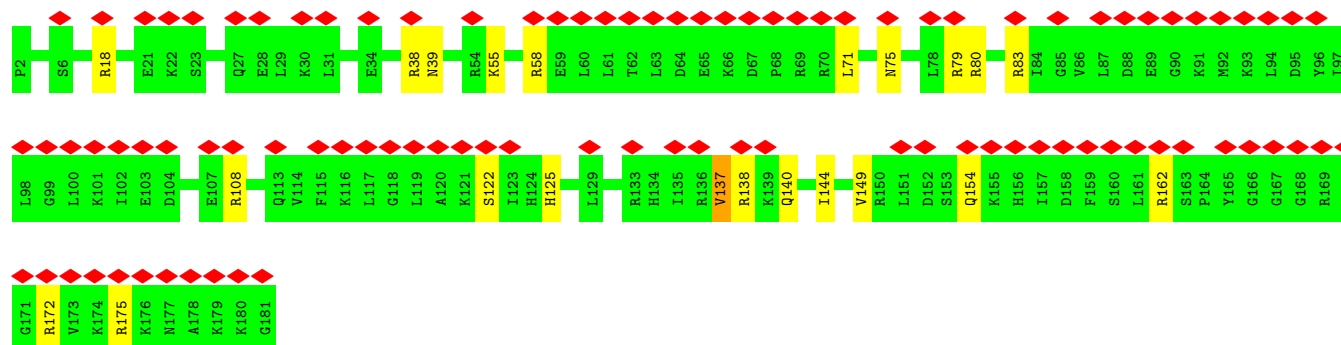
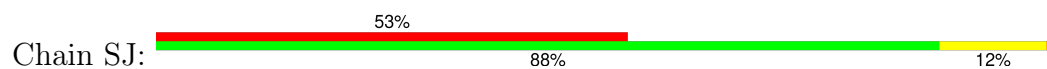


• Molecule 69: 40S ribosomal protein S6

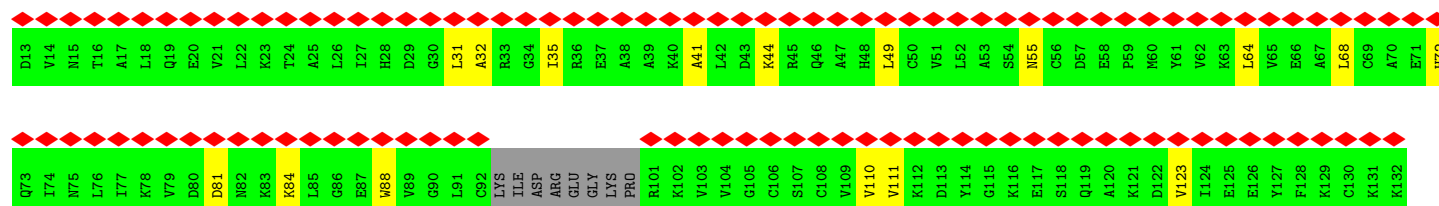
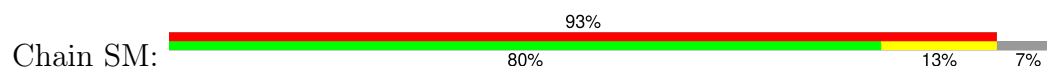




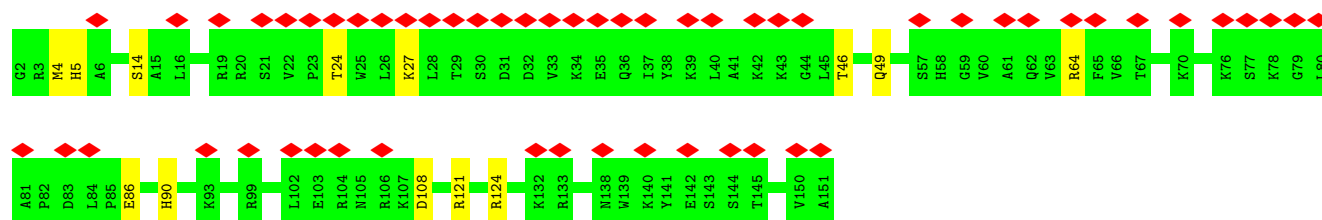
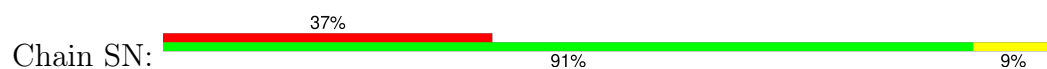
• Molecule 70: 40S ribosomal protein S9



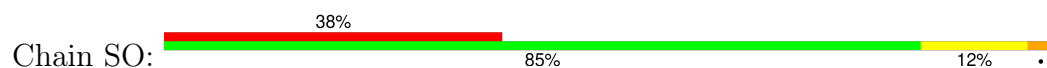
• Molecule 71: 40S ribosomal protein S12

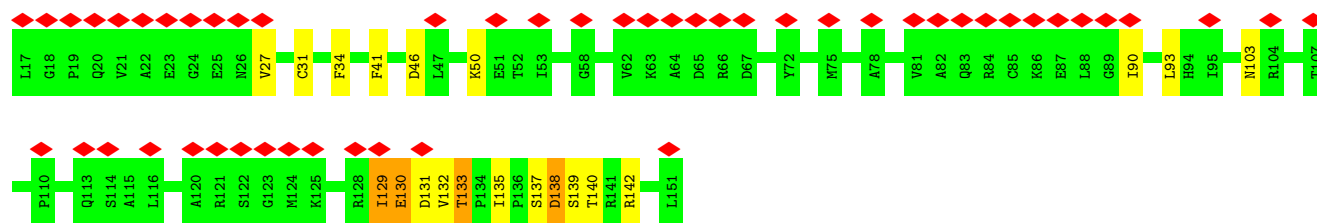


• Molecule 72: 40S ribosomal protein S13

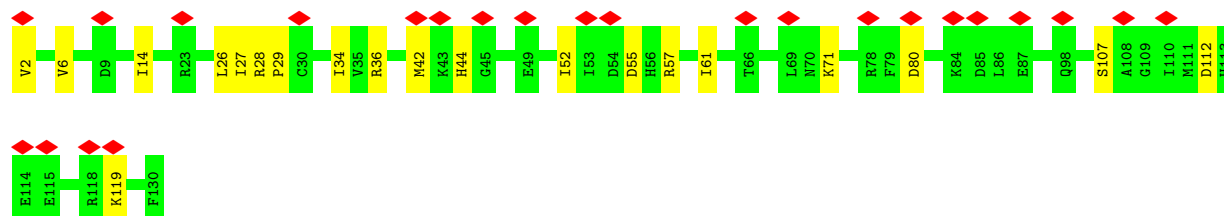
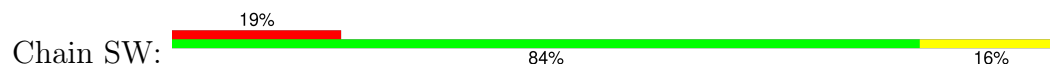


• Molecule 73: 40S ribosomal protein S14

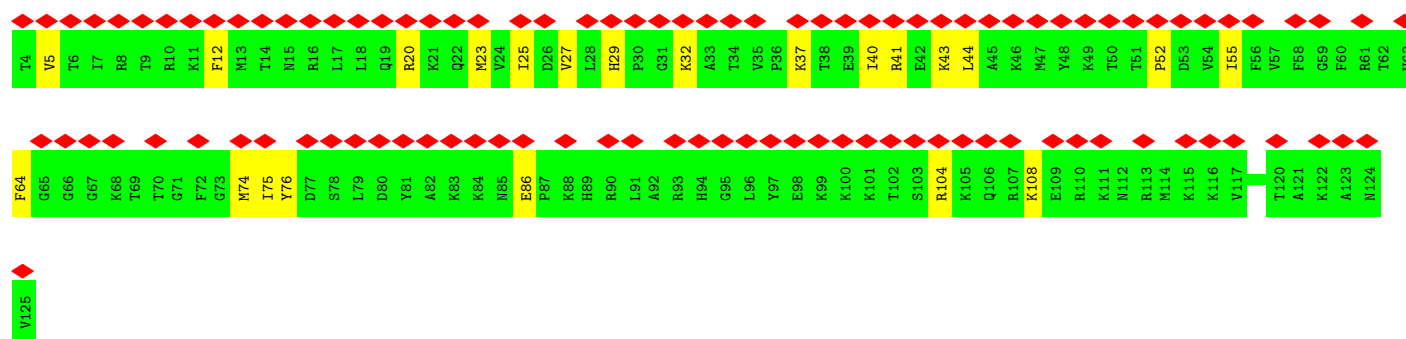
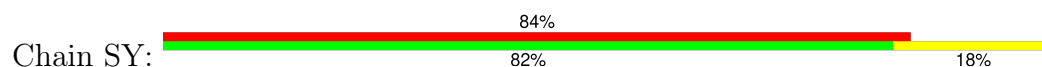




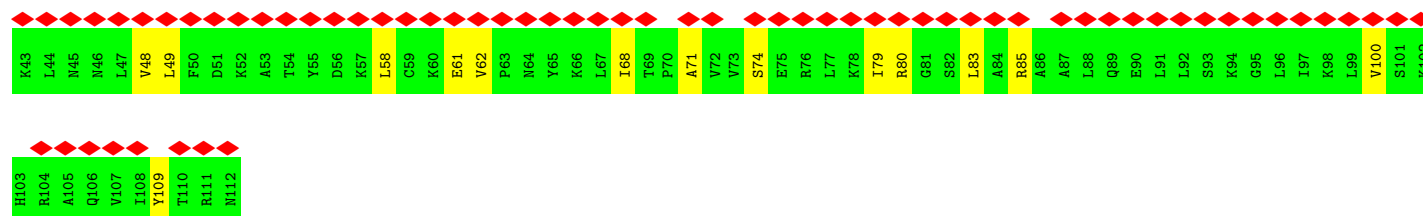
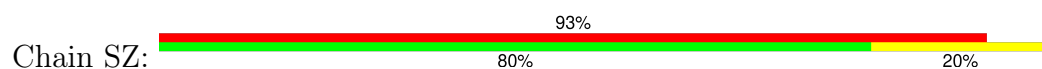
• Molecule 74: 40S ribosomal protein S15a



• Molecule 75: 40S ribosomal protein S24

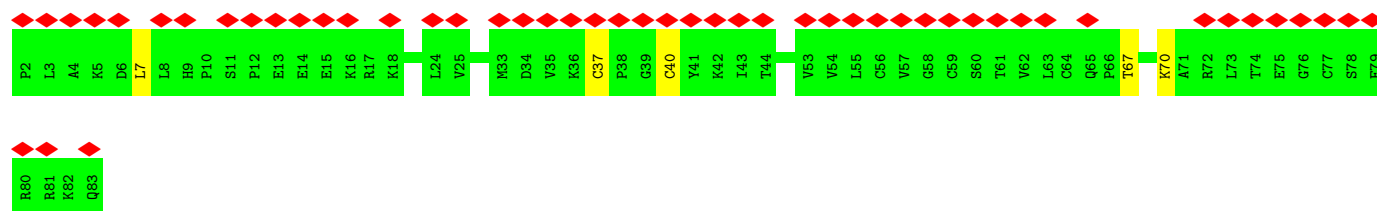


• Molecule 76: 40S ribosomal protein S25

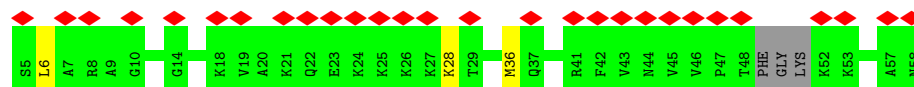
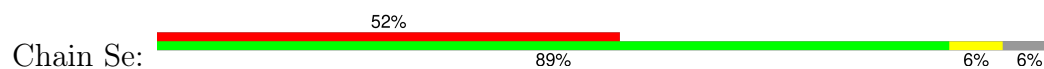


• Molecule 77: 40S ribosomal protein S27

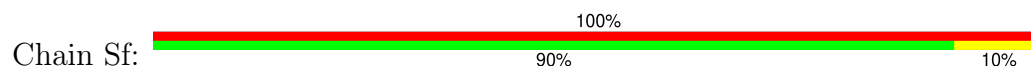




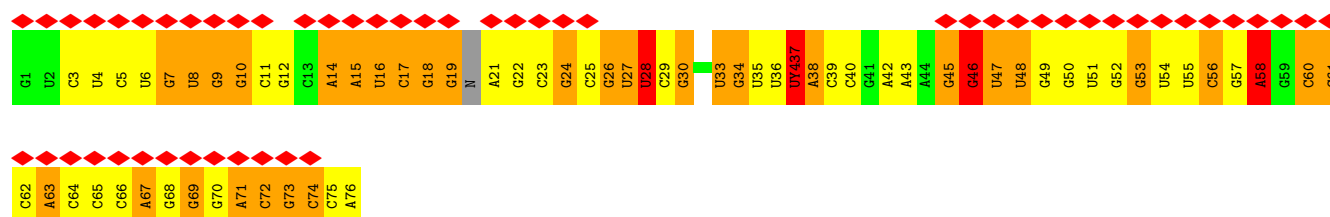
• Molecule 78: 40S ribosomal protein S30



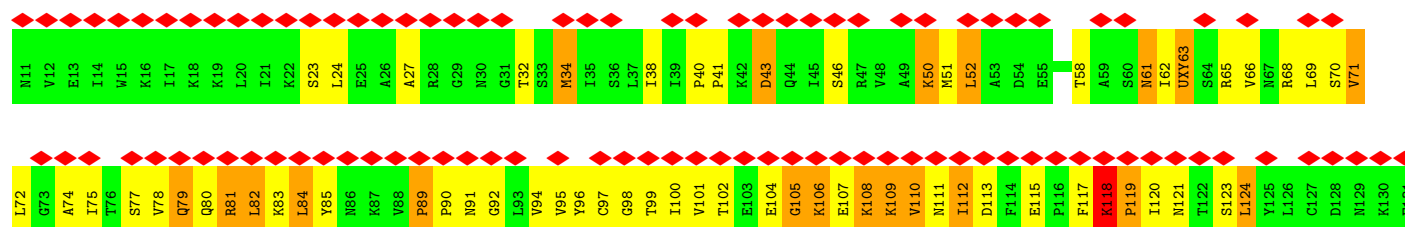
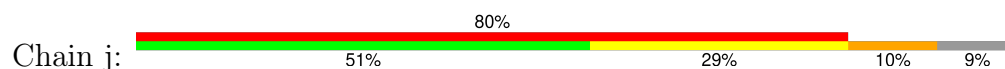
• Molecule 79: 40S ribosomal protein S27a

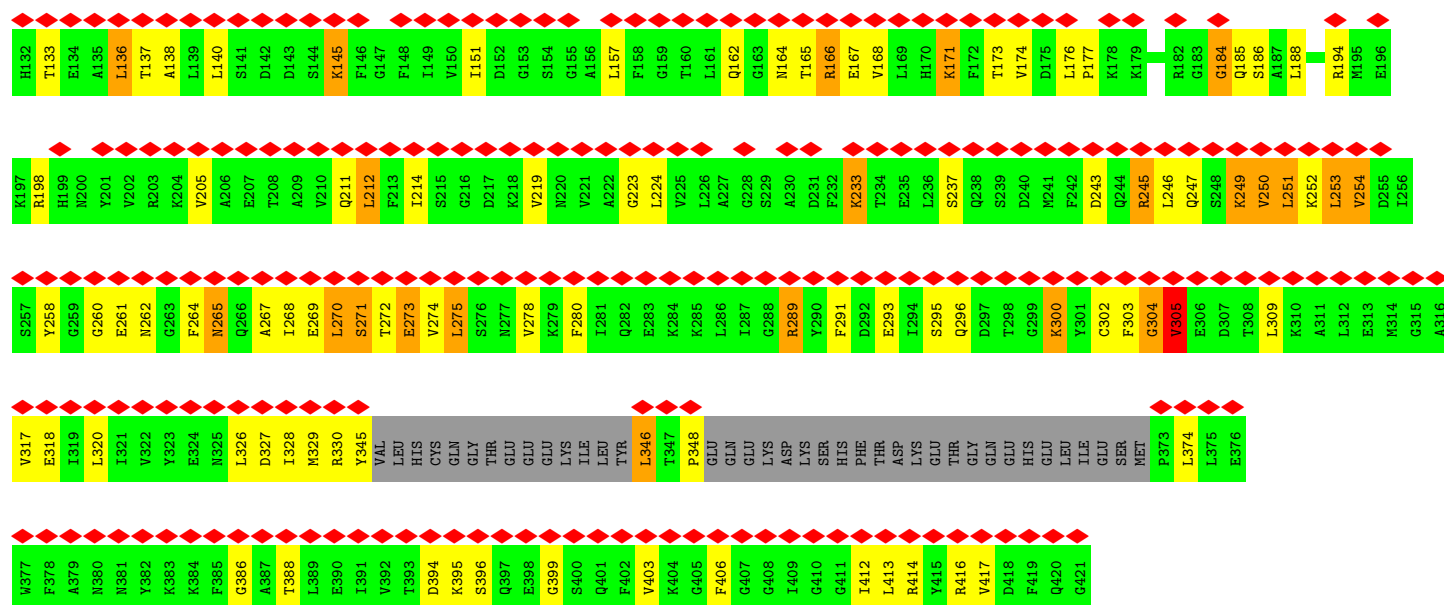


• Molecule 80: P-tRNA



• Molecule 81: Eukaryotic peptide chain release factor subunit 1





- Molecule 82: mRNA



- Molecule 83: Stalled Nascent chain



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 57324                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.260                     | Depositor |
| Minimum map value                    | -0.089                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.009                     | Depositor |
| Recommended contour level            | 0.04                      | Depositor |
| Map size ( $\text{\AA}$ )            | 494.5, 494.5, 494.5       | wwPDB     |
| Map dimensions                       | 430, 430, 430             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.15, 1.15, 1.15          | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, IAS, OMC, M2G, ACE, OMU, MVM, B8N, 1MA, G7M, UR3, 5MC, MEQ, 1MG, UY4, UY1, PSU, OMG, ZN, K, 6MZ, MA6, MG, A2M, 2MG, MLZ, H2U, UXY

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   | LA    | 0.76         | 0/1936         | 0.78        | 2/2596 (0.1%)    |
| 2   | LB    | 0.70         | 1/3265 (0.0%)  | 0.69        | 0/4370           |
| 3   | L5    | 0.77         | 4/81383 (0.0%) | 0.53        | 10/126935 (0.0%) |
| 4   | L7    | 0.72         | 0/2862         | 0.46        | 0/4459           |
| 5   | L8    | 0.71         | 0/3612         | 0.47        | 0/5627           |
| 6   | LC    | 0.72         | 0/2898         | 0.71        | 0/3891           |
| 7   | LD    | 0.60         | 0/2403         | 0.61        | 0/3219           |
| 8   | LE    | 0.57         | 0/1942         | 0.76        | 1/2606 (0.0%)    |
| 9   | LF    | 0.74         | 0/1916         | 0.78        | 0/2553           |
| 10  | LG    | 0.62         | 0/1971         | 0.77        | 1/2651 (0.0%)    |
| 11  | LH    | 0.64         | 0/1537         | 0.69        | 0/2066           |
| 12  | LI    | 0.61         | 0/1716         | 0.66        | 0/2291           |
| 13  | LJ    | 0.58         | 0/1433         | 0.81        | 1/1915 (0.1%)    |
| 14  | LL    | 0.66         | 0/1680         | 0.78        | 0/2249           |
| 15  | LM    | 0.64         | 0/1161         | 0.69        | 0/1554           |
| 16  | LN    | 0.81         | 0/1746         | 0.82        | 0/2338           |
| 17  | LO    | 0.75         | 0/1682         | 0.73        | 1/2250 (0.0%)    |
| 18  | LP    | 0.72         | 0/1268         | 0.70        | 0/1701           |
| 19  | LQ    | 0.75         | 0/1537         | 0.75        | 2/2052 (0.1%)    |
| 20  | LR    | 0.65         | 0/1582         | 0.71        | 0/2091           |
| 21  | LS    | 0.70         | 0/1493         | 0.66        | 0/2003           |
| 22  | LT    | 0.70         | 0/1326         | 0.67        | 0/1770           |
| 23  | LU    | 0.49         | 0/839          | 0.78        | 0/1126           |
| 24  | LV    | 0.66         | 0/993          | 0.74        | 0/1332           |
| 25  | LW    | 0.54         | 0/1030         | 0.71        | 0/1364           |
| 26  | LX    | 0.60         | 0/1002         | 0.62        | 0/1345           |
| 27  | LY    | 0.66         | 0/1132         | 0.76        | 0/1504           |
| 28  | LZ    | 0.62         | 0/1130         | 0.73        | 0/1507           |
| 29  | La    | 0.76         | 0/1191         | 0.74        | 2/1591 (0.1%)    |
| 30  | Lb    | 0.61         | 0/895          | 0.73        | 0/1182           |
| 31  | Lc    | 0.64         | 0/774          | 0.69        | 0/1038           |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 32  | Ld    | 0.66         | 0/903          | 0.74        | 0/1216         |
| 33  | Le    | 0.75         | 0/1071         | 0.74        | 0/1429         |
| 34  | Lf    | 0.76         | 0/895          | 0.78        | 0/1198         |
| 35  | Lg    | 0.70         | 0/916          | 0.70        | 0/1220         |
| 36  | Lh    | 0.60         | 0/1023         | 0.66        | 0/1351         |
| 37  | Li    | 0.57         | 0/843          | 0.66        | 0/1115         |
| 38  | Lj    | 0.75         | 0/731          | 0.78        | 0/966          |
| 39  | Lk    | 0.53         | 0/575          | 0.67        | 0/761          |
| 40  | Ll    | 0.70         | 0/454          | 0.76        | 0/599          |
| 41  | Lm    | 0.62         | 0/425          | 0.61        | 0/561          |
| 42  | Ln    | 0.71         | 0/231          | 0.97        | 1/294 (0.3%)   |
| 43  | Lo    | 0.66         | 0/887          | 0.76        | 0/1170         |
| 44  | Lp    | 0.68         | 0/718          | 0.69        | 0/953          |
| 45  | Lr    | 0.70         | 0/1017         | 0.77        | 0/1364         |
| 46  | S2    | 0.80         | 6/36169 (0.0%) | 0.42        | 3/56356 (0.0%) |
| 47  | SA    | 0.39         | 0/1742         | 0.57        | 0/2367         |
| 48  | SB    | 0.45         | 0/1745         | 0.56        | 0/2335         |
| 49  | SD    | 0.34         | 0/1773         | 0.52        | 0/2387         |
| 50  | SE    | 0.43         | 1/2092 (0.0%)  | 0.56        | 0/2816         |
| 51  | SF    | 0.37         | 0/1491         | 0.58        | 0/2003         |
| 52  | SH    | 0.36         | 0/1512         | 0.62        | 0/2025         |
| 53  | SI    | 0.48         | 0/1651         | 0.63        | 0/2200         |
| 54  | SK    | 0.31         | 0/823          | 0.55        | 0/1111         |
| 55  | SL    | 0.53         | 0/1164         | 0.60        | 1/1558 (0.1%)  |
| 56  | SP    | 0.33         | 0/1097         | 0.56        | 0/1467         |
| 57  | SQ    | 0.35         | 0/1134         | 0.62        | 1/1517 (0.1%)  |
| 58  | SR    | 0.34         | 0/1078         | 0.65        | 1/1447 (0.1%)  |
| 59  | SS    | 0.36         | 0/1202         | 0.58        | 0/1610         |
| 60  | ST    | 0.36         | 0/1113         | 0.56        | 0/1493         |
| 61  | SU    | 0.32         | 0/808          | 0.62        | 0/1085         |
| 62  | SV    | 0.43         | 0/644          | 0.59        | 0/862          |
| 63  | SX    | 0.47         | 0/1097         | 0.61        | 0/1464         |
| 64  | Sa    | 0.49         | 0/805          | 0.67        | 0/1079         |
| 65  | Sc    | 0.35         | 0/481          | 0.60        | 0/643          |
| 66  | Sd    | 0.41         | 0/470          | 0.59        | 0/623          |
| 67  | Sg    | 0.29         | 0/2493         | 0.64        | 1/3394 (0.0%)  |
| 68  | SC    | 0.43         | 0/1755         | 0.59        | 0/2371         |
| 69  | SG    | 0.34         | 0/1871         | 0.59        | 2/2492 (0.1%)  |
| 70  | SJ    | 0.37         | 0/1524         | 0.54        | 0/2035         |
| 71  | SM    | 0.23         | 0/868          | 0.55        | 0/1165         |
| 72  | SN    | 0.47         | 0/1232         | 0.53        | 0/1656         |
| 73  | SO    | 0.54         | 1/1014 (0.1%)  | 0.59        | 0/1358         |
| 74  | SW    | 0.50         | 0/1051         | 0.58        | 0/1406         |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 75  | SY    | 0.35         | 0/1019           | 0.53        | 0/1354           |
| 76  | SZ    | 0.35         | 0/565            | 0.64        | 2/759 (0.3%)     |
| 77  | Sb    | 0.42         | 0/653            | 0.51        | 0/876            |
| 78  | Se    | 0.32         | 0/410            | 0.53        | 0/539            |
| 79  | Sf    | 0.31         | 0/525            | 0.68        | 0/695            |
| 80  | Bv    | 0.41         | 0/1527           | 0.60        | 0/2373           |
| 81  | j     | 0.36         | 0/2954           | 1.03        | 11/3968 (0.3%)   |
| 82  | k     | 0.37         | 0/300            | 0.63        | 0/463            |
| 83  | NC    | 0.34         | 0/178            | 0.91        | 0/243            |
| All | All   | 0.69         | 13/222054 (0.0%) | 0.58        | 43/324968 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | LA    | 0                   | 1                   |
| 7   | LD    | 0                   | 1                   |
| 8   | LE    | 0                   | 1                   |
| 11  | LH    | 0                   | 1                   |
| 13  | LJ    | 0                   | 1                   |
| 21  | LS    | 0                   | 1                   |
| 22  | LT    | 0                   | 1                   |
| 23  | LU    | 0                   | 1                   |
| 29  | La    | 0                   | 1                   |
| 34  | Lf    | 0                   | 2                   |
| 36  | Lh    | 0                   | 1                   |
| 38  | Lj    | 0                   | 1                   |
| 45  | Lr    | 0                   | 1                   |
| 46  | S2    | 1                   | 0                   |
| 52  | SH    | 0                   | 1                   |
| 63  | SX    | 0                   | 1                   |
| 70  | SJ    | 0                   | 1                   |
| 74  | SW    | 0                   | 1                   |
| All | All   | 1                   | 18                  |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 46  | S2    | 970 | G    | C6-N1 | 59.89 | 2.59        | 1.39     |
| 46  | S2    | 970 | G    | N1-C2 | 56.13 | 2.50        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 46  | S2    | 970  | G    | N3-C4 | 46.92 | 2.29        | 1.35     |
| 46  | S2    | 970  | G    | C2-N3 | 46.80 | 2.26        | 1.32     |
| 46  | S2    | 970  | G    | C5-C6 | 45.50 | 2.33        | 1.42     |
| 46  | S2    | 970  | G    | C5-C4 | 40.80 | 2.19        | 1.38     |
| 3   | L5    | 3690 | A    | N1-C2 | 36.65 | 2.07        | 1.34     |
| 3   | L5    | 3690 | A    | C2-N3 | 35.87 | 2.05        | 1.33     |
| 3   | L5    | 3690 | A    | C6-N1 | 22.39 | 1.80        | 1.35     |
| 3   | L5    | 3690 | A    | N3-C4 | 20.62 | 1.76        | 1.34     |
| 73  | SO    | 140  | THR  | C-N   | -7.93 | 1.23        | 1.33     |
| 50  | SE    | 149  | TYR  | C-O   | 7.37  | 1.27        | 1.23     |
| 2   | LB    | 16   | PHE  | C-N   | -5.70 | 1.25        | 1.33     |

All (43) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 3   | L5    | 3690 | A    | N1-C2-N3   | -39.65 | 10.36       | 129.30   |
| 81  | j     | 303  | PHE  | N-CA-C     | 29.86  | 150.60      | 113.88   |
| 81  | j     | 304  | GLY  | N-CA-C     | 20.76  | 145.00      | 113.86   |
| 81  | j     | 305  | VAL  | N-CA-CB    | 18.35  | 141.51      | 111.23   |
| 3   | L5    | 3690 | A    | C6-N1-C2   | 14.75  | 162.85      | 118.60   |
| 3   | L5    | 3690 | A    | C2-N3-C4   | 14.19  | 153.17      | 110.60   |
| 81  | j     | 303  | PHE  | CB-CA-C    | -10.04 | 92.77       | 109.03   |
| 10  | LG    | 217  | LYS  | N-CA-C     | -8.37  | 103.66      | 114.04   |
| 81  | j     | 118  | LYS  | CA-C-N     | 8.27   | 130.18      | 119.84   |
| 81  | j     | 118  | LYS  | C-N-CA     | 8.27   | 130.18      | 119.84   |
| 3   | L5    | 3690 | A    | N3-C4-N9   | 7.90   | 151.11      | 127.40   |
| 81  | j     | 89   | PRO  | CA-C-N     | -7.62  | 111.76      | 119.92   |
| 81  | j     | 89   | PRO  | C-N-CA     | -7.62  | 111.76      | 119.92   |
| 3   | L5    | 3690 | A    | C4-C5-C6   | -7.50  | 94.51       | 117.00   |
| 81  | j     | 43   | ASP  | N-CA-C     | 7.38   | 121.21      | 110.28   |
| 81  | j     | 305  | VAL  | N-CA-C     | -7.33  | 94.09       | 109.34   |
| 67  | Sg    | 294  | ASP  | N-CA-C     | -6.80  | 106.18      | 114.75   |
| 3   | L5    | 3690 | A    | N3-C4-C5   | -6.51  | 107.27      | 126.80   |
| 76  | SZ    | 61   | GLU  | CA-C-N     | 6.42   | 124.28      | 120.24   |
| 76  | SZ    | 61   | GLU  | C-N-CA     | 6.42   | 124.28      | 120.24   |
| 8   | LE    | 177  | GLY  | N-CA-C     | -6.19  | 99.72       | 112.34   |
| 57  | SQ    | 113  | ILE  | N-CA-C     | -5.87  | 107.14      | 111.90   |
| 3   | L5    | 3887 | A    | N9-C1'-C2' | -5.66  | 105.51      | 114.00   |
| 69  | SG    | 180  | VAL  | CA-C-N     | 5.62   | 142.97      | 121.95   |
| 69  | SG    | 180  | VAL  | C-N-CA     | 5.62   | 142.97      | 121.95   |
| 29  | La    | 23   | GLY  | CA-C-N     | 5.48   | 132.01      | 121.54   |
| 29  | La    | 23   | GLY  | C-N-CA     | 5.48   | 132.01      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | LJ    | 10   | ASN  | N-CA-C      | 5.45  | 121.86      | 109.81   |
| 55  | SL    | 4    | ILE  | N-CA-C      | -5.42 | 107.07      | 113.42   |
| 17  | LO    | 110  | PRO  | N-CA-C      | 5.38  | 117.26      | 110.70   |
| 58  | SR    | 124  | VAL  | N-CA-C      | -5.37 | 107.51      | 112.83   |
| 3   | L5    | 397  | C    | C2'-C3'-O3' | 5.33  | 121.69      | 113.70   |
| 3   | L5    | 2662 | G    | P-O3'-C3'   | 5.31  | 128.16      | 120.20   |
| 81  | j     | 254  | VAL  | N-CA-C      | 5.29  | 116.20      | 108.58   |
| 3   | L5    | 4570 | G    | P-O3'-C3'   | 5.21  | 128.02      | 120.20   |
| 46  | S2    | 688  | U    | P-O3'-C3'   | 5.18  | 127.97      | 120.20   |
| 46  | S2    | 970  | G    | N7-C8-N9    | 5.10  | 128.40      | 113.10   |
| 42  | Ln    | 10   | MET  | CB-CG-SD    | -5.09 | 97.42       | 112.70   |
| 19  | LQ    | 76   | GLU  | CA-C-N      | 5.07  | 129.61      | 122.46   |
| 19  | LQ    | 76   | GLU  | C-N-CA      | 5.07  | 129.61      | 122.46   |
| 1   | LA    | 179  | ILE  | CA-C-N      | 5.04  | 131.16      | 121.54   |
| 1   | LA    | 179  | ILE  | C-N-CA      | 5.04  | 131.16      | 121.54   |
| 46  | S2    | 970  | G    | C4-C5-N7    | -5.01 | 95.78       | 110.80   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 46  | S2    | 1248 | B8N  | C33  |

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | LA    | 246 | LEU  | Peptide |
| 7   | LD    | 43  | LYS  | Peptide |
| 8   | LE    | 176 | THR  | Peptide |
| 11  | LH    | 173 | ARG  | Peptide |
| 13  | LJ    | 10  | ASN  | Peptide |
| 21  | LS    | 5   | GLY  | Peptide |
| 22  | LT    | 80  | VAL  | Peptide |
| 23  | LU    | 97  | ARG  | Peptide |
| 29  | La    | 23  | GLY  | Peptide |
| 34  | Lf    | 103 | VAL  | Peptide |
| 34  | Lf    | 106 | TYR  | Peptide |
| 36  | Lh    | 86  | LYS  | Peptide |
| 38  | Lj    | 39  | TYR  | Peptide |
| 45  | Lr    | 20  | ARG  | Peptide |
| 52  | SH    | 11  | PRO  | Peptide |
| 70  | SJ    | 137 | VAL  | Peptide |
| 74  | SW    | 28  | ARG  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 63  | SX    | 86  | PRO  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | LA    | 1898  | 0        | 1993     | 19      | 0            |
| 2   | LB    | 3197  | 0        | 3338     | 24      | 0            |
| 3   | L5    | 75317 | 0        | 38138    | 322     | 0            |
| 4   | L7    | 2562  | 0        | 1295     | 5       | 0            |
| 5   | L8    | 3298  | 0        | 1673     | 10      | 0            |
| 6   | LC    | 2855  | 0        | 3030     | 21      | 0            |
| 7   | LD    | 2357  | 0        | 2386     | 21      | 0            |
| 8   | LE    | 1904  | 0        | 2055     | 30      | 0            |
| 9   | LF    | 1878  | 0        | 2009     | 13      | 0            |
| 10  | LG    | 1935  | 0        | 2087     | 21      | 0            |
| 11  | LH    | 1518  | 0        | 1601     | 13      | 0            |
| 12  | LI    | 1677  | 0        | 1721     | 13      | 0            |
| 13  | LJ    | 1410  | 0        | 1441     | 19      | 0            |
| 14  | LL    | 1649  | 0        | 1760     | 15      | 0            |
| 15  | LM    | 1138  | 0        | 1204     | 5       | 0            |
| 16  | LN    | 1701  | 0        | 1749     | 20      | 0            |
| 17  | LO    | 1650  | 0        | 1794     | 13      | 0            |
| 18  | LP    | 1242  | 0        | 1269     | 15      | 0            |
| 19  | LQ    | 1513  | 0        | 1628     | 18      | 0            |
| 20  | LR    | 1566  | 0        | 1729     | 16      | 0            |
| 21  | LS    | 1453  | 0        | 1490     | 10      | 0            |
| 22  | LT    | 1298  | 0        | 1366     | 12      | 0            |
| 23  | LU    | 825   | 0        | 850      | 16      | 0            |
| 24  | LV    | 979   | 0        | 1039     | 9       | 0            |
| 25  | LW    | 1015  | 0        | 1079     | 14      | 0            |
| 26  | LX    | 985   | 0        | 1066     | 6       | 0            |
| 27  | LY    | 1115  | 0        | 1205     | 13      | 0            |
| 28  | LZ    | 1107  | 0        | 1182     | 11      | 0            |
| 29  | La    | 1162  | 0        | 1213     | 8       | 0            |
| 30  | Lb    | 882   | 0        | 962      | 5       | 0            |
| 31  | Lc    | 764   | 0        | 804      | 6       | 0            |
| 32  | Ld    | 888   | 0        | 930      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | Le    | 1053  | 0        | 1147     | 9       | 0            |
| 34  | Lf    | 876   | 0        | 912      | 6       | 0            |
| 35  | Lg    | 906   | 0        | 998      | 5       | 0            |
| 36  | Lh    | 1015  | 0        | 1148     | 9       | 0            |
| 37  | Li    | 832   | 0        | 917      | 3       | 0            |
| 38  | Lj    | 713   | 0        | 751      | 8       | 0            |
| 39  | Lk    | 569   | 0        | 637      | 8       | 0            |
| 40  | Ll    | 444   | 0        | 483      | 8       | 0            |
| 41  | Lm    | 430   | 0        | 466      | 8       | 0            |
| 42  | Ln    | 230   | 0        | 274      | 1       | 0            |
| 43  | Lo    | 870   | 0        | 944      | 11      | 0            |
| 44  | Lp    | 708   | 0        | 756      | 8       | 0            |
| 45  | Lr    | 1002  | 0        | 1068     | 10      | 0            |
| 46  | S2    | 34012 | 0        | 17222    | 178     | 0            |
| 47  | SA    | 1705  | 0        | 1706     | 15      | 0            |
| 48  | SB    | 1718  | 0        | 1791     | 16      | 0            |
| 49  | SD    | 1745  | 0        | 1839     | 22      | 0            |
| 50  | SE    | 2050  | 0        | 2156     | 22      | 0            |
| 51  | SF    | 1471  | 0        | 1524     | 15      | 0            |
| 52  | SH    | 1490  | 0        | 1583     | 9       | 0            |
| 53  | SI    | 1624  | 0        | 1703     | 14      | 0            |
| 54  | SK    | 799   | 0        | 823      | 11      | 0            |
| 55  | SL    | 1144  | 0        | 1206     | 8       | 0            |
| 56  | SP    | 1075  | 0        | 1123     | 15      | 0            |
| 57  | SQ    | 1117  | 0        | 1185     | 13      | 0            |
| 58  | SR    | 1064  | 0        | 1118     | 14      | 0            |
| 59  | SS    | 1184  | 0        | 1244     | 13      | 0            |
| 60  | ST    | 1094  | 0        | 1120     | 10      | 0            |
| 61  | SU    | 798   | 0        | 868      | 9       | 0            |
| 62  | SV    | 639   | 0        | 638      | 6       | 0            |
| 63  | SX    | 1080  | 0        | 1147     | 6       | 0            |
| 64  | Sa    | 792   | 0        | 841      | 9       | 0            |
| 65  | Sc    | 479   | 0        | 507      | 9       | 0            |
| 66  | Sd    | 459   | 0        | 448      | 4       | 0            |
| 67  | Sg    | 2436  | 0        | 2393     | 44      | 0            |
| 68  | SC    | 1715  | 0        | 1804     | 19      | 0            |
| 69  | SG    | 1848  | 0        | 2000     | 23      | 0            |
| 70  | SJ    | 1499  | 0        | 1618     | 16      | 0            |
| 71  | SM    | 860   | 0        | 876      | 8       | 0            |
| 72  | SN    | 1208  | 0        | 1294     | 9       | 0            |
| 73  | SO    | 1010  | 0        | 1033     | 17      | 0            |
| 74  | SW    | 1034  | 0        | 1080     | 13      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 75  | SY    | 1002   | 0        | 1075     | 14      | 0            |
| 76  | SZ    | 559    | 0        | 616      | 10      | 0            |
| 77  | Sb    | 640    | 0        | 665      | 3       | 0            |
| 78  | Se    | 407    | 0        | 453      | 2       | 0            |
| 79  | Sf    | 515    | 0        | 524      | 5       | 0            |
| 80  | Bv    | 1621   | 0        | 815      | 91      | 0            |
| 81  | j     | 2930   | 0        | 2985     | 221     | 0            |
| 82  | k     | 270    | 0        | 139      | 19      | 0            |
| 83  | NC    | 177    | 0        | 209      | 14      | 0            |
| 84  | Bv    | 2      | 0        | 0        | 0       | 0            |
| 84  | L5    | 145    | 0        | 0        | 0       | 0            |
| 84  | L7    | 5      | 0        | 0        | 0       | 0            |
| 84  | L8    | 2      | 0        | 0        | 0       | 0            |
| 84  | S2    | 35     | 0        | 0        | 0       | 0            |
| 84  | k     | 1      | 0        | 0        | 0       | 0            |
| 85  | L5    | 31     | 0        | 0        | 0       | 0            |
| 86  | Lg    | 1      | 0        | 0        | 0       | 0            |
| 86  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 86  | Lm    | 1      | 0        | 0        | 0       | 0            |
| 86  | Lo    | 1      | 0        | 0        | 0       | 0            |
| 86  | Lp    | 1      | 0        | 0        | 0       | 0            |
| 86  | Sa    | 1      | 0        | 0        | 0       | 0            |
| 86  | Sd    | 1      | 0        | 0        | 0       | 0            |
| 86  | Sf    | 1      | 0        | 0        | 0       | 0            |
| 87  | Bv    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 211887 | 0        | 158958   | 1431    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 3:L5:3690:A:C4 | 3:L5:3690:A:N3   | 1.76                     | 1.51              |
| 3:L5:3690:A:N1 | 3:L5:3690:A:C6   | 1.80                     | 1.48              |
| 3:L5:1968:G:N2 | 81:j:414:ARG:NH1 | 1.65                     | 1.43              |
| 3:L5:3690:A:N3 | 3:L5:3690:A:C6   | 1.98                     | 1.32              |
| 3:L5:3690:A:C4 | 3:L5:3690:A:N1   | 1.96                     | 1.32              |
| 46:S2:970:G:C5 | 46:S2:970:G:C4   | 2.20                     | 1.28              |
| 81:j:327:ASP:O | 81:j:348:PRO:CD  | 1.86                     | 1.23              |
| 3:L5:3690:A:N3 | 3:L5:3690:A:C2   | 2.05                     | 1.22              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L5:3690:A:N1    | 3:L5:3690:A:C2    | 2.07                     | 1.21              |
| 81:j:166:ARG:NH2  | 81:j:265:ASN:HD22 | 1.38                     | 1.20              |
| 81:j:291:PHE:HE1  | 81:j:406:PHE:CE2  | 1.58                     | 1.20              |
| 3:L5:3690:A:N1    | 46:S2:970:G:N1    | 1.91                     | 1.19              |
| 46:S2:970:G:C5    | 46:S2:970:G:C6    | 2.33                     | 1.17              |
| 43:Lo:105:GLN:O   | 80:Bv:19:G:N1     | 1.82                     | 1.13              |
| 56:SP:138:SER:HB3 | 81:j:110:VAL:HG22 | 1.20                     | 1.11              |
| 81:j:327:ASP:HB3  | 81:j:348:PRO:HG2  | 1.32                     | 1.10              |
| 81:j:89:PRO:HB2   | 81:j:115:GLU:OE2  | 1.51                     | 1.09              |
| 46:S2:626:G:N2    | 82:k:1060:U:O2    | 1.89                     | 1.06              |
| 81:j:327:ASP:O    | 81:j:348:PRO:HD2  | 1.57                     | 1.05              |
| 3:L5:1968:G:N2    | 81:j:414:ARG:HH12 | 1.35                     | 1.04              |
| 46:S2:970:G:N3    | 46:S2:970:G:C2    | 2.26                     | 1.04              |
| 43:Lo:105:GLN:O   | 80:Bv:19:G:C2     | 2.13                     | 1.02              |
| 46:S2:970:G:C4    | 46:S2:970:G:N3    | 2.29                     | 1.00              |
| 81:j:291:PHE:CE1  | 81:j:406:PHE:HE2  | 1.79                     | 1.00              |
| 81:j:233:LYS:HG2  | 81:j:253:LEU:CD2  | 1.92                     | 0.99              |
| 80:Bv:7:G:C2      | 80:Bv:67:A:C2     | 2.50                     | 0.98              |
| 81:j:291:PHE:CE1  | 81:j:406:PHE:CE2  | 2.50                     | 0.98              |
| 81:j:327:ASP:HB3  | 81:j:348:PRO:CG   | 1.93                     | 0.98              |
| 81:j:166:ARG:NH2  | 81:j:265:ASN:ND2  | 2.12                     | 0.98              |
| 81:j:289:ARG:HG3  | 81:j:289:ARG:HH11 | 1.29                     | 0.97              |
| 80:Bv:53:G:C2     | 80:Bv:62:C:C2     | 2.52                     | 0.97              |
| 81:j:271:SER:O    | 81:j:275:LEU:HD22 | 1.65                     | 0.96              |
| 3:L5:1968:G:C2    | 81:j:414:ARG:NH1  | 2.35                     | 0.94              |
| 81:j:291:PHE:HE1  | 81:j:406:PHE:HE2  | 0.95                     | 0.94              |
| 81:j:166:ARG:HH22 | 81:j:265:ASN:HD22 | 1.12                     | 0.94              |
| 81:j:327:ASP:O    | 81:j:348:PRO:HD3  | 1.64                     | 0.94              |
| 81:j:89:PRO:CB    | 81:j:115:GLU:OE2  | 2.16                     | 0.93              |
| 80:Bv:52:G:N2     | 80:Bv:63:A:C5     | 2.37                     | 0.93              |
| 3:L5:1968:G:H22   | 81:j:414:ARG:HH12 | 1.10                     | 0.92              |
| 80:Bv:53:G:N2     | 80:Bv:62:C:C2     | 2.38                     | 0.92              |
| 80:Bv:52:G:N1     | 80:Bv:63:A:C6     | 2.38                     | 0.91              |
| 81:j:233:LYS:CG   | 81:j:253:LEU:HD23 | 2.04                     | 0.88              |
| 3:L5:3690:A:C2    | 46:S2:970:G:N1    | 2.42                     | 0.88              |
| 81:j:50:LYS:O     | 81:j:50:LYS:HD3   | 1.75                     | 0.87              |
| 81:j:40:PRO:CD    | 81:j:123:SER:OG   | 2.23                     | 0.86              |
| 81:j:219:VAL:HG21 | 81:j:249:LYS:HD2  | 1.58                     | 0.86              |
| 3:L5:3690:A:N3    | 46:S2:970:G:N1    | 2.23                     | 0.86              |
| 3:L5:3690:A:N1    | 46:S2:970:G:C6    | 2.45                     | 0.85              |
| 81:j:245:ARG:HB2  | 81:j:245:ARG:NH1  | 1.91                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 56:SP:142:ILE:HD12 | 81:j:23:SER:OG    | 1.76                     | 0.85              |
| 80:Bv:7:G:N2       | 80:Bv:67:A:N3     | 2.25                     | 0.84              |
| 81:j:233:LYS:CG    | 81:j:253:LEU:CD2  | 2.55                     | 0.84              |
| 81:j:329:MET:O     | 81:j:345:TYR:HA   | 1.77                     | 0.84              |
| 81:j:40:PRO:HA     | 81:j:120:ILE:CD1  | 2.08                     | 0.83              |
| 80:Bv:28:PSU:H6    | 80:Bv:28:PSU:H5'  | 1.44                     | 0.83              |
| 80:Bv:52:G:C2      | 80:Bv:63:A:C6     | 2.66                     | 0.83              |
| 81:j:233:LYS:HG3   | 81:j:253:LEU:HD23 | 1.57                     | 0.82              |
| 81:j:327:ASP:CB    | 81:j:348:PRO:HG2  | 2.10                     | 0.82              |
| 3:L5:1968:G:H21    | 81:j:414:ARG:NH1  | 1.74                     | 0.81              |
| 2:LB:315:ASN:HD21  | 2:LB:326:VAL:H    | 1.26                     | 0.81              |
| 81:j:40:PRO:HD3    | 81:j:123:SER:OG   | 1.81                     | 0.81              |
| 57:SQ:146:ARG:HH22 | 80:Bv:34:G:H5''   | 1.46                     | 0.81              |
| 3:L5:3690:A:C2     | 46:S2:970:G:C4    | 2.69                     | 0.81              |
| 46:S2:970:G:N1     | 46:S2:970:G:C2    | 2.50                     | 0.80              |
| 3:L5:3690:A:C2     | 46:S2:970:G:C2    | 2.69                     | 0.80              |
| 81:j:38:ILE:HG12   | 81:j:94:VAL:HG13  | 1.62                     | 0.80              |
| 3:L5:1968:G:N2     | 81:j:414:ARG:HH11 | 1.78                     | 0.80              |
| 81:j:100:ILE:HD12  | 81:j:100:ILE:O    | 1.83                     | 0.79              |
| 3:L5:3690:A:C2     | 46:S2:970:G:C6    | 2.71                     | 0.79              |
| 81:j:34:MET:HA     | 81:j:34:MET:HE2   | 1.65                     | 0.78              |
| 81:j:90:PRO:O      | 81:j:91:ASN:HB2   | 1.83                     | 0.78              |
| 81:j:289:ARG:HG3   | 81:j:289:ARG:NH1  | 1.97                     | 0.78              |
| 82:k:1058:A:H8     | 82:k:1058:A:H5''  | 1.49                     | 0.77              |
| 80:Bv:60:C:H5'     | 80:Bv:61:C:H5     | 1.50                     | 0.77              |
| 81:j:166:ARG:HH21  | 81:j:265:ASN:HD22 | 1.31                     | 0.77              |
| 81:j:330:ARG:HA    | 81:j:345:TYR:CD1  | 2.19                     | 0.77              |
| 3:L5:4422:U:N3     | 83:NC:727:PRO:HD2 | 2.00                     | 0.77              |
| 81:j:219:VAL:CG1   | 81:j:246:LEU:HD23 | 2.15                     | 0.76              |
| 3:L5:3690:A:N3     | 46:S2:970:G:C2    | 2.53                     | 0.76              |
| 81:j:27:ALA:HB1    | 81:j:100:ILE:HG21 | 1.67                     | 0.76              |
| 3:L5:3690:A:N1     | 3:L5:3690:A:C5    | 2.51                     | 0.76              |
| 81:j:289:ARG:HD2   | 81:j:412:ILE:HD13 | 1.65                     | 0.76              |
| 37:Li:2:ALA:N      | 37:Li:5:TYR:HH    | 1.84                     | 0.76              |
| 3:L5:3690:A:C2     | 46:S2:970:G:C5    | 2.74                     | 0.76              |
| 80:Bv:52:G:N1      | 80:Bv:63:A:N6     | 2.33                     | 0.76              |
| 80:Bv:50:G:N2      | 80:Bv:64:C:O2     | 2.18                     | 0.75              |
| 81:j:330:ARG:HB2   | 81:j:345:TYR:CE1  | 2.21                     | 0.75              |
| 81:j:289:ARG:O     | 81:j:289:ARG:HD3  | 1.86                     | 0.75              |
| 81:j:166:ARG:HH22  | 81:j:265:ASN:ND2  | 1.78                     | 0.75              |
| 3:L5:3690:A:N1     | 46:S2:970:G:C2    | 2.55                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 80:Bv:28:PSU:H5'  | 80:Bv:28:PSU:C6   | 2.22                     | 0.74              |
| 81:j:136:LEU:N    | 81:j:136:LEU:HD23 | 2.02                     | 0.74              |
| 80:Bv:52:G:N2     | 80:Bv:63:A:C4     | 2.55                     | 0.74              |
| 81:j:40:PRO:HA    | 81:j:120:ILE:HD11 | 1.68                     | 0.74              |
| 80:Bv:7:G:N2      | 80:Bv:67:A:C2     | 2.54                     | 0.74              |
| 81:j:118:LYS:O    | 81:j:118:LYS:HG2  | 1.88                     | 0.74              |
| 81:j:219:VAL:HG12 | 81:j:246:LEU:HD23 | 1.70                     | 0.74              |
| 46:S2:940:U:H3    | 46:S2:1002:U:H3   | 1.36                     | 0.74              |
| 81:j:258:TYR:CD1  | 81:j:262:ASN:ND2  | 2.56                     | 0.73              |
| 81:j:291:PHE:HE1  | 81:j:406:PHE:CD2  | 2.05                     | 0.73              |
| 46:S2:626:G:N7    | 82:k:1059:U:C5    | 2.56                     | 0.73              |
| 82:k:1058:A:H8    | 82:k:1058:A:C5'   | 2.01                     | 0.73              |
| 3:L5:4422:U:C6    | 81:j:185:MEQ:HE1  | 2.23                     | 0.72              |
| 73:SO:103:ASN:OD1 | 73:SO:139:SER:OG  | 2.06                     | 0.72              |
| 81:j:330:ARG:HB2  | 81:j:345:TYR:HE1  | 1.53                     | 0.72              |
| 81:j:50:LYS:HD3   | 81:j:50:LYS:C     | 2.15                     | 0.72              |
| 81:j:81:ARG:HD2   | 81:j:113:ASP:CG   | 2.14                     | 0.72              |
| 3:L5:3690:A:N3    | 46:S2:970:G:C4    | 2.57                     | 0.72              |
| 81:j:91:ASN:HA    | 81:j:119:PRO:HA   | 1.72                     | 0.72              |
| 80:Bv:61:C:H2'    | 80:Bv:62:C:H6     | 1.53                     | 0.72              |
| 81:j:110:VAL:HG13 | 81:j:112:ILE:HD12 | 1.72                     | 0.72              |
| 80:Bv:4:U:H3      | 80:Bv:69:G:H1     | 1.36                     | 0.72              |
| 81:j:34:MET:CE    | 81:j:98:GLY:HA3   | 2.20                     | 0.72              |
| 56:SP:138:SER:CB  | 81:j:110:VAL:HG22 | 2.12                     | 0.71              |
| 81:j:254:VAL:HG11 | 81:j:270:LEU:HB3  | 1.72                     | 0.71              |
| 50:SE:125:LYS:H   | 50:SE:142:HIS:HD2 | 1.35                     | 0.71              |
| 81:j:107:GLU:O    | 81:j:107:GLU:HG3  | 1.90                     | 0.71              |
| 12:LI:38:ARG:HD2  | 12:LI:83:ASP:HB2  | 1.73                     | 0.71              |
| 81:j:243:ASP:OD2  | 81:j:245:ARG:NH1  | 2.24                     | 0.71              |
| 3:L5:3689:G:H4'   | 3:L5:3690:A:H5'   | 1.73                     | 0.70              |
| 81:j:151:ILE:HD12 | 81:j:205:VAL:HG11 | 1.73                     | 0.70              |
| 81:j:219:VAL:HG12 | 81:j:246:LEU:CD2  | 2.21                     | 0.70              |
| 46:S2:970:G:N1    | 46:S2:970:G:C6    | 2.59                     | 0.70              |
| 81:j:74:ALA:O     | 81:j:78:VAL:HG12  | 1.92                     | 0.70              |
| 80:Bv:58:1MA:O2'  | 80:Bv:60:C:OP2    | 2.09                     | 0.69              |
| 3:L5:2456:C:H5    | 3:L5:2458:G:H1    | 1.39                     | 0.69              |
| 81:j:245:ARG:HB2  | 81:j:245:ARG:HH11 | 1.57                     | 0.69              |
| 80:Bv:52:G:C2     | 80:Bv:63:A:C5     | 2.81                     | 0.69              |
| 3:L5:3690:A:C2    | 46:S2:970:G:N3    | 2.61                     | 0.68              |
| 49:SD:64:ARG:HH12 | 54:SK:73:ASN:HD21 | 1.41                     | 0.68              |
| 81:j:171:LYS:HG3  | 81:j:171:LYS:O    | 1.92                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L5:1799:C:H5''   | 30:Lb:56:LYS:HE3   | 1.76                     | 0.68              |
| 80:Bv:53:G:C2      | 80:Bv:62:C:O2      | 2.46                     | 0.68              |
| 80:Bv:60:C:C5'     | 80:Bv:61:C:H5      | 2.06                     | 0.67              |
| 3:L5:681:C:H4'     | 45:Lr:85:ASN:HD22  | 1.59                     | 0.67              |
| 22:LT:43:LYS:O     | 22:LT:58:HIS:ND1   | 2.26                     | 0.67              |
| 46:S2:928:G:H1     | 46:S2:1013:U:H3    | 1.40                     | 0.67              |
| 81:j:41:PRO:HB3    | 81:j:91:ASN:N      | 2.10                     | 0.67              |
| 3:L5:2285:U:OP1    | 6:LC:204:ARG:NH2   | 2.27                     | 0.67              |
| 81:j:91:ASN:HA     | 81:j:119:PRO:CA    | 2.25                     | 0.67              |
| 81:j:317:VAL:HG21  | 81:j:320:LEU:HB2   | 1.77                     | 0.67              |
| 3:L5:4074:C:N3     | 3:L5:4090:U:O2'    | 2.28                     | 0.67              |
| 13:LJ:3:GLN:HE21   | 13:LJ:8:LYS:HG3    | 1.59                     | 0.67              |
| 81:j:91:ASN:CA     | 81:j:119:PRO:HA    | 2.25                     | 0.66              |
| 83:NC:718:LEU:HD12 | 83:NC:718:LEU:O    | 1.94                     | 0.66              |
| 81:j:346:LEU:N     | 81:j:346:LEU:HD12  | 2.10                     | 0.66              |
| 3:L5:3690:A:N3     | 46:S2:970:G:C5     | 2.64                     | 0.66              |
| 3:L5:3916:C:H1'    | 16:LN:125:SER:HB3  | 1.78                     | 0.66              |
| 81:j:291:PHE:CE1   | 81:j:406:PHE:CD2   | 2.82                     | 0.66              |
| 73:SO:103:ASN:HB3  | 73:SO:142:ARG:HG2  | 1.77                     | 0.66              |
| 3:L5:1957:A:O2'    | 3:L5:2004:A:N6     | 2.28                     | 0.65              |
| 3:L5:366:G:OP2     | 38:Lj:52:LYS:NZ    | 2.27                     | 0.65              |
| 3:L5:2470:G:O2'    | 3:L5:2483:G:N2     | 2.29                     | 0.65              |
| 56:SP:41:GLN:HG3   | 56:SP:84:ILE:HD12  | 1.78                     | 0.65              |
| 13:LJ:117:ILE:HG22 | 13:LJ:118:LYS:HG2  | 1.79                     | 0.65              |
| 24:LV:13:LYS:HD2   | 24:LV:128:LEU:HD11 | 1.78                     | 0.65              |
| 3:L5:4075:G:H22    | 3:L5:4089:C:H2'    | 1.61                     | 0.65              |
| 42:Ln:15:ARG:HH12  | 46:S2:1182:A:H5''  | 1.61                     | 0.65              |
| 80:Bv:52:G:C4      | 80:Bv:53:G:C8      | 2.85                     | 0.65              |
| 81:j:327:ASP:HB3   | 81:j:348:PRO:CD    | 2.27                     | 0.64              |
| 81:j:91:ASN:HA     | 81:j:119:PRO:CB    | 2.27                     | 0.64              |
| 3:L5:3690:A:N3     | 46:S2:970:G:N3     | 2.45                     | 0.64              |
| 81:j:41:PRO:HD3    | 81:j:91:ASN:O      | 1.96                     | 0.64              |
| 3:L5:4518:A:C8     | 80:Bv:74:C:C6      | 2.86                     | 0.64              |
| 46:S2:1396:A:O2'   | 46:S2:1398:G:N7    | 2.29                     | 0.64              |
| 3:L5:1340:G:N7     | 19:LQ:104:ARG:NH2  | 2.41                     | 0.64              |
| 81:j:243:ASP:CG    | 81:j:245:ARG:HH12  | 2.06                     | 0.64              |
| 3:L5:1795:C:OP1    | 22:LT:110:LYS:NZ   | 2.32                     | 0.63              |
| 47:SA:77:ILE:HG12  | 47:SA:99:ILE:HB    | 1.79                     | 0.63              |
| 23:LU:45:GLU:HG3   | 23:LU:46:ARG:HG3   | 1.80                     | 0.63              |
| 82:k:1058:A:H5''   | 82:k:1058:A:C8     | 2.32                     | 0.63              |
| 3:L5:1511:A2M:H62  | 3:L5:1638:G:H22    | 1.46                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L5:4875:G:N2     | 17:LO:106:ASP:O    | 2.32                     | 0.63              |
| 27:LY:34:LEU:HD23  | 27:LY:38:LEU:HB3   | 1.78                     | 0.63              |
| 46:S2:4:C:H1'      | 70:SJ:18:ARG:HH12  | 1.64                     | 0.63              |
| 24:LV:87:SER:OG    | 25:LW:19:ARG:NH1   | 2.31                     | 0.63              |
| 35:Lg:82:MET:HE1   | 35:Lg:90:ARG:HD3   | 1.80                     | 0.63              |
| 46:S2:1265:A:H2    | 46:S2:1517:G:H22   | 1.47                     | 0.63              |
| 46:S2:925:G:H1     | 46:S2:1017:U:H3    | 1.46                     | 0.63              |
| 81:j:330:ARG:CB    | 81:j:345:TYR:CE1   | 2.81                     | 0.63              |
| 81:j:75:ILE:HG22   | 81:j:79:GLN:NE2    | 2.14                     | 0.63              |
| 81:j:300:LYS:HD2   | 81:j:300:LYS:N     | 2.13                     | 0.63              |
| 23:LU:24:ASP:HB3   | 23:LU:111:GLU:HG3  | 1.81                     | 0.63              |
| 75:SY:76:TYR:OH    | 75:SY:86:GLU:OE2   | 2.17                     | 0.63              |
| 3:L5:2043:G:H5''   | 17:LO:128:ARG:HH11 | 1.64                     | 0.62              |
| 43:Lo:45:GLN:HE22  | 43:Lo:52:THR:H     | 1.46                     | 0.62              |
| 3:L5:1688:A:OP2    | 3:L5:2083:G:N2     | 2.32                     | 0.62              |
| 3:L5:4385:A:OP1    | 12:LI:154:ARG:NH2  | 2.32                     | 0.62              |
| 3:L5:964:C:OP2     | 8:LE:59:ARG:NH1    | 2.32                     | 0.62              |
| 3:L5:1255:G:N7     | 30:Lb:111:ARG:NH2  | 2.48                     | 0.62              |
| 3:L5:2356:U:H1'    | 32:Ld:39:LYS:HE3   | 1.81                     | 0.62              |
| 80:Bv:53:G:N1      | 80:Bv:62:C:N3      | 2.48                     | 0.62              |
| 3:L5:1742:C:N4     | 3:L5:1763:A:N1     | 2.43                     | 0.62              |
| 31:Lc:22:MET:SD    | 31:Lc:22:MET:N     | 2.72                     | 0.62              |
| 45:Lr:39:ARG:O     | 45:Lr:103:ARG:NH1  | 2.32                     | 0.62              |
| 46:S2:522:A:N7     | 70:SJ:38:ARG:NH2   | 2.47                     | 0.62              |
| 3:L5:3887:A:N6     | 83:NC:726:ASN:HD22 | 1.97                     | 0.62              |
| 50:SE:133:THR:HG22 | 50:SE:134:LYS:HD2  | 1.82                     | 0.62              |
| 81:j:289:ARG:HE    | 81:j:412:ILE:HG21  | 1.65                     | 0.62              |
| 75:SY:55:ILE:HG12  | 75:SY:75:ILE:HG12  | 1.81                     | 0.61              |
| 3:L5:2689:C:OP1    | 23:LU:101:ARG:NH2  | 2.32                     | 0.61              |
| 27:LY:4:ASN:HB3    | 27:LY:7:VAL:HG22   | 1.80                     | 0.61              |
| 80:Bv:6:U:C2'      | 80:Bv:7:G:H5'      | 2.30                     | 0.61              |
| 83:NC:718:LEU:O    | 83:NC:722:ILE:HG12 | 1.99                     | 0.61              |
| 3:L5:3568:G:N2     | 3:L5:3569:G:N7     | 2.48                     | 0.61              |
| 28:LZ:5:MET:O      | 28:LZ:28:ASN:ND2   | 2.34                     | 0.61              |
| 50:SE:80:ILE:HD12  | 50:SE:81:THR:HG23  | 1.81                     | 0.61              |
| 67:Sg:5:MET:HG2    | 67:Sg:312:VAL:HA   | 1.82                     | 0.61              |
| 25:LW:97:LYS:NZ    | 69:SG:145:PHE:O    | 2.31                     | 0.61              |
| 46:S2:659:G:HO2'   | 46:S2:662:G:HO2'   | 1.48                     | 0.61              |
| 3:L5:2461:G:N2     | 3:L5:2489:G:O2'    | 2.33                     | 0.61              |
| 3:L5:3690:A:N3     | 46:S2:970:G:C6     | 2.67                     | 0.61              |
| 56:SP:123:TYR:OH   | 59:SS:124:ARG:NH1  | 2.34                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:626:G:C8     | 82:k:1059:U:C5     | 2.89                     | 0.61              |
| 46:S2:824:C:H1'    | 70:SJ:144:ILE:HG21 | 1.81                     | 0.61              |
| 2:LB:95:THR:HG22   | 3:L5:4875:G:H4'    | 1.82                     | 0.61              |
| 3:L5:2240:A:H61    | 9:LF:27:GLU:HB3    | 1.64                     | 0.61              |
| 48:SB:83:LYS:HE3   | 48:SB:106:THR:HG22 | 1.80                     | 0.61              |
| 81:j:166:ARG:HH21  | 81:j:265:ASN:ND2   | 1.91                     | 0.61              |
| 81:j:237:SER:O     | 81:j:247:GLN:OE1   | 2.19                     | 0.61              |
| 51:SF:49:LEU:HD12  | 57:SQ:50:LYS:HG2   | 1.81                     | 0.61              |
| 80:Bv:60:C:H5'     | 80:Bv:61:C:C5      | 2.35                     | 0.61              |
| 3:L5:3802:G:N2     | 3:L5:3802:G:OP2    | 2.32                     | 0.60              |
| 17:LO:61:ARG:HD3   | 17:LO:66:PRO:HB3   | 1.82                     | 0.60              |
| 80:Bv:52:G:H2'     | 80:Bv:53:G:O4'     | 2.00                     | 0.60              |
| 23:LU:47:ILE:HG21  | 23:LU:56:LEU:HD13  | 1.84                     | 0.60              |
| 38:Lj:33:THR:HA    | 38:Lj:40:PRO:HD3   | 1.83                     | 0.60              |
| 3:L5:1388:C:H2'    | 3:L5:1389:C:H4'    | 1.81                     | 0.60              |
| 81:j:75:ILE:HA     | 81:j:78:VAL:CG1    | 2.31                     | 0.60              |
| 3:L5:145:C:OP2     | 10:LG:197:LYS:NZ   | 2.34                     | 0.60              |
| 16:LN:124:ASP:HB3  | 16:LN:127:TYR:H    | 1.64                     | 0.60              |
| 73:SO:132:VAL:HG23 | 73:SO:132:VAL:O    | 2.01                     | 0.60              |
| 81:j:121:ASN:HB3   | 81:j:164:ASN:HB3   | 1.83                     | 0.60              |
| 3:L5:4053:U:OP1    | 10:LG:249:ARG:NH2  | 2.34                     | 0.60              |
| 67:Sg:216:ALA:HB3  | 67:Sg:230:LEU:HB3  | 1.82                     | 0.60              |
| 3:L5:2893:G:N2     | 3:L5:3565:G:O6     | 2.35                     | 0.60              |
| 3:L5:1490:A:H4'    | 3:L5:1491:G:H5'    | 1.83                     | 0.60              |
| 46:S2:626:G:N2     | 82:k:1060:U:C2     | 2.69                     | 0.60              |
| 80:Bv:50:G:H2'     | 80:Bv:51:U:H6      | 1.66                     | 0.60              |
| 8:LE:256:GLN:O     | 8:LE:260:LYS:NZ    | 2.34                     | 0.60              |
| 46:S2:140:C:H42    | 46:S2:313:A:H61    | 1.50                     | 0.60              |
| 67:Sg:313:THR:HG22 | 67:Sg:314:ILE:HD12 | 1.82                     | 0.60              |
| 3:L5:1342:G:OP1    | 19:LQ:108:ARG:NH1  | 2.33                     | 0.59              |
| 10:LG:114:LEU:HD22 | 10:LG:117:ARG:HH21 | 1.67                     | 0.59              |
| 54:SK:14:LEU:HA    | 54:SK:17:LYS:HG2   | 1.85                     | 0.59              |
| 75:SY:25:ILE:HG21  | 75:SY:40:ILE:HD11  | 1.85                     | 0.59              |
| 6:LC:204:ARG:NH2   | 6:LC:205:ARG:O     | 2.34                     | 0.59              |
| 38:Lj:34:CYS:HB3   | 38:Lj:39:TYR:H     | 1.67                     | 0.59              |
| 80:Bv:6:U:O2'      | 80:Bv:7:G:H5'      | 2.02                     | 0.59              |
| 80:Bv:52:G:C6      | 80:Bv:63:A:N6      | 2.70                     | 0.59              |
| 83:NC:707:ILE:HB   | 83:NC:710:ILE:HG13 | 1.85                     | 0.59              |
| 67:Sg:297:THR:HG22 | 67:Sg:311:GLN:HG2  | 1.84                     | 0.59              |
| 81:j:300:LYS:HB3   | 81:j:413:LEU:O     | 2.01                     | 0.59              |
| 6:LC:337:ARG:NH2   | 8:LE:55:GLY:O      | 2.36                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:LD:50:ARG:NH2   | 7:LD:72:ASP:OD2    | 2.36                     | 0.59              |
| 36:Lh:86:LYS:O    | 36:Lh:92:ARG:NH1   | 2.36                     | 0.59              |
| 46:S2:1597:C:OP2  | 76:SZ:85:ARG:NH2   | 2.35                     | 0.59              |
| 48:SB:83:LYS:HE2  | 73:SO:130:GLU:OE1  | 2.03                     | 0.59              |
| 1:LA:116:LEU:HB2  | 1:LA:126:LEU:HB2   | 1.83                     | 0.59              |
| 59:SS:34:LYS:HG2  | 59:SS:103:LEU:HD23 | 1.85                     | 0.59              |
| 71:SM:41:ALA:HA   | 71:SM:44:LYS:HB2   | 1.84                     | 0.59              |
| 81:j:91:ASN:HA    | 81:j:119:PRO:HB3   | 1.85                     | 0.59              |
| 28:LZ:12:LEU:HB2  | 28:LZ:81:MET:HB3   | 1.82                     | 0.58              |
| 46:S2:1239:U:H5'' | 56:SP:124:LYS:HD2  | 1.85                     | 0.58              |
| 46:S2:1550:G:H3'  | 46:S2:1579:A:H61   | 1.68                     | 0.58              |
| 67:Sg:238:ALA:H   | 67:Sg:251:ALA:HB3  | 1.67                     | 0.58              |
| 3:L5:4669:U:OP2   | 41:Lm:111:ARG:NH2  | 2.36                     | 0.58              |
| 46:S2:1147:C:OP1  | 64:Sa:6:ARG:NH2    | 2.35                     | 0.58              |
| 7:LD:41:LYS:NZ    | 22:LT:32:ARG:O     | 2.36                     | 0.58              |
| 46:S2:1467:C:OP1  | 58:SR:2:GLY:N      | 2.37                     | 0.58              |
| 2:LB:218:ASP:OD2  | 2:LB:348:ARG:NH1   | 2.37                     | 0.58              |
| 3:L5:929:G:OP1    | 9:LF:245:ARG:NH1   | 2.35                     | 0.58              |
| 3:L5:4103:C:OP1   | 10:LG:37:LYS:NZ    | 2.36                     | 0.58              |
| 46:S2:943:U:OP2   | 48:SB:216:LYS:NZ   | 2.34                     | 0.58              |
| 47:SA:41:ARG:HE   | 47:SA:45:GLY:HA2   | 1.69                     | 0.58              |
| 80:Bv:37:UY4:N08  | 80:Bv:37:UY4:N1    | 2.51                     | 0.58              |
| 46:S2:1123:C:OP1  | 48:SB:151:ARG:NH1  | 2.37                     | 0.58              |
| 46:S2:1314:U:H4'  | 54:SK:8:ARG:HH12   | 1.68                     | 0.58              |
| 3:L5:1968:G:H21   | 81:j:414:ARG:HH11  | 1.43                     | 0.58              |
| 63:SX:93:PHE:O    | 63:SX:140:ARG:NH2  | 2.33                     | 0.58              |
| 80:Bv:53:G:N2     | 80:Bv:62:C:O2      | 2.37                     | 0.58              |
| 46:S2:601:OMG:HN1 | 46:S2:621:OMC:H5   | 1.51                     | 0.58              |
| 81:j:40:PRO:HA    | 81:j:120:ILE:HD12  | 1.83                     | 0.58              |
| 81:j:318:GLU:O    | 81:j:388:THR:OG1   | 2.22                     | 0.58              |
| 82:k:1058:A:C5'   | 82:k:1058:A:C8     | 2.86                     | 0.58              |
| 3:L5:1426:C:H5'   | 9:LF:34:ARG:HH12   | 1.69                     | 0.58              |
| 46:S2:157:U:O2'   | 46:S2:159:A2M:N7   | 2.31                     | 0.58              |
| 72:SN:46:THR:H    | 72:SN:49:GLN:HE21  | 1.50                     | 0.58              |
| 75:SY:5:VAL:O     | 75:SY:43:LYS:NZ    | 2.37                     | 0.58              |
| 3:L5:4422:U:C6    | 81:j:185:MEQ:CE    | 2.87                     | 0.57              |
| 46:S2:583:A:OP1   | 70:SJ:162:ARG:NH2  | 2.37                     | 0.57              |
| 81:j:168:VAL:HG23 | 81:j:168:VAL:O     | 2.04                     | 0.57              |
| 3:L5:1957:A:H5''  | 3:L5:2002:U:H3     | 1.69                     | 0.57              |
| 3:L5:2645:G:N2    | 3:L5:2663:A:OP2    | 2.31                     | 0.57              |
| 8:LE:192:LYS:HE2  | 34:Lf:107:PRO:HB3  | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:192:LYS:HB3   | 1:LA:193:ARG:HE    | 1.69                     | 0.57              |
| 56:SP:142:ILE:CD1  | 81:j:23:SER:OG     | 2.50                     | 0.57              |
| 3:L5:4840:G:H2'    | 21:LS:169:THR:HG22 | 1.87                     | 0.57              |
| 4:L7:7:G:OP1       | 7:LD:33:ARG:NH2    | 2.38                     | 0.57              |
| 22:LT:48:VAL:HG21  | 22:LT:94:GLU:HG2   | 1.86                     | 0.57              |
| 81:j:117:PHE:CZ    | 81:j:140:LEU:HD22  | 2.39                     | 0.57              |
| 81:j:304:GLY:O     | 81:j:305:VAL:HG22  | 2.03                     | 0.57              |
| 3:L5:63:G:OP2      | 16:LN:169:ARG:NH1  | 2.34                     | 0.57              |
| 16:LN:138:PHE:HA   | 16:LN:143:ARG:HD2  | 1.86                     | 0.57              |
| 67:Sg:7:LEU:HD23   | 67:Sg:9:GLY:H      | 1.70                     | 0.57              |
| 67:Sg:11:LEU:HB2   | 67:Sg:307:VAL:HB   | 1.86                     | 0.57              |
| 81:j:254:VAL:CG1   | 81:j:270:LEU:HB3   | 2.34                     | 0.57              |
| 3:L5:700:C:OP1     | 34:Lf:89:ARG:NH1   | 2.38                     | 0.57              |
| 3:L5:3887:A:H61    | 83:NC:726:ASN:ND2  | 2.02                     | 0.57              |
| 34:Lf:36:ARG:NH2   | 34:Lf:79:GLY:O     | 2.34                     | 0.57              |
| 81:j:289:ARG:NE    | 81:j:412:ILE:HG21  | 2.19                     | 0.57              |
| 3:L5:3668:G:O2'    | 3:L5:3797:UY1:OP2  | 2.21                     | 0.57              |
| 3:L5:4075:G:OP1    | 35:Lg:114:GLN:NE2  | 2.38                     | 0.57              |
| 46:S2:1488:C:O2'   | 46:S2:1490:OMG:OP2 | 2.23                     | 0.57              |
| 51:SF:58:ALA:HB3   | 51:SF:62:ARG:HH12  | 1.68                     | 0.57              |
| 81:j:302:CYS:SG    | 81:j:413:LEU:HD21  | 2.45                     | 0.57              |
| 3:L5:1259:C:H5''   | 9:LF:34:ARG:HG2    | 1.87                     | 0.57              |
| 53:SI:101:ILE:HD12 | 53:SI:190:LEU:HD11 | 1.87                     | 0.57              |
| 52:SH:144:ILE:HG23 | 74:SW:52:ILE:HB    | 1.86                     | 0.57              |
| 18:LP:48:LEU:HD21  | 18:LP:91:LEU:HB3   | 1.87                     | 0.56              |
| 20:LR:182:GLU:HG2  | 20:LR:183:GLU:HG3  | 1.87                     | 0.56              |
| 80:Bv:5:C:H2'      | 80:Bv:6:U:H6       | 1.70                     | 0.56              |
| 3:L5:109:G:OP2     | 14:LL:74:ARG:NH2   | 2.38                     | 0.56              |
| 3:L5:1432:U:O4     | 3:L5:2087:A:N6     | 2.37                     | 0.56              |
| 46:S2:1564:C:OP1   | 60:ST:121:ARG:NH1  | 2.38                     | 0.56              |
| 52:SH:51:ILE:HG21  | 52:SH:179:LYS:HG2  | 1.87                     | 0.56              |
| 71:SM:49:LEU:HD22  | 71:SM:123:VAL:HG11 | 1.88                     | 0.56              |
| 1:LA:116:LEU:HD11  | 1:LA:148:VAL:HG11  | 1.86                     | 0.56              |
| 2:LB:10:ARG:HH22   | 2:LB:265:SER:HB2   | 1.70                     | 0.56              |
| 3:L5:2395:U:OP1    | 40:Ll:42:ARG:NH2   | 2.38                     | 0.56              |
| 3:L5:2549:G:N2     | 3:L5:2552:A:OP2    | 2.39                     | 0.56              |
| 3:L5:4260:U:OP1    | 43:Lo:9[B]:ARG:NH1 | 2.38                     | 0.56              |
| 11:LH:51:LYS:HG2   | 11:LH:52:LYS:HG2   | 1.87                     | 0.56              |
| 46:S2:71:G:O6      | 69:SG:170:ARG:NH2  | 2.35                     | 0.56              |
| 56:SP:38:SER:OG    | 56:SP:41:GLN:NE2   | 2.39                     | 0.56              |
| 67:Sg:256:ILE:HB   | 67:Sg:270:LEU:HB2  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:j:34:MET:HE2   | 81:j:98:GLY:HA3    | 1.87                     | 0.56              |
| 81:j:280:PHE:HE1  | 81:j:395:LYS:HG3   | 1.70                     | 0.56              |
| 3:L5:148:G:H3'    | 16:LN:49:ARG:HH12  | 1.71                     | 0.56              |
| 53:SI:65:PHE:HD2  | 53:SI:104:ILE:HD13 | 1.70                     | 0.56              |
| 69:SG:54:GLY:O    | 69:SG:110:ASN:ND2  | 2.38                     | 0.56              |
| 3:L5:3690:A:C6    | 46:S2:970:G:N1     | 2.74                     | 0.56              |
| 25:LW:93:LYS:O    | 25:LW:101:ARG:NH2  | 2.37                     | 0.56              |
| 7:LD:181:PRO:HD2  | 7:LD:195:HIS:HD2   | 1.70                     | 0.56              |
| 3:L5:353:A:N6     | 40:LI:37:TYR:O     | 2.35                     | 0.56              |
| 6:LC:221:PHE:O    | 6:LC:223:ASN:N     | 2.39                     | 0.56              |
| 12:LI:38:ARG:HG3  | 12:LI:41:ALA:HB2   | 1.88                     | 0.56              |
| 50:SE:11:ARG:NH2  | 50:SE:21:ASP:O     | 2.37                     | 0.56              |
| 65:Sc:29:GLN:HG2  | 65:Sc:45:ASN:HB3   | 1.87                     | 0.56              |
| 75:SY:20:ARG:NH2  | 75:SY:74:MET:SD    | 2.79                     | 0.56              |
| 81:j:63:UXY:C06   | 82:k:1059:U:H5'    | 2.36                     | 0.56              |
| 3:L5:398:A:O2'    | 3:L5:401:A:OP1     | 2.23                     | 0.56              |
| 3:L5:2835:G:O2'   | 3:L5:3817:U:O4     | 2.19                     | 0.56              |
| 18:LP:109:VAL:HA  | 18:LP:112:LEU:HD13 | 1.88                     | 0.56              |
| 46:S2:847:A:OP1   | 50:SE:108:ARG:NH2  | 2.38                     | 0.56              |
| 65:Sc:29:GLN:HE22 | 65:Sc:67:ARG:HD3   | 1.71                     | 0.56              |
| 3:L5:2588:A:N6    | 3:L5:2731:A:OP2    | 2.36                     | 0.56              |
| 20:LR:39:GLN:OE1  | 20:LR:42:ARG:NH2   | 2.39                     | 0.56              |
| 46:S2:1398:G:O2'  | 67:Sg:88:ARG:NH2   | 2.39                     | 0.56              |
| 80:Bv:52:G:H1     | 80:Bv:63:A:N6      | 2.04                     | 0.56              |
| 3:L5:4455:C:O2'   | 41:Lm:114:LYS:NZ   | 2.37                     | 0.56              |
| 13:LJ:64:ARG:NH2  | 13:LJ:65:ASN:OD1   | 2.38                     | 0.56              |
| 49:SD:33:GLY:HA3  | 49:SD:53:THR:HG22  | 1.87                     | 0.56              |
| 3:L5:2685:G:H21   | 35:Lg:28:ASN:HD21  | 1.55                     | 0.55              |
| 64:Sa:44:ILE:HD13 | 73:SO:129:ILE:HG21 | 1.87                     | 0.55              |
| 68:SC:211:LYS:HG2 | 68:SC:215:MET:HE2  | 1.88                     | 0.55              |
| 11:LH:93:ARG:HD2  | 11:LH:143:GLU:HB3  | 1.89                     | 0.55              |
| 33:Le:92:ASN:ND2  | 33:Le:119:ALA:O    | 2.36                     | 0.55              |
| 3:L5:4073:G:H22   | 3:L5:4091:C:H4'    | 1.71                     | 0.55              |
| 23:LU:41:GLN:HA   | 23:LU:44:GLN:HB3   | 1.87                     | 0.55              |
| 46:S2:463:C:O2'   | 46:S2:466:G:O6     | 2.23                     | 0.55              |
| 49:SD:226:GLN:NE2 | 67:Sg:224:GLY:O    | 2.39                     | 0.55              |
| 79:Sf:95:ARG:NH1  | 79:Sf:96:LYS:O     | 2.40                     | 0.55              |
| 81:j:40:PRO:CG    | 81:j:123:SER:OG    | 2.54                     | 0.55              |
| 81:j:58:THR:O     | 81:j:61:ASN:OD1    | 2.25                     | 0.55              |
| 3:L5:296:A:OP2    | 16:LN:15:GLN:NE2   | 2.40                     | 0.55              |
| 7:LD:197:LYS:HB3  | 7:LD:202:GLN:HB2   | 1.89                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LL:201:GLU:O    | 14:LL:205:GLN:NE2  | 2.39                     | 0.55              |
| 62:SV:15:ARG:NH1   | 62:SV:33:GLN:OE1   | 2.40                     | 0.55              |
| 77:Sb:37:CYS:HB2   | 77:Sb:40:CYS:HB2   | 1.88                     | 0.55              |
| 80:Bv:35:U:H2'     | 80:Bv:36:U:H6      | 1.72                     | 0.55              |
| 81:j:219:VAL:HG11  | 81:j:246:LEU:HD23  | 1.89                     | 0.55              |
| 3:L5:35:U:O2'      | 3:L5:1512:A:N1     | 2.39                     | 0.55              |
| 28:LZ:100:VAL:HG23 | 28:LZ:106:LEU:HD23 | 1.89                     | 0.55              |
| 3:L5:1643:U:OP2    | 29:La:26:ARG:NH1   | 2.40                     | 0.55              |
| 3:L5:2726:C:H5''   | 44:Lp:69:TRP:HH2   | 1.71                     | 0.55              |
| 5:L8:71:A:OP1      | 27:LY:27:ARG:NH2   | 2.37                     | 0.55              |
| 18:LP:119:VAL:HG12 | 18:LP:146:ILE:HG12 | 1.89                     | 0.55              |
| 23:LU:20:LYS:H     | 23:LU:73:THR:HA    | 1.71                     | 0.55              |
| 81:j:95:VAL:HG22   | 81:j:113:ASP:HB2   | 1.89                     | 0.55              |
| 14:LL:50:PRO:HB3   | 14:LL:150:LEU:HB3  | 1.87                     | 0.55              |
| 47:SA:89:LYS:NZ    | 58:SR:82:ASP:OD2   | 2.35                     | 0.55              |
| 49:SD:22:ASN:OD1   | 49:SD:34:TYR:OH    | 2.21                     | 0.55              |
| 81:j:91:ASN:O      | 81:j:120:ILE:HG13  | 2.06                     | 0.55              |
| 81:j:327:ASP:HB3   | 81:j:348:PRO:HD2   | 1.88                     | 0.55              |
| 3:L5:1505:A:OP1    | 29:La:27:LYS:NZ    | 2.30                     | 0.55              |
| 67:Sg:87:LEU:HB2   | 67:Sg:101:PHE:HB2  | 1.89                     | 0.55              |
| 67:Sg:174:VAL:HB   | 67:Sg:188:HIS:HB2  | 1.87                     | 0.55              |
| 75:SY:41:ARG:NH2   | 75:SY:52:PRO:O     | 2.40                     | 0.55              |
| 81:j:75:ILE:HA     | 81:j:78:VAL:HG12   | 1.89                     | 0.55              |
| 3:L5:1949:A:N6     | 3:L5:2013:A:O2'    | 2.39                     | 0.55              |
| 3:L5:3690:A:N1     | 46:S2:970:G:C5     | 2.74                     | 0.55              |
| 39:Lk:5:ILE:HD11   | 39:Lk:43:TYR:HB3   | 1.89                     | 0.55              |
| 48:SB:138:PHE:O    | 48:SB:213:ARG:N    | 2.35                     | 0.55              |
| 62:SV:53:TYR:OH    | 62:SV:76:ASP:OD2   | 2.25                     | 0.54              |
| 80:Bv:62:C:O2      | 80:Bv:62:C:H2'     | 2.07                     | 0.54              |
| 3:L5:1446:A:OP1    | 19:LQ:65:ARG:NH2   | 2.35                     | 0.54              |
| 22:LT:49:GLN:HA    | 22:LT:52:MET:HE3   | 1.90                     | 0.54              |
| 29:La:72:THR:HG22  | 29:La:110:LYS:HB3  | 1.89                     | 0.54              |
| 3:L5:1981:C:H2'    | 3:L5:1982:G:H4'    | 1.89                     | 0.54              |
| 3:L5:3696:A:OP2    | 3:L5:3714:G:N2     | 2.38                     | 0.54              |
| 52:SH:6:ALA:N      | 52:SH:43:LEU:O     | 2.40                     | 0.54              |
| 81:j:330:ARG:CG    | 81:j:345:TYR:CE1   | 2.90                     | 0.54              |
| 81:j:394:ASP:HB3   | 81:j:403:VAL:HG21  | 1.89                     | 0.54              |
| 48:SB:175:GLU:O    | 48:SB:179:ASN:ND2  | 2.41                     | 0.54              |
| 75:SY:12:PHE:HD1   | 75:SY:23:MET:HG2   | 1.72                     | 0.54              |
| 81:j:247:GLN:HA    | 81:j:250:VAL:HG23  | 1.89                     | 0.54              |
| 3:L5:3887:A:H61    | 83:NC:726:ASN:HD22 | 1.54                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:LS:95:ARG:NH2   | 21:LS:112:ASP:OD2  | 2.41                     | 0.54              |
| 74:SW:26:LEU:HG    | 77:Sb:7:LEU:HD23   | 1.89                     | 0.54              |
| 80:Bv:28:PSU:C6    | 80:Bv:28:PSU:C5'   | 2.91                     | 0.54              |
| 81:j:78:VAL:HG23   | 81:j:95:VAL:HG11   | 1.90                     | 0.54              |
| 68:SC:103:LYS:HD2  | 68:SC:133:TYR:HE2  | 1.73                     | 0.54              |
| 1:LA:137:ILE:HD11  | 1:LA:149:LYS:HB2   | 1.89                     | 0.54              |
| 15:LM:41:PRO:HG3   | 15:LM:73:VAL:HG23  | 1.88                     | 0.54              |
| 19:LQ:15:ARG:NH1   | 19:LQ:52:PHE:O     | 2.40                     | 0.54              |
| 58:SR:28:PHE:HA    | 58:SR:55:THR:HG21  | 1.88                     | 0.54              |
| 3:L5:2598:A:H5'    | 3:L5:2675:G:H4'    | 1.90                     | 0.54              |
| 74:SW:44:HIS:NE2   | 74:SW:112:ASP:OD2  | 2.40                     | 0.54              |
| 81:j:77:SER:OG     | 81:j:97:CYS:SG     | 2.66                     | 0.54              |
| 81:j:214:ILE:HD13  | 81:j:245:ARG:NH2   | 2.22                     | 0.54              |
| 3:L5:2745:G:O2'    | 3:L5:2752:A:N3     | 2.34                     | 0.54              |
| 7:LD:50:ARG:NH1    | 7:LD:147:ASP:OD2   | 2.41                     | 0.54              |
| 11:LH:106:GLN:HB2  | 11:LH:111:LEU:HB3  | 1.90                     | 0.54              |
| 57:SQ:53:GLU:OE1   | 57:SQ:85:ARG:NH2   | 2.38                     | 0.54              |
| 81:j:327:ASP:O     | 81:j:348:PRO:CG    | 2.53                     | 0.54              |
| 3:L5:4269:PSU:OP1  | 30:Lb:33:LYS:NZ    | 2.41                     | 0.54              |
| 46:S2:156:G:OP1    | 69:SG:2:LYS:NZ     | 2.40                     | 0.54              |
| 67:Sg:130:LYS:HG2  | 67:Sg:141:THR:HB   | 1.90                     | 0.54              |
| 20:LR:109:TYR:OH   | 20:LR:139:MET:SD   | 2.62                     | 0.53              |
| 68:SC:81:ILE:HG21  | 68:SC:88:ILE:HD11  | 1.90                     | 0.53              |
| 80:Bv:24:G:H2'     | 80:Bv:25:C:O4'     | 2.08                     | 0.53              |
| 2:LB:30:LYS:NZ     | 3:L5:4687:A:OP2    | 2.40                     | 0.53              |
| 3:L5:88:A:N7       | 19:LQ:173:LYS:NZ   | 2.55                     | 0.53              |
| 3:L5:4489:C:C4     | 81:j:188:LEU:HD12  | 2.43                     | 0.53              |
| 7:LD:62:CYS:HB3    | 7:LD:105:LEU:HD22  | 1.90                     | 0.53              |
| 3:L5:2237:C:N4     | 3:L5:2238:G:O6     | 2.41                     | 0.53              |
| 3:L5:4263:PSU:O2'  | 43:Lo:81:ARG:NH2   | 2.42                     | 0.53              |
| 3:L5:4422:U:H3     | 83:NC:727:PRO:HD2  | 1.72                     | 0.53              |
| 3:L5:4557:G:OP1    | 17:LO:61:ARG:NH1   | 2.41                     | 0.53              |
| 8:LE:262:LYS:HG3   | 8:LE:268:GLN:HE21  | 1.73                     | 0.53              |
| 13:LJ:129:ASP:OD1  | 13:LJ:129:ASP:N    | 2.42                     | 0.53              |
| 52:SH:144:ILE:HD11 | 52:SH:152:ARG:HD3  | 1.91                     | 0.53              |
| 80:Bv:71:A:H2'     | 80:Bv:72:C:C6      | 2.44                     | 0.53              |
| 10:LG:200:THR:HG22 | 10:LG:201:THR:HG23 | 1.91                     | 0.53              |
| 45:Lr:53:PRO:HD3   | 45:Lr:117:ILE:HD11 | 1.90                     | 0.53              |
| 46:S2:1401:A:N6    | 46:S2:1441:U:O2'   | 2.41                     | 0.53              |
| 51:SF:167:LYS:HA   | 76:SZ:71:ALA:HB1   | 1.91                     | 0.53              |
| 53:SI:22:HIS:ND1   | 53:SI:23:LYS:O     | 2.35                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 67:Sg:124:SER:OG  | 67:Sg:126:ASP:OD1 | 2.24                     | 0.53              |
| 67:Sg:127:LYS:HE3 | 67:Sg:149:GLU:HA  | 1.89                     | 0.53              |
| 82:k:1059:U:H3'   | 82:k:1059:U:O2    | 2.08                     | 0.53              |
| 3:L5:1656:A:N3    | 3:L5:1839:U:O2'   | 2.42                     | 0.53              |
| 3:L5:3642:A:N6    | 3:L5:4138:G:O2'   | 2.40                     | 0.53              |
| 3:L5:4848:C:N4    | 8:LE:181:LEU:O    | 2.41                     | 0.53              |
| 8:LE:179:LEU:HD12 | 8:LE:183:ARG:HA   | 1.90                     | 0.53              |
| 80:Bv:5:C:H2'     | 80:Bv:6:U:C6      | 2.44                     | 0.53              |
| 81:j:40:PRO:HG3   | 81:j:123:SER:OG   | 2.08                     | 0.53              |
| 3:L5:731:G:O6     | 3:L5:910:C:N4     | 2.42                     | 0.53              |
| 8:LE:138:ARG:HH21 | 8:LE:170:SER:HA   | 1.72                     | 0.53              |
| 33:Le:26:ASP:N    | 33:Le:26:ASP:OD1  | 2.42                     | 0.53              |
| 46:S2:626:G:C8    | 82:k:1059:U:C4    | 2.96                     | 0.53              |
| 48:SB:146:ARG:HB2 | 48:SB:149:GLN:HB2 | 1.90                     | 0.53              |
| 52:SH:40:LEU:HA   | 52:SH:43:LEU:HD13 | 1.89                     | 0.53              |
| 67:Sg:42:MET:HG3  | 67:Sg:56:GLN:HB3  | 1.90                     | 0.53              |
| 3:L5:1685:C:H42   | 19:LQ:45:GLN:HE22 | 1.56                     | 0.53              |
| 13:LJ:56:THR:HG21 | 80:Bv:57:G:H5'    | 1.90                     | 0.53              |
| 15:LM:100:ARG:HA  | 15:LM:103:LYS:HG2 | 1.90                     | 0.53              |
| 25:LW:74:ARG:HD2  | 46:S2:1748:G:H5'  | 1.90                     | 0.53              |
| 80:Bv:42:A:H2'    | 80:Bv:43:A:C8     | 2.43                     | 0.53              |
| 81:j:254:VAL:HG21 | 81:j:271:SER:OG   | 2.08                     | 0.53              |
| 3:L5:2682:A:H4'   | 39:Lk:26:LYS:HE2  | 1.91                     | 0.53              |
| 11:LH:186:THR:O   | 11:LH:189:GLN:NE2 | 2.42                     | 0.53              |
| 19:LQ:39:THR:HG22 | 19:LQ:41:SER:H    | 1.74                     | 0.53              |
| 39:Lk:10:ASP:N    | 39:Lk:10:ASP:OD1  | 2.41                     | 0.53              |
| 80:Bv:52:G:C5     | 80:Bv:53:G:N7     | 2.77                     | 0.53              |
| 3:L5:2332:G:N7    | 29:La:9:ARG:NH2   | 2.57                     | 0.53              |
| 2:LB:246:ARG:NH2  | 3:L5:4495:C:OP1   | 2.42                     | 0.52              |
| 3:L5:1167:U:OP2   | 7:LD:289:ARG:NH2  | 2.37                     | 0.52              |
| 3:L5:2798:G:N1    | 3:L5:2801:C:OP2   | 2.40                     | 0.52              |
| 3:L5:3602:C:O2    | 20:LR:82:LYS:NZ   | 2.39                     | 0.52              |
| 61:SU:17:ILE:HD13 | 61:SU:94:PRO:HD3  | 1.91                     | 0.52              |
| 64:Sa:80:HIS:CE1  | 82:k:1049:U:O2    | 2.62                     | 0.52              |
| 81:j:280:PHE:HE1  | 81:j:395:LYS:CB   | 2.21                     | 0.52              |
| 11:LH:59:LYS:HE3  | 11:LH:66:GLU:HB3  | 1.91                     | 0.52              |
| 54:SK:49:MET:HG2  | 54:SK:52:LEU:HD12 | 1.91                     | 0.52              |
| 69:SG:121:ILE:HB  | 69:SG:124:LEU:HB2 | 1.91                     | 0.52              |
| 72:SN:86:GLU:O    | 72:SN:90:HIS:ND1  | 2.37                     | 0.52              |
| 80:Bv:56:C:H2'    | 80:Bv:56:C:O2     | 2.09                     | 0.52              |
| 81:j:252:LYS:HD2  | 81:j:274:VAL:HG21 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L5:1968:G:H1    | 81:j:386:GLY:HA2  | 1.74                     | 0.52              |
| 6:LC:221:PHE:HD2  | 6:LC:229:LEU:HD21 | 1.75                     | 0.52              |
| 47:SA:76:VAL:HG12 | 47:SA:123:VAL:HB  | 1.91                     | 0.52              |
| 59:SS:86:ARG:NH2  | 59:SS:110:ASP:OD2 | 2.43                     | 0.52              |
| 80:Bv:61:C:H2'    | 80:Bv:62:C:C6     | 2.38                     | 0.52              |
| 3:L5:1633:A:O2'   | 38:Lj:49:TRP:O    | 2.26                     | 0.52              |
| 3:L5:1968:G:C2    | 81:j:414:ARG:CZ   | 2.91                     | 0.52              |
| 61:SU:70:CYS:SG   | 61:SU:71:GLY:N    | 2.82                     | 0.52              |
| 80:Bv:11:C:H2'    | 80:Bv:12:G:C8     | 2.44                     | 0.52              |
| 3:L5:1351:U:OP2   | 14:LL:36:ARG:NH1  | 2.38                     | 0.52              |
| 3:L5:2290:C:H5''  | 33:Le:104:SER:HB3 | 1.92                     | 0.52              |
| 3:L5:2613:U:O4    | 23:LU:97:ARG:NH1  | 2.43                     | 0.52              |
| 20:LR:172:ARG:HA  | 20:LR:175:GLU:HG3 | 1.92                     | 0.52              |
| 81:j:326:LEU:HD13 | 81:j:328:ILE:HD12 | 1.92                     | 0.52              |
| 82:k:1051:C:H2'   | 82:k:1051:C:O2    | 2.08                     | 0.52              |
| 23:LU:40:GLU:HB2  | 23:LU:63:ILE:HG21 | 1.92                     | 0.52              |
| 46:S2:813:A:OP1   | 50:SE:16:LYS:NZ   | 2.43                     | 0.52              |
| 46:S2:870:A:H62   | 46:S2:916:A:H5'   | 1.75                     | 0.52              |
| 46:S2:984:C:O2    | 73:SO:138:IAS:HB3 | 2.10                     | 0.52              |
| 56:SP:18:ARG:NH1  | 59:SS:88:LYS:O    | 2.43                     | 0.52              |
| 67:Sg:201:SER:OG  | 67:Sg:203:ASP:O   | 2.25                     | 0.52              |
| 2:LB:35:ASP:OD2   | 2:LB:193:LYS:NZ   | 2.42                     | 0.52              |
| 3:L5:1939:G:H4'   | 21:LS:93:MET:HG2  | 1.92                     | 0.52              |
| 38:Lj:27:TYR:HA   | 38:Lj:34:CYS:HA   | 1.92                     | 0.52              |
| 66:Sd:6:LEU:HA    | 66:Sd:9:SER:HB3   | 1.92                     | 0.52              |
| 3:L5:97:G:OP1     | 14:LL:16:LYS:NZ   | 2.43                     | 0.52              |
| 3:L5:134:G:H2'    | 3:L5:135:G:H8     | 1.74                     | 0.52              |
| 3:L5:390:G:H1'    | 18:LP:97:ASN:HD21 | 1.74                     | 0.52              |
| 3:L5:4958:G:H22   | 3:L5:5023:A:H2    | 1.58                     | 0.52              |
| 13:LJ:93:GLU:HG3  | 13:LJ:173:ILE:HB  | 1.92                     | 0.52              |
| 21:LS:115:ALA:O   | 21:LS:118:ARG:NH2 | 2.43                     | 0.52              |
| 25:LW:80:ARG:NH1  | 46:S2:167:G:O2'   | 2.42                     | 0.52              |
| 46:S2:819:G:OP1   | 70:SJ:79:ARG:NH2  | 2.42                     | 0.52              |
| 46:S2:1036:A:N3   | 46:S2:1844:U:O2'  | 2.41                     | 0.52              |
| 3:L5:3925:G:H1    | 3:L5:4045:U:H3    | 1.58                     | 0.52              |
| 3:L5:4263:PSU:OP2 | 3:L5:4299:G:O2'   | 2.27                     | 0.52              |
| 26:LX:114:LYS:NZ  | 26:LX:120:ASP:OD1 | 2.42                     | 0.52              |
| 36:Lh:105:LYS:HA  | 36:Lh:108:GLN:HG2 | 1.90                     | 0.52              |
| 80:Bv:21:A:H2'    | 80:Bv:46:G7M:O6   | 2.10                     | 0.52              |
| 81:j:252:LYS:CD   | 81:j:274:VAL:HG21 | 2.40                     | 0.52              |
| 81:j:330:ARG:CA   | 81:j:345:TYR:CD1  | 2.92                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:L5:2097:C:N4    | 3:L5:2098:G:N7     | 2.58                     | 0.52              |
| 9:LF:213:LEU:HB3  | 9:LF:247:MET:HG2   | 1.91                     | 0.52              |
| 16:LN:64:ILE:HD11 | 16:LN:106:ALA:HB2  | 1.92                     | 0.52              |
| 20:LR:77:GLY:O    | 20:LR:81:ARG:NE    | 2.43                     | 0.52              |
| 46:S2:951:C:O2'   | 73:SO:50:LYS:NZ    | 2.35                     | 0.52              |
| 58:SR:37:GLU:OE1  | 67:Sg:106:LYS:NZ   | 2.43                     | 0.52              |
| 81:j:41:PRO:HB3   | 81:j:91:ASN:C      | 2.35                     | 0.52              |
| 1:LA:72:ARG:NH2   | 3:L5:4062:G:O6     | 2.43                     | 0.51              |
| 13:LJ:95:ARG:NH1  | 13:LJ:176:PRO:O    | 2.43                     | 0.51              |
| 20:LR:44:LEU:HD22 | 20:LR:49:LEU:HD22  | 1.91                     | 0.51              |
| 21:LS:45:TRP:HA   | 21:LS:48:VAL:HG12  | 1.90                     | 0.51              |
| 57:SQ:85:ARG:NH2  | 57:SQ:116:ASP:OD2  | 2.38                     | 0.51              |
| 63:SX:28:LYS:HE2  | 63:SX:32:LEU:HD11  | 1.92                     | 0.51              |
| 3:L5:3749:PSU:O2' | 80:Bv:12:G:O2'     | 2.16                     | 0.51              |
| 10:LG:63:LEU:HD11 | 16:LN:29:GLN:HG3   | 1.91                     | 0.51              |
| 46:S2:444:G:N2    | 46:S2:447:A:OP2    | 2.43                     | 0.51              |
| 81:j:89:PRO:CG    | 81:j:115:GLU:OE2   | 2.58                     | 0.51              |
| 81:j:177:PRO:HG2  | 81:j:194:ARG:HB2   | 1.92                     | 0.51              |
| 81:j:346:LEU:N    | 81:j:346:LEU:CD1   | 2.73                     | 0.51              |
| 3:L5:2305:G:O6    | 33:Le:19:LYS:NZ    | 2.42                     | 0.51              |
| 13:LJ:108:GLY:HA2 | 13:LJ:129:ASP:HA   | 1.92                     | 0.51              |
| 24:LV:112:MET:HE2 | 24:LV:135:ASN:HD22 | 1.76                     | 0.51              |
| 27:LY:4:ASN:HD22  | 27:LY:5:PRO:HD2    | 1.76                     | 0.51              |
| 43:Lo:6:LYS:HE3   | 43:Lo:94:GLY:HA3   | 1.92                     | 0.51              |
| 46:S2:643:A:OP1   | 70:SJ:39:ASN:ND2   | 2.43                     | 0.51              |
| 78:Se:28:LYS:HD2  | 78:Se:36:MET:HE3   | 1.92                     | 0.51              |
| 81:j:416:ARG:NH1  | 81:j:417:VAL:O     | 2.44                     | 0.51              |
| 3:L5:1857:C:H2'   | 3:L5:1858:A2M:H8   | 1.91                     | 0.51              |
| 3:L5:1963:G:OP1   | 3:L5:1965:C:N4     | 2.43                     | 0.51              |
| 3:L5:3887:A:N6    | 83:NC:726:ASN:ND2  | 2.59                     | 0.51              |
| 3:L5:50:C:H5''    | 14:LL:20:ARG:HH22  | 1.76                     | 0.51              |
| 3:L5:415:U:OP1    | 18:LP:34:GLN:NE2   | 2.43                     | 0.51              |
| 3:L5:2418:A:OP1   | 40:Ll:41:ARG:NH1   | 2.33                     | 0.51              |
| 6:LC:318:PRO:HG2  | 9:LF:155:TYR:HB3   | 1.93                     | 0.51              |
| 31:Lc:38:ILE:HG21 | 31:Lc:63:TYR:HB3   | 1.92                     | 0.51              |
| 48:SB:26:SER:O    | 48:SB:51:ARG:NH2   | 2.40                     | 0.51              |
| 60:ST:76:THR:HB   | 60:ST:94:ARG:HB3   | 1.93                     | 0.51              |
| 80:Bv:64:C:H2'    | 80:Bv:65:C:C6      | 2.45                     | 0.51              |
| 81:j:243:ASP:CG   | 81:j:245:ARG:NH1   | 2.67                     | 0.51              |
| 81:j:289:ARG:CD   | 81:j:412:ILE:HD13  | 2.38                     | 0.51              |
| 3:L5:748:G:N1     | 3:L5:893:C:N3      | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:L8:94:G:C5       | 38:Lj:84:PRO:HG3   | 2.46                     | 0.51              |
| 6:LC:149:GLU:OE2   | 45:Lr:71:ARG:NH2   | 2.41                     | 0.51              |
| 46:S2:462:OMC:HM22 | 46:S2:463:C:H5'    | 1.93                     | 0.51              |
| 2:LB:224:LYS:NZ    | 3:L5:4596:A:OP2    | 2.36                     | 0.51              |
| 3:L5:27:C:OP1      | 16:LN:193:ARG:NH1  | 2.44                     | 0.51              |
| 3:L5:1851:G:OP2    | 12:LI:14:ASN:ND2   | 2.43                     | 0.51              |
| 5:L8:51:U:OP2      | 40:Ll:21:ARG:NH2   | 2.44                     | 0.51              |
| 23:LU:56:LEU:HD12  | 23:LU:61:VAL:HG23  | 1.93                     | 0.51              |
| 50:SE:31:PRO:HA    | 50:SE:81:THR:HB    | 1.93                     | 0.51              |
| 81:j:82:LEU:CD1    | 81:j:82:LEU:N      | 2.73                     | 0.51              |
| 81:j:219:VAL:HG21  | 81:j:249:LYS:CD    | 2.37                     | 0.51              |
| 3:L5:2004:A:H5''   | 3:L5:2005:C:H5     | 1.76                     | 0.51              |
| 10:LG:99:ALA:HB1   | 10:LG:136:LEU:HD11 | 1.93                     | 0.51              |
| 46:S2:1593:C:O2    | 60:ST:12:GLN:NE2   | 2.44                     | 0.51              |
| 69:SG:48:TYR:HE2   | 69:SG:121:ILE:HD11 | 1.76                     | 0.51              |
| 81:j:41:PRO:HB3    | 81:j:92:GLY:N      | 2.26                     | 0.51              |
| 81:j:245:ARG:HB2   | 81:j:245:ARG:CZ    | 2.41                     | 0.51              |
| 40:Ll:21:ARG:HH12  | 40:Ll:24:PRO:HG3   | 1.75                     | 0.51              |
| 46:S2:1454:A:OP2   | 58:SR:49:LYS:NZ    | 2.44                     | 0.51              |
| 46:S2:1549:U:OP1   | 66:Sd:34:TYR:OH    | 2.28                     | 0.51              |
| 10:LG:193:LEU:HD12 | 10:LG:194:VAL:HG13 | 1.91                     | 0.51              |
| 22:LT:25:VAL:HG22  | 22:LT:45:MET:HE1   | 1.92                     | 0.51              |
| 26:LX:89:LYS:HG2   | 26:LX:95:THR:HG23  | 1.93                     | 0.51              |
| 45:Lr:56:ASP:OD2   | 45:Lr:58:LYS:NZ    | 2.42                     | 0.51              |
| 46:S2:1354:G:N2    | 46:S2:1357:A:OP2   | 2.41                     | 0.51              |
| 80:Bv:65:C:H2'     | 80:Bv:66:C:H6      | 1.76                     | 0.51              |
| 81:j:233:LYS:HG2   | 81:j:253:LEU:HD22  | 1.85                     | 0.51              |
| 2:LB:77:THR:OG1    | 2:LB:335:GLY:O     | 2.26                     | 0.50              |
| 43:Lo:45:GLN:NE2   | 43:Lo:52:THR:OG1   | 2.44                     | 0.50              |
| 81:j:38:ILE:HD12   | 81:j:124:LEU:CD2   | 2.41                     | 0.50              |
| 81:j:91:ASN:CB     | 81:j:119:PRO:HA    | 2.41                     | 0.50              |
| 25:LW:105:ARG:NH2  | 69:SG:150:GLU:O    | 2.31                     | 0.50              |
| 35:Lg:16:ALA:HA    | 35:Lg:19:LYS:HE2   | 1.93                     | 0.50              |
| 46:S2:814:PSU:OP1  | 50:SE:22:LYS:NZ    | 2.44                     | 0.50              |
| 46:S2:1091:C:HO2'  | 74:SW:2:VAL:N      | 2.09                     | 0.50              |
| 81:j:34:MET:HA     | 81:j:34:MET:CE     | 2.40                     | 0.50              |
| 81:j:110:VAL:HG12  | 81:j:110:VAL:O     | 2.11                     | 0.50              |
| 3:L5:4071:G:H2'    | 3:L5:4072:G:C8     | 2.47                     | 0.50              |
| 8:LE:161:ARG:NH2   | 8:LE:273:SER:OG    | 2.44                     | 0.50              |
| 13:LJ:95:ARG:HH12  | 13:LJ:176:PRO:HG2  | 1.74                     | 0.50              |
| 47:SA:80:ARG:HH22  | 47:SA:166:LYS:HA   | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:SD:225:GLU:HB3  | 67:Sg:187:ASN:HB3  | 1.93                     | 0.50              |
| 54:SK:80:ARG:NH1   | 54:SK:89:ILE:O     | 2.45                     | 0.50              |
| 80:Bv:63:A:H2'     | 80:Bv:64:C:C6      | 2.46                     | 0.50              |
| 81:j:145:LYS:HG2   | 81:j:162:GLN:HG3   | 1.92                     | 0.50              |
| 81:j:289:ARG:HD3   | 81:j:289:ARG:C     | 2.36                     | 0.50              |
| 27:LY:91:ASN:HB2   | 27:LY:93:THR:HG22  | 1.93                     | 0.50              |
| 81:j:81:ARG:HG2    | 81:j:111:ASN:HD21  | 1.76                     | 0.50              |
| 81:j:176:LEU:HD13  | 81:j:198:ARG:HG2   | 1.93                     | 0.50              |
| 3:L5:1269:G:OP2    | 8:LE:128:HIS:NE2   | 2.45                     | 0.50              |
| 57:SQ:146:ARG:NH2  | 80:Bv:34:G:H5''    | 2.23                     | 0.50              |
| 60:ST:124:THR:OG1  | 60:ST:127:GLY:N    | 2.44                     | 0.50              |
| 77:Sb:67:THR:OG1   | 77:Sb:70:LYS:O     | 2.29                     | 0.50              |
| 81:j:254:VAL:CG2   | 81:j:271:SER:OG    | 2.60                     | 0.50              |
| 3:L5:24:G:N7       | 38:Lj:46:LYS:NZ    | 2.60                     | 0.50              |
| 3:L5:4259:U:HO2'   | 3:L5:4290:G:HO2'   | 1.52                     | 0.50              |
| 46:S2:1050:A:H62   | 46:S2:1068:G:H21   | 1.58                     | 0.50              |
| 46:S2:1291:A:O2'   | 79:Sf:140:TYR:OH   | 2.24                     | 0.50              |
| 3:L5:74:G:H5'      | 14:LL:59:VAL:HG13  | 1.93                     | 0.50              |
| 3:L5:1389:C:O2'    | 3:L5:1403:G:N2     | 2.45                     | 0.50              |
| 27:LY:109:LEU:HD22 | 27:LY:115:ARG:HH21 | 1.77                     | 0.50              |
| 44:Lp:38:THR:HA    | 44:Lp:45:THR:HA    | 1.93                     | 0.50              |
| 46:S2:374:G:OP1    | 55:SL:59:LYS:NZ    | 2.43                     | 0.50              |
| 58:SR:106:LEU:HD23 | 58:SR:109:LEU:HD23 | 1.94                     | 0.50              |
| 3:L5:259:G:H2'     | 3:L5:260:G:H8      | 1.76                     | 0.50              |
| 14:LL:64:VAL:HA    | 14:LL:67:HIS:CD2   | 2.47                     | 0.50              |
| 27:LY:82:ILE:HB    | 27:LY:85:VAL:HG22  | 1.93                     | 0.50              |
| 46:S2:594:A:H61    | 46:S2:643:A:H5''   | 1.76                     | 0.50              |
| 80:Bv:53:G:C2      | 80:Bv:62:C:N3      | 2.79                     | 0.50              |
| 3:L5:1585:C:H2'    | 3:L5:1586:A:H8     | 1.76                     | 0.50              |
| 8:LE:180:VAL:HG21  | 8:LE:258:LEU:HD21  | 1.92                     | 0.50              |
| 8:LE:264:ILE:HD11  | 8:LE:267:LEU:HD22  | 1.94                     | 0.50              |
| 49:SD:76:ARG:HB2   | 54:SK:22:VAL:HG11  | 1.94                     | 0.50              |
| 70:SJ:55:LYS:HG2   | 70:SJ:58:ARG:HH21  | 1.76                     | 0.50              |
| 11:LH:118:LEU:HD11 | 11:LH:167:VAL:HG22 | 1.94                     | 0.49              |
| 21:LS:77:ASN:HD21  | 21:LS:98:ARG:HH11  | 1.60                     | 0.49              |
| 80:Bv:3:C:H2'      | 80:Bv:4:U:H6       | 1.77                     | 0.49              |
| 3:L5:1945:A:O2'    | 3:L5:2012:A:N1     | 2.45                     | 0.49              |
| 3:L5:4605:A:H3'    | 3:L5:4606:PSU:H4'  | 1.93                     | 0.49              |
| 38:Lj:60:GLY:HA2   | 38:Lj:64:MET:HE3   | 1.95                     | 0.49              |
| 47:SA:128:ARG:NH2  | 47:SA:151:ASP:O    | 2.42                     | 0.49              |
| 63:SX:109:GLY:O    | 63:SX:119:ARG:NH1  | 2.40                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:Bv:27:PSU:H2'   | 80:Bv:28:PSU:C6    | 2.47                     | 0.49              |
| 80:Bv:33:U:H2'     | 80:Bv:35:U:OP2     | 2.12                     | 0.49              |
| 81:j:102:THR:HG22  | 81:j:106:LYS:O     | 2.12                     | 0.49              |
| 81:j:330:ARG:HG3   | 81:j:345:TYR:CE1   | 2.47                     | 0.49              |
| 3:L5:3690:A:C4     | 46:S2:970:G:C4     | 3.00                     | 0.49              |
| 48:SB:65:ARG:NH2   | 73:SO:46:ASP:OD2   | 2.46                     | 0.49              |
| 67:Sg:163:PRO:HB2  | 67:Sg:179:LEU:HB3  | 1.95                     | 0.49              |
| 69:SG:142:ARG:HB2  | 69:SG:147:LEU:HB2  | 1.93                     | 0.49              |
| 45:Lr:51:VAL:HG12  | 45:Lr:62:VAL:HG22  | 1.93                     | 0.49              |
| 68:SC:81:ILE:HG23  | 68:SC:86:LEU:HB2   | 1.93                     | 0.49              |
| 80:Bv:53:G:N2      | 80:Bv:62:C:H1'     | 2.27                     | 0.49              |
| 80:Bv:71:A:H2'     | 80:Bv:72:C:H6      | 1.76                     | 0.49              |
| 3:L5:1486:C:OP1    | 19:LQ:150:ARG:NH2  | 2.46                     | 0.49              |
| 3:L5:2305:G:N2     | 3:L5:2308:G:OP2    | 2.41                     | 0.49              |
| 3:L5:4076:A:OP2    | 35:Lg:115:LYS:NZ   | 2.42                     | 0.49              |
| 25:LW:44:ARG:HD3   | 25:LW:49:ILE:HD11  | 1.94                     | 0.49              |
| 46:S2:114:G:N7     | 55:SL:69:ARG:NH2   | 2.60                     | 0.49              |
| 46:S2:818:A:OP1    | 70:SJ:80:ARG:NH2   | 2.44                     | 0.49              |
| 46:S2:1030:A:H2'   | 46:S2:1031:A2M:H8  | 1.95                     | 0.49              |
| 43:Lo:105:GLN:O    | 80:Bv:19:G:N2      | 2.43                     | 0.49              |
| 67:Sg:31:ILE:HG12  | 67:Sg:45:LEU:HD21  | 1.95                     | 0.49              |
| 80:Bv:36:U:H2'     | 80:Bv:36:U:O2      | 2.11                     | 0.49              |
| 3:L5:2654:C:OP2    | 20:LR:103:ARG:NH1  | 2.45                     | 0.49              |
| 39:Lk:26:LYS:HB2   | 39:Lk:69:LEU:HD12  | 1.93                     | 0.49              |
| 46:S2:10:G:O2'     | 68:SC:113:GLN:OE1  | 2.28                     | 0.49              |
| 46:S2:309:G:OP2    | 53:SI:55:TYR:OH    | 2.23                     | 0.49              |
| 46:S2:354:U:OP1    | 55:SL:90:ARG:NH1   | 2.45                     | 0.49              |
| 46:S2:1628:C:OP1   | 60:ST:38:LYS:NZ    | 2.38                     | 0.49              |
| 54:SK:85:LEU:HB3   | 54:SK:89:ILE:HD11  | 1.94                     | 0.49              |
| 81:j:136:LEU:N     | 81:j:136:LEU:CD2   | 2.73                     | 0.49              |
| 81:j:273:GLU:OE1   | 81:j:273:GLU:HA    | 2.08                     | 0.49              |
| 3:L5:1419:G:O2'    | 3:L5:1439:A:N6     | 2.46                     | 0.49              |
| 3:L5:1728:G:O6     | 4:L7:103:A:O2'     | 2.24                     | 0.49              |
| 3:L5:3576:G:O2'    | 3:L5:3577:C:O4'    | 2.30                     | 0.49              |
| 17:LO:8:VAL:HG12   | 17:LO:117:ARG:HG3  | 1.93                     | 0.49              |
| 25:LW:80:ARG:NH2   | 69:SG:129:VAL:O    | 2.36                     | 0.49              |
| 46:S2:508:A:H3'    | 46:S2:509:OMG:H8   | 1.78                     | 0.49              |
| 51:SF:128:ILE:HG21 | 65:Sc:68:LEU:HD22  | 1.94                     | 0.49              |
| 54:SK:3:MET:HE1    | 54:SK:48:ALA:HB2   | 1.95                     | 0.49              |
| 62:SV:16:LYS:H     | 68:SC:259:THR:HG21 | 1.77                     | 0.49              |
| 71:SM:68:LEU:O     | 71:SM:72:HIS:ND1   | 2.41                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L5:1679:C:H4'    | 19:LQ:143:ARG:HH12 | 1.76                     | 0.49              |
| 3:L5:2394:G:O6     | 40:Ll:2:SER:N      | 2.46                     | 0.49              |
| 6:LC:79:VAL:HG11   | 6:LC:86:ARG:HG3    | 1.95                     | 0.49              |
| 12:LI:207:ASP:OD1  | 12:LI:210:ARG:NH2  | 2.45                     | 0.49              |
| 46:S2:26:U:H2'     | 46:S2:27:A2M:H8    | 1.93                     | 0.49              |
| 65:Sc:20:ARG:HG2   | 65:Sc:28:THR:HB    | 1.95                     | 0.49              |
| 10:LG:55:VAL:HG12  | 26:LX:44:PRO:HA    | 1.93                     | 0.49              |
| 45:Lr:26:SER:OG    | 45:Lr:28:GLU:OE1   | 2.23                     | 0.49              |
| 51:SF:125:SER:O    | 51:SF:136:ARG:NH2  | 2.46                     | 0.49              |
| 52:SH:170:VAL:HG13 | 52:SH:187:PHE:HB2  | 1.95                     | 0.49              |
| 68:SC:108:LYS:HE3  | 68:SC:233:LEU:HD13 | 1.94                     | 0.49              |
| 81:j:62:ILE:HG23   | 82:k:1059:U:OP1    | 2.13                     | 0.49              |
| 3:L5:2338:OMC:HM22 | 3:L5:2339:U:H5'    | 1.94                     | 0.48              |
| 80:Bv:3:C:H2'      | 80:Bv:4:U:C6       | 2.48                     | 0.48              |
| 80:Bv:39:C:H2'     | 80:Bv:40:C:H6      | 1.77                     | 0.48              |
| 80:Bv:53:G:N2      | 80:Bv:62:C:N1      | 2.60                     | 0.48              |
| 1:LA:114:CYS:HB2   | 1:LA:169:VAL:HG13  | 1.96                     | 0.48              |
| 1:LA:117:GLU:HG2   | 1:LA:124:GLY:H     | 1.79                     | 0.48              |
| 55:SL:66:VAL:HG11  | 55:SL:141:ASN:HD22 | 1.78                     | 0.48              |
| 58:SR:37:GLU:OE2   | 67:Sg:127:LYS:NZ   | 2.46                     | 0.48              |
| 81:j:269:GLU:O     | 81:j:269:GLU:HG2   | 2.13                     | 0.48              |
| 2:LB:161:ARG:HA    | 2:LB:184:GLN:HA    | 1.95                     | 0.48              |
| 46:S2:191:A:N6     | 46:S2:208:G:O2'    | 2.46                     | 0.48              |
| 46:S2:571:U:H5''   | 75:SY:37:LYS:HG3   | 1.95                     | 0.48              |
| 46:S2:1737:G:OP1   | 69:SG:94:ARG:NH2   | 2.43                     | 0.48              |
| 51:SF:102:LEU:HD11 | 76:SZ:100:VAL:HG21 | 1.95                     | 0.48              |
| 59:SS:5:ILE:HA     | 76:SZ:49:LEU:HD13  | 1.95                     | 0.48              |
| 67:Sg:35:SER:OG    | 67:Sg:36:ARG:N     | 2.47                     | 0.48              |
| 80:Bv:10:2MG:H2'   | 80:Bv:11:C:C6      | 2.49                     | 0.48              |
| 81:j:32:THR:HG21   | 82:k:1058:A:H1'    | 1.94                     | 0.48              |
| 3:L5:1237:C:N3     | 3:L5:1247:G:N1     | 2.49                     | 0.48              |
| 19:LQ:122:THR:OG1  | 19:LQ:124:ASP:OD1  | 2.25                     | 0.48              |
| 29:La:132:ARG:HA   | 29:La:135:GLU:HG2  | 1.94                     | 0.48              |
| 46:S2:1650:A:H5''  | 57:SQ:139:ALA:HB2  | 1.95                     | 0.48              |
| 69:SG:32:MET:HE3   | 69:SG:54:GLY:HA3   | 1.95                     | 0.48              |
| 1:LA:123:ARG:NH1   | 3:L5:4061:U:OP1    | 2.46                     | 0.48              |
| 59:SS:132:ARG:HB2  | 59:SS:134:GLN:HE22 | 1.78                     | 0.48              |
| 79:Sf:107:LYS:HG3  | 79:Sf:117:LEU:HD21 | 1.95                     | 0.48              |
| 80:Bv:17:C:O2      | 80:Bv:17:C:O2'     | 2.27                     | 0.48              |
| 3:L5:3575:A:N1     | 55:SL:3:ASP:N      | 2.61                     | 0.48              |
| 3:L5:4616:U:OP2    | 20:LR:62:ARG:NH2   | 2.44                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:LI:152:LEU:HB3  | 12:LI:165:ILE:HD12 | 1.96                     | 0.48              |
| 58:SR:36:GLU:OE1   | 58:SR:47:ARG:NH1   | 2.46                     | 0.48              |
| 70:SJ:71:LEU:O     | 70:SJ:75:ASN:ND2   | 2.46                     | 0.48              |
| 3:L5:414:G:OP1     | 18:LP:62:ARG:NH2   | 2.47                     | 0.48              |
| 3:L5:2653:U:OP2    | 20:LR:124:TYR:OH   | 2.29                     | 0.48              |
| 15:LM:20:HIS:CD2   | 15:LM:48:GLN:HE22  | 2.32                     | 0.48              |
| 33:Le:85:LEU:HD21  | 33:Le:115:ALA:HB2  | 1.95                     | 0.48              |
| 46:S2:984:C:O2'    | 73:SO:138:IAS:OD1  | 2.18                     | 0.48              |
| 57:SQ:16:LYS:HG3   | 57:SQ:17:LYS:H     | 1.79                     | 0.48              |
| 72:SN:24:THR:O     | 72:SN:27:LYS:NZ    | 2.40                     | 0.48              |
| 80:Bv:51:U:N3      | 80:Bv:52:G:N7      | 2.61                     | 0.48              |
| 49:SD:167:TYR:OH   | 49:SD:202:LYS:O    | 2.29                     | 0.48              |
| 58:SR:115:SER:OG   | 58:SR:116:ASN:N    | 2.46                     | 0.48              |
| 81:j:71:VAL:HG21   | 82:k:1058:A:C2     | 2.48                     | 0.48              |
| 81:j:328:ILE:HG22  | 81:j:374:LEU:HD13  | 1.95                     | 0.48              |
| 23:LU:25:CYS:O     | 23:LU:68:SER:OG    | 2.30                     | 0.48              |
| 24:LV:35:LYS:HB2   | 24:LV:67:LYS:HG3   | 1.94                     | 0.48              |
| 50:SE:102:ILE:HD12 | 50:SE:239:PRO:HD3  | 1.96                     | 0.48              |
| 56:SP:85:ILE:HG22  | 56:SP:112:ILE:HD12 | 1.95                     | 0.48              |
| 81:j:71:VAL:O      | 81:j:75:ILE:HG13   | 2.14                     | 0.48              |
| 4:L7:11:A:O2'      | 4:L7:13:A:OP2      | 2.30                     | 0.48              |
| 17:LO:9:LEU:HD23   | 17:LO:118:MET:HB2  | 1.95                     | 0.48              |
| 53:SI:83:TYR:HB3   | 53:SI:101:ILE:HB   | 1.95                     | 0.48              |
| 81:j:90:PRO:O      | 81:j:91:ASN:CB     | 2.56                     | 0.48              |
| 81:j:300:LYS:N     | 81:j:300:LYS:CD    | 2.77                     | 0.48              |
| 1:LA:198:ARG:NH1   | 3:L5:3667:U:OP2    | 2.47                     | 0.47              |
| 14:LL:46:ILE:HB    | 14:LL:49:ARG:HB2   | 1.95                     | 0.47              |
| 46:S2:1485:U:OP1   | 49:SD:151:LYS:NZ   | 2.46                     | 0.47              |
| 46:S2:1598:G:N7    | 76:SZ:85:ARG:NH1   | 2.52                     | 0.47              |
| 67:Sg:230:LEU:HD21 | 67:Sg:259:TRP:CG   | 2.49                     | 0.47              |
| 3:L5:1883:A:OP1    | 9:LF:223:LYS:NZ    | 2.44                     | 0.47              |
| 3:L5:3869:A:N6     | 3:L5:4540:G:O2'    | 2.47                     | 0.47              |
| 13:LJ:143:ASP:OD1  | 13:LJ:143:ASP:N    | 2.47                     | 0.47              |
| 27:LY:19:PHE:O     | 27:LY:26:ARG:NH2   | 2.47                     | 0.47              |
| 44:Lp:38:THR:HB    | 44:Lp:45:THR:HG22  | 1.96                     | 0.47              |
| 46:S2:1679:A:H3'   | 51:SF:60:ARG:HD2   | 1.95                     | 0.47              |
| 71:SM:32:ALA:HB3   | 71:SM:110:VAL:HB   | 1.97                     | 0.47              |
| 81:j:330:ARG:HA    | 81:j:345:TYR:HD1   | 1.76                     | 0.47              |
| 3:L5:1432:U:H3     | 3:L5:2089:G:H1     | 1.62                     | 0.47              |
| 3:L5:2099:G:O2'    | 3:L5:2237:C:N4     | 2.42                     | 0.47              |
| 5:L8:60:G:OP1      | 26:LX:68:ARG:NH2   | 2.43                     | 0.47              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 17:LO:113:ASP:OD1    | 17:LO:113:ASP:N    | 2.46                     | 0.47              |
| 46:S2:1386:A:OP2     | 49:SD:160:SER:OG   | 2.31                     | 0.47              |
| 70:SJ:137:VAL:O      | 70:SJ:140:GLN:N    | 2.44                     | 0.47              |
| 3:L5:955:C:O2'       | 3:L5:956:C:O4'     | 2.31                     | 0.47              |
| 3:L5:1389:C:O2       | 3:L5:1402:G:N1     | 2.44                     | 0.47              |
| 3:L5:2078:C:O2       | 3:L5:2081:G:O2'    | 2.28                     | 0.47              |
| 3:L5:4341:G:OP1      | 43:Lo:59:LYS:NZ    | 2.47                     | 0.47              |
| 6:LC:95:MET:SD       | 6:LC:95:MET:N      | 2.87                     | 0.47              |
| 50:SE:131:VAL:HA     | 50:SE:137:PRO:HA   | 1.95                     | 0.47              |
| 56:SP:29:SER:OG      | 56:SP:32:GLN:OE1   | 2.28                     | 0.47              |
| 67:Sg:120:ILE:HB     | 67:Sg:132:TRP:HB2  | 1.96                     | 0.47              |
| 80:Bv:18:G:C4        | 80:Bv:58:1MA:C2    | 3.02                     | 0.47              |
| 22:LT:116:LYS:O      | 22:LT:120:LYS:NZ   | 2.35                     | 0.47              |
| 47:SA:141:ASN:ND2    | 68:SC:85:SER:O     | 2.41                     | 0.47              |
| 49:SD:16:ILE:HD11    | 66:Sd:36:LEU:HD23  | 1.97                     | 0.47              |
| 81:j:75:ILE:HG22     | 81:j:79:GLN:HE22   | 1.77                     | 0.47              |
| 2:LB:170:LEU:O       | 2:LB:328:ASN:ND2   | 2.45                     | 0.47              |
| 16:LN:46:ASP:OD1     | 16:LN:46:ASP:N     | 2.47                     | 0.47              |
| 41:Lm:79:GLU:HB3     | 41:Lm:82:LEU:HB2   | 1.96                     | 0.47              |
| 48:SB:122:GLU:HG2    | 48:SB:140:VAL:HG23 | 1.96                     | 0.47              |
| 55:SL:16:ILE:HG23    | 55:SL:34:PRO:HG2   | 1.96                     | 0.47              |
| 79:Sf:133:ALA:N      | 79:Sf:140:TYR:O    | 2.47                     | 0.47              |
| 1:LA:116:LEU:HD23    | 1:LA:164:ALA:HB2   | 1.96                     | 0.47              |
| 1:LA:207:VAL:HG23    | 1:LA:208:GLU:HG3   | 1.97                     | 0.47              |
| 3:L5:2256:C:H42      | 19:LQ:21:GLN:HE22  | 1.61                     | 0.47              |
| 3:L5:4089:C:H5''     | 3:L5:4090:U:H5     | 1.79                     | 0.47              |
| 3:L5:4249:A:H5'      | 3:L5:4251:A:H1'    | 1.96                     | 0.47              |
| 4:L7:110:G:O6        | 7:LD:21:ARG:NH1    | 2.48                     | 0.47              |
| 12:LI:31:ILE:HB      | 12:LI:66:GLU:HB3   | 1.97                     | 0.47              |
| 46:S2:290:U:O2'      | 46:S2:292:A:N7     | 2.41                     | 0.47              |
| 46:S2:1018:U:O2'     | 72:SN:86:GLU:OE2   | 2.30                     | 0.47              |
| 59:SS:101:ASN:O      | 59:SS:105:ASN:N    | 2.41                     | 0.47              |
| 68:SC:114:LYS:HD3    | 68:SC:121:ARG:HE   | 1.80                     | 0.47              |
| 71:SM:31:LEU:HD11    | 71:SM:111:VAL:HA   | 1.96                     | 0.47              |
| 80:Bv:52:G:C6        | 80:Bv:53:G:C5      | 3.03                     | 0.47              |
| 80:Bv:53:G:N1        | 80:Bv:62:C:C2      | 2.82                     | 0.47              |
| 81:j:100:ILE:HD12    | 81:j:100:ILE:C     | 2.38                     | 0.47              |
| 3:L5:155:A:H5''      | 3:L5:156:C:H2'     | 1.96                     | 0.47              |
| 10:LG:137[A]:ARG:HD2 | 10:LG:146:LEU:HD11 | 1.97                     | 0.47              |
| 18:LP:128:ARG:HH11   | 18:LP:136:ILE:HG21 | 1.79                     | 0.47              |
| 19:LQ:154:LYS:O      | 19:LQ:163:THR:OG1  | 2.30                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:Lc:22:MET:HE2  | 31:Lc:85:CYS:HB2   | 1.96                     | 0.47              |
| 53:SI:120:PRO:HB3 | 53:SI:123:ARG:HD2  | 1.97                     | 0.47              |
| 80:Bv:8:U:H1'     | 80:Bv:48:U:O2'     | 2.15                     | 0.47              |
| 81:j:68:ARG:O     | 81:j:72:LEU:HG     | 2.14                     | 0.47              |
| 81:j:243:ASP:OD1  | 81:j:245:ARG:NH1   | 2.48                     | 0.47              |
| 3:L5:2348:G:O6    | 18:LP:25:HIS:ND1   | 2.48                     | 0.47              |
| 3:L5:2567:U:OP1   | 28:LZ:36:ARG:NH2   | 2.48                     | 0.47              |
| 46:S2:1597:C:H4'  | 46:S2:1603:G:C6    | 2.50                     | 0.47              |
| 46:S2:1657:G:H1   | 46:S2:1667:U:H3    | 1.63                     | 0.47              |
| 52:SH:91:HIS:HE1  | 52:SH:168:HIS:HD2  | 1.62                     | 0.47              |
| 81:j:89:PRO:O     | 81:j:90:PRO:C      | 2.54                     | 0.47              |
| 3:L5:4711:G:H2'   | 3:L5:4712:G:H8     | 1.80                     | 0.47              |
| 23:LU:28:PRO:HB3  | 23:LU:100:LEU:HD21 | 1.96                     | 0.47              |
| 80:Bv:18:G:C2     | 80:Bv:58:1MA:C5    | 3.02                     | 0.47              |
| 3:L5:4575:A:C2    | 81:j:295:SER:O     | 2.68                     | 0.46              |
| 22:LT:115:LYS:HA  | 22:LT:118:GLU:HG2  | 1.97                     | 0.46              |
| 62:SV:1:MET:HB2   | 68:SC:254:ASP:HB3  | 1.97                     | 0.46              |
| 74:SW:52:ILE:HG12 | 74:SW:61:ILE:HG12  | 1.97                     | 0.46              |
| 81:j:61:ASN:OD1   | 81:j:61:ASN:N      | 2.48                     | 0.46              |
| 81:j:157:LEU:HD13 | 81:j:260:GLY:O     | 2.15                     | 0.46              |
| 3:L5:1186:G:H2'   | 3:L5:1187:G:C8     | 2.50                     | 0.46              |
| 14:LL:126:LEU:N   | 14:LL:138:ASP:OD2  | 2.38                     | 0.46              |
| 25:LW:72:THR:O    | 25:LW:73:ARG:NE    | 2.43                     | 0.46              |
| 27:LY:54:GLU:HB2  | 27:LY:108:ARG:HG2  | 1.97                     | 0.46              |
| 40:Ll:42:ARG:HG2  | 40:Ll:47:THR:HG23  | 1.96                     | 0.46              |
| 67:Sg:44:LYS:HB3  | 67:Sg:54:ILE:HB    | 1.97                     | 0.46              |
| 81:j:280:PHE:HE1  | 81:j:395:LYS:CG    | 2.28                     | 0.46              |
| 3:L5:6:C:H5''     | 10:LG:197:LYS:HB3  | 1.97                     | 0.46              |
| 3:L5:1266:A:O2'   | 6:LC:323:ARG:NH2   | 2.48                     | 0.46              |
| 3:L5:1673:C:O2'   | 30:Lb:18:ARG:NH2   | 2.49                     | 0.46              |
| 3:L5:4906:G:OP2   | 8:LE:188:ARG:NH1   | 2.36                     | 0.46              |
| 7:LD:200:MET:HB3  | 7:LD:237:GLU:HG3   | 1.97                     | 0.46              |
| 12:LI:54:SER:OG   | 12:LI:130:HIS:O    | 2.34                     | 0.46              |
| 20:LR:151:ARG:NH2 | 55:SL:119:ASP:OD2  | 2.46                     | 0.46              |
| 46:S2:380:G:OP1   | 53:SI:56:ARG:NH2   | 2.48                     | 0.46              |
| 71:SM:55:ASN:ND2  | 71:SM:81:ASP:OD1   | 2.46                     | 0.46              |
| 81:j:289:ARG:CD   | 81:j:289:ARG:C     | 2.89                     | 0.46              |
| 8:LE:141:ARG:HB2  | 8:LE:191:GLN:HE21  | 1.80                     | 0.46              |
| 9:LF:116:GLN:HB3  | 9:LF:119:ASN:ND2   | 2.30                     | 0.46              |
| 10:LG:58:PRO:HD3  | 26:LX:46:PHE:CG    | 2.50                     | 0.46              |
| 46:S2:943:U:H1'   | 73:SO:137:SER:HB3  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:1551:U:OP1   | 49:SD:9:ARG:NH1    | 2.47                     | 0.46              |
| 49:SD:23:GLU:OE2   | 49:SD:27:ARG:NE    | 2.49                     | 0.46              |
| 81:j:233:LYS:HG2   | 81:j:253:LEU:HD21  | 1.90                     | 0.46              |
| 1:LA:101:VAL:HG22  | 1:LA:165:VAL:HG22  | 1.97                     | 0.46              |
| 3:L5:706:G:H5''    | 6:LC:316:LYS:HG2   | 1.98                     | 0.46              |
| 3:L5:4714:G:H22    | 3:L5:4920:A:H2     | 1.63                     | 0.46              |
| 46:S2:525:A:H2'    | 46:S2:526:A:H8     | 1.81                     | 0.46              |
| 46:S2:1720:U:H5''  | 46:S2:1721:U:H5''  | 1.96                     | 0.46              |
| 74:SW:14:ILE:HG13  | 74:SW:27:ILE:HD11  | 1.98                     | 0.46              |
| 79:Sf:133:ALA:H    | 79:Sf:140:TYR:H    | 1.62                     | 0.46              |
| 81:j:280:PHE:CE1   | 81:j:395:LYS:CB    | 2.99                     | 0.46              |
| 2:LB:49:TYR:OH     | 2:LB:168:MET:SD    | 2.73                     | 0.46              |
| 3:L5:2262:G:H2'    | 3:L5:2263:A:C8     | 2.51                     | 0.46              |
| 5:L8:152:U:O2'     | 10:LG:160:ASP:OD2  | 2.33                     | 0.46              |
| 46:S2:1351:G:O2'   | 46:S2:1378:A:N1    | 2.47                     | 0.46              |
| 60:ST:113:VAL:HG12 | 60:ST:123:LEU:HD23 | 1.98                     | 0.46              |
| 76:SZ:68:ILE:HB    | 76:SZ:109:TYR:HB2  | 1.98                     | 0.46              |
| 81:j:84:LEU:N      | 81:j:84:LEU:CD2    | 2.79                     | 0.46              |
| 6:LC:218:ILE:O     | 6:LC:222:ARG:HB2   | 2.15                     | 0.46              |
| 9:LF:105:VAL:HG13  | 9:LF:136:VAL:HG12  | 1.98                     | 0.46              |
| 50:SE:183:VAL:HG21 | 50:SE:218:PHE:HE2  | 1.80                     | 0.46              |
| 80:Bv:27:PSU:H2'   | 80:Bv:28:PSU:H6    | 1.81                     | 0.46              |
| 3:L5:1577:C:H4'    | 3:L5:2844:A:H5'    | 1.97                     | 0.46              |
| 3:L5:4099:G:O2'    | 28:LZ:136:PHE:OXT  | 2.33                     | 0.46              |
| 3:L5:4422:U:C6     | 81:j:185:MEQ:NE2   | 2.84                     | 0.46              |
| 8:LE:190:HIS:HD2   | 8:LE:192:LYS:HG2   | 1.80                     | 0.46              |
| 46:S2:553:U:O4     | 46:S2:554:A:N6     | 2.49                     | 0.46              |
| 46:S2:1866:A:C6    | 64:Sa:87:ARG:HD2   | 2.50                     | 0.46              |
| 81:j:78:VAL:HG22   | 81:j:78:VAL:O      | 2.16                     | 0.46              |
| 81:j:219:VAL:O     | 81:j:219:VAL:HG23  | 2.16                     | 0.46              |
| 5:L8:109:C:O2'     | 5:L8:111:U:OP2     | 2.29                     | 0.46              |
| 46:S2:989:C:O2     | 64:Sa:32:LYS:NZ    | 2.48                     | 0.46              |
| 83:NC:705:LEU:HD12 | 83:NC:705:LEU:N    | 2.31                     | 0.46              |
| 3:L5:50:C:H5'      | 14:LL:20:ARG:HH12  | 1.81                     | 0.46              |
| 3:L5:120:A:H2'     | 3:L5:146:A:H61     | 1.81                     | 0.46              |
| 3:L5:675:G:H5''    | 8:LE:100:LYS:HD3   | 1.98                     | 0.46              |
| 3:L5:3676:U:H5''   | 3:L5:3677:G:H5'    | 1.98                     | 0.46              |
| 7:LD:256:LYS:HD2   | 7:LD:257:PRO:HD2   | 1.97                     | 0.46              |
| 14:LL:48:PRO:HB2   | 36:Lh:120:ALA:HB2  | 1.97                     | 0.46              |
| 17:LO:61:ARG:HA    | 17:LO:70:PRO:HD2   | 1.97                     | 0.46              |
| 20:LR:98:ARG:NH1   | 20:LR:132:PHE:O    | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:Sa:44:ILE:CD1   | 73:SO:129:ILE:HG21 | 2.46                     | 0.46              |
| 67:Sg:10:THR:HB    | 67:Sg:306:LEU:HD12 | 1.96                     | 0.46              |
| 74:SW:80:ASP:OD1   | 74:SW:80:ASP:N     | 2.49                     | 0.46              |
| 80:Bv:26:M2G:H2'   | 80:Bv:27:PSU:H6    | 1.80                     | 0.46              |
| 80:Bv:63:A:H2'     | 80:Bv:64:C:H6      | 1.81                     | 0.46              |
| 2:LB:10:ARG:NH1    | 2:LB:265:SER:O     | 2.39                     | 0.45              |
| 3:L5:1671:A:OP1    | 29:La:47:LYS:NZ    | 2.37                     | 0.45              |
| 3:L5:1957:A:H2     | 3:L5:2005:C:H42    | 1.64                     | 0.45              |
| 50:SE:253:ASP:HA   | 50:SE:256:LEU:HB2  | 1.98                     | 0.45              |
| 69:SG:57:ASP:HA    | 69:SG:106:LEU:HA   | 1.99                     | 0.45              |
| 69:SG:181:THR:HG22 | 69:SG:183:ARG:H    | 1.81                     | 0.45              |
| 81:j:102:THR:HG22  | 81:j:106:LYS:HB3   | 1.98                     | 0.45              |
| 3:L5:4988:C:H2'    | 3:L5:4989:C:H4'    | 1.97                     | 0.45              |
| 6:LC:94:ASN:HD22   | 6:LC:102:PHE:HB2   | 1.81                     | 0.45              |
| 6:LC:209:ILE:HD13  | 6:LC:251:ILE:HB    | 1.98                     | 0.45              |
| 46:S2:935:G:O2'    | 72:SN:108:ASP:OD1  | 2.28                     | 0.45              |
| 50:SE:152:PRO:O    | 50:SE:155:LYS:NZ   | 2.49                     | 0.45              |
| 81:j:84:LEU:N      | 81:j:84:LEU:HD23   | 2.31                     | 0.45              |
| 14:LL:63:THR:HG23  | 14:LL:65:ARG:H     | 1.81                     | 0.45              |
| 25:LW:86:SER:OG    | 25:LW:87:LEU:N     | 2.49                     | 0.45              |
| 41:Lm:92:ASP:OD1   | 41:Lm:126:LYS:NZ   | 2.38                     | 0.45              |
| 1:LA:67:TYR:OH     | 3:L5:4065:G:N7     | 2.41                     | 0.45              |
| 10:LG:95:LEU:HD23  | 10:LG:184:ILE:HD12 | 1.99                     | 0.45              |
| 12:LI:86:HIS:HB3   | 12:LI:139:ARG:HG2  | 1.98                     | 0.45              |
| 16:LN:60:VAL:HG23  | 16:LN:134:LEU:HB2  | 1.99                     | 0.45              |
| 47:SA:51:LEU:HA    | 47:SA:54:THR:HG22  | 1.99                     | 0.45              |
| 61:SU:67:LYS:HB2   | 61:SU:78:ASP:HB2   | 1.98                     | 0.45              |
| 73:SO:34:PHE:HB3   | 73:SO:41:PHE:HB2   | 1.98                     | 0.45              |
| 3:L5:2888:G:H1     | 3:L5:3577:C:H42    | 1.63                     | 0.45              |
| 3:L5:3651:G:H4'    | 16:LN:67:ARG:HH12  | 1.82                     | 0.45              |
| 3:L5:3690:A:C6     | 46:S2:970:G:C6     | 3.05                     | 0.45              |
| 46:S2:512:A2M:HM'2 | 46:S2:513:G:H5'    | 1.99                     | 0.45              |
| 67:Sg:72:SER:OG    | 67:Sg:74:ASP:OD1   | 2.32                     | 0.45              |
| 3:L5:1268:G:N1     | 8:LE:128:HIS:HB2   | 2.31                     | 0.45              |
| 3:L5:4488:A:OP1    | 3:L5:4490:G:O2'    | 2.31                     | 0.45              |
| 8:LE:88:VAL:HA     | 8:LE:89:LEU:HA     | 1.79                     | 0.45              |
| 12:LI:61:SER:HA    | 12:LI:126:VAL:HG12 | 1.99                     | 0.45              |
| 46:S2:1808:U:H2'   | 46:S2:1809:A:C8    | 2.51                     | 0.45              |
| 56:SP:135:ALA:O    | 56:SP:139:SER:OG   | 2.33                     | 0.45              |
| 68:SC:198:ALA:HB3  | 68:SC:221:ASP:HB3  | 1.97                     | 0.45              |
| 47:SA:104:THR:O    | 47:SA:107:THR:OG1  | 2.24                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:SQ:58:LEU:O    | 57:SQ:62:ARG:NH2   | 2.49                     | 0.45              |
| 67:Sg:107:ASP:N   | 67:Sg:107:ASP:OD1  | 2.49                     | 0.45              |
| 70:SJ:140:GLN:NE2 | 75:SY:64:PHE:O     | 2.45                     | 0.45              |
| 71:SM:35:ILE:HD11 | 71:SM:64:LEU:HD22  | 1.99                     | 0.45              |
| 71:SM:84:LYS:HG2  | 71:SM:88:TRP:HZ3   | 1.82                     | 0.45              |
| 3:L5:2474:G:N1    | 3:L5:2479:C:O2     | 2.45                     | 0.45              |
| 3:L5:4869:G:H1    | 3:L5:4882:C:H42    | 1.64                     | 0.45              |
| 6:LC:333:MLZ:HCM3 | 8:LE:55:GLY:H      | 1.82                     | 0.45              |
| 7:LD:119:TYR:OH   | 7:LD:139:PRO:O     | 2.34                     | 0.45              |
| 18:LP:7:ASP:N     | 18:LP:7:ASP:OD1    | 2.50                     | 0.45              |
| 21:LS:127:MET:HA  | 22:LT:153:PRO:HD2  | 1.98                     | 0.45              |
| 46:S2:1587:G:N2   | 46:S2:1587:G:OP1   | 2.50                     | 0.45              |
| 50:SE:204:SER:OG  | 50:SE:205:PHE:N    | 2.50                     | 0.45              |
| 53:SI:118:ALA:HB2 | 53:SI:141:ARG:HH22 | 1.82                     | 0.45              |
| 70:SJ:172:ARG:HA  | 70:SJ:175:ARG:HE   | 1.82                     | 0.45              |
| 3:L5:1859:G:O2'   | 3:L5:4189:A:N3     | 2.48                     | 0.45              |
| 34:Lf:11:PHE:HB2  | 34:Lf:101:ILE:HD12 | 1.99                     | 0.45              |
| 34:Lf:33:VAL:HG23 | 34:Lf:38:GLU:HB3   | 1.98                     | 0.45              |
| 81:j:62:ILE:HA    | 82:k:1059:U:OP1    | 2.16                     | 0.45              |
| 3:L5:79:C:OP1     | 16:LN:194:ARG:NH2  | 2.50                     | 0.45              |
| 3:L5:153:G:N2     | 3:L5:154:U:O4      | 2.50                     | 0.45              |
| 3:L5:391:A2M:HM'3 | 18:LP:104:LEU:HD23 | 1.99                     | 0.45              |
| 3:L5:1808:G:H21   | 3:L5:1809:U:H5'    | 1.81                     | 0.45              |
| 3:L5:4190:6MZ:H2' | 3:L5:4192:G:H5''   | 1.99                     | 0.45              |
| 8:LE:136:HIS:O    | 8:LE:138:ARG:NH1   | 2.50                     | 0.45              |
| 41:Lm:94:MET:HG2  | 41:Lm:105:PRO:HA   | 1.99                     | 0.45              |
| 46:S2:172:OMU:OP1 | 46:S2:314:U:O2'    | 2.35                     | 0.45              |
| 46:S2:919:A:OP2   | 72:SN:64:ARG:NH2   | 2.47                     | 0.45              |
| 58:SR:92:ASP:OD1  | 58:SR:92:ASP:N     | 2.50                     | 0.45              |
| 83:NC:707:ILE:HB  | 83:NC:710:ILE:CD1  | 2.47                     | 0.45              |
| 3:L5:1163:C:O3'   | 7:LD:268:ARG:NH2   | 2.50                     | 0.44              |
| 7:LD:156:GLY:HA2  | 7:LD:181:PRO:HG3   | 1.99                     | 0.44              |
| 9:LF:96:ARG:HD2   | 9:LF:139:TYR:CE2   | 2.52                     | 0.44              |
| 17:LO:190:ASP:HA  | 17:LO:193:THR:HG22 | 2.00                     | 0.44              |
| 20:LR:148:ASP:O   | 20:LR:152:LYS:NZ   | 2.46                     | 0.44              |
| 46:S2:507:G:OP2   | 75:SY:104:ARG:NH2  | 2.50                     | 0.44              |
| 3:L5:1367:G:N2    | 3:L5:1368:U:O4     | 2.41                     | 0.44              |
| 3:L5:2768:G:O2'   | 40:Ll:3:SER:O      | 2.30                     | 0.44              |
| 3:L5:3790:G:O2'   | 3:L5:3793:U:OP2    | 2.31                     | 0.44              |
| 13:LJ:55:TYR:HA   | 13:LJ:64:ARG:HB3   | 1.99                     | 0.44              |
| 15:LM:50:MET:HE2  | 15:LM:50:MET:HB3   | 1.79                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LP:45:THR:HG22  | 18:LP:49:LYS:HE3   | 1.98                     | 0.44              |
| 46:S2:1333:U:H5'   | 49:SD:147:ALA:HB2  | 1.99                     | 0.44              |
| 51:SF:24:SER:O     | 51:SF:107:ASN:ND2  | 2.41                     | 0.44              |
| 64:Sa:40:VAL:HG22  | 64:Sa:42:ARG:H     | 1.82                     | 0.44              |
| 73:SO:138:IAS:OD1  | 73:SO:139:SER:O    | 2.36                     | 0.44              |
| 81:j:280:PHE:CE1   | 81:j:395:LYS:HB2   | 2.52                     | 0.44              |
| 46:S2:165:G:OP2    | 46:S2:165:G:N2     | 2.35                     | 0.44              |
| 46:S2:1536:G:H2'   | 46:S2:1537:A:C8    | 2.53                     | 0.44              |
| 51:SF:137:GLN:HG2  | 65:Sc:68:LEU:HD21  | 1.98                     | 0.44              |
| 69:SG:55:GLY:N     | 69:SG:63:MET:SD    | 2.82                     | 0.44              |
| 74:SW:55:ASP:O     | 74:SW:57:ARG:NH1   | 2.48                     | 0.44              |
| 80:Bv:50:G:N1      | 80:Bv:64:C:N3      | 2.54                     | 0.44              |
| 3:L5:1561:G:OP2    | 20:LR:92:LYS:NZ    | 2.50                     | 0.44              |
| 46:S2:65:C:O2'     | 46:S2:67:C:OP2     | 2.35                     | 0.44              |
| 46:S2:1401:A:H2'   | 46:S2:1402:A:C8    | 2.53                     | 0.44              |
| 46:S2:1863:A:OP2   | 64:Sa:4:LYS:NZ     | 2.47                     | 0.44              |
| 56:SP:111:MET:HE2  | 59:SS:117:ILE:HB   | 2.00                     | 0.44              |
| 13:LJ:104:ASN:HD22 | 13:LJ:134:LEU:H    | 1.64                     | 0.44              |
| 46:S2:1228:A:H2'   | 46:S2:1229:G:C8    | 2.53                     | 0.44              |
| 53:SI:76:THR:OG1   | 53:SI:77:ARG:N     | 2.50                     | 0.44              |
| 59:SS:84:LEU:O     | 59:SS:87:GLN:NE2   | 2.49                     | 0.44              |
| 70:SJ:122:SER:H    | 70:SJ:125:HIS:HB3  | 1.82                     | 0.44              |
| 3:L5:2692:G:H22    | 3:L5:2697:C:H5     | 1.64                     | 0.44              |
| 3:L5:2732:A:H2'    | 3:L5:2733:A:C8     | 2.53                     | 0.44              |
| 46:S2:30:C:O2'     | 46:S2:596:U:OP1    | 2.34                     | 0.44              |
| 46:S2:116:OMU:HN3  | 46:S2:347:G:H1     | 1.66                     | 0.44              |
| 51:SF:70:GLU:HA    | 51:SF:73:THR:HG22  | 2.00                     | 0.44              |
| 67:Sg:198:VAL:HG12 | 67:Sg:209:SER:HA   | 1.99                     | 0.44              |
| 68:SC:196:ILE:HB   | 68:SC:223:TYR:HB2  | 1.98                     | 0.44              |
| 68:SC:275:LYS:HG3  | 68:SC:276:THR:HG23 | 2.00                     | 0.44              |
| 16:LN:200:LEU:HD22 | 16:LN:204:ARG:HH11 | 1.83                     | 0.44              |
| 3:L5:1957:A:H5''   | 3:L5:2002:U:N3     | 2.33                     | 0.44              |
| 3:L5:2096:G:H22    | 3:L5:2239:G:H1     | 1.66                     | 0.44              |
| 3:L5:2562:U:OP1    | 28:LZ:48:ARG:NH2   | 2.51                     | 0.44              |
| 3:L5:5031:U:OP1    | 18:LP:43:LYS:NZ    | 2.36                     | 0.44              |
| 10:LG:247:VAL:HA   | 10:LG:250:ILE:HG12 | 2.00                     | 0.44              |
| 12:LI:54:SER:HB3   | 12:LI:135:ILE:HD11 | 2.00                     | 0.44              |
| 41:Lm:93:LYS:HD3   | 41:Lm:102:ARG:HG2  | 2.00                     | 0.44              |
| 67:Sg:167:SER:OG   | 67:Sg:175:LYS:O    | 2.33                     | 0.44              |
| 76:SZ:58:LEU:HD12  | 76:SZ:62:VAL:HG21  | 1.99                     | 0.44              |
| 3:L5:681:C:OP2     | 8:LE:111:LYS:NZ    | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:LE:190:HIS:CD2   | 8:LE:192:LYS:HG2   | 2.53                     | 0.44              |
| 22:LT:45:MET:HE2   | 22:LT:45:MET:HB3   | 1.85                     | 0.44              |
| 23:LU:105:ASN:OD1  | 23:LU:106:SER:N    | 2.50                     | 0.44              |
| 46:S2:658:U:O2     | 63:SX:17:ARG:NH1   | 2.49                     | 0.44              |
| 50:SE:151:ASP:OD2  | 69:SG:216:ARG:NH2  | 2.50                     | 0.44              |
| 60:ST:2:PRO:HB2    | 60:ST:3:GLY:H      | 1.65                     | 0.44              |
| 80:Bv:39:C:C2      | 80:Bv:40:C:C5      | 3.06                     | 0.44              |
| 81:j:82:LEU:N      | 81:j:82:LEU:HD13   | 2.33                     | 0.44              |
| 81:j:95:VAL:HG22   | 81:j:113:ASP:CB    | 2.47                     | 0.44              |
| 1:LA:57:PRO:HB3    | 44:Lp:54:ILE:HD11  | 2.00                     | 0.43              |
| 3:L5:4422:U:C5     | 81:j:185:MEQ:HE1   | 2.53                     | 0.43              |
| 3:L5:4422:U:C1'    | 81:j:185:MEQ:HE21  | 2.31                     | 0.43              |
| 6:LC:209:ILE:HB    | 6:LC:229:LEU:HD23  | 1.99                     | 0.43              |
| 14:LL:90:VAL:O     | 14:LL:93:THR:OG1   | 2.31                     | 0.43              |
| 46:S2:507:G:OP1    | 75:SY:108:LYS:NZ   | 2.40                     | 0.43              |
| 46:S2:878:G:H22    | 46:S2:908:A:H2     | 1.66                     | 0.43              |
| 81:j:223:GLY:HA3   | 81:j:251:LEU:HD22  | 1.98                     | 0.43              |
| 3:L5:240:A:H5''    | 27:LY:3:PHE:HD2    | 1.83                     | 0.43              |
| 3:L5:1743:U:O2'    | 3:L5:1745:G:OP1    | 2.36                     | 0.43              |
| 3:L5:4441:PSU:OP1  | 11:LH:168:LYS:NZ   | 2.47                     | 0.43              |
| 3:L5:4442:G:O2'    | 41:Lm:100:TYR:O    | 2.32                     | 0.43              |
| 3:L5:4710:C:H4'    | 3:L5:4711:G:H5'    | 2.00                     | 0.43              |
| 3:L5:4900:C:H2'    | 3:L5:4901:G:C8     | 2.53                     | 0.43              |
| 21:LS:88:SER:OG    | 21:LS:89:GLY:N     | 2.51                     | 0.43              |
| 46:S2:434:G:OP2    | 53:SI:25:ARG:NH1   | 2.46                     | 0.43              |
| 46:S2:1083:A:N3    | 46:S2:1859:A:O2'   | 2.47                     | 0.43              |
| 47:SA:65:ILE:HG23  | 47:SA:74:VAL:HG21  | 2.00                     | 0.43              |
| 50:SE:19:MET:SD    | 50:SE:108:ARG:NH1  | 2.91                     | 0.43              |
| 58:SR:25:GLY:H     | 58:SR:31:ASN:HD21  | 1.66                     | 0.43              |
| 75:SY:29:HIS:HB2   | 75:SY:32:LYS:HB2   | 1.99                     | 0.43              |
| 80:Bv:18:G:C1'     | 80:Bv:58:1MA:C2    | 3.01                     | 0.43              |
| 2:LB:165:HIS:HB3   | 2:LB:180:LEU:HD23  | 1.99                     | 0.43              |
| 3:L5:3730:G:H21    | 3:L5:3754:A:H8     | 1.64                     | 0.43              |
| 16:LN:135:ILE:HG23 | 16:LN:142:ILE:HD13 | 1.98                     | 0.43              |
| 20:LR:98:ARG:HH22  | 20:LR:130:ASN:ND2  | 2.16                     | 0.43              |
| 46:S2:64:A:OP1     | 69:SG:177:GLN:NE2  | 2.48                     | 0.43              |
| 47:SA:24:HIS:HB3   | 47:SA:51:LEU:HD21  | 2.00                     | 0.43              |
| 49:SD:75:LYS:HE2   | 54:SK:21:MET:HA    | 1.99                     | 0.43              |
| 50:SE:126:VAL:HG22 | 50:SE:139:LEU:HD21 | 1.99                     | 0.43              |
| 63:SX:68:LYS:HG3   | 78:Se:6:LEU:HD22   | 2.00                     | 0.43              |
| 72:SN:5:HIS:HD2    | 72:SN:121:ARG:HH21 | 1.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 81:j:104:GLU:O     | 81:j:105:GLY:O     | 2.36                     | 0.43              |
| 81:j:264:PHE:O     | 81:j:264:PHE:CD1   | 2.70                     | 0.43              |
| 2:LB:14:LEU:HA     | 2:LB:17:LEU:HD13   | 2.00                     | 0.43              |
| 2:LB:80:GLU:OE1    | 2:LB:323:TYR:OH    | 2.27                     | 0.43              |
| 3:L5:259:G:H2'     | 3:L5:260:G:C8      | 2.54                     | 0.43              |
| 6:LC:8:ILE:HD13    | 6:LC:151:PRO:HD2   | 2.00                     | 0.43              |
| 6:LC:292:ILE:HG23  | 19:LQ:128:LEU:HD11 | 2.00                     | 0.43              |
| 25:LW:76:VAL:HG12  | 25:LW:77:LYS:H     | 1.83                     | 0.43              |
| 47:SA:10:MET:HE1   | 58:SR:109:LEU:HD11 | 2.00                     | 0.43              |
| 52:SH:152:ARG:HH21 | 74:SW:36:ARG:HH21  | 1.67                     | 0.43              |
| 56:SP:18:ARG:HD3   | 59:SS:88:LYS:HG2   | 2.01                     | 0.43              |
| 80:Bv:66:C:O2      | 80:Bv:66:C:H2'     | 2.19                     | 0.43              |
| 81:j:305:VAL:HG11  | 81:j:328:ILE:HD13  | 2.00                     | 0.43              |
| 3:L5:441:G:H1      | 3:L5:1284:U:H3     | 1.66                     | 0.43              |
| 3:L5:1489:G:H1     | 19:LQ:89:ASP:HA    | 1.83                     | 0.43              |
| 11:LH:142:ASP:OD1  | 11:LH:142:ASP:N    | 2.49                     | 0.43              |
| 32:Ld:68:LEU:HD23  | 32:Ld:108:TYR:HB2  | 2.00                     | 0.43              |
| 61:SU:21:ARG:HD3   | 61:SU:88:LEU:HD23  | 2.01                     | 0.43              |
| 69:SG:2:LYS:HD3    | 69:SG:15:LEU:HD21  | 2.00                     | 0.43              |
| 70:SJ:79:ARG:NH1   | 70:SJ:83:ARG:HH21  | 2.16                     | 0.43              |
| 81:j:211:GLN:O     | 81:j:212:LEU:CD1   | 2.66                     | 0.43              |
| 81:j:258:TYR:CE1   | 81:j:262:ASN:ND2   | 2.85                     | 0.43              |
| 3:L5:2617:U:O4     | 23:LU:89:LYS:NZ    | 2.51                     | 0.43              |
| 3:L5:4582:C:C2     | 11:LH:120:GLU:HB2  | 2.53                     | 0.43              |
| 6:LC:284:MET:HE2   | 6:LC:287:THR:HA    | 1.99                     | 0.43              |
| 50:SE:136:ILE:HD13 | 50:SE:148:ARG:HH11 | 1.82                     | 0.43              |
| 61:SU:17:ILE:HD13  | 61:SU:93:SER:HA    | 2.00                     | 0.43              |
| 68:SC:180:VAL:HG23 | 68:SC:197:PRO:HG3  | 1.99                     | 0.43              |
| 3:L5:2309:G:OP1    | 33:Le:36:ARG:NH1   | 2.40                     | 0.43              |
| 3:L5:3697:A2M:O5'  | 3:L5:3697:A2M:H8   | 2.18                     | 0.43              |
| 3:L5:4981:A:H2     | 3:L5:4998:G:H21    | 1.64                     | 0.43              |
| 13:LJ:15:LEU:HD12  | 13:LJ:134:LEU:HG   | 2.01                     | 0.43              |
| 13:LJ:18:ARG:HD2   | 13:LJ:135:GLY:HA3  | 2.01                     | 0.43              |
| 13:LJ:174:ILE:HG22 | 13:LJ:175:LEU:H    | 1.83                     | 0.43              |
| 32:Ld:24:GLU:HG3   | 32:Ld:122:VAL:HG21 | 1.99                     | 0.43              |
| 46:S2:67:C:C5      | 69:SG:162:LEU:HB3  | 2.54                     | 0.43              |
| 46:S2:155:G:H4'    | 69:SG:15:LEU:HD13  | 2.00                     | 0.43              |
| 46:S2:1808:U:H2'   | 46:S2:1809:A:H8    | 1.83                     | 0.43              |
| 67:Sg:129:ILE:HD12 | 67:Sg:154:VAL:HG11 | 2.00                     | 0.43              |
| 81:j:224:LEU:HD12  | 81:j:250:VAL:HG22  | 2.01                     | 0.43              |
| 3:L5:4235:U:OP1    | 7:LD:12:TYR:OH     | 2.28                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:LN:5:LYS:HG3    | 37:Li:40:VAL:HG11  | 2.00                     | 0.43              |
| 23:LU:33:ILE:H     | 23:LU:33:ILE:HG13  | 1.67                     | 0.43              |
| 46:S2:428:OMU:H2'  | 46:S2:428:OMU:H6   | 1.77                     | 0.43              |
| 74:SW:42:MET:HE2   | 74:SW:42:MET:HB3   | 1.90                     | 0.43              |
| 80:Bv:27:PSU:H5'   | 81:j:46:SER:OG     | 2.19                     | 0.43              |
| 81:j:24:LEU:HD13   | 81:j:96:TYR:CD2    | 2.53                     | 0.43              |
| 81:j:108:LYS:HD3   | 81:j:109:LYS:H     | 1.84                     | 0.43              |
| 1:LA:247:ARG:NH2   | 1:LA:248:GLY:O     | 2.52                     | 0.43              |
| 3:L5:3620:U:H5     | 3:L5:3625:A:N7     | 2.17                     | 0.43              |
| 13:LJ:120:ASP:OD1  | 13:LJ:120:ASP:N    | 2.50                     | 0.43              |
| 32:Ld:93:ASN:ND2   | 32:Ld:98:SER:OG    | 2.52                     | 0.43              |
| 36:Lh:35:LYS:HA    | 36:Lh:44:LEU:HD21  | 2.01                     | 0.43              |
| 48:SB:38:MET:SD    | 48:SB:38:MET:N     | 2.91                     | 0.43              |
| 54:SK:49:MET:HB2   | 54:SK:49:MET:HE3   | 1.85                     | 0.43              |
| 67:Sg:140:TYR:OH   | 67:Sg:181:ASN:O    | 2.37                     | 0.43              |
| 68:SC:263:LYS:HG3  | 68:SC:268:GLU:HB3  | 2.01                     | 0.43              |
| 81:j:75:ILE:CA     | 81:j:78:VAL:HG12   | 2.48                     | 0.43              |
| 81:j:118:LYS:HA    | 81:j:119:PRO:HD2   | 1.66                     | 0.43              |
| 81:j:293:GLU:OE1   | 81:j:293:GLU:HA    | 2.18                     | 0.43              |
| 83:NC:711:LEU:HD12 | 83:NC:711:LEU:N    | 2.34                     | 0.43              |
| 3:L5:731:G:N2      | 3:L5:911:C:H42     | 2.17                     | 0.43              |
| 46:S2:1495:G:N2    | 66:Sd:42:CYS:SG    | 2.84                     | 0.43              |
| 46:S2:1610:G:N2    | 59:SS:85:ASN:OD1   | 2.52                     | 0.43              |
| 48:SB:52:THR:HG23  | 48:SB:57:ILE:HA    | 2.00                     | 0.43              |
| 50:SE:124:CYS:HB3  | 50:SE:141:THR:HB   | 2.00                     | 0.43              |
| 81:j:62:ILE:HB     | 81:j:68:ARG:HB2    | 2.01                     | 0.43              |
| 81:j:267:ALA:O     | 81:j:271:SER:HB2   | 2.19                     | 0.43              |
| 3:L5:2089:G:N2     | 3:L5:2090:G:O6     | 2.43                     | 0.42              |
| 3:L5:4479:U:O3'    | 24:LV:46:LYS:NZ    | 2.52                     | 0.42              |
| 9:LF:95:ILE:O      | 9:LF:223:LYS:HD2   | 2.19                     | 0.42              |
| 11:LH:42:ASN:HD21  | 17:LO:131:PRO:HB2  | 1.84                     | 0.42              |
| 46:S2:42:A:O2'     | 46:S2:98:C:OP1     | 2.30                     | 0.42              |
| 46:S2:656:G:H5'    | 46:S2:662:G:N2     | 2.34                     | 0.42              |
| 48:SB:38:MET:HB2   | 48:SB:186:ASN:HD21 | 1.83                     | 0.42              |
| 53:SI:78:ILE:HA    | 53:SI:104:ILE:HG22 | 2.01                     | 0.42              |
| 67:Sg:128:THR:OG1  | 67:Sg:141:THR:OG1  | 2.34                     | 0.42              |
| 2:LB:384:GLU:OE2   | 25:LW:14:TYR:OH    | 2.33                     | 0.42              |
| 3:L5:299:G:OP2     | 3:L5:299:G:N2      | 2.41                     | 0.42              |
| 3:L5:2469:C:H2'    | 3:L5:2470:G:H4'    | 2.01                     | 0.42              |
| 10:LG:59:ARG:HB3   | 10:LG:62:ARG:HH21  | 1.83                     | 0.42              |
| 46:S2:436:OMG:HM22 | 46:S2:437:G:H5'    | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:SK:19:GLY:HA2   | 54:SK:71:LEU:HD12  | 2.01                     | 0.42              |
| 59:SS:75:ARG:HH11  | 59:SS:95:TYR:HB2   | 1.85                     | 0.42              |
| 69:SG:139:SER:HA   | 69:SG:142:ARG:HG2  | 2.01                     | 0.42              |
| 75:SY:23:MET:HE1   | 75:SY:44:LEU:HD22  | 2.01                     | 0.42              |
| 81:j:136:LEU:C     | 81:j:138:ALA:H     | 2.25                     | 0.42              |
| 2:LB:247:GLY:HA2   | 3:L5:2825:G:H5'    | 2.02                     | 0.42              |
| 3:L5:4462:U:O2'    | 3:L5:4482:U:O2     | 2.34                     | 0.42              |
| 3:L5:4500:UR3:O2'  | 81:j:184:GLY:N     | 2.48                     | 0.42              |
| 28:LZ:41:ALA:HB2   | 28:LZ:77:TYR:HE1   | 1.83                     | 0.42              |
| 46:S2:1156:U:OP1   | 74:SW:71:LYS:NZ    | 2.53                     | 0.42              |
| 47:SA:123:VAL:HG22 | 47:SA:145:ILE:HB   | 2.02                     | 0.42              |
| 58:SR:106:LEU:HA   | 58:SR:109:LEU:HB3  | 2.01                     | 0.42              |
| 73:SO:137:SER:O    | 73:SO:137:SER:OG   | 2.30                     | 0.42              |
| 3:L5:4139:G:H4'    | 3:L5:4141:C:C2     | 2.55                     | 0.42              |
| 3:L5:4168:G:N2     | 80:Bv:73:G:O2'     | 2.43                     | 0.42              |
| 3:L5:4534:A:H5''   | 17:LO:68:ARG:HH12  | 1.85                     | 0.42              |
| 3:L5:4859:A:H3'    | 3:L5:4860:C:H5'    | 2.01                     | 0.42              |
| 8:LE:157:HIS:HB3   | 8:LE:160:LYS:HG3   | 2.01                     | 0.42              |
| 28:LZ:99:ASP:HB2   | 28:LZ:102:ARG:HE   | 1.84                     | 0.42              |
| 31:Lc:24:SER:O     | 31:Lc:24:SER:OG    | 2.35                     | 0.42              |
| 46:S2:1156:U:O4    | 68:SC:194:ARG:NH1  | 2.51                     | 0.42              |
| 53:SI:113:TYR:OH   | 53:SI:156:ALA:O    | 2.37                     | 0.42              |
| 57:SQ:19:ALA:HB2   | 57:SQ:75:GLY:HA3   | 2.01                     | 0.42              |
| 57:SQ:97:GLN:HB2   | 57:SQ:105:LYS:HD3  | 2.00                     | 0.42              |
| 61:SU:23:THR:HG22  | 61:SU:88:LEU:HG    | 2.02                     | 0.42              |
| 73:SO:133:THR:O    | 73:SO:135:ILE:HG12 | 2.20                     | 0.42              |
| 80:Bv:14:A:C2'     | 80:Bv:15:A:H5'     | 2.49                     | 0.42              |
| 81:j:38:ILE:HD12   | 81:j:124:LEU:HD23  | 2.00                     | 0.42              |
| 81:j:219:VAL:HG12  | 81:j:246:LEU:HD21  | 2.00                     | 0.42              |
| 1:LA:2:GLY:HA2     | 1:LA:207:VAL:HG12  | 2.01                     | 0.42              |
| 3:L5:2367:G:N2     | 3:L5:2411:OMG:H5'  | 2.35                     | 0.42              |
| 6:LC:61:GLN:H      | 6:LC:61:GLN:HG2    | 1.66                     | 0.42              |
| 7:LD:110:LEU:O     | 7:LD:115:MET:N     | 2.52                     | 0.42              |
| 8:LE:284:HIS:CD2   | 8:LE:285:LYS:HG3   | 2.55                     | 0.42              |
| 13:LJ:101:ASP:OD1  | 13:LJ:101:ASP:N    | 2.52                     | 0.42              |
| 15:LM:104:MET:HE3  | 15:LM:109:ARG:HG2  | 2.01                     | 0.42              |
| 21:LS:41:LYS:HD2   | 21:LS:61:ILE:HG13  | 2.00                     | 0.42              |
| 28:LZ:103:ASP:N    | 28:LZ:103:ASP:OD1  | 2.52                     | 0.42              |
| 36:Lh:105:LYS:HG2  | 36:Lh:108:GLN:HE21 | 1.84                     | 0.42              |
| 47:SA:159:ILE:HD11 | 62:SV:34:MET:HE1   | 2.01                     | 0.42              |
| 49:SD:105:LEU:HD13 | 49:SD:122:VAL:HG21 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:Sg:14:HIS:CE1   | 67:Sg:18:VAL:HG22  | 2.54                     | 0.42              |
| 1:LA:150:LEU:HD23  | 3:L5:3640:G:C5     | 2.54                     | 0.42              |
| 3:L5:4507:C:H2'    | 3:L5:4508:G:C8     | 2.55                     | 0.42              |
| 10:LG:58:PRO:HG2   | 10:LG:61:ILE:HD12  | 2.02                     | 0.42              |
| 46:S2:1628:C:H2'   | 46:S2:1629:C:C6    | 2.55                     | 0.42              |
| 67:Sg:29:ASP:HB2   | 67:Sg:45:LEU:HB2   | 2.02                     | 0.42              |
| 81:j:75:ILE:HG22   | 81:j:75:ILE:O      | 2.20                     | 0.42              |
| 1:LA:133:TYR:HB3   | 1:LA:168:VAL:HG12  | 2.02                     | 0.42              |
| 3:L5:1501:U:H2'    | 3:L5:1502:A:C8     | 2.55                     | 0.42              |
| 3:L5:2856:U:O2'    | 3:L5:2868:A:N7     | 2.47                     | 0.42              |
| 3:L5:4250:A:N6     | 7:LD:28:THR:O      | 2.52                     | 0.42              |
| 17:LO:125:LYS:HG3  | 17:LO:129:LEU:HD12 | 2.01                     | 0.42              |
| 29:La:75:LEU:HD12  | 29:La:78:LEU:HD22  | 2.01                     | 0.42              |
| 36:Lh:80:PRO:HD2   | 36:Lh:83:LEU:HD12  | 2.02                     | 0.42              |
| 36:Lh:82:ASP:OD1   | 36:Lh:82:ASP:N     | 2.52                     | 0.42              |
| 65:Sc:20:ARG:HA    | 65:Sc:28:THR:HA    | 2.01                     | 0.42              |
| 74:SW:6:VAL:HG12   | 74:SW:34:ILE:HD11  | 2.00                     | 0.42              |
| 81:j:41:PRO:CB     | 81:j:91:ASN:N      | 2.81                     | 0.42              |
| 81:j:120:ILE:HG13  | 81:j:120:ILE:H     | 1.67                     | 0.42              |
| 81:j:264:PHE:CE1   | 81:j:268:ILE:HD11  | 2.54                     | 0.42              |
| 2:LB:224:LYS:HG3   | 2:LB:340:THR:HG22  | 2.02                     | 0.42              |
| 3:L5:1081:G:H1     | 3:L5:1188:U:H3     | 1.66                     | 0.42              |
| 3:L5:2365:G:O2'    | 3:L5:2367:G:N7     | 2.52                     | 0.42              |
| 3:L5:4493:A2M:H5'' | 3:L5:4494:G:H5'    | 2.01                     | 0.42              |
| 3:L5:4575:A:N6     | 81:j:296:GLN:HG2   | 2.35                     | 0.42              |
| 7:LD:61:ILE:HG23   | 7:LD:79:TYR:HE1    | 1.84                     | 0.42              |
| 8:LE:223:ARG:HA    | 8:LE:224:LYS:HA    | 1.81                     | 0.42              |
| 22:LT:28:ALA:HA    | 22:LT:31:MET:HG2   | 2.02                     | 0.42              |
| 24:LV:65:VAL:HG22  | 24:LV:73:ARG:HA    | 2.01                     | 0.42              |
| 34:Lf:66:LYS:HE3   | 34:Lf:66:LYS:HB3   | 1.87                     | 0.42              |
| 37:Li:65:LYS:HG3   | 37:Li:68:ARG:HB3   | 2.01                     | 0.42              |
| 46:S2:987:A:C6     | 48:SB:120:MET:HE1  | 2.55                     | 0.42              |
| 46:S2:1123:C:O2'   | 48:SB:148:ASN:OD1  | 2.29                     | 0.42              |
| 48:SB:47:THR:OG1   | 48:SB:65:ARG:NH2   | 2.53                     | 0.42              |
| 52:SH:87:PHE:HB3   | 52:SH:90:LYS:HG3   | 2.02                     | 0.42              |
| 60:ST:12:GLN:HG2   | 60:ST:16:ARG:HH12  | 1.84                     | 0.42              |
| 67:Sg:40:ILE:HB    | 67:Sg:59:LEU:HB2   | 2.01                     | 0.42              |
| 3:L5:2468:G:H1     | 3:L5:2484:C:H42    | 1.68                     | 0.42              |
| 5:L8:21:C:OP1      | 6:LC:195:LYS:NZ    | 2.52                     | 0.42              |
| 18:LP:10:ASN:OD1   | 18:LP:10:ASN:N     | 2.50                     | 0.42              |
| 33:Le:43:ASN:HD22  | 33:Le:44:ARG:N     | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:28:U:H2'     | 46:S2:29:G:H8      | 1.85                     | 0.42              |
| 46:S2:1740:C:OP1   | 53:SI:44:HIS:ND1   | 2.47                     | 0.42              |
| 49:SD:115:VAL:HG11 | 49:SD:142:LEU:HD22 | 2.02                     | 0.42              |
| 80:Bv:38:A:H2'     | 80:Bv:39:C:O4'     | 2.20                     | 0.42              |
| 11:LH:135:SER:HB3  | 11:LH:145:ILE:HG23 | 2.02                     | 0.42              |
| 16:LN:123:GLU:HG2  | 16:LN:128:LYS:HG3  | 2.02                     | 0.42              |
| 28:LZ:74:VAL:HG13  | 28:LZ:101:PHE:HE2  | 1.85                     | 0.42              |
| 44:Lp:22:LEU:HD23  | 44:Lp:25:MET:HE3   | 2.02                     | 0.42              |
| 46:S2:491:C:O2'    | 46:S2:493:A:N7     | 2.49                     | 0.42              |
| 46:S2:628:A:H2'    | 49:SD:145:GLN:HE22 | 1.83                     | 0.42              |
| 46:S2:1256:G:H8    | 61:SU:66:ARG:HB2   | 1.84                     | 0.42              |
| 51:SF:163:PHE:CD2  | 51:SF:164:ARG:HG3  | 2.55                     | 0.42              |
| 56:SP:103:ASN:OD1  | 56:SP:120:SER:OG   | 2.33                     | 0.42              |
| 64:Sa:36:ILE:HB    | 64:Sa:73:TYR:HB2   | 2.02                     | 0.42              |
| 67:Sg:166:VAL:HG12 | 67:Sg:176:VAL:HG22 | 2.01                     | 0.42              |
| 76:SZ:79:ILE:HB    | 76:SZ:83:LEU:HD12  | 2.01                     | 0.42              |
| 80:Bv:52:G:C6      | 80:Bv:53:G:N7      | 2.88                     | 0.42              |
| 81:j:52:LEU:HB3    | 81:j:79:GLN:NE2    | 2.34                     | 0.42              |
| 3:L5:732:C:N3      | 3:L5:911:C:N4      | 2.66                     | 0.41              |
| 3:L5:4971:U:H4'    | 3:L5:4972:A:H5'    | 2.01                     | 0.41              |
| 10:LG:199:CYS:SG   | 10:LG:200:THR:N    | 2.93                     | 0.41              |
| 13:LJ:56:THR:HG21  | 80:Bv:57:G:C5'     | 2.49                     | 0.41              |
| 14:LL:81:LEU:HD12  | 14:LL:86:ILE:HG13  | 2.02                     | 0.41              |
| 21:LS:15:ARG:HD2   | 21:LS:16:CYS:O     | 2.19                     | 0.41              |
| 26:LX:43:SER:HA    | 26:LX:44:PRO:HD3   | 1.93                     | 0.41              |
| 46:S2:932:G:O2'    | 46:S2:934:G:OP2    | 2.35                     | 0.41              |
| 65:Sc:12:ALA:HB1   | 65:Sc:32:VAL:HB    | 2.02                     | 0.41              |
| 3:L5:1805:G:O2'    | 3:L5:1807:C:OP2    | 2.31                     | 0.41              |
| 3:L5:4667:U:H4'    | 41:Lm:104:HIS:CD2  | 2.55                     | 0.41              |
| 8:LE:176:THR:OG1   | 8:LE:177:GLY:O     | 2.28                     | 0.41              |
| 8:LE:267:LEU:HG    | 8:LE:271:LEU:HD13  | 2.02                     | 0.41              |
| 10:LG:39:PHE:CD1   | 10:LG:47:PRO:HD3   | 2.56                     | 0.41              |
| 46:S2:1551:U:P     | 49:SD:9:ARG:HH12   | 2.42                     | 0.41              |
| 61:SU:20:ILE:HD13  | 61:SU:98:VAL:HG21  | 2.03                     | 0.41              |
| 81:j:85:TYR:HE2    | 81:j:113:ASP:OD1   | 2.03                     | 0.41              |
| 83:NC:707:ILE:HB   | 83:NC:710:ILE:CG1  | 2.51                     | 0.41              |
| 3:L5:678:U:H1'     | 8:LE:94:LYS:HE2    | 2.01                     | 0.41              |
| 3:L5:1564:G:OP1    | 44:Lp:17:ARG:NH1   | 2.49                     | 0.41              |
| 3:L5:4339:A:H5''   | 43:Lo:65:LYS:HD2   | 2.02                     | 0.41              |
| 12:LI:87:MET:HB3   | 12:LI:87:MET:HE2   | 1.84                     | 0.41              |
| 24:LV:43:LYS:HD3   | 24:LV:60:MET:HE3   | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:Lk:13:LEU:HA    | 39:Lk:16:ARG:HG2   | 2.01                     | 0.41              |
| 46:S2:860:G:N2     | 74:SW:107:SER:OG   | 2.51                     | 0.41              |
| 46:S2:1570:G:O2'   | 46:S2:1614:A:O2'   | 2.37                     | 0.41              |
| 47:SA:122:LEU:HB3  | 47:SA:144:THR:HG22 | 2.02                     | 0.41              |
| 49:SD:53:THR:HG23  | 49:SD:54:ARG:HD3   | 2.02                     | 0.41              |
| 80:Bv:18:G:N2      | 80:Bv:57:G:H2'     | 2.36                     | 0.41              |
| 1:LA:180:LEU:HD11  | 44:Lp:26:VAL:HG21  | 2.02                     | 0.41              |
| 3:L5:299:G:O6      | 16:LN:12:ARG:NH1   | 2.54                     | 0.41              |
| 44:Lp:51:ALA:HB3   | 44:Lp:54:ILE:HD13  | 2.03                     | 0.41              |
| 46:S2:145:G:H2'    | 46:S2:146:G:C8     | 2.55                     | 0.41              |
| 46:S2:525:A:H2'    | 46:S2:526:A:C8     | 2.55                     | 0.41              |
| 46:S2:1473:G:N1    | 46:S2:1476:A:OP2   | 2.52                     | 0.41              |
| 2:LB:92:TYR:HB2    | 2:LB:159:VAL:HB    | 2.01                     | 0.41              |
| 3:L5:360:G:N2      | 3:L5:363:A:OP2     | 2.36                     | 0.41              |
| 3:L5:1949:A:H2     | 3:L5:2011:G:H21    | 1.68                     | 0.41              |
| 3:L5:2006:C:H2'    | 3:L5:2007:U:C4     | 2.56                     | 0.41              |
| 3:L5:4230:U:H2'    | 3:L5:4231:C:C6     | 2.55                     | 0.41              |
| 3:L5:4511:G:N2     | 3:L5:4514:A:OP2    | 2.42                     | 0.41              |
| 8:LE:261:ILE:HG23  | 8:LE:267:LEU:HD23  | 2.03                     | 0.41              |
| 11:LH:165:THR:HG21 | 11:LH:179:ILE:HD12 | 2.03                     | 0.41              |
| 23:LU:63:ILE:HG23  | 23:LU:70:ILE:HG23  | 2.02                     | 0.41              |
| 46:S2:643:A:OP1    | 70:SJ:38:ARG:NH1   | 2.51                     | 0.41              |
| 46:S2:1401:A:H4'   | 61:SU:52:GLY:HA3   | 2.03                     | 0.41              |
| 46:S2:1415:C:H2'   | 46:S2:1416:C:C6    | 2.56                     | 0.41              |
| 49:SD:103:GLU:HA   | 49:SD:106:ARG:HG2  | 2.02                     | 0.41              |
| 67:Sg:57:ARG:HE    | 67:Sg:95:GLY:HA3   | 1.85                     | 0.41              |
| 7:LD:108:ARG:CZ    | 7:LD:253:TYR:HB2   | 2.50                     | 0.41              |
| 8:LE:128:HIS:O     | 8:LE:128:HIS:ND1   | 2.54                     | 0.41              |
| 17:LO:25:LYS:HD2   | 17:LO:25:LYS:HA    | 1.87                     | 0.41              |
| 46:S2:453:C:O2'    | 69:SG:92:ARG:O     | 2.33                     | 0.41              |
| 46:S2:1160:U:O4    | 63:SX:2:GLY:N      | 2.53                     | 0.41              |
| 46:S2:1277:C:H2'   | 46:S2:1278:A:H8    | 1.85                     | 0.41              |
| 51:SF:128:ILE:HD13 | 65:Sc:68:LEU:HD22  | 2.03                     | 0.41              |
| 67:Sg:83:TRP:HA    | 67:Sg:107:ASP:HB2  | 2.03                     | 0.41              |
| 67:Sg:231:ASP:OD1  | 67:Sg:232:GLY:N    | 2.54                     | 0.41              |
| 68:SC:192:LEU:HG   | 68:SC:227:ARG:HB3  | 2.02                     | 0.41              |
| 73:SO:27:VAL:HG23  | 73:SO:90:ILE:HA    | 2.02                     | 0.41              |
| 76:SZ:48:VAL:HG12  | 76:SZ:80:ARG:HD2   | 2.02                     | 0.41              |
| 76:SZ:74:SER:OG    | 76:SZ:79:ILE:O     | 2.28                     | 0.41              |
| 2:LB:231:VAL:HG21  | 2:LB:251:VAL:HG23  | 2.03                     | 0.41              |
| 2:LB:285:TYR:CD1   | 2:LB:363:ILE:HD13  | 2.56                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:L5:1564:G:H5'   | 3:L5:1565:U:H5''   | 2.03                     | 0.41              |
| 3:L5:3736:G:H1    | 3:L5:3746:C:H42    | 1.68                     | 0.41              |
| 3:L5:3795:A:O2'   | 3:L5:3798:G:N3     | 2.41                     | 0.41              |
| 4:L7:48:G:OP1     | 7:LD:226:TYR:OH    | 2.38                     | 0.41              |
| 31:Lc:48:LEU:HD21 | 31:Lc:60:ILE:HG21  | 2.03                     | 0.41              |
| 36:Lh:69:LEU:HD12 | 36:Lh:73:TYR:HE2   | 1.86                     | 0.41              |
| 80:Bv:45:G:O2'    | 80:Bv:46:G7M:H5'   | 2.21                     | 0.41              |
| 3:L5:2470:G:N1    | 3:L5:2482:U:O2     | 2.47                     | 0.41              |
| 10:LG:132:ARG:HA  | 10:LG:133:PRO:HD3  | 1.81                     | 0.41              |
| 49:SD:135:GLU:HG3 | 49:SD:157:MET:HE3  | 2.02                     | 0.41              |
| 51:SF:41:VAL:HG13 | 51:SF:68:ILE:HG22  | 2.02                     | 0.41              |
| 80:Bv:30:G:H5''   | 80:Bv:30:G:C8      | 2.56                     | 0.41              |
| 2:LB:242:ARG:NH2  | 3:L5:2843:C:O2     | 2.48                     | 0.41              |
| 3:L5:95:G:OP2     | 29:La:34:ASN:ND2   | 2.53                     | 0.41              |
| 3:L5:730:G:O2'    | 3:L5:731:G:O4'     | 2.39                     | 0.41              |
| 3:L5:2386:G:O2'   | 3:L5:2809:G:O2'    | 2.38                     | 0.41              |
| 3:L5:2893:G:H2'   | 3:L5:2895:U:H1'    | 2.02                     | 0.41              |
| 7:LD:51:MET:HE3   | 7:LD:105:LEU:HD23  | 2.03                     | 0.41              |
| 18:LP:6:LEU:HD23  | 18:LP:6:LEU:HA     | 1.92                     | 0.41              |
| 18:LP:108:ASP:OD1 | 18:LP:108:ASP:N    | 2.54                     | 0.41              |
| 19:LQ:72:LEU:HD13 | 19:LQ:72:LEU:HA    | 1.94                     | 0.41              |
| 19:LQ:159:PRO:HA  | 19:LQ:160:HIS:HA   | 1.75                     | 0.41              |
| 22:LT:81:LYS:HB2  | 30:Lb:16:TRP:CZ3   | 2.56                     | 0.41              |
| 24:LV:39:ILE:HG12 | 24:LV:61:VAL:HG11  | 2.02                     | 0.41              |
| 28:LZ:90:PRO:O    | 28:LZ:117:LYS:NZ   | 2.47                     | 0.41              |
| 45:Lr:89:THR:HG21 | 45:Lr:118:LEU:HD11 | 2.02                     | 0.41              |
| 46:S2:626:G:N7    | 82:k:1059:U:C6     | 2.88                     | 0.41              |
| 46:S2:1112:U:H2'  | 46:S2:1113:A:C8    | 2.55                     | 0.41              |
| 46:S2:1550:G:O2'  | 46:S2:1558:C:O2    | 2.34                     | 0.41              |
| 46:S2:1579:A:O2'  | 46:S2:1581:C:OP2   | 2.32                     | 0.41              |
| 49:SD:60:GLY:HA3  | 49:SD:65:ARG:H     | 1.85                     | 0.41              |
| 53:SI:46:VAL:HG21 | 53:SI:56:ARG:HE    | 1.85                     | 0.41              |
| 57:SQ:31:LEU:HD11 | 57:SQ:33:LYS:HE3   | 2.03                     | 0.41              |
| 59:SS:38:ARG:O    | 59:SS:42:HIS:ND1   | 2.41                     | 0.41              |
| 68:SC:169:TYR:OH  | 68:SC:175:GLY:O    | 2.36                     | 0.41              |
| 75:SY:27:VAL:HG12 | 75:SY:29:HIS:HD2   | 1.85                     | 0.41              |
| 80:Bv:60:C:C5'    | 80:Bv:61:C:C5      | 2.96                     | 0.41              |
| 81:j:34:MET:HE1   | 81:j:98:GLY:C      | 2.46                     | 0.41              |
| 81:j:102:THR:CG2  | 81:j:106:LYS:HB3   | 2.50                     | 0.41              |
| 81:j:309:LEU:HD11 | 81:j:345:TYR:CE2   | 2.56                     | 0.41              |
| 3:L5:113:A:N1     | 3:L5:268:G:O2'     | 2.51                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:L5:2646:A:N1      | 3:L5:2659:C:O2'    | 2.46                     | 0.41              |
| 3:L5:3858:G:O2'     | 3:L5:3860:G:OP2    | 2.32                     | 0.41              |
| 3:L5:4114:C:O2      | 3:L5:4117:G:N2     | 2.37                     | 0.41              |
| 3:L5:4265:U:OP1     | 43:Lo:13:LYS:NZ    | 2.45                     | 0.41              |
| 5:L8:75:OMG:OP2     | 27:LY:74:TYR:OH    | 2.35                     | 0.41              |
| 19:LQ:82:VAL:HG11   | 19:LQ:86:ILE:HD11  | 2.02                     | 0.41              |
| 46:S2:1426:U:H1'    | 60:ST:5:THR:HG21   | 2.03                     | 0.41              |
| 46:S2:1830:U:C4     | 82:k:1054:A:H5''   | 2.56                     | 0.41              |
| 67:Sg:59:LEU:HD23   | 67:Sg:90:TRP:CD2   | 2.56                     | 0.41              |
| 69:SG:7:PHE:HD1     | 69:SG:113:ILE:HB   | 1.86                     | 0.41              |
| 3:L5:1308:G:H2'     | 3:L5:3855:A:N7     | 2.35                     | 0.40              |
| 9:LF:157:ARG:NH2    | 9:LF:212:LYS:O     | 2.55                     | 0.40              |
| 13:LJ:3:GLN:HG3     | 13:LJ:8:LYS:HD2    | 2.03                     | 0.40              |
| 39:Lk:5:ILE:HG22    | 39:Lk:7:GLU:H      | 1.86                     | 0.40              |
| 46:S2:867:OMG:H5''  | 55:SL:149:ALA:HB2  | 2.03                     | 0.40              |
| 57:SQ:58:LEU:HB3    | 57:SQ:62:ARG:HD2   | 2.02                     | 0.40              |
| 60:ST:114:GLU:HG3   | 60:ST:124:THR:HG22 | 2.02                     | 0.40              |
| 67:Sg:3:GLU:HG2     | 67:Sg:314:ILE:HG22 | 2.03                     | 0.40              |
| 81:j:211:GLN:O      | 81:j:212:LEU:HD12  | 2.21                     | 0.40              |
| 3:L5:67:C:OP2       | 3:L5:303:G:N2      | 2.54                     | 0.40              |
| 3:L5:1428:C:N4      | 3:L5:2091:G:H1     | 2.17                     | 0.40              |
| 3:L5:1744:U:H5      | 3:L5:4225:A:H5'    | 1.86                     | 0.40              |
| 9:LF:144:TYR:CE2    | 9:LF:237:GLU:HB2   | 2.56                     | 0.40              |
| 16:LN:104:GLU:HA    | 16:LN:160:GLU:HG3  | 2.03                     | 0.40              |
| 23:LU:88:LYS:HD2    | 23:LU:97:ARG:HH12  | 1.86                     | 0.40              |
| 24:LV:87:SER:HG     | 25:LW:19:ARG:HH11  | 1.64                     | 0.40              |
| 25:LW:78:PHE:CE2    | 69:SG:8:PRO:HB2    | 2.57                     | 0.40              |
| 39:Lk:12:LEU:HA     | 39:Lk:12:LEU:HD23  | 1.85                     | 0.40              |
| 39:Lk:12:LEU:HD21   | 39:Lk:56:LEU:HD11  | 2.02                     | 0.40              |
| 45:Lr:85:ASN:OD1    | 45:Lr:85:ASN:N     | 2.54                     | 0.40              |
| 46:S2:1391:OMC:HM22 | 46:S2:1392:U:H5'   | 2.04                     | 0.40              |
| 50:SE:36:HIS:CD2    | 50:SE:85:GLY:HA3   | 2.56                     | 0.40              |
| 51:SF:27:ASP:OD1    | 51:SF:27:ASP:N     | 2.55                     | 0.40              |
| 67:Sg:32:LEU:HG     | 67:Sg:71:ILE:HD11  | 2.03                     | 0.40              |
| 68:SC:167:ARG:HG3   | 68:SC:219:ILE:HD13 | 2.02                     | 0.40              |
| 3:L5:4165:G:O2'     | 3:L5:4412:PSU:OP1  | 2.30                     | 0.40              |
| 3:L5:4357:C:OP2     | 3:L5:4502:PSU:O2'  | 2.40                     | 0.40              |
| 5:L8:141:C:H2'      | 5:L8:142:U:C6      | 2.56                     | 0.40              |
| 11:LH:103:VAL:HG11  | 11:LH:144:LEU:HD21 | 2.04                     | 0.40              |
| 19:LQ:122:THR:H     | 19:LQ:125:GLN:HE21 | 1.69                     | 0.40              |
| 27:LY:44:VAL:HG21   | 27:LY:119:LEU:HD12 | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:Lc:47:ILE:HD12  | 31:Lc:94:LEU:HD11  | 2.02                     | 0.40              |
| 33:Le:6:PRO:HG3    | 33:Le:73:GLY:HA3   | 2.03                     | 0.40              |
| 45:Lr:107:ARG:NH1  | 45:Lr:108:MET:HE2  | 2.36                     | 0.40              |
| 46:S2:1466:G:H5'   | 58:SR:4:VAL:HG22   | 2.02                     | 0.40              |
| 51:SF:144:LEU:HD23 | 65:Sc:49:PRO:HG2   | 2.04                     | 0.40              |
| 70:SJ:108:ARG:HH22 | 70:SJ:154:GLN:HE21 | 1.70                     | 0.40              |
| 72:SN:4:MET:HE3    | 72:SN:124:ARG:CZ   | 2.51                     | 0.40              |
| 81:j:274:VAL:O     | 81:j:278:VAL:HG23  | 2.21                     | 0.40              |
| 2:LB:220:ILE:HB    | 2:LB:346:THR:HB    | 2.03                     | 0.40              |
| 3:L5:4422:U:C5     | 81:j:185:MEQ:CE    | 3.05                     | 0.40              |
| 3:L5:4711:G:H2'    | 3:L5:4712:G:C8     | 2.55                     | 0.40              |
| 16:LN:49:ARG:HH11  | 16:LN:49:ARG:HD2   | 1.70                     | 0.40              |
| 20:LR:98:ARG:HD2   | 20:LR:133:LYS:O    | 2.21                     | 0.40              |
| 27:LY:99:ILE:HG21  | 27:LY:99:ILE:HD13  | 1.90                     | 0.40              |
| 46:S2:1098:C:H2'   | 46:S2:1099:G:C8    | 2.56                     | 0.40              |
| 50:SE:182:MET:HE2  | 50:SE:192:ILE:HD11 | 2.03                     | 0.40              |
| 62:SV:16:LYS:HG2   | 62:SV:23:ILE:HD13  | 2.02                     | 0.40              |
| 73:SO:31:CYS:HB2   | 73:SO:93:LEU:HD13  | 2.03                     | 0.40              |
| 81:j:396:SER:HG    | 81:j:399:GLY:H     | 1.68                     | 0.40              |
| 83:NC:726:ASN:HA   | 83:NC:727:PRO:HD3  | 1.91                     | 0.40              |
| 3:L5:4411:A:H5''   | 12:LI:114:GLY:HA2  | 2.04                     | 0.40              |
| 3:L5:4489:C:N4     | 81:j:188:LEU:HD12  | 2.37                     | 0.40              |
| 5:L8:96:C:H5''     | 36:Lh:66:LYS:HG2   | 2.04                     | 0.40              |
| 10:LG:223:ARG:HG3  | 10:LG:227:ASN:HB2  | 2.04                     | 0.40              |
| 33:Le:35:TRP:CZ2   | 33:Le:56:PRO:HD2   | 2.57                     | 0.40              |
| 46:S2:1016:U:H5''  | 72:SN:14:SER:HB3   | 2.03                     | 0.40              |
| 46:S2:1543:U:OP1   | 57:SQ:37:ARG:NH2   | 2.54                     | 0.40              |
| 50:SE:253:ASP:O    | 50:SE:257:ALA:N    | 2.44                     | 0.40              |
| 80:Bv:26:M2G:H2'   | 80:Bv:27:PSU:C6    | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | LA    | 246/248 (99%)  | 229 (93%) | 17 (7%)  | 0        | 100         | 100 |
| 2   | LB    | 394/396 (100%) | 379 (96%) | 15 (4%)  | 0        | 100         | 100 |
| 6   | LC    | 355/358 (99%)  | 340 (96%) | 14 (4%)  | 1 (0%)   | 36          | 66  |
| 7   | LD    | 288/290 (99%)  | 275 (96%) | 13 (4%)  | 0        | 100         | 100 |
| 8   | LE    | 232/247 (94%)  | 206 (89%) | 26 (11%) | 0        | 100         | 100 |
| 9   | LF    | 224/225 (100%) | 212 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 10  | LG    | 240/241 (100%) | 223 (93%) | 17 (7%)  | 0        | 100         | 100 |
| 11  | LH    | 188/190 (99%)  | 171 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 12  | LI    | 203/213 (95%)  | 191 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 13  | LJ    | 174/176 (99%)  | 154 (88%) | 20 (12%) | 0        | 100         | 100 |
| 14  | LL    | 202/204 (99%)  | 182 (90%) | 20 (10%) | 0        | 100         | 100 |
| 15  | LM    | 137/139 (99%)  | 127 (93%) | 9 (7%)   | 1 (1%)   | 18          | 47  |
| 16  | LN    | 201/203 (99%)  | 193 (96%) | 5 (2%)   | 3 (2%)   | 8           | 28  |
| 17  | LO    | 199/201 (99%)  | 193 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 18  | LP    | 151/153 (99%)  | 143 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 19  | LQ    | 185/187 (99%)  | 176 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 20  | LR    | 185/187 (99%)  | 176 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 21  | LS    | 173/175 (99%)  | 160 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 22  | LT    | 157/159 (99%)  | 149 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 23  | LU    | 99/101 (98%)   | 85 (86%)  | 14 (14%) | 0        | 100         | 100 |
| 24  | LV    | 129/131 (98%)  | 122 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 25  | LW    | 122/124 (98%)  | 108 (88%) | 14 (12%) | 0        | 100         | 100 |
| 26  | LX    | 118/120 (98%)  | 111 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 27  | LY    | 132/134 (98%)  | 129 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 28  | LZ    | 133/135 (98%)  | 120 (90%) | 13 (10%) | 0        | 100         | 100 |
| 29  | La    | 145/147 (99%)  | 136 (94%) | 8 (6%)   | 1 (1%)   | 18          | 47  |
| 30  | Lb    | 105/121 (87%)  | 95 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 31  | Lc    | 96/98 (98%)    | 88 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 32  | Ld    | 105/107 (98%)  | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 33  | Le    | 126/128 (98%)  | 118 (94%) | 7 (6%)   | 1 (1%)   | 16          | 44  |
| 34  | Lf    | 107/109 (98%)  | 98 (92%)  | 8 (8%)   | 1 (1%)   | 14          | 41  |
| 35  | Lg    | 112/114 (98%)  | 110 (98%) | 2 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 36  | Lh    | 120/122 (98%) | 116 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 37  | Li    | 100/102 (98%) | 98 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 38  | Lj    | 85/86 (99%)   | 78 (92%)  | 6 (7%)   | 1 (1%)   | 10          | 34  |
| 39  | Lk    | 67/69 (97%)   | 61 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 40  | Ll    | 48/50 (96%)   | 42 (88%)  | 6 (12%)  | 0        | 100         | 100 |
| 41  | Lm    | 49/52 (94%)   | 47 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 42  | Ln    | 22/24 (92%)   | 21 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 43  | Lo    | 104/105 (99%) | 99 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 44  | Lp    | 89/91 (98%)   | 83 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 45  | Lr    | 123/125 (98%) | 113 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 47  | SA    | 214/216 (99%) | 199 (93%) | 14 (6%)  | 1 (0%)   | 24          | 55  |
| 48  | SB    | 209/211 (99%) | 201 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 49  | SD    | 222/224 (99%) | 210 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 50  | SE    | 256/258 (99%) | 244 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 51  | SF    | 181/189 (96%) | 168 (93%) | 12 (7%)  | 1 (1%)   | 21          | 51  |
| 52  | SH    | 181/189 (96%) | 167 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 53  | SI    | 193/205 (94%) | 185 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 54  | SK    | 93/95 (98%)   | 83 (89%)  | 10 (11%) | 0        | 100         | 100 |
| 55  | SL    | 136/150 (91%) | 130 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 56  | SP    | 129/131 (98%) | 126 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 57  | SQ    | 138/140 (99%) | 130 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 58  | SR    | 129/131 (98%) | 119 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 59  | SS    | 141/143 (99%) | 133 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 60  | ST    | 139/141 (99%) | 129 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 61  | SU    | 98/100 (98%)  | 94 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 62  | SV    | 82/84 (98%)   | 79 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 63  | SX    | 137/139 (99%) | 131 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 64  | Sa    | 97/99 (98%)   | 92 (95%)  | 4 (4%)   | 1 (1%)   | 12          | 38  |
| 65  | Sc    | 59/61 (97%)   | 54 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 66  | Sd    | 53/55 (96%)   | 52 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 67  | Sg    | 311/313 (99%) | 271 (87%) | 40 (13%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 68  | SC    | 219/220 (100%)    | 212 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 69  | SG    | 226/228 (99%)     | 212 (94%)   | 14 (6%)  | 0        | 100         | 100 |
| 70  | SJ    | 178/180 (99%)     | 174 (98%)   | 3 (2%)   | 1 (1%)   | 21          | 51  |
| 71  | SM    | 108/120 (90%)     | 102 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 72  | SN    | 148/150 (99%)     | 145 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 73  | SO    | 131/135 (97%)     | 121 (92%)   | 10 (8%)  | 0        | 100         | 100 |
| 74  | SW    | 127/129 (98%)     | 121 (95%)   | 5 (4%)   | 1 (1%)   | 16          | 44  |
| 75  | SY    | 120/122 (98%)     | 117 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 76  | SZ    | 68/70 (97%)       | 68 (100%)   | 0        | 0        | 100         | 100 |
| 77  | Sb    | 80/82 (98%)       | 75 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 78  | Se    | 47/54 (87%)       | 44 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| 79  | Sf    | 61/63 (97%)       | 50 (82%)    | 11 (18%) | 0        | 100         | 100 |
| 81  | j     | 365/411 (89%)     | 325 (89%)   | 34 (9%)  | 6 (2%)   | 7           | 27  |
| 83  | NC    | 23/25 (92%)       | 22 (96%)    | 0        | 1 (4%)   | 2           | 7   |
| All | All   | 11569/11850 (98%) | 10840 (94%) | 708 (6%) | 21 (0%)  | 44          | 72  |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | LC    | 222 | ARG  |
| 16  | LN    | 124 | ASP  |
| 29  | La    | 24  | LYS  |
| 81  | j     | 305 | VAL  |
| 33  | Le    | 73  | GLY  |
| 47  | SA    | 12  | GLU  |
| 51  | SF    | 80  | GLY  |
| 81  | j     | 105 | GLY  |
| 15  | LM    | 32  | ASP  |
| 34  | Lf    | 107 | PRO  |
| 64  | Sa    | 47  | ALA  |
| 81  | j     | 118 | LYS  |
| 38  | Lj    | 40  | PRO  |
| 81  | j     | 119 | PRO  |
| 83  | NC    | 727 | PRO  |
| 70  | SJ    | 138 | ARG  |
| 16  | LN    | 84  | PRO  |
| 81  | j     | 184 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74  | SW    | 29  | PRO  |
| 16  | LN    | 83  | LYS  |
| 81  | j     | 250 | VAL  |

### 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   | LA    | 190/190 (100%) | 184 (97%)  | 6 (3%)   | 34          | 70  |
| 2   | LB    | 345/345 (100%) | 344 (100%) | 1 (0%)   | 86          | 95  |
| 6   | LC    | 298/298 (100%) | 298 (100%) | 0        | 100         | 100 |
| 7   | LD    | 244/245 (100%) | 244 (100%) | 0        | 100         | 100 |
| 8   | LE    | 209/220 (95%)  | 208 (100%) | 1 (0%)   | 81          | 93  |
| 9   | LF    | 195/194 (100%) | 194 (100%) | 1 (0%)   | 81          | 93  |
| 10  | LG    | 204/205 (100%) | 204 (100%) | 0        | 100         | 100 |
| 11  | LH    | 169/169 (100%) | 166 (98%)  | 3 (2%)   | 51          | 82  |
| 12  | LI    | 177/180 (98%)  | 176 (99%)  | 1 (1%)   | 78          | 92  |
| 13  | LJ    | 148/148 (100%) | 146 (99%)  | 2 (1%)   | 59          | 85  |
| 14  | LL    | 170/170 (100%) | 167 (98%)  | 3 (2%)   | 51          | 82  |
| 15  | LM    | 118/118 (100%) | 116 (98%)  | 2 (2%)   | 53          | 83  |
| 16  | LN    | 171/171 (100%) | 171 (100%) | 0        | 100         | 100 |
| 17  | LO    | 173/173 (100%) | 173 (100%) | 0        | 100         | 100 |
| 18  | LP    | 134/134 (100%) | 133 (99%)  | 1 (1%)   | 76          | 91  |
| 19  | LQ    | 164/164 (100%) | 162 (99%)  | 2 (1%)   | 63          | 87  |
| 20  | LR    | 166/166 (100%) | 165 (99%)  | 1 (1%)   | 78          | 92  |
| 21  | LS    | 156/156 (100%) | 155 (99%)  | 1 (1%)   | 78          | 92  |
| 22  | LT    | 139/139 (100%) | 139 (100%) | 0        | 100         | 100 |
| 23  | LU    | 91/91 (100%)   | 91 (100%)  | 0        | 100         | 100 |
| 24  | LV    | 101/101 (100%) | 99 (98%)   | 2 (2%)   | 48          | 80  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 25  | LW    | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 68          | 88  |
| 26  | LX    | 108/108 (100%) | 106 (98%)  | 2 (2%)   | 50          | 81  |
| 27  | LY    | 124/124 (100%) | 122 (98%)  | 2 (2%)   | 55          | 83  |
| 28  | LZ    | 117/117 (100%) | 114 (97%)  | 3 (3%)   | 40          | 75  |
| 29  | La    | 120/120 (100%) | 119 (99%)  | 1 (1%)   | 73          | 90  |
| 30  | Lb    | 89/100 (89%)   | 89 (100%)  | 0        | 100         | 100 |
| 31  | Lc    | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 32  | Ld    | 98/98 (100%)   | 96 (98%)   | 2 (2%)   | 48          | 80  |
| 33  | Le    | 114/114 (100%) | 112 (98%)  | 2 (2%)   | 51          | 82  |
| 34  | Lf    | 88/88 (100%)   | 87 (99%)   | 1 (1%)   | 65          | 87  |
| 35  | Lg    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 36  | Lh    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 37  | Li    | 86/86 (100%)   | 86 (100%)  | 0        | 100         | 100 |
| 38  | Lj    | 74/73 (101%)   | 74 (100%)  | 0        | 100         | 100 |
| 39  | Lk    | 64/64 (100%)   | 64 (100%)  | 0        | 100         | 100 |
| 40  | Ll    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 41  | Lm    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 42  | Ln    | 23/23 (100%)   | 23 (100%)  | 0        | 100         | 100 |
| 43  | Lo    | 94/93 (101%)   | 94 (100%)  | 0        | 100         | 100 |
| 44  | Lp    | 74/74 (100%)   | 74 (100%)  | 0        | 100         | 100 |
| 45  | Lr    | 109/109 (100%) | 108 (99%)  | 1 (1%)   | 70          | 89  |
| 47  | SA    | 180/180 (100%) | 180 (100%) | 0        | 100         | 100 |
| 48  | SB    | 193/193 (100%) | 193 (100%) | 0        | 100         | 100 |
| 49  | SD    | 188/188 (100%) | 188 (100%) | 0        | 100         | 100 |
| 50  | SE    | 221/221 (100%) | 221 (100%) | 0        | 100         | 100 |
| 51  | SF    | 158/159 (99%)  | 156 (99%)  | 2 (1%)   | 61          | 86  |
| 52  | SH    | 165/169 (98%)  | 165 (100%) | 0        | 100         | 100 |
| 53  | SI    | 172/178 (97%)  | 172 (100%) | 0        | 100         | 100 |
| 54  | SK    | 86/86 (100%)   | 84 (98%)   | 2 (2%)   | 44          | 78  |
| 55  | SL    | 126/134 (94%)  | 126 (100%) | 0        | 100         | 100 |
| 56  | SP    | 117/117 (100%) | 117 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|-------------|-----|
| 57  | SQ    | 116/116 (100%)    | 116 (100%) | 0        | 100         | 100 |
| 58  | SR    | 119/119 (100%)    | 118 (99%)  | 1 (1%)   | 73          | 90  |
| 59  | SS    | 124/124 (100%)    | 123 (99%)  | 1 (1%)   | 73          | 90  |
| 60  | ST    | 111/111 (100%)    | 111 (100%) | 0        | 100         | 100 |
| 61  | SU    | 93/93 (100%)      | 92 (99%)   | 1 (1%)   | 65          | 87  |
| 62  | SV    | 67/67 (100%)      | 66 (98%)   | 1 (2%)   | 57          | 84  |
| 63  | SX    | 111/111 (100%)    | 111 (100%) | 0        | 100         | 100 |
| 64  | Sa    | 86/86 (100%)      | 86 (100%)  | 0        | 100         | 100 |
| 65  | Sc    | 54/54 (100%)      | 54 (100%)  | 0        | 100         | 100 |
| 66  | Sd    | 48/48 (100%)      | 48 (100%)  | 0        | 100         | 100 |
| 67  | Sg    | 272/272 (100%)    | 271 (100%) | 1 (0%)   | 84          | 94  |
| 68  | SC    | 187/186 (100%)    | 187 (100%) | 0        | 100         | 100 |
| 69  | SG    | 199/199 (100%)    | 199 (100%) | 0        | 100         | 100 |
| 70  | SJ    | 160/160 (100%)    | 159 (99%)  | 1 (1%)   | 78          | 92  |
| 71  | SM    | 93/102 (91%)      | 93 (100%)  | 0        | 100         | 100 |
| 72  | SN    | 130/130 (100%)    | 130 (100%) | 0        | 100         | 100 |
| 73  | SO    | 104/104 (100%)    | 100 (96%)  | 4 (4%)   | 29          | 64  |
| 74  | SW    | 112/112 (100%)    | 111 (99%)  | 1 (1%)   | 70          | 89  |
| 75  | SY    | 107/107 (100%)    | 107 (100%) | 0        | 100         | 100 |
| 76  | SZ    | 62/62 (100%)      | 62 (100%)  | 0        | 100         | 100 |
| 77  | Sb    | 74/74 (100%)      | 74 (100%)  | 0        | 100         | 100 |
| 78  | Se    | 42/44 (96%)       | 42 (100%)  | 0        | 100         | 100 |
| 79  | Sf    | 56/56 (100%)      | 56 (100%)  | 0        | 100         | 100 |
| 81  | j     | 317/353 (90%)     | 264 (83%)  | 53 (17%) | 2           | 8   |
| 83  | NC    | 19/19 (100%)      | 18 (95%)   | 1 (5%)   | 20          | 52  |
| All | All   | 10100/10189 (99%) | 9989 (99%) | 111 (1%) | 63          | 87  |

All (111) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LA    | 45  | VAL  |
| 1   | LA    | 89  | TYR  |
| 1   | LA    | 136 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LA    | 143 | THR  |
| 1   | LA    | 175 | ILE  |
| 1   | LA    | 207 | VAL  |
| 2   | LB    | 101 | THR  |
| 8   | LE    | 149 | ILE  |
| 9   | LF    | 109 | LEU  |
| 11  | LH    | 57  | VAL  |
| 11  | LH    | 112 | VAL  |
| 11  | LH    | 126 | VAL  |
| 12  | LI    | 7   | ARG  |
| 13  | LJ    | 43  | LEU  |
| 13  | LJ    | 83  | LEU  |
| 14  | LL    | 59  | VAL  |
| 14  | LL    | 70  | VAL  |
| 14  | LL    | 124 | LEU  |
| 15  | LM    | 25  | VAL  |
| 15  | LM    | 38  | VAL  |
| 18  | LP    | 24  | VAL  |
| 19  | LQ    | 72  | LEU  |
| 19  | LQ    | 83  | VAL  |
| 20  | LR    | 137 | ILE  |
| 21  | LS    | 90  | THR  |
| 24  | LV    | 15  | ARG  |
| 24  | LV    | 65  | VAL  |
| 25  | LW    | 76  | VAL  |
| 26  | LX    | 97  | VAL  |
| 26  | LX    | 138 | VAL  |
| 27  | LY    | 55  | VAL  |
| 27  | LY    | 79  | VAL  |
| 28  | LZ    | 74  | VAL  |
| 28  | LZ    | 91  | LEU  |
| 28  | LZ    | 96  | VAL  |
| 29  | La    | 56  | VAL  |
| 32  | Ld    | 64  | ILE  |
| 32  | Ld    | 84  | ILE  |
| 33  | Le    | 13  | VAL  |
| 33  | Le    | 113 | GLU  |
| 34  | Lf    | 33  | VAL  |
| 45  | Lr    | 117 | ILE  |
| 51  | SF    | 41  | VAL  |
| 51  | SF    | 83  | ASN  |
| 54  | SK    | 15  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | SK    | 40  | VAL  |
| 58  | SR    | 117 | LEU  |
| 59  | SS    | 50  | ILE  |
| 61  | SU    | 40  | ILE  |
| 62  | SV    | 1   | MET  |
| 67  | Sg    | 46  | THR  |
| 70  | SJ    | 149 | VAL  |
| 73  | SO    | 129 | ILE  |
| 73  | SO    | 130 | GLU  |
| 73  | SO    | 131 | ASP  |
| 73  | SO    | 133 | THR  |
| 74  | SW    | 119 | LYS  |
| 81  | j     | 34  | MET  |
| 81  | j     | 43  | ASP  |
| 81  | j     | 50  | LYS  |
| 81  | j     | 51  | MET  |
| 81  | j     | 52  | LEU  |
| 81  | j     | 61  | ASN  |
| 81  | j     | 65  | ARG  |
| 81  | j     | 66  | VAL  |
| 81  | j     | 69  | LEU  |
| 81  | j     | 70  | SER  |
| 81  | j     | 71  | VAL  |
| 81  | j     | 79  | GLN  |
| 81  | j     | 80  | GLN  |
| 81  | j     | 81  | ARG  |
| 81  | j     | 82  | LEU  |
| 81  | j     | 83  | LYS  |
| 81  | j     | 84  | LEU  |
| 81  | j     | 99  | THR  |
| 81  | j     | 101 | VAL  |
| 81  | j     | 106 | LYS  |
| 81  | j     | 108 | LYS  |
| 81  | j     | 109 | LYS  |
| 81  | j     | 110 | VAL  |
| 81  | j     | 112 | ILE  |
| 81  | j     | 118 | LYS  |
| 81  | j     | 124 | LEU  |
| 81  | j     | 133 | THR  |
| 81  | j     | 136 | LEU  |
| 81  | j     | 137 | THR  |
| 81  | j     | 145 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | j     | 165 | THR  |
| 81  | j     | 166 | ARG  |
| 81  | j     | 167 | GLU  |
| 81  | j     | 171 | LYS  |
| 81  | j     | 173 | THR  |
| 81  | j     | 174 | VAL  |
| 81  | j     | 186 | SER  |
| 81  | j     | 212 | LEU  |
| 81  | j     | 233 | LYS  |
| 81  | j     | 245 | ARG  |
| 81  | j     | 249 | LYS  |
| 81  | j     | 251 | LEU  |
| 81  | j     | 253 | LEU  |
| 81  | j     | 261 | GLU  |
| 81  | j     | 265 | ASN  |
| 81  | j     | 270 | LEU  |
| 81  | j     | 271 | SER  |
| 81  | j     | 272 | THR  |
| 81  | j     | 273 | GLU  |
| 81  | j     | 275 | LEU  |
| 81  | j     | 289 | ARG  |
| 81  | j     | 300 | LYS  |
| 81  | j     | 346 | LEU  |
| 83  | NC    | 718 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LA    | 22  | HIS  |
| 1   | LA    | 38  | HIS  |
| 1   | LA    | 97  | ASN  |
| 1   | LA    | 215 | ASN  |
| 1   | LA    | 216 | HIS  |
| 2   | LB    | 138 | GLN  |
| 2   | LB    | 245 | HIS  |
| 2   | LB    | 315 | ASN  |
| 6   | LC    | 310 | HIS  |
| 7   | LD    | 63  | GLN  |
| 7   | LD    | 195 | HIS  |
| 7   | LD    | 229 | ASN  |
| 7   | LD    | 244 | HIS  |
| 7   | LD    | 250 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | LE    | 190 | HIS  |
| 8   | LE    | 191 | GLN  |
| 8   | LE    | 245 | GLN  |
| 8   | LE    | 268 | GLN  |
| 8   | LE    | 279 | ASN  |
| 9   | LF    | 63  | GLN  |
| 9   | LF    | 119 | ASN  |
| 10  | LG    | 46  | GLN  |
| 10  | LG    | 90  | GLN  |
| 10  | LG    | 206 | GLN  |
| 11  | LH    | 42  | ASN  |
| 11  | LH    | 106 | GLN  |
| 11  | LH    | 116 | ASN  |
| 11  | LH    | 140 | GLN  |
| 11  | LH    | 156 | ASN  |
| 12  | LI    | 14  | ASN  |
| 12  | LI    | 147 | HIS  |
| 13  | LJ    | 3   | GLN  |
| 13  | LJ    | 104 | ASN  |
| 14  | LL    | 6   | ASN  |
| 14  | LL    | 205 | GLN  |
| 15  | LM    | 20  | HIS  |
| 16  | LN    | 37  | HIS  |
| 16  | LN    | 139 | HIS  |
| 16  | LN    | 156 | HIS  |
| 17  | LO    | 42  | ASN  |
| 17  | LO    | 173 | GLN  |
| 17  | LO    | 180 | GLN  |
| 17  | LO    | 184 | ASN  |
| 17  | LO    | 199 | HIS  |
| 18  | LP    | 34  | GLN  |
| 18  | LP    | 97  | ASN  |
| 18  | LP    | 133 | HIS  |
| 19  | LQ    | 21  | GLN  |
| 19  | LQ    | 45  | GLN  |
| 20  | LR    | 7   | GLN  |
| 20  | LR    | 130 | ASN  |
| 21  | LS    | 37  | HIS  |
| 21  | LS    | 77  | ASN  |
| 22  | LT    | 114 | GLN  |
| 22  | LT    | 127 | GLN  |
| 23  | LU    | 50  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | LV    | 135 | ASN  |
| 25  | LW    | 79  | GLN  |
| 26  | LX    | 107 | HIS  |
| 27  | LY    | 4   | ASN  |
| 27  | LY    | 18  | HIS  |
| 27  | LY    | 96  | HIS  |
| 27  | LY    | 127 | GLN  |
| 28  | LZ    | 78  | ASN  |
| 28  | LZ    | 127 | ASN  |
| 29  | La    | 28  | HIS  |
| 29  | La    | 60  | HIS  |
| 29  | La    | 62  | HIS  |
| 29  | La    | 93  | ASN  |
| 30  | Lb    | 19  | ASN  |
| 30  | Lb    | 60  | ASN  |
| 31  | Lc    | 72  | HIS  |
| 32  | Ld    | 18  | ASN  |
| 32  | Ld    | 79  | ASN  |
| 32  | Ld    | 93  | ASN  |
| 32  | Ld    | 116 | ASN  |
| 33  | Le    | 43  | ASN  |
| 33  | Le    | 52  | GLN  |
| 33  | Le    | 102 | ASN  |
| 33  | Le    | 107 | ASN  |
| 34  | Lf    | 80  | ASN  |
| 34  | Lf    | 99  | HIS  |
| 35  | Lg    | 3   | GLN  |
| 35  | Lg    | 28  | ASN  |
| 35  | Lg    | 100 | GLN  |
| 36  | Lh    | 108 | GLN  |
| 37  | Li    | 12  | ASN  |
| 37  | Li    | 92  | ASN  |
| 43  | Lo    | 19  | GLN  |
| 43  | Lo    | 45  | GLN  |
| 43  | Lo    | 51  | GLN  |
| 43  | Lo    | 105 | GLN  |
| 44  | Lp    | 56  | HIS  |
| 45  | Lr    | 41  | ASN  |
| 45  | Lr    | 100 | ASN  |
| 47  | SA    | 50  | ASN  |
| 47  | SA    | 193 | HIS  |
| 48  | SB    | 101 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | SB    | 124 | HIS  |
| 48  | SB    | 179 | ASN  |
| 48  | SB    | 186 | ASN  |
| 48  | SB    | 208 | HIS  |
| 49  | SD    | 145 | GLN  |
| 50  | SE    | 112 | HIS  |
| 50  | SE    | 142 | HIS  |
| 50  | SE    | 157 | ASN  |
| 50  | SE    | 188 | ASN  |
| 50  | SE    | 197 | ASN  |
| 51  | SF    | 74  | ASN  |
| 51  | SF    | 83  | ASN  |
| 51  | SF    | 118 | ASN  |
| 52  | SH    | 91  | HIS  |
| 52  | SH    | 114 | GLN  |
| 53  | SI    | 52  | ASN  |
| 53  | SI    | 84  | ASN  |
| 53  | SI    | 165 | GLN  |
| 53  | SI    | 181 | GLN  |
| 54  | SK    | 7   | ASN  |
| 54  | SK    | 39  | ASN  |
| 54  | SK    | 50  | GLN  |
| 54  | SK    | 73  | ASN  |
| 55  | SL    | 11  | GLN  |
| 55  | SL    | 65  | ASN  |
| 56  | SP    | 41  | GLN  |
| 57  | SQ    | 35  | ASN  |
| 58  | SR    | 56  | HIS  |
| 59  | SS    | 101 | ASN  |
| 59  | SS    | 135 | HIS  |
| 65  | Sc    | 29  | GLN  |
| 66  | Sd    | 28  | HIS  |
| 67  | Sg    | 143 | GLN  |
| 67  | Sg    | 162 | ASN  |
| 67  | Sg    | 191 | HIS  |
| 67  | Sg    | 215 | GLN  |
| 67  | Sg    | 222 | ASN  |
| 67  | Sg    | 226 | HIS  |
| 68  | SC    | 115 | GLN  |
| 68  | SC    | 136 | HIS  |
| 69  | SG    | 59  | GLN  |
| 69  | SG    | 155 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 69  | SG    | 163 | ASN  |
| 69  | SG    | 202 | ASN  |
| 69  | SG    | 227 | GLN  |
| 70  | SJ    | 154 | GLN  |
| 71  | SM    | 28  | HIS  |
| 71  | SM    | 48  | HIS  |
| 71  | SM    | 119 | GLN  |
| 72  | SN    | 5   | HIS  |
| 72  | SN    | 49  | GLN  |
| 73  | SO    | 32  | HIS  |
| 73  | SO    | 83  | GLN  |
| 74  | SW    | 98  | GLN  |
| 77  | Sb    | 19  | HIS  |
| 78  | Se    | 58  | ASN  |
| 81  | j     | 79  | GLN  |
| 81  | j     | 80  | GLN  |
| 81  | j     | 121 | ASN  |
| 81  | j     | 211 | GLN  |
| 81  | j     | 265 | ASN  |
| 81  | j     | 420 | GLN  |
| 83  | NC    | 726 | ASN  |
| 83  | NC    | 728 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 3   | L5    | 3486/3510 (99%) | 799 (22%)         | 14 (0%)         |
| 4   | L7    | 119/120 (99%)   | 19 (15%)          | 0               |
| 46  | S2    | 1577/1590 (99%) | 326 (20%)         | 10 (0%)         |
| 5   | L8    | 154/155 (99%)   | 27 (17%)          | 1 (0%)          |
| 80  | Bv    | 73/76 (96%)     | 41 (56%)          | 0               |
| 82  | k     | 12/13 (92%)     | 7 (58%)           | 0               |
| All | All   | 5421/5464 (99%) | 1219 (22%)        | 25 (0%)         |

All (1219) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 8   | U    |
| 3   | L5    | 12  | A    |
| 3   | L5    | 13  | U    |
| 3   | L5    | 17  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 21  | G    |
| 3   | L5    | 25  | A    |
| 3   | L5    | 30  | C    |
| 3   | L5    | 39  | A    |
| 3   | L5    | 42  | A    |
| 3   | L5    | 44  | A    |
| 3   | L5    | 56  | A    |
| 3   | L5    | 58  | G    |
| 3   | L5    | 59  | A    |
| 3   | L5    | 64  | A    |
| 3   | L5    | 65  | A    |
| 3   | L5    | 66  | A    |
| 3   | L5    | 72  | C    |
| 3   | L5    | 74  | G    |
| 3   | L5    | 75  | G    |
| 3   | L5    | 91  | G    |
| 3   | L5    | 95  | G    |
| 3   | L5    | 98  | A    |
| 3   | L5    | 104 | G    |
| 3   | L5    | 108 | A    |
| 3   | L5    | 109 | G    |
| 3   | L5    | 110 | C    |
| 3   | L5    | 117 | C    |
| 3   | L5    | 119 | G    |
| 3   | L5    | 120 | A    |
| 3   | L5    | 121 | A    |
| 3   | L5    | 147 | U    |
| 3   | L5    | 149 | U    |
| 3   | L5    | 156 | C    |
| 3   | L5    | 162 | A    |
| 3   | L5    | 168 | U    |
| 3   | L5    | 169 | C    |
| 3   | L5    | 197 | U    |
| 3   | L5    | 206 | U    |
| 3   | L5    | 207 | C    |
| 3   | L5    | 222 | G    |
| 3   | L5    | 229 | G    |
| 3   | L5    | 230 | U    |
| 3   | L5    | 231 | G    |
| 3   | L5    | 250 | G    |
| 3   | L5    | 254 | G    |
| 3   | L5    | 269 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 271 | G    |
| 3   | L5    | 288 | U    |
| 3   | L5    | 297 | A    |
| 3   | L5    | 306 | G    |
| 3   | L5    | 307 | U    |
| 3   | L5    | 331 | C    |
| 3   | L5    | 332 | G    |
| 3   | L5    | 344 | A    |
| 3   | L5    | 351 | A    |
| 3   | L5    | 354 | A    |
| 3   | L5    | 376 | A    |
| 3   | L5    | 378 | G    |
| 3   | L5    | 379 | A    |
| 3   | L5    | 390 | G    |
| 3   | L5    | 392 | G    |
| 3   | L5    | 398 | A    |
| 3   | L5    | 400 | G    |
| 3   | L5    | 401 | A    |
| 3   | L5    | 403 | G    |
| 3   | L5    | 404 | G    |
| 3   | L5    | 405 | C    |
| 3   | L5    | 422 | G    |
| 3   | L5    | 423 | U    |
| 3   | L5    | 440 | C    |
| 3   | L5    | 441 | G    |
| 3   | L5    | 442 | C    |
| 3   | L5    | 443 | A    |
| 3   | L5    | 444 | G    |
| 3   | L5    | 445 | U    |
| 3   | L5    | 452 | G    |
| 3   | L5    | 458 | U    |
| 3   | L5    | 459 | U    |
| 3   | L5    | 474 | G    |
| 3   | L5    | 476 | C    |
| 3   | L5    | 498 | G    |
| 3   | L5    | 501 | U    |
| 3   | L5    | 661 | G    |
| 3   | L5    | 664 | C    |
| 3   | L5    | 665 | G    |
| 3   | L5    | 676 | C    |
| 3   | L5    | 677 | A    |
| 3   | L5    | 678 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 681 | C    |
| 3   | L5    | 687 | C    |
| 3   | L5    | 688 | G    |
| 3   | L5    | 694 | G    |
| 3   | L5    | 695 | C    |
| 3   | L5    | 699 | G    |
| 3   | L5    | 721 | G    |
| 3   | L5    | 722 | G    |
| 3   | L5    | 729 | C    |
| 3   | L5    | 730 | G    |
| 3   | L5    | 731 | G    |
| 3   | L5    | 733 | G    |
| 3   | L5    | 737 | A    |
| 3   | L5    | 740 | G    |
| 3   | L5    | 744 | C    |
| 3   | L5    | 745 | U    |
| 3   | L5    | 748 | G    |
| 3   | L5    | 899 | G    |
| 3   | L5    | 901 | U    |
| 3   | L5    | 902 | A    |
| 3   | L5    | 904 | A    |
| 3   | L5    | 905 | G    |
| 3   | L5    | 910 | C    |
| 3   | L5    | 911 | C    |
| 3   | L5    | 913 | G    |
| 3   | L5    | 919 | A    |
| 3   | L5    | 920 | G    |
| 3   | L5    | 921 | C    |
| 3   | L5    | 922 | A    |
| 3   | L5    | 923 | C    |
| 3   | L5    | 930 | A    |
| 3   | L5    | 932 | U    |
| 3   | L5    | 946 | G    |
| 3   | L5    | 947 | A    |
| 3   | L5    | 948 | G    |
| 3   | L5    | 949 | C    |
| 3   | L5    | 950 | G    |
| 3   | L5    | 951 | A    |
| 3   | L5    | 952 | G    |
| 3   | L5    | 953 | A    |
| 3   | L5    | 957 | G    |
| 3   | L5    | 958 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 959  | C    |
| 3   | L5    | 1057 | G    |
| 3   | L5    | 1059 | C    |
| 3   | L5    | 1061 | G    |
| 3   | L5    | 1062 | G    |
| 3   | L5    | 1083 | C    |
| 3   | L5    | 1157 | G    |
| 3   | L5    | 1162 | A    |
| 3   | L5    | 1167 | U    |
| 3   | L5    | 1168 | C    |
| 3   | L5    | 1169 | C    |
| 3   | L5    | 1170 | C    |
| 3   | L5    | 1189 | C    |
| 3   | L5    | 1190 | G    |
| 3   | L5    | 1197 | C    |
| 3   | L5    | 1198 | G    |
| 3   | L5    | 1202 | C    |
| 3   | L5    | 1203 | C    |
| 3   | L5    | 1204 | G    |
| 3   | L5    | 1206 | G    |
| 3   | L5    | 1228 | C    |
| 3   | L5    | 1249 | G    |
| 3   | L5    | 1253 | G    |
| 3   | L5    | 1259 | C    |
| 3   | L5    | 1260 | G    |
| 3   | L5    | 1264 | G    |
| 3   | L5    | 1266 | A    |
| 3   | L5    | 1267 | C    |
| 3   | L5    | 1271 | G    |
| 3   | L5    | 1272 | U    |
| 3   | L5    | 1274 | G    |
| 3   | L5    | 1280 | G    |
| 3   | L5    | 1281 | A    |
| 3   | L5    | 1282 | C    |
| 3   | L5    | 1283 | G    |
| 3   | L5    | 1288 | C    |
| 3   | L5    | 1289 | U    |
| 3   | L5    | 1290 | A    |
| 3   | L5    | 1301 | C    |
| 3   | L5    | 1303 | OMG  |
| 3   | L5    | 1311 | A    |
| 3   | L5    | 1313 | A2M  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1314 | C    |
| 3   | L5    | 1315 | G    |
| 3   | L5    | 1324 | A    |
| 3   | L5    | 1341 | A    |
| 3   | L5    | 1345 | G    |
| 3   | L5    | 1346 | G    |
| 3   | L5    | 1347 | G    |
| 3   | L5    | 1352 | C    |
| 3   | L5    | 1357 | G    |
| 3   | L5    | 1364 | G    |
| 3   | L5    | 1365 | C    |
| 3   | L5    | 1366 | C    |
| 3   | L5    | 1367 | G    |
| 3   | L5    | 1374 | A    |
| 3   | L5    | 1380 | G    |
| 3   | L5    | 1381 | G    |
| 3   | L5    | 1384 | A    |
| 3   | L5    | 1385 | A    |
| 3   | L5    | 1386 | G    |
| 3   | L5    | 1389 | C    |
| 3   | L5    | 1404 | C    |
| 3   | L5    | 1407 | A    |
| 3   | L5    | 1412 | G    |
| 3   | L5    | 1422 | G    |
| 3   | L5    | 1424 | C    |
| 3   | L5    | 1426 | C    |
| 3   | L5    | 1428 | C    |
| 3   | L5    | 1430 | A    |
| 3   | L5    | 1431 | G    |
| 3   | L5    | 1432 | U    |
| 3   | L5    | 1444 | G    |
| 3   | L5    | 1445 | C    |
| 3   | L5    | 1469 | G    |
| 3   | L5    | 1470 | C    |
| 3   | L5    | 1480 | G    |
| 3   | L5    | 1484 | A    |
| 3   | L5    | 1485 | G    |
| 3   | L5    | 1489 | G    |
| 3   | L5    | 1493 | G    |
| 3   | L5    | 1505 | A    |
| 3   | L5    | 1514 | A    |
| 3   | L5    | 1521 | A2M  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1534 | A    |
| 3   | L5    | 1536 | G    |
| 3   | L5    | 1550 | A    |
| 3   | L5    | 1551 | A    |
| 3   | L5    | 1553 | C    |
| 3   | L5    | 1565 | U    |
| 3   | L5    | 1578 | U    |
| 3   | L5    | 1583 | U    |
| 3   | L5    | 1611 | G    |
| 3   | L5    | 1612 | OMG  |
| 3   | L5    | 1618 | A    |
| 3   | L5    | 1620 | G    |
| 3   | L5    | 1621 | A    |
| 3   | L5    | 1625 | A    |
| 3   | L5    | 1627 | C    |
| 3   | L5    | 1629 | A    |
| 3   | L5    | 1637 | A    |
| 3   | L5    | 1641 | G    |
| 3   | L5    | 1643 | U    |
| 3   | L5    | 1648 | C    |
| 3   | L5    | 1650 | C    |
| 3   | L5    | 1663 | C    |
| 3   | L5    | 1664 | PSU  |
| 3   | L5    | 1666 | A    |
| 3   | L5    | 1668 | G    |
| 3   | L5    | 1684 | G    |
| 3   | L5    | 1686 | A    |
| 3   | L5    | 1687 | G    |
| 3   | L5    | 1690 | C    |
| 3   | L5    | 1691 | C    |
| 3   | L5    | 1692 | G    |
| 3   | L5    | 1694 | C    |
| 3   | L5    | 1707 | C    |
| 3   | L5    | 1713 | U    |
| 3   | L5    | 1716 | A    |
| 3   | L5    | 1718 | C    |
| 3   | L5    | 1721 | G    |
| 3   | L5    | 1727 | C    |
| 3   | L5    | 1729 | A    |
| 3   | L5    | 1737 | G    |
| 3   | L5    | 1744 | U    |
| 3   | L5    | 1762 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1774 | A    |
| 3   | L5    | 1784 | G    |
| 3   | L5    | 1791 | A    |
| 3   | L5    | 1792 | A    |
| 3   | L5    | 1797 | G    |
| 3   | L5    | 1802 | G    |
| 3   | L5    | 1808 | G    |
| 3   | L5    | 1809 | U    |
| 3   | L5    | 1823 | G    |
| 3   | L5    | 1824 | A    |
| 3   | L5    | 1829 | G    |
| 3   | L5    | 1842 | G    |
| 3   | L5    | 1854 | A    |
| 3   | L5    | 1856 | G    |
| 3   | L5    | 1865 | G    |
| 3   | L5    | 1869 | U    |
| 3   | L5    | 1870 | G    |
| 3   | L5    | 1876 | U    |
| 3   | L5    | 1879 | A    |
| 3   | L5    | 1884 | A    |
| 3   | L5    | 1887 | C    |
| 3   | L5    | 1903 | G    |
| 3   | L5    | 1905 | U    |
| 3   | L5    | 1906 | G    |
| 3   | L5    | 1907 | C    |
| 3   | L5    | 1908 | C    |
| 3   | L5    | 1909 | G    |
| 3   | L5    | 1912 | G    |
| 3   | L5    | 1918 | C    |
| 3   | L5    | 1919 | A    |
| 3   | L5    | 1922 | C    |
| 3   | L5    | 1923 | C    |
| 3   | L5    | 1934 | U    |
| 3   | L5    | 1935 | G    |
| 3   | L5    | 1938 | G    |
| 3   | L5    | 1946 | U    |
| 3   | L5    | 1947 | A    |
| 3   | L5    | 1948 | G    |
| 3   | L5    | 1949 | A    |
| 3   | L5    | 1953 | C    |
| 3   | L5    | 1954 | A    |
| 3   | L5    | 1957 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1958 | C    |
| 3   | L5    | 1961 | U    |
| 3   | L5    | 1962 | G    |
| 3   | L5    | 1963 | G    |
| 3   | L5    | 1964 | C    |
| 3   | L5    | 1965 | C    |
| 3   | L5    | 1966 | A    |
| 3   | L5    | 1967 | U    |
| 3   | L5    | 1968 | G    |
| 3   | L5    | 1969 | G    |
| 3   | L5    | 1970 | A    |
| 3   | L5    | 1971 | A    |
| 3   | L5    | 1972 | G    |
| 3   | L5    | 1974 | C    |
| 3   | L5    | 1976 | G    |
| 3   | L5    | 1977 | A    |
| 3   | L5    | 1978 | A    |
| 3   | L5    | 1979 | U    |
| 3   | L5    | 1980 | C    |
| 3   | L5    | 1982 | G    |
| 3   | L5    | 1983 | C    |
| 3   | L5    | 1985 | A    |
| 3   | L5    | 1986 | A    |
| 3   | L5    | 1987 | G    |
| 3   | L5    | 1988 | G    |
| 3   | L5    | 1989 | A    |
| 3   | L5    | 1990 | G    |
| 3   | L5    | 1991 | U    |
| 3   | L5    | 1992 | G    |
| 3   | L5    | 1993 | U    |
| 3   | L5    | 1994 | G    |
| 3   | L5    | 1996 | A    |
| 3   | L5    | 1998 | C    |
| 3   | L5    | 1999 | A    |
| 3   | L5    | 2000 | A    |
| 3   | L5    | 2001 | C    |
| 3   | L5    | 2002 | U    |
| 3   | L5    | 2005 | C    |
| 3   | L5    | 2007 | U    |
| 3   | L5    | 2009 | C    |
| 3   | L5    | 2011 | G    |
| 3   | L5    | 2012 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2013 | A    |
| 3   | L5    | 2020 | A    |
| 3   | L5    | 2027 | A    |
| 3   | L5    | 2031 | U    |
| 3   | L5    | 2032 | G    |
| 3   | L5    | 2033 | G    |
| 3   | L5    | 2035 | U    |
| 3   | L5    | 2036 | G    |
| 3   | L5    | 2042 | G    |
| 3   | L5    | 2043 | G    |
| 3   | L5    | 2056 | A    |
| 3   | L5    | 2058 | A    |
| 3   | L5    | 2071 | C    |
| 3   | L5    | 2072 | G    |
| 3   | L5    | 2076 | G    |
| 3   | L5    | 2077 | U    |
| 3   | L5    | 2079 | G    |
| 3   | L5    | 2080 | A    |
| 3   | L5    | 2081 | G    |
| 3   | L5    | 2082 | A    |
| 3   | L5    | 2083 | G    |
| 3   | L5    | 2084 | U    |
| 3   | L5    | 2085 | G    |
| 3   | L5    | 2088 | C    |
| 3   | L5    | 2089 | G    |
| 3   | L5    | 2093 | G    |
| 3   | L5    | 2095 | G    |
| 3   | L5    | 2097 | C    |
| 3   | L5    | 2099 | G    |
| 3   | L5    | 2239 | G    |
| 3   | L5    | 2240 | A    |
| 3   | L5    | 2242 | C    |
| 3   | L5    | 2243 | C    |
| 3   | L5    | 2245 | C    |
| 3   | L5    | 2246 | G    |
| 3   | L5    | 2253 | C    |
| 3   | L5    | 2255 | A    |
| 3   | L5    | 2276 | C    |
| 3   | L5    | 2281 | G    |
| 3   | L5    | 2284 | G    |
| 3   | L5    | 2287 | A    |
| 3   | L5    | 2288 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2292 | U    |
| 3   | L5    | 2293 | G    |
| 3   | L5    | 2300 | A    |
| 3   | L5    | 2318 | G    |
| 3   | L5    | 2320 | G    |
| 3   | L5    | 2324 | C    |
| 3   | L5    | 2329 | G    |
| 3   | L5    | 2333 | C    |
| 3   | L5    | 2335 | G    |
| 3   | L5    | 2338 | OMC  |
| 3   | L5    | 2344 | G    |
| 3   | L5    | 2347 | A    |
| 3   | L5    | 2351 | OMG  |
| 3   | L5    | 2369 | A    |
| 3   | L5    | 2376 | A    |
| 3   | L5    | 2382 | A    |
| 3   | L5    | 2383 | A    |
| 3   | L5    | 2384 | G    |
| 3   | L5    | 2389 | G    |
| 3   | L5    | 2397 | C    |
| 3   | L5    | 2403 | G    |
| 3   | L5    | 2404 | A    |
| 3   | L5    | 2405 | A    |
| 3   | L5    | 2408 | G    |
| 3   | L5    | 2409 | OMC  |
| 3   | L5    | 2412 | U    |
| 3   | L5    | 2424 | C    |
| 3   | L5    | 2428 | C    |
| 3   | L5    | 2434 | U    |
| 3   | L5    | 2437 | G    |
| 3   | L5    | 2440 | A    |
| 3   | L5    | 2451 | C    |
| 3   | L5    | 2452 | C    |
| 3   | L5    | 2461 | G    |
| 3   | L5    | 2462 | G    |
| 3   | L5    | 2465 | C    |
| 3   | L5    | 2470 | G    |
| 3   | L5    | 2471 | A    |
| 3   | L5    | 2472 | U    |
| 3   | L5    | 2474 | G    |
| 3   | L5    | 2475 | C    |
| 3   | L5    | 2476 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2477 | U    |
| 3   | L5    | 2478 | C    |
| 3   | L5    | 2480 | G    |
| 3   | L5    | 2489 | G    |
| 3   | L5    | 2490 | G    |
| 3   | L5    | 2491 | C    |
| 3   | L5    | 2492 | C    |
| 3   | L5    | 2493 | G    |
| 3   | L5    | 2498 | A    |
| 3   | L5    | 2500 | A    |
| 3   | L5    | 2506 | U    |
| 3   | L5    | 2507 | C    |
| 3   | L5    | 2516 | A    |
| 3   | L5    | 2520 | C    |
| 3   | L5    | 2524 | A    |
| 3   | L5    | 2531 | G    |
| 3   | L5    | 2533 | G    |
| 3   | L5    | 2534 | G    |
| 3   | L5    | 2541 | U    |
| 3   | L5    | 2543 | G    |
| 3   | L5    | 2551 | G    |
| 3   | L5    | 2552 | A    |
| 3   | L5    | 2553 | G    |
| 3   | L5    | 2560 | A    |
| 3   | L5    | 2564 | C    |
| 3   | L5    | 2567 | U    |
| 3   | L5    | 2570 | C    |
| 3   | L5    | 2574 | A    |
| 3   | L5    | 2576 | C    |
| 3   | L5    | 2588 | A    |
| 3   | L5    | 2605 | G    |
| 3   | L5    | 2614 | C    |
| 3   | L5    | 2625 | G    |
| 3   | L5    | 2639 | G    |
| 3   | L5    | 2640 | C    |
| 3   | L5    | 2646 | A    |
| 3   | L5    | 2649 | G    |
| 3   | L5    | 2656 | C    |
| 3   | L5    | 2657 | C    |
| 3   | L5    | 2660 | G    |
| 3   | L5    | 2663 | A    |
| 3   | L5    | 2674 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2681 | G    |
| 3   | L5    | 2682 | A    |
| 3   | L5    | 2683 | A    |
| 3   | L5    | 2684 | A    |
| 3   | L5    | 2694 | U    |
| 3   | L5    | 2697 | C    |
| 3   | L5    | 2698 | G    |
| 3   | L5    | 2699 | G    |
| 3   | L5    | 2708 | G    |
| 3   | L5    | 2711 | G    |
| 3   | L5    | 2713 | G    |
| 3   | L5    | 2726 | C    |
| 3   | L5    | 2729 | G    |
| 3   | L5    | 2730 | A    |
| 3   | L5    | 2733 | A    |
| 3   | L5    | 2741 | G    |
| 3   | L5    | 2743 | G    |
| 3   | L5    | 2747 | G    |
| 3   | L5    | 2748 | U    |
| 3   | L5    | 2750 | U    |
| 3   | L5    | 2756 | U    |
| 3   | L5    | 2757 | C    |
| 3   | L5    | 2775 | U    |
| 3   | L5    | 2776 | A    |
| 3   | L5    | 2777 | U    |
| 3   | L5    | 2786 | G    |
| 3   | L5    | 2801 | C    |
| 3   | L5    | 2802 | A2M  |
| 3   | L5    | 2813 | U    |
| 3   | L5    | 2814 | G    |
| 3   | L5    | 2815 | U    |
| 3   | L5    | 2816 | U    |
| 3   | L5    | 2825 | G    |
| 3   | L5    | 2829 | G    |
| 3   | L5    | 2837 | A    |
| 3   | L5    | 2842 | G    |
| 3   | L5    | 2843 | C    |
| 3   | L5    | 2854 | C    |
| 3   | L5    | 2862 | C    |
| 3   | L5    | 2864 | G    |
| 3   | L5    | 2879 | C    |
| 3   | L5    | 2881 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2884 | G    |
| 3   | L5    | 2889 | G    |
| 3   | L5    | 2890 | G    |
| 3   | L5    | 2891 | U    |
| 3   | L5    | 2892 | C    |
| 3   | L5    | 2893 | G    |
| 3   | L5    | 2894 | G    |
| 3   | L5    | 2895 | U    |
| 3   | L5    | 2897 | G    |
| 3   | L5    | 3564 | G    |
| 3   | L5    | 3565 | G    |
| 3   | L5    | 3566 | C    |
| 3   | L5    | 3567 | C    |
| 3   | L5    | 3570 | C    |
| 3   | L5    | 3571 | G    |
| 3   | L5    | 3574 | U    |
| 3   | L5    | 3575 | A    |
| 3   | L5    | 3576 | G    |
| 3   | L5    | 3583 | A    |
| 3   | L5    | 3584 | C    |
| 3   | L5    | 3594 | G    |
| 3   | L5    | 3595 | U    |
| 3   | L5    | 3597 | C    |
| 3   | L5    | 3605 | G    |
| 3   | L5    | 3609 | A    |
| 3   | L5    | 3614 | A    |
| 3   | L5    | 3623 | U    |
| 3   | L5    | 3625 | A    |
| 3   | L5    | 3627 | A    |
| 3   | L5    | 3641 | A    |
| 3   | L5    | 3643 | G    |
| 3   | L5    | 3652 | C    |
| 3   | L5    | 3653 | G    |
| 3   | L5    | 3670 | G    |
| 3   | L5    | 3689 | G    |
| 3   | L5    | 3690 | A    |
| 3   | L5    | 3691 | A    |
| 3   | L5    | 3692 | U    |
| 3   | L5    | 3693 | G    |
| 3   | L5    | 3706 | A    |
| 3   | L5    | 3708 | U    |
| 3   | L5    | 3714 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 3715 | A    |
| 3   | L5    | 3727 | A    |
| 3   | L5    | 3729 | G    |
| 3   | L5    | 3732 | G    |
| 3   | L5    | 3745 | A    |
| 3   | L5    | 3750 | C    |
| 3   | L5    | 3755 | G    |
| 3   | L5    | 3756 | G    |
| 3   | L5    | 3764 | A2M  |
| 3   | L5    | 3765 | U    |
| 3   | L5    | 3767 | C    |
| 3   | L5    | 3780 | U    |
| 3   | L5    | 3781 | U    |
| 3   | L5    | 3790 | G    |
| 3   | L5    | 3791 | C    |
| 3   | L5    | 3793 | U    |
| 3   | L5    | 3796 | A    |
| 3   | L5    | 3797 | UY1  |
| 3   | L5    | 3798 | G    |
| 3   | L5    | 3803 | A    |
| 3   | L5    | 3817 | U    |
| 3   | L5    | 3819 | U    |
| 3   | L5    | 3846 | A2M  |
| 3   | L5    | 3855 | A    |
| 3   | L5    | 3856 | A    |
| 3   | L5    | 3857 | C    |
| 3   | L5    | 3858 | G    |
| 3   | L5    | 3861 | C    |
| 3   | L5    | 3864 | G    |
| 3   | L5    | 3869 | A    |
| 3   | L5    | 3876 | G    |
| 3   | L5    | 3880 | A    |
| 3   | L5    | 3881 | A    |
| 3   | L5    | 3885 | A    |
| 3   | L5    | 3886 | G    |
| 3   | L5    | 3887 | A    |
| 3   | L5    | 3894 | U    |
| 3   | L5    | 3895 | G    |
| 3   | L5    | 3899 | PSU  |
| 3   | L5    | 3901 | G    |
| 3   | L5    | 3905 | C    |
| 3   | L5    | 3917 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 3918 | G    |
| 3   | L5    | 3921 | A    |
| 3   | L5    | 3922 | A    |
| 3   | L5    | 3923 | G    |
| 3   | L5    | 3926 | A    |
| 3   | L5    | 3927 | C    |
| 3   | L5    | 4051 | A    |
| 3   | L5    | 4054 | G    |
| 3   | L5    | 4064 | G    |
| 3   | L5    | 4075 | G    |
| 3   | L5    | 4076 | A    |
| 3   | L5    | 4087 | C    |
| 3   | L5    | 4089 | C    |
| 3   | L5    | 4090 | U    |
| 3   | L5    | 4091 | C    |
| 3   | L5    | 4092 | G    |
| 3   | L5    | 4093 | C    |
| 3   | L5    | 4094 | U    |
| 3   | L5    | 4096 | C    |
| 3   | L5    | 4098 | G    |
| 3   | L5    | 4099 | G    |
| 3   | L5    | 4104 | A    |
| 3   | L5    | 4110 | C    |
| 3   | L5    | 4114 | C    |
| 3   | L5    | 4120 | G    |
| 3   | L5    | 4132 | C    |
| 3   | L5    | 4133 | U    |
| 3   | L5    | 4136 | G    |
| 3   | L5    | 4138 | G    |
| 3   | L5    | 4140 | A    |
| 3   | L5    | 4153 | G    |
| 3   | L5    | 4154 | G    |
| 3   | L5    | 4161 | G    |
| 3   | L5    | 4173 | A    |
| 3   | L5    | 4182 | A    |
| 3   | L5    | 4192 | G    |
| 3   | L5    | 4193 | C    |
| 3   | L5    | 4195 | G    |
| 3   | L5    | 4199 | U    |
| 3   | L5    | 4203 | A    |
| 3   | L5    | 4207 | C    |
| 3   | L5    | 4212 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4219 | G    |
| 3   | L5    | 4221 | A    |
| 3   | L5    | 4224 | G    |
| 3   | L5    | 4227 | A    |
| 3   | L5    | 4228 | C    |
| 3   | L5    | 4235 | U    |
| 3   | L5    | 4236 | G    |
| 3   | L5    | 4238 | A    |
| 3   | L5    | 4243 | A    |
| 3   | L5    | 4250 | A    |
| 3   | L5    | 4251 | A    |
| 3   | L5    | 4256 | C    |
| 3   | L5    | 4261 | G    |
| 3   | L5    | 4263 | PSU  |
| 3   | L5    | 4265 | U    |
| 3   | L5    | 4274 | A    |
| 3   | L5    | 4275 | G    |
| 3   | L5    | 4276 | OMU  |
| 3   | L5    | 4284 | C    |
| 3   | L5    | 4289 | C    |
| 3   | L5    | 4296 | G    |
| 3   | L5    | 4299 | G    |
| 3   | L5    | 4300 | G    |
| 3   | L5    | 4302 | C    |
| 3   | L5    | 4309 | A    |
| 3   | L5    | 4319 | C    |
| 3   | L5    | 4320 | C    |
| 3   | L5    | 4324 | U    |
| 3   | L5    | 4334 | G    |
| 3   | L5    | 4343 | G    |
| 3   | L5    | 4346 | A    |
| 3   | L5    | 4347 | G    |
| 3   | L5    | 4348 | A    |
| 3   | L5    | 4349 | A    |
| 3   | L5    | 4350 | A    |
| 3   | L5    | 4351 | A    |
| 3   | L5    | 4357 | C    |
| 3   | L5    | 4361 | G    |
| 3   | L5    | 4364 | A    |
| 3   | L5    | 4375 | G    |
| 3   | L5    | 4390 | PSU  |
| 3   | L5    | 4392 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4394 | A    |
| 3   | L5    | 4396 | C    |
| 3   | L5    | 4397 | G    |
| 3   | L5    | 4400 | G    |
| 3   | L5    | 4407 | U    |
| 3   | L5    | 4411 | A    |
| 3   | L5    | 4414 | C    |
| 3   | L5    | 4418 | G    |
| 3   | L5    | 4419 | A    |
| 3   | L5    | 4420 | U    |
| 3   | L5    | 4422 | U    |
| 3   | L5    | 4433 | U    |
| 3   | L5    | 4434 | A    |
| 3   | L5    | 4435 | U    |
| 3   | L5    | 4436 | C    |
| 3   | L5    | 4445 | G    |
| 3   | L5    | 4470 | PSU  |
| 3   | L5    | 4482 | U    |
| 3   | L5    | 4483 | A    |
| 3   | L5    | 4485 | G    |
| 3   | L5    | 4488 | A    |
| 3   | L5    | 4489 | C    |
| 3   | L5    | 4490 | G    |
| 3   | L5    | 4494 | G    |
| 3   | L5    | 4515 | G    |
| 3   | L5    | 4518 | A    |
| 3   | L5    | 4519 | G    |
| 3   | L5    | 4524 | G    |
| 3   | L5    | 4530 | C    |
| 3   | L5    | 4537 | G    |
| 3   | L5    | 4543 | G    |
| 3   | L5    | 4545 | G    |
| 3   | L5    | 4559 | A    |
| 3   | L5    | 4560 | A    |
| 3   | L5    | 4570 | G    |
| 3   | L5    | 4571 | U    |
| 3   | L5    | 4587 | G    |
| 3   | L5    | 4605 | A    |
| 3   | L5    | 4606 | PSU  |
| 3   | L5    | 4607 | OMG  |
| 3   | L5    | 4617 | G    |
| 3   | L5    | 4626 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4627 | U    |
| 3   | L5    | 4638 | U    |
| 3   | L5    | 4640 | C    |
| 3   | L5    | 4649 | G    |
| 3   | L5    | 4654 | A    |
| 3   | L5    | 4657 | A    |
| 3   | L5    | 4663 | C    |
| 3   | L5    | 4664 | G    |
| 3   | L5    | 4665 | C    |
| 3   | L5    | 4677 | A    |
| 3   | L5    | 4678 | A    |
| 3   | L5    | 4679 | U    |
| 3   | L5    | 4698 | U    |
| 3   | L5    | 4709 | G    |
| 3   | L5    | 4710 | C    |
| 3   | L5    | 4711 | G    |
| 3   | L5    | 4714 | G    |
| 3   | L5    | 4719 | G    |
| 3   | L5    | 4723 | G    |
| 3   | L5    | 4726 | C    |
| 3   | L5    | 4728 | C    |
| 3   | L5    | 4730 | G    |
| 3   | L5    | 4733 | A    |
| 3   | L5    | 4734 | G    |
| 3   | L5    | 4832 | G    |
| 3   | L5    | 4835 | G    |
| 3   | L5    | 4836 | C    |
| 3   | L5    | 4838 | G    |
| 3   | L5    | 4840 | G    |
| 3   | L5    | 4847 | U    |
| 3   | L5    | 4848 | C    |
| 3   | L5    | 4853 | U    |
| 3   | L5    | 4854 | G    |
| 3   | L5    | 4860 | C    |
| 3   | L5    | 4861 | G    |
| 3   | L5    | 4864 | G    |
| 3   | L5    | 4865 | C    |
| 3   | L5    | 4866 | G    |
| 3   | L5    | 4875 | G    |
| 3   | L5    | 4877 | G    |
| 3   | L5    | 4879 | C    |
| 3   | L5    | 4888 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4893 | C    |
| 3   | L5    | 4896 | G    |
| 3   | L5    | 4899 | A    |
| 3   | L5    | 4902 | C    |
| 3   | L5    | 4903 | A    |
| 3   | L5    | 4906 | G    |
| 3   | L5    | 4908 | A    |
| 3   | L5    | 4912 | U    |
| 3   | L5    | 4915 | U    |
| 3   | L5    | 4916 | G    |
| 3   | L5    | 4925 | G    |
| 3   | L5    | 4926 | G    |
| 3   | L5    | 4928 | G    |
| 3   | L5    | 4931 | A    |
| 3   | L5    | 4932 | A    |
| 3   | L5    | 4940 | G    |
| 3   | L5    | 4941 | U    |
| 3   | L5    | 4950 | U    |
| 3   | L5    | 4953 | U    |
| 3   | L5    | 4954 | U    |
| 3   | L5    | 4956 | U    |
| 3   | L5    | 4979 | A    |
| 3   | L5    | 4982 | G    |
| 3   | L5    | 4985 | G    |
| 3   | L5    | 4987 | U    |
| 3   | L5    | 4988 | C    |
| 3   | L5    | 4989 | C    |
| 3   | L5    | 4990 | C    |
| 3   | L5    | 4994 | C    |
| 3   | L5    | 4996 | G    |
| 3   | L5    | 4999 | A    |
| 3   | L5    | 5005 | U    |
| 3   | L5    | 5006 | G    |
| 3   | L5    | 5015 | C    |
| 3   | L5    | 5019 | C    |
| 3   | L5    | 5020 | G    |
| 3   | L5    | 5023 | A    |
| 3   | L5    | 5026 | A    |
| 3   | L5    | 5034 | U    |
| 4   | L7    | 10   | C    |
| 4   | L7    | 13   | A    |
| 4   | L7    | 22   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L7    | 25  | G    |
| 4   | L7    | 33  | U    |
| 4   | L7    | 38  | U    |
| 4   | L7    | 42  | A    |
| 4   | L7    | 43  | U    |
| 4   | L7    | 49  | A    |
| 4   | L7    | 50  | A    |
| 4   | L7    | 53  | U    |
| 4   | L7    | 54  | A    |
| 4   | L7    | 64  | G    |
| 4   | L7    | 76  | U    |
| 4   | L7    | 97  | G    |
| 4   | L7    | 98  | G    |
| 4   | L7    | 100 | A    |
| 4   | L7    | 110 | G    |
| 4   | L7    | 111 | C    |
| 5   | L8    | 25  | G    |
| 5   | L8    | 34  | U    |
| 5   | L8    | 35  | C    |
| 5   | L8    | 48  | A    |
| 5   | L8    | 52  | A    |
| 5   | L8    | 59  | A    |
| 5   | L8    | 62  | A    |
| 5   | L8    | 63  | U    |
| 5   | L8    | 82  | A    |
| 5   | L8    | 84  | A    |
| 5   | L8    | 85  | U    |
| 5   | L8    | 86  | U    |
| 5   | L8    | 97  | A    |
| 5   | L8    | 103 | A    |
| 5   | L8    | 104 | A    |
| 5   | L8    | 105 | C    |
| 5   | L8    | 110 | U    |
| 5   | L8    | 111 | U    |
| 5   | L8    | 112 | G    |
| 5   | L8    | 114 | G    |
| 5   | L8    | 124 | U    |
| 5   | L8    | 125 | C    |
| 5   | L8    | 126 | C    |
| 5   | L8    | 127 | U    |
| 5   | L8    | 150 | C    |
| 5   | L8    | 153 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L8    | 156 | U    |
| 46  | S2    | 3   | C    |
| 46  | S2    | 4   | C    |
| 46  | S2    | 17  | C    |
| 46  | S2    | 23  | G    |
| 46  | S2    | 25  | A    |
| 46  | S2    | 26  | U    |
| 46  | S2    | 33  | G    |
| 46  | S2    | 41  | G    |
| 46  | S2    | 44  | U    |
| 46  | S2    | 45  | A    |
| 46  | S2    | 46  | A    |
| 46  | S2    | 56  | G    |
| 46  | S2    | 58  | C    |
| 46  | S2    | 59  | U    |
| 46  | S2    | 65  | C    |
| 46  | S2    | 67  | C    |
| 46  | S2    | 68  | A    |
| 46  | S2    | 79  | A    |
| 46  | S2    | 99  | A2M  |
| 46  | S2    | 103 | A    |
| 46  | S2    | 113 | G    |
| 46  | S2    | 115 | U    |
| 46  | S2    | 116 | OMU  |
| 46  | S2    | 120 | U    |
| 46  | S2    | 126 | G    |
| 46  | S2    | 141 | A    |
| 46  | S2    | 142 | C    |
| 46  | S2    | 143 | U    |
| 46  | S2    | 154 | U    |
| 46  | S2    | 155 | G    |
| 46  | S2    | 158 | A    |
| 46  | S2    | 160 | U    |
| 46  | S2    | 163 | U    |
| 46  | S2    | 167 | G    |
| 46  | S2    | 168 | C    |
| 46  | S2    | 172 | OMU  |
| 46  | S2    | 175 | A    |
| 46  | S2    | 182 | C    |
| 46  | S2    | 183 | G    |
| 46  | S2    | 184 | G    |
| 46  | S2    | 187 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 188 | C    |
| 46  | S2    | 189 | U    |
| 46  | S2    | 190 | G    |
| 46  | S2    | 191 | A    |
| 46  | S2    | 192 | C    |
| 46  | S2    | 200 | G    |
| 46  | S2    | 202 | G    |
| 46  | S2    | 209 | A    |
| 46  | S2    | 293 | C    |
| 46  | S2    | 302 | A    |
| 46  | S2    | 305 | U    |
| 46  | S2    | 306 | C    |
| 46  | S2    | 307 | G    |
| 46  | S2    | 309 | G    |
| 46  | S2    | 318 | A    |
| 46  | S2    | 319 | C    |
| 46  | S2    | 320 | G    |
| 46  | S2    | 322 | C    |
| 46  | S2    | 335 | G    |
| 46  | S2    | 338 | G    |
| 46  | S2    | 339 | A    |
| 46  | S2    | 347 | G    |
| 46  | S2    | 360 | A    |
| 46  | S2    | 362 | C    |
| 46  | S2    | 364 | A    |
| 46  | S2    | 368 | U    |
| 46  | S2    | 369 | C    |
| 46  | S2    | 370 | G    |
| 46  | S2    | 377 | G    |
| 46  | S2    | 381 | C    |
| 46  | S2    | 382 | C    |
| 46  | S2    | 383 | G    |
| 46  | S2    | 385 | G    |
| 46  | S2    | 386 | C    |
| 46  | S2    | 400 | C    |
| 46  | S2    | 408 | A    |
| 46  | S2    | 409 | C    |
| 46  | S2    | 420 | G    |
| 46  | S2    | 426 | A    |
| 46  | S2    | 428 | OMU  |
| 46  | S2    | 429 | C    |
| 46  | S2    | 438 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 441 | C    |
| 46  | S2    | 447 | A    |
| 46  | S2    | 448 | A    |
| 46  | S2    | 449 | A    |
| 46  | S2    | 450 | C    |
| 46  | S2    | 464 | A    |
| 46  | S2    | 465 | A    |
| 46  | S2    | 467 | G    |
| 46  | S2    | 471 | G    |
| 46  | S2    | 472 | C    |
| 46  | S2    | 473 | A    |
| 46  | S2    | 474 | G    |
| 46  | S2    | 482 | G    |
| 46  | S2    | 487 | U    |
| 46  | S2    | 488 | U    |
| 46  | S2    | 492 | C    |
| 46  | S2    | 516 | A    |
| 46  | S2    | 518 | G    |
| 46  | S2    | 525 | A    |
| 46  | S2    | 532 | C    |
| 46  | S2    | 534 | G    |
| 46  | S2    | 536 | A    |
| 46  | S2    | 550 | C    |
| 46  | S2    | 551 | U    |
| 46  | S2    | 555 | A    |
| 46  | S2    | 559 | G    |
| 46  | S2    | 560 | A    |
| 46  | S2    | 568 | C    |
| 46  | S2    | 574 | A    |
| 46  | S2    | 576 | A2M  |
| 46  | S2    | 585 | C    |
| 46  | S2    | 587 | A    |
| 46  | S2    | 589 | G    |
| 46  | S2    | 590 | A2M  |
| 46  | S2    | 591 | U    |
| 46  | S2    | 594 | A    |
| 46  | S2    | 598 | G    |
| 46  | S2    | 605 | A    |
| 46  | S2    | 606 | G    |
| 46  | S2    | 608 | C    |
| 46  | S2    | 614 | C    |
| 46  | S2    | 617 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 620 | G    |
| 46  | S2    | 621 | OMC  |
| 46  | S2    | 629 | A    |
| 46  | S2    | 631 | U    |
| 46  | S2    | 632 | C    |
| 46  | S2    | 637 | U    |
| 46  | S2    | 643 | A    |
| 46  | S2    | 644 | OMG  |
| 46  | S2    | 658 | U    |
| 46  | S2    | 659 | G    |
| 46  | S2    | 660 | C    |
| 46  | S2    | 662 | G    |
| 46  | S2    | 664 | A    |
| 46  | S2    | 668 | A2M  |
| 46  | S2    | 669 | A    |
| 46  | S2    | 670 | A    |
| 46  | S2    | 671 | A    |
| 46  | S2    | 672 | A    |
| 46  | S2    | 673 | G    |
| 46  | S2    | 683 | OMG  |
| 46  | S2    | 687 | C    |
| 46  | S2    | 688 | U    |
| 46  | S2    | 689 | U    |
| 46  | S2    | 800 | U    |
| 46  | S2    | 808 | A    |
| 46  | S2    | 809 | A    |
| 46  | S2    | 821 | G    |
| 46  | S2    | 822 | PSU  |
| 46  | S2    | 823 | U    |
| 46  | S2    | 827 | A    |
| 46  | S2    | 830 | A    |
| 46  | S2    | 841 | G    |
| 46  | S2    | 847 | A    |
| 46  | S2    | 848 | U    |
| 46  | S2    | 870 | A    |
| 46  | S2    | 875 | A    |
| 46  | S2    | 877 | C    |
| 46  | S2    | 878 | G    |
| 46  | S2    | 909 | G    |
| 46  | S2    | 910 | G    |
| 46  | S2    | 913 | A    |
| 46  | S2    | 914 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 916  | A    |
| 46  | S2    | 917  | U    |
| 46  | S2    | 920  | A    |
| 46  | S2    | 921  | G    |
| 46  | S2    | 933  | G    |
| 46  | S2    | 934  | G    |
| 46  | S2    | 943  | U    |
| 46  | S2    | 955  | A    |
| 46  | S2    | 970  | G    |
| 46  | S2    | 971  | G    |
| 46  | S2    | 985  | G    |
| 46  | S2    | 990  | A    |
| 46  | S2    | 991  | G    |
| 46  | S2    | 992  | A    |
| 46  | S2    | 999  | G    |
| 46  | S2    | 1017 | U    |
| 46  | S2    | 1023 | A    |
| 46  | S2    | 1041 | G    |
| 46  | S2    | 1049 | A    |
| 46  | S2    | 1058 | A    |
| 46  | S2    | 1067 | C    |
| 46  | S2    | 1069 | U    |
| 46  | S2    | 1078 | C    |
| 46  | S2    | 1083 | A    |
| 46  | S2    | 1085 | C    |
| 46  | S2    | 1096 | G    |
| 46  | S2    | 1112 | U    |
| 46  | S2    | 1126 | G    |
| 46  | S2    | 1130 | G    |
| 46  | S2    | 1149 | A    |
| 46  | S2    | 1150 | A    |
| 46  | S2    | 1153 | C    |
| 46  | S2    | 1154 | U    |
| 46  | S2    | 1166 | G    |
| 46  | S2    | 1171 | G    |
| 46  | S2    | 1172 | U    |
| 46  | S2    | 1195 | A    |
| 46  | S2    | 1207 | G    |
| 46  | S2    | 1211 | G    |
| 46  | S2    | 1215 | C    |
| 46  | S2    | 1224 | G    |
| 46  | S2    | 1242 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1244 | PSU  |
| 46  | S2    | 1250 | A    |
| 46  | S2    | 1251 | A    |
| 46  | S2    | 1253 | A    |
| 46  | S2    | 1254 | C    |
| 46  | S2    | 1256 | G    |
| 46  | S2    | 1257 | G    |
| 46  | S2    | 1259 | A    |
| 46  | S2    | 1261 | C    |
| 46  | S2    | 1265 | A    |
| 46  | S2    | 1269 | G    |
| 46  | S2    | 1273 | C    |
| 46  | S2    | 1274 | G    |
| 46  | S2    | 1275 | G    |
| 46  | S2    | 1284 | A    |
| 46  | S2    | 1285 | G    |
| 46  | S2    | 1286 | G    |
| 46  | S2    | 1295 | A    |
| 46  | S2    | 1301 | A    |
| 46  | S2    | 1302 | G    |
| 46  | S2    | 1303 | C    |
| 46  | S2    | 1308 | U    |
| 46  | S2    | 1312 | G    |
| 46  | S2    | 1315 | U    |
| 46  | S2    | 1319 | U    |
| 46  | S2    | 1341 | C    |
| 46  | S2    | 1342 | U    |
| 46  | S2    | 1371 | U    |
| 46  | S2    | 1372 | U    |
| 46  | S2    | 1378 | A    |
| 46  | S2    | 1395 | C    |
| 46  | S2    | 1396 | A    |
| 46  | S2    | 1397 | U    |
| 46  | S2    | 1402 | A    |
| 46  | S2    | 1406 | G    |
| 46  | S2    | 1412 | C    |
| 46  | S2    | 1414 | A    |
| 46  | S2    | 1422 | G    |
| 46  | S2    | 1428 | G    |
| 46  | S2    | 1439 | A    |
| 46  | S2    | 1442 | OMU  |
| 46  | S2    | 1447 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1454 | A    |
| 46  | S2    | 1462 | U    |
| 46  | S2    | 1463 | U    |
| 46  | S2    | 1464 | C    |
| 46  | S2    | 1466 | G    |
| 46  | S2    | 1476 | A    |
| 46  | S2    | 1477 | U    |
| 46  | S2    | 1478 | U    |
| 46  | S2    | 1480 | A    |
| 46  | S2    | 1488 | C    |
| 46  | S2    | 1489 | A    |
| 46  | S2    | 1490 | OMG  |
| 46  | S2    | 1493 | C    |
| 46  | S2    | 1496 | U    |
| 46  | S2    | 1498 | A    |
| 46  | S2    | 1507 | G    |
| 46  | S2    | 1520 | G    |
| 46  | S2    | 1521 | C    |
| 46  | S2    | 1522 | A    |
| 46  | S2    | 1523 | C    |
| 46  | S2    | 1533 | A    |
| 46  | S2    | 1564 | C    |
| 46  | S2    | 1570 | G    |
| 46  | S2    | 1574 | C    |
| 46  | S2    | 1575 | G    |
| 46  | S2    | 1580 | A    |
| 46  | S2    | 1585 | U    |
| 46  | S2    | 1587 | G    |
| 46  | S2    | 1588 | A    |
| 46  | S2    | 1601 | A    |
| 46  | S2    | 1604 | G    |
| 46  | S2    | 1612 | G    |
| 46  | S2    | 1621 | U    |
| 46  | S2    | 1623 | A    |
| 46  | S2    | 1629 | C    |
| 46  | S2    | 1636 | G    |
| 46  | S2    | 1637 | A    |
| 46  | S2    | 1638 | G    |
| 46  | S2    | 1660 | C    |
| 46  | S2    | 1661 | A    |
| 46  | S2    | 1665 | G    |
| 46  | S2    | 1671 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1675 | A    |
| 46  | S2    | 1680 | G    |
| 46  | S2    | 1695 | A    |
| 46  | S2    | 1698 | C    |
| 46  | S2    | 1699 | A    |
| 46  | S2    | 1703 | OMC  |
| 46  | S2    | 1721 | U    |
| 46  | S2    | 1722 | G    |
| 46  | S2    | 1726 | G    |
| 46  | S2    | 1729 | U    |
| 46  | S2    | 1732 | G    |
| 46  | S2    | 1744 | G    |
| 46  | S2    | 1749 | G    |
| 46  | S2    | 1785 | C    |
| 46  | S2    | 1786 | U    |
| 46  | S2    | 1824 | A    |
| 46  | S2    | 1825 | A    |
| 46  | S2    | 1826 | G    |
| 46  | S2    | 1829 | G    |
| 46  | S2    | 1831 | A    |
| 46  | S2    | 1835 | A    |
| 46  | S2    | 1836 | G    |
| 46  | S2    | 1849 | G    |
| 46  | S2    | 1850 | MA6  |
| 46  | S2    | 1851 | MA6  |
| 46  | S2    | 1852 | C    |
| 46  | S2    | 1861 | G    |
| 46  | S2    | 1862 | G    |
| 46  | S2    | 1863 | A    |
| 46  | S2    | 1864 | U    |
| 46  | S2    | 1865 | C    |
| 46  | S2    | 1867 | U    |
| 46  | S2    | 1869 | A    |
| 80  | Bv    | 7    | G    |
| 80  | Bv    | 8    | U    |
| 80  | Bv    | 9    | 1MG  |
| 80  | Bv    | 14   | A    |
| 80  | Bv    | 15   | A    |
| 80  | Bv    | 16   | H2U  |
| 80  | Bv    | 17   | C    |
| 80  | Bv    | 18   | G    |
| 80  | Bv    | 19   | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 80  | Bv    | 22   | G    |
| 80  | Bv    | 23   | C    |
| 80  | Bv    | 24   | G    |
| 80  | Bv    | 28   | PSU  |
| 80  | Bv    | 29   | C    |
| 80  | Bv    | 30   | G    |
| 80  | Bv    | 33   | U    |
| 80  | Bv    | 34   | G    |
| 80  | Bv    | 37   | UY4  |
| 80  | Bv    | 38   | A    |
| 80  | Bv    | 45   | G    |
| 80  | Bv    | 46   | G7M  |
| 80  | Bv    | 47   | H2U  |
| 80  | Bv    | 48   | U    |
| 80  | Bv    | 49   | G    |
| 80  | Bv    | 53   | G    |
| 80  | Bv    | 54   | U    |
| 80  | Bv    | 56   | C    |
| 80  | Bv    | 58   | 1MA  |
| 80  | Bv    | 60   | C    |
| 80  | Bv    | 61   | C    |
| 80  | Bv    | 63   | A    |
| 80  | Bv    | 67   | A    |
| 80  | Bv    | 68   | G    |
| 80  | Bv    | 69   | G    |
| 80  | Bv    | 70   | G    |
| 80  | Bv    | 71   | A    |
| 80  | Bv    | 72   | C    |
| 80  | Bv    | 73   | G    |
| 80  | Bv    | 74   | C    |
| 80  | Bv    | 75   | C    |
| 80  | Bv    | 76   | A    |
| 82  | k     | 1051 | C    |
| 82  | k     | 1056 | U    |
| 82  | k     | 1057 | A    |
| 82  | k     | 1058 | A    |
| 82  | k     | 1059 | U    |
| 82  | k     | 1060 | U    |
| 82  | k     | 1061 | U    |

All (25) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 167  | C    |
| 3   | L5    | 397  | C    |
| 3   | L5    | 1620 | G    |
| 3   | L5    | 1908 | C    |
| 3   | L5    | 2006 | C    |
| 3   | L5    | 2403 | G    |
| 3   | L5    | 2662 | G    |
| 3   | L5    | 2747 | G    |
| 3   | L5    | 3593 | G    |
| 3   | L5    | 3652 | C    |
| 3   | L5    | 4348 | A    |
| 3   | L5    | 4570 | G    |
| 3   | L5    | 4641 | C    |
| 3   | L5    | 4878 | G    |
| 5   | L8    | 83   | C    |
| 46  | S2    | 140  | C    |
| 46  | S2    | 407  | G    |
| 46  | S2    | 688  | U    |
| 46  | S2    | 1129 | G    |
| 46  | S2    | 1253 | A    |
| 46  | S2    | 1394 | G    |
| 46  | S2    | 1395 | C    |
| 46  | S2    | 1637 | A    |
| 46  | S2    | 1679 | A    |
| 46  | S2    | 1824 | A    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | A2M  | L5    | 3804 | 3    | 22,25,26     | 0.40 | 0           | 30,36,39    | 0.55 | 0           |
| 3   | OMG  | L5    | 1612 | 84,3 | 23,26,27     | 1.37 | 4 (17%)     | 32,38,41    | 2.09 | 8 (25%)     |
| 3   | PSU  | L5    | 4966 | 3    | 18,21,22     | 1.80 | 5 (27%)     | 21,30,33    | 2.16 | 4 (19%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | OMC  | S2    | 621  | 46    | 19,22,23     | 0.96 | 2 (10%)  | 25,31,34    | 1.62 | 5 (20%)  |
| 46  | PSU  | S2    | 1625 | 46    | 18,21,22     | 1.44 | 4 (22%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 46  | OMC  | S2    | 1391 | 46    | 19,22,23     | 0.84 | 0        | 25,31,34    | 1.03 | 1 (4%)   |
| 3   | PSU  | L5    | 1768 | 3     | 18,21,22     | 1.59 | 5 (27%)  | 21,30,33    | 2.22 | 3 (14%)  |
| 46  | PSU  | S2    | 34   | 46    | 18,21,22     | 1.49 | 4 (22%)  | 21,30,33    | 2.15 | 5 (23%)  |
| 3   | PSU  | L5    | 3694 | 3     | 18,21,22     | 1.52 | 4 (22%)  | 21,30,33    | 2.07 | 4 (19%)  |
| 46  | PSU  | S2    | 105  | 46    | 18,21,22     | 1.57 | 4 (22%)  | 21,30,33    | 2.13 | 4 (19%)  |
| 46  | 4AC  | S2    | 1337 | 46    | 21,24,25     | 1.21 | 2 (9%)   | 28,34,37    | 2.60 | 9 (32%)  |
| 3   | PSU  | L5    | 4331 | 3     | 18,21,22     | 1.80 | 5 (27%)  | 21,30,33    | 2.14 | 5 (23%)  |
| 46  | PSU  | S2    | 406  | 46    | 18,21,22     | 1.64 | 5 (27%)  | 21,30,33    | 2.23 | 5 (23%)  |
| 3   | 2MG  | L5    | 1504 | 3     | 23,26,27     | 1.42 | 6 (26%)  | 33,38,41    | 2.45 | 9 (27%)  |
| 46  | A2M  | S2    | 1678 | 46    | 22,25,26     | 0.30 | 0        | 30,36,39    | 0.44 | 0        |
| 3   | OMC  | L5    | 3848 | 3     | 19,22,23     | 0.96 | 1 (5%)   | 25,31,34    | 0.95 | 1 (4%)   |
| 3   | PSU  | L5    | 4549 | 3     | 18,21,22     | 1.70 | 5 (27%)  | 21,30,33    | 2.39 | 6 (28%)  |
| 3   | OMG  | L5    | 4593 | 3     | 23,26,27     | 1.32 | 3 (13%)  | 32,38,41    | 2.14 | 6 (18%)  |
| 3   | A2M  | L5    | 4493 | 84,3  | 22,25,26     | 0.36 | 0        | 30,36,39    | 0.67 | 1 (3%)   |
| 3   | PSU  | L5    | 4323 | 3     | 18,21,22     | 1.78 | 5 (27%)  | 21,30,33    | 2.43 | 5 (23%)  |
| 3   | A2M  | L5    | 2802 | 3     | 22,25,26     | 0.37 | 0        | 30,36,39    | 0.77 | 2 (6%)   |
| 46  | A2M  | S2    | 484  | 46    | 22,25,26     | 0.31 | 0        | 30,36,39    | 0.57 | 0        |
| 46  | PSU  | S2    | 1177 | 46    | 18,21,22     | 1.61 | 4 (22%)  | 21,30,33    | 1.95 | 4 (19%)  |
| 3   | PSU  | L5    | 4390 | 3     | 18,21,22     | 1.35 | 3 (16%)  | 21,30,33    | 2.02 | 4 (19%)  |
| 3   | OMG  | L5    | 4362 | 3     | 23,26,27     | 1.48 | 6 (26%)  | 32,38,41    | 2.09 | 7 (21%)  |
| 3   | A2M  | L5    | 3697 | 3     | 22,25,26     | 0.33 | 0        | 30,36,39    | 0.54 | 0        |
| 46  | OMG  | S2    | 1328 | 46    | 23,26,27     | 1.26 | 3 (13%)  | 32,38,41    | 2.01 | 6 (18%)  |
| 3   | PSU  | L5    | 4522 | 3     | 18,21,22     | 1.86 | 5 (27%)  | 21,30,33    | 2.47 | 5 (23%)  |
| 3   | A2M  | L5    | 3846 | 3     | 22,25,26     | 0.35 | 0        | 30,36,39    | 0.73 | 2 (6%)   |
| 3   | PSU  | L5    | 4401 | 3     | 18,21,22     | 1.72 | 5 (27%)  | 21,30,33    | 2.25 | 4 (19%)  |
| 3   | PSU  | L5    | 1731 | 3     | 18,21,22     | 1.70 | 4 (22%)  | 21,30,33    | 2.31 | 3 (14%)  |
| 3   | PSU  | L5    | 4373 | 3     | 18,21,22     | 1.67 | 5 (27%)  | 21,30,33    | 2.09 | 4 (19%)  |
| 3   | OMG  | L5    | 3878 | 3     | 23,26,27     | 1.45 | 4 (17%)  | 32,38,41    | 2.11 | 8 (25%)  |
| 3   | PSU  | L5    | 3743 | 3     | 18,21,22     | 1.60 | 4 (22%)  | 21,30,33    | 2.13 | 4 (19%)  |
| 3   | UR3  | L5    | 4500 | 3     | 19,22,23     | 1.07 | 1 (5%)   | 26,32,35    | 2.00 | 6 (23%)  |
| 46  | A2M  | S2    | 27   | 46,84 | 22,25,26     | 0.36 | 0        | 30,36,39    | 0.48 | 0        |
| 46  | PSU  | S2    | 109  | 46    | 18,21,22     | 1.52 | 4 (22%)  | 21,30,33    | 2.17 | 4 (19%)  |
| 46  | OMU  | S2    | 121  | 46    | 19,22,23     | 1.35 | 3 (15%)  | 25,31,34    | 1.92 | 4 (16%)  |
| 3   | A2M  | L5    | 2350 | 84,3  | 22,25,26     | 0.46 | 0        | 30,36,39    | 0.46 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | A2M  | L5    | 1521 | 3    | 22,25,26     | 0.41 | 0        | 30,36,39    | 0.49 | 0        |
| 3   | PSU  | L5    | 1664 | 3    | 18,21,22     | 1.74 | 5 (27%)  | 21,30,33    | 2.44 | 6 (28%)  |
| 46  | PSU  | S2    | 1643 | 46   | 18,21,22     | 1.51 | 5 (27%)  | 21,30,33    | 2.07 | 4 (19%)  |
| 3   | OMC  | L5    | 2352 | 3    | 19,22,23     | 0.88 | 2 (10%)  | 25,31,34    | 0.73 | 0        |
| 3   | OMU  | L5    | 4590 | 3    | 19,22,23     | 1.64 | 3 (15%)  | 25,31,34    | 1.80 | 6 (24%)  |
| 3   | OMG  | L5    | 3723 | 3    | 23,26,27     | 1.41 | 4 (17%)  | 32,38,41    | 1.94 | 7 (21%)  |
| 3   | UY1  | L5    | 3797 | 84,3 | 19,22,23     | 1.58 | 5 (26%)  | 21,31,34    | 2.01 | 4 (19%)  |
| 3   | PSU  | L5    | 4427 | 3    | 18,21,22     | 1.71 | 5 (27%)  | 21,30,33    | 2.44 | 5 (23%)  |
| 46  | PSU  | S2    | 1081 | 46   | 18,21,22     | 1.62 | 5 (27%)  | 21,30,33    | 2.26 | 5 (23%)  |
| 3   | PSU  | L5    | 4266 | 3    | 18,21,22     | 1.57 | 4 (22%)  | 21,30,33    | 2.19 | 4 (19%)  |
| 46  | 6MZ  | S2    | 1832 | 46   | 22,25,26     | 1.52 | 5 (22%)  | 29,36,39    | 2.35 | 11 (37%) |
| 46  | PSU  | S2    | 1045 | 46   | 18,21,22     | 1.51 | 3 (16%)  | 21,30,33    | 2.26 | 4 (19%)  |
| 3   | A2M  | L5    | 389  | 3    | 22,25,26     | 0.40 | 0        | 30,36,39    | 0.67 | 1 (3%)   |
| 3   | OMG  | L5    | 3771 | 3    | 23,26,27     | 1.33 | 3 (13%)  | 32,38,41    | 2.16 | 9 (28%)  |
| 46  | OMU  | S2    | 172  | 46   | 19,22,23     | 1.31 | 4 (21%)  | 25,31,34    | 1.96 | 5 (20%)  |
| 46  | MA6  | S2    | 1851 | 46   | 23,26,27     | 1.51 | 5 (21%)  | 33,38,41    | 2.32 | 10 (30%) |
| 3   | OMG  | L5    | 2863 | 3    | 23,26,27     | 1.35 | 5 (21%)  | 32,38,41    | 2.12 | 8 (25%)  |
| 46  | PSU  | S2    | 801  | 46   | 18,21,22     | 1.52 | 4 (22%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 3   | PSU  | L5    | 4269 | 3    | 18,21,22     | 1.75 | 4 (22%)  | 21,30,33    | 1.97 | 4 (19%)  |
| 80  | H2U  | Bv    | 47   | 80   | 18,21,22     | 1.02 | 2 (11%)  | 19,30,33    | 1.35 | 3 (15%)  |
| 3   | PSU  | L5    | 3709 | 3    | 18,21,22     | 1.47 | 4 (22%)  | 21,30,33    | 2.17 | 4 (19%)  |
| 46  | PSU  | S2    | 1174 | 46   | 18,21,22     | 1.60 | 5 (27%)  | 21,30,33    | 2.32 | 4 (19%)  |
| 3   | OMU  | L5    | 4197 | 3    | 19,22,23     | 1.48 | 4 (21%)  | 25,31,34    | 2.00 | 6 (24%)  |
| 3   | PSU  | L5    | 1670 | 3    | 18,21,22     | 1.97 | 4 (22%)  | 21,30,33    | 2.15 | 3 (14%)  |
| 3   | OMU  | L5    | 4468 | 3    | 19,22,23     | 1.53 | 4 (21%)  | 25,31,34    | 1.96 | 5 (20%)  |
| 3   | PSU  | L5    | 1569 | 3    | 18,21,22     | 1.71 | 5 (27%)  | 21,30,33    | 2.19 | 4 (19%)  |
| 3   | PSU  | L5    | 4598 | 3    | 18,21,22     | 1.78 | 5 (27%)  | 21,30,33    | 2.38 | 4 (19%)  |
| 46  | OMU  | S2    | 1326 | 46   | 19,22,23     | 1.31 | 4 (21%)  | 25,31,34    | 2.03 | 7 (28%)  |
| 3   | PSU  | L5    | 4263 | 3    | 18,21,22     | 1.77 | 6 (33%)  | 21,30,33    | 2.21 | 4 (19%)  |
| 3   | OMU  | L5    | 3904 | 3    | 19,22,23     | 1.81 | 4 (21%)  | 25,31,34    | 2.12 | 8 (32%)  |
| 3   | OMG  | L5    | 1303 | 3    | 23,26,27     | 1.56 | 6 (26%)  | 32,38,41    | 2.03 | 5 (15%)  |
| 3   | OMC  | L5    | 3787 | 3    | 19,22,23     | 0.99 | 2 (10%)  | 25,31,34    | 1.08 | 2 (8%)   |
| 3   | A2M  | L5    | 2774 | 84,3 | 22,25,26     | 0.37 | 0        | 30,36,39    | 0.74 | 1 (3%)   |
| 46  | A2M  | S2    | 159  | 46   | 22,25,26     | 0.24 | 0        | 30,36,39    | 0.38 | 0        |
| 3   | PSU  | L5    | 4975 | 3    | 18,21,22     | 1.65 | 4 (22%)  | 21,30,33    | 2.30 | 3 (14%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | A2M  | S2    | 99   | 46    | 22,25,26     | 0.33 | 0        | 30,36,39    | 0.63 | 0        |
| 46  | OMU  | S2    | 116  | 46    | 19,22,23     | 1.29 | 3 (15%)  | 25,31,34    | 1.84 | 6 (24%)  |
| 46  | OMG  | S2    | 509  | 46,84 | 23,26,27     | 1.29 | 3 (13%)  | 32,38,41    | 2.00 | 6 (18%)  |
| 3   | OMC  | L5    | 4506 | 3     | 19,22,23     | 1.00 | 2 (10%)  | 25,31,34    | 1.03 | 1 (4%)   |
| 3   | OMG  | L5    | 2411 | 3     | 23,26,27     | 1.40 | 4 (17%)  | 32,38,41    | 1.81 | 6 (18%)  |
| 3   | OMG  | L5    | 4588 | 3     | 23,26,27     | 1.35 | 5 (21%)  | 32,38,41    | 2.08 | 8 (25%)  |
| 80  | UY4  | Bv    | 37   | 80    | 31,34,35     | 1.86 | 8 (25%)  | 43,49,52    | 2.06 | 13 (30%) |
| 3   | OMG  | L5    | 4469 | 3     | 23,26,27     | 1.34 | 4 (17%)  | 32,38,41    | 1.96 | 6 (18%)  |
| 3   | A2M  | L5    | 3809 | 3     | 22,25,26     | 0.39 | 0        | 30,36,39    | 0.53 | 0        |
| 3   | A2M  | L5    | 3764 | 3     | 22,25,26     | 0.38 | 0        | 30,36,39    | 0.85 | 0        |
| 3   | OMC  | L5    | 2409 | 84,3  | 19,22,23     | 1.00 | 2 (10%)  | 25,31,34    | 1.15 | 2 (8%)   |
| 80  | 1MA  | Bv    | 58   | 80    | 21,25,26     | 1.40 | 4 (19%)  | 30,37,40    | 1.79 | 5 (16%)  |
| 3   | 6MZ  | L5    | 4190 | 3     | 22,25,26     | 1.49 | 4 (18%)  | 29,36,39    | 2.15 | 8 (27%)  |
| 46  | PSU  | S2    | 815  | 46    | 18,21,22     | 1.50 | 4 (22%)  | 21,30,33    | 2.11 | 3 (14%)  |
| 3   | A2M  | L5    | 1511 | 3     | 22,25,26     | 0.54 | 0        | 30,36,39    | 0.82 | 0        |
| 3   | A2M  | L5    | 2388 | 84,3  | 22,25,26     | 0.36 | 0        | 30,36,39    | 0.54 | 0        |
| 3   | PSU  | L5    | 3832 | 84,3  | 18,21,22     | 1.82 | 4 (22%)  | 21,30,33    | 2.09 | 4 (19%)  |
| 46  | PSU  | S2    | 1692 | 46    | 18,21,22     | 1.67 | 5 (27%)  | 21,30,33    | 2.25 | 5 (23%)  |
| 46  | PSU  | S2    | 1445 | 46    | 18,21,22     | 1.44 | 4 (22%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 80  | PSU  | Bv    | 28   | 80    | 18,21,22     | 1.41 | 3 (16%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 3   | OMC  | L5    | 4426 | 3     | 19,22,23     | 1.01 | 2 (10%)  | 25,31,34    | 0.96 | 1 (4%)   |
| 46  | MA6  | S2    | 1850 | 46    | 23,26,27     | 1.49 | 5 (21%)  | 33,38,41    | 2.16 | 10 (30%) |
| 3   | PSU  | L5    | 2402 | 3     | 18,21,22     | 1.62 | 4 (22%)  | 21,30,33    | 2.45 | 5 (23%)  |
| 3   | PSU  | L5    | 4491 | 84,3  | 18,21,22     | 1.85 | 5 (27%)  | 21,30,33    | 2.40 | 6 (28%)  |
| 46  | PSU  | S2    | 863  | 46    | 18,21,22     | 1.58 | 5 (27%)  | 21,30,33    | 2.13 | 4 (19%)  |
| 46  | PSU  | S2    | 1244 | 46    | 18,21,22     | 1.43 | 4 (22%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 81  | MEQ  | j     | 185  | 81    | 8,9,10       | 0.47 | 0        | 5,10,12     | 0.48 | 0        |
| 3   | PSU  | L5    | 3618 | 3     | 18,21,22     | 2.02 | 5 (27%)  | 21,30,33    | 2.32 | 5 (23%)  |
| 3   | PSU  | L5    | 2495 | 3     | 18,21,22     | 1.61 | 4 (22%)  | 21,30,33    | 2.10 | 4 (19%)  |
| 80  | PSU  | Bv    | 27   | 80    | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.09 | 4 (19%)  |
| 3   | PSU  | L5    | 1523 | 3     | 18,21,22     | 1.94 | 5 (27%)  | 21,30,33    | 2.26 | 4 (19%)  |
| 46  | A2M  | S2    | 166  | 46    | 22,25,26     | 0.36 | 0        | 30,36,39    | 0.57 | 0        |
| 46  | OMG  | S2    | 436  | 46    | 23,26,27     | 1.26 | 4 (17%)  | 32,38,41    | 2.17 | 8 (25%)  |
| 3   | PSU  | L5    | 3741 | 3     | 18,21,22     | 1.55 | 5 (27%)  | 21,30,33    | 2.36 | 5 (23%)  |
| 3   | 5MC  | L5    | 3761 | 3     | 19,22,23     | 1.24 | 2 (10%)  | 26,32,35    | 1.71 | 6 (23%)  |
| 46  | G7M  | S2    | 1639 | 46,80 | 23,26,27     | 1.57 | 4 (17%)  | 34,39,42    | 1.67 | 5 (14%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | PSU  | S2    | 1238 | 46    | 18,21,22     | 1.55 | 4 (22%)  | 21,30,33    | 2.09 | 3 (14%)  |
| 46  | B8N  | S2    | 1248 | 46    | 25,29,30     | 1.44 | 4 (16%)  | 28,42,45    | 1.64 | 6 (21%)  |
| 46  | PSU  | S2    | 1367 | 46    | 18,21,22     | 1.51 | 4 (22%)  | 21,30,33    | 2.14 | 3 (14%)  |
| 3   | PSU  | L5    | 3747 | 3     | 18,21,22     | 1.65 | 5 (27%)  | 21,30,33    | 2.19 | 4 (19%)  |
| 3   | OMG  | L5    | 4607 | 3     | 23,26,27     | 1.50 | 5 (21%)  | 32,38,41    | 2.01 | 8 (25%)  |
| 3   | PSU  | L5    | 3899 | 84,3  | 18,21,22     | 1.88 | 5 (27%)  | 21,30,33    | 2.48 | 5 (23%)  |
| 3   | PSU  | L5    | 4606 | 3     | 18,21,22     | 1.59 | 4 (22%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 3   | A2M  | L5    | 1858 | 84,3  | 22,25,26     | 0.53 | 0        | 30,36,39    | 0.72 | 1 (3%)   |
| 3   | PSU  | L5    | 3616 | 3     | 18,21,22     | 2.02 | 5 (27%)  | 21,30,33    | 2.38 | 5 (23%)  |
| 3   | OMC  | L5    | 1327 | 3     | 19,22,23     | 0.95 | 2 (10%)  | 25,31,34    | 0.88 | 1 (4%)   |
| 46  | OMC  | S2    | 462  | 46    | 19,22,23     | 0.83 | 0        | 25,31,34    | 1.06 | 2 (8%)   |
| 46  | OMU  | S2    | 1804 | 46    | 19,22,23     | 1.35 | 4 (21%)  | 25,31,34    | 1.93 | 6 (24%)  |
| 81  | UXY  | j     | 63   | 81    | 7,9,10       | 0.75 | 0        | 7,10,12     | 1.36 | 1 (14%)  |
| 3   | OMC  | L5    | 3680 | 3     | 19,22,23     | 1.03 | 2 (10%)  | 25,31,34    | 0.80 | 0        |
| 3   | PSU  | L5    | 4643 | 3     | 18,21,22     | 1.82 | 5 (27%)  | 21,30,33    | 2.11 | 3 (14%)  |
| 46  | A2M  | S2    | 468  | 46    | 22,25,26     | 0.32 | 0        | 30,36,39    | 0.54 | 0        |
| 46  | OMC  | S2    | 174  | 46    | 19,22,23     | 0.87 | 1 (5%)   | 25,31,34    | 0.96 | 1 (4%)   |
| 46  | PSU  | S2    | 814  | 46    | 18,21,22     | 1.54 | 4 (22%)  | 21,30,33    | 2.12 | 4 (19%)  |
| 3   | OMC  | L5    | 3820 | 3     | 19,22,23     | 1.16 | 2 (10%)  | 25,31,34    | 1.45 | 4 (16%)  |
| 80  | H2U  | Bv    | 16   | 80    | 18,21,22     | 1.01 | 2 (11%)  | 19,30,33    | 1.26 | 3 (15%)  |
| 41  | MLZ  | Lm    | 98   | 41    | 8,9,10       | 0.89 | 0        | 4,9,11      | 0.75 | 0        |
| 3   | PSU  | L5    | 1847 | 3     | 18,21,22     | 1.70 | 5 (27%)  | 21,30,33    | 2.30 | 5 (23%)  |
| 3   | PSU  | L5    | 4441 | 3     | 18,21,22     | 1.71 | 5 (27%)  | 21,30,33    | 2.35 | 4 (19%)  |
| 3   | PSU  | L5    | 1779 | 3     | 18,21,22     | 1.65 | 4 (22%)  | 21,30,33    | 1.97 | 4 (19%)  |
| 3   | PSU  | L5    | 2619 | 3     | 18,21,22     | 1.67 | 5 (27%)  | 21,30,33    | 2.27 | 5 (23%)  |
| 3   | OMG  | L5    | 3606 | 3     | 23,26,27     | 1.43 | 5 (21%)  | 32,38,41    | 1.89 | 7 (21%)  |
| 3   | PSU  | L5    | 3830 | 3     | 18,21,22     | 1.77 | 5 (27%)  | 21,30,33    | 2.17 | 6 (28%)  |
| 3   | 1MA  | L5    | 1309 | 84,3  | 21,25,26     | 1.54 | 6 (28%)  | 30,37,40    | 1.71 | 6 (20%)  |
| 3   | OMG  | L5    | 2351 | 3     | 23,26,27     | 1.34 | 4 (17%)  | 32,38,41    | 2.23 | 8 (25%)  |
| 3   | PSU  | L5    | 1769 | 3     | 18,21,22     | 1.65 | 5 (27%)  | 21,30,33    | 2.39 | 4 (19%)  |
| 3   | PSU  | L5    | 4659 | 3     | 18,21,22     | 1.82 | 5 (27%)  | 21,30,33    | 2.34 | 6 (28%)  |
| 5   | OMG  | L8    | 75   | 5     | 23,26,27     | 1.33 | 4 (17%)  | 32,38,41    | 1.96 | 7 (21%)  |
| 80  | 2MG  | Bv    | 10   | 80    | 23,26,27     | 1.26 | 4 (17%)  | 33,38,41    | 2.29 | 9 (27%)  |
| 3   | OMU  | L5    | 2824 | 3     | 19,22,23     | 1.47 | 4 (21%)  | 25,31,34    | 2.14 | 4 (16%)  |
| 46  | A2M  | S2    | 668  | 46,84 | 22,25,26     | 0.44 | 0        | 30,36,39    | 0.81 | 2 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | OMU  | S2    | 1288 | 46   | 19,22,23     | 1.31 | 4 (21%)  | 25,31,34    | 1.79 | 4 (16%)  |
| 6   | MLZ  | LC    | 333  | 6    | 8,9,10       | 0.94 | 0        | 4,9,11      | 0.68 | 0        |
| 3   | OMG  | L5    | 364  | 3    | 23,26,27     | 1.52 | 5 (21%)  | 32,38,41    | 2.25 | 9 (28%)  |
| 3   | OMC  | L5    | 2791 | 3    | 19,22,23     | 1.03 | 2 (10%)  | 25,31,34    | 0.91 | 1 (4%)   |
| 80  | PSU  | Bv    | 55   | 80   | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 2.14 | 5 (23%)  |
| 5   | PSU  | L8    | 55   | 5    | 18,21,22     | 1.55 | 5 (27%)  | 21,30,33    | 2.26 | 4 (19%)  |
| 3   | OMC  | L5    | 3866 | 3    | 19,22,23     | 0.93 | 1 (5%)   | 25,31,34    | 0.94 | 1 (4%)   |
| 46  | A2M  | S2    | 576  | 46   | 22,25,26     | 0.25 | 0        | 30,36,39    | 0.56 | 0        |
| 3   | PSU  | L5    | 3823 | 3    | 18,21,22     | 1.74 | 5 (27%)  | 21,30,33    | 2.48 | 4 (19%)  |
| 80  | M2G  | Bv    | 26   | 80   | 24,27,28     | 1.31 | 4 (16%)  | 33,40,43    | 2.01 | 7 (21%)  |
| 46  | PSU  | S2    | 649  | 46   | 18,21,22     | 1.60 | 4 (22%)  | 21,30,33    | 2.16 | 4 (19%)  |
| 46  | OMC  | S2    | 1703 | 46   | 19,22,23     | 0.88 | 2 (10%)  | 25,31,34    | 1.21 | 2 (8%)   |
| 3   | OMG  | L5    | 4464 | 3    | 23,26,27     | 1.48 | 5 (21%)  | 32,38,41    | 2.03 | 8 (25%)  |
| 3   | OMG  | L5    | 4340 | 3    | 23,26,27     | 1.38 | 6 (26%)  | 32,38,41    | 2.08 | 8 (25%)  |
| 46  | PSU  | S2    | 572  | 46   | 18,21,22     | 1.44 | 4 (22%)  | 21,30,33    | 2.21 | 5 (23%)  |
| 46  | A2M  | S2    | 590  | 46   | 22,25,26     | 0.30 | 0        | 30,36,39    | 0.70 | 1 (3%)   |
| 3   | A2M  | L5    | 1313 | 3    | 22,25,26     | 1.68 | 5 (22%)  | 30,36,39    | 2.25 | 10 (33%) |
| 3   | OMG  | L5    | 4166 | 80,3 | 23,26,27     | 1.41 | 4 (17%)  | 32,38,41    | 2.10 | 9 (28%)  |
| 46  | PSU  | S2    | 609  | 46   | 18,21,22     | 1.45 | 4 (22%)  | 21,30,33    | 2.14 | 3 (14%)  |
| 46  | PSU  | S2    | 1004 | 46   | 18,21,22     | 1.56 | 5 (27%)  | 21,30,33    | 2.24 | 3 (14%)  |
| 3   | PSU  | L5    | 4282 | 3    | 18,21,22     | 1.69 | 4 (22%)  | 21,30,33    | 2.34 | 5 (23%)  |
| 46  | A2M  | S2    | 512  | 46   | 22,25,26     | 0.33 | 0        | 30,36,39    | 0.64 | 0        |
| 46  | PSU  | S2    | 119  | 46   | 18,21,22     | 1.49 | 5 (27%)  | 21,30,33    | 2.04 | 5 (23%)  |
| 3   | A2M  | L5    | 3703 | 3    | 22,25,26     | 0.30 | 0        | 30,36,39    | 0.50 | 0        |
| 46  | OMC  | S2    | 517  | 46   | 19,22,23     | 0.84 | 1 (5%)   | 25,31,34    | 0.80 | 1 (4%)   |
| 46  | OMG  | S2    | 601  | 46   | 23,26,27     | 1.38 | 4 (17%)  | 32,38,41    | 1.76 | 5 (15%)  |
| 46  | PSU  | S2    | 686  | 46   | 18,21,22     | 1.56 | 5 (27%)  | 21,30,33    | 2.27 | 5 (23%)  |
| 46  | PSU  | S2    | 822  | 46   | 18,21,22     | 1.52 | 5 (27%)  | 21,30,33    | 2.16 | 4 (19%)  |
| 46  | OMU  | S2    | 428  | 46   | 19,22,23     | 1.24 | 3 (15%)  | 25,31,34    | 1.82 | 5 (20%)  |
| 46  | PSU  | S2    | 1347 | 46   | 18,21,22     | 1.44 | 4 (22%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 3   | OMC  | L5    | 2848 | 3    | 19,22,23     | 0.97 | 2 (10%)  | 25,31,34    | 0.61 | 0        |
| 73  | IAS  | SO    | 138  | 73   | 6,7,8        | 1.30 | 1 (16%)  | 3,8,10      | 1.21 | 0        |
| 3   | OMU  | L5    | 4276 | 3    | 19,22,23     | 1.58 | 4 (21%)  | 25,31,34    | 1.92 | 6 (24%)  |
| 3   | PSU  | L5    | 4546 | 3    | 18,21,22     | 1.59 | 5 (27%)  | 21,30,33    | 2.27 | 3 (14%)  |
| 3   | PSU  | L5    | 4412 | 3    | 18,21,22     | 1.66 | 5 (27%)  | 21,30,33    | 2.28 | 4 (19%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | OMG  | S2    | 1490 | 46   | 23,26,27     | 1.32 | 5 (21%)  | 32,38,41    | 2.21 | 7 (21%)  |
| 46  | PSU  | S2    | 93   | 46   | 18,21,22     | 1.47 | 4 (22%)  | 21,30,33    | 2.07 | 4 (19%)  |
| 3   | PSU  | L5    | 4502 | 3    | 18,21,22     | 1.78 | 6 (33%)  | 21,30,33    | 2.01 | 5 (23%)  |
| 3   | A2M  | L5    | 4541 | 3    | 22,25,26     | 0.41 | 0        | 30,36,39    | 0.44 | 0        |
| 46  | PSU  | S2    | 218  | 46   | 18,21,22     | 1.47 | 4 (22%)  | 21,30,33    | 2.14 | 5 (23%)  |
| 3   | OMG  | L5    | 1509 | 3    | 23,26,27     | 1.48 | 6 (26%)  | 32,38,41    | 2.20 | 8 (25%)  |
| 3   | OMC  | L5    | 2338 | 3    | 19,22,23     | 1.07 | 2 (10%)  | 25,31,34    | 1.47 | 3 (12%)  |
| 3   | PSU  | L5    | 3737 | 3    | 18,21,22     | 1.63 | 4 (22%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 46  | OMG  | S2    | 683  | 46   | 23,26,27     | 1.29 | 3 (13%)  | 32,38,41    | 2.02 | 7 (21%)  |
| 46  | 4AC  | S2    | 1842 | 46   | 21,24,25     | 1.12 | 3 (14%)  | 28,34,37    | 2.93 | 7 (25%)  |
| 46  | OMU  | S2    | 1442 | 46   | 19,22,23     | 1.36 | 4 (21%)  | 25,31,34    | 1.87 | 4 (16%)  |
| 80  | 1MG  | Bv    | 9    | 80   | 23,26,27     | 1.25 | 3 (13%)  | 33,39,42    | 1.80 | 5 (15%)  |
| 46  | PSU  | S2    | 1046 | 46   | 18,21,22     | 1.59 | 5 (27%)  | 21,30,33    | 2.03 | 4 (19%)  |
| 46  | A2M  | S2    | 1031 | 46   | 22,25,26     | 0.32 | 0        | 30,36,39    | 0.55 | 0        |
| 5   | PSU  | L8    | 69   | 5    | 18,21,22     | 1.60 | 5 (27%)  | 21,30,33    | 2.39 | 4 (19%)  |
| 3   | PSU  | L5    | 4470 | 3    | 18,21,22     | 1.60 | 6 (33%)  | 21,30,33    | 2.33 | 3 (14%)  |
| 3   | PSU  | L5    | 3749 | 3    | 18,21,22     | 1.64 | 4 (22%)  | 21,30,33    | 2.13 | 3 (14%)  |
| 3   | A2M  | L5    | 3739 | 3    | 22,25,26     | 0.29 | 0        | 30,36,39    | 0.54 | 0        |
| 3   | 5MC  | L5    | 4417 | 3    | 19,22,23     | 1.22 | 1 (5%)   | 26,32,35    | 2.09 | 7 (26%)  |
| 3   | PSU  | L5    | 3713 | 3    | 18,21,22     | 1.46 | 5 (27%)  | 21,30,33    | 2.25 | 5 (23%)  |
| 3   | PSU  | L5    | 4937 | 3    | 18,21,22     | 1.60 | 5 (27%)  | 21,30,33    | 2.03 | 5 (23%)  |
| 46  | PSU  | S2    | 866  | 46   | 18,21,22     | 1.47 | 4 (22%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 3   | PSU  | L5    | 3674 | 3    | 18,21,22     | 1.84 | 5 (27%)  | 21,30,33    | 2.24 | 5 (23%)  |
| 3   | PSU  | L5    | 4393 | 3    | 18,21,22     | 1.62 | 4 (22%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 46  | OMG  | S2    | 644  | 46   | 23,26,27     | 1.28 | 4 (17%)  | 32,38,41    | 1.97 | 6 (18%)  |
| 46  | PSU  | S2    | 1136 | 46   | 18,21,22     | 1.50 | 3 (16%)  | 21,30,33    | 2.16 | 5 (23%)  |
| 46  | PSU  | S2    | 1232 | 46   | 18,21,22     | 1.62 | 4 (22%)  | 21,30,33    | 2.16 | 3 (14%)  |
| 46  | PSU  | S2    | 966  | 46   | 18,21,22     | 1.51 | 4 (22%)  | 21,30,33    | 2.19 | 5 (23%)  |
| 46  | A2M  | S2    | 1383 | 46   | 22,25,26     | 0.32 | 0        | 30,36,39    | 0.65 | 0        |
| 3   | OMC  | L5    | 2811 | 3    | 19,22,23     | 0.93 | 2 (10%)  | 25,31,34    | 0.88 | 1 (4%)   |
| 46  | OMG  | S2    | 867  | 46   | 23,26,27     | 1.23 | 3 (13%)  | 32,38,41    | 1.92 | 6 (18%)  |
| 3   | A2M  | L5    | 391  | 3    | 22,25,26     | 0.41 | 0        | 30,36,39    | 0.59 | 0        |
| 3   | OMG  | L5    | 4198 | 3    | 23,26,27     | 1.30 | 5 (21%)  | 32,38,41    | 2.02 | 7 (21%)  |
| 46  | PSU  | S2    | 651  | 46   | 18,21,22     | 1.51 | 4 (22%)  | 21,30,33    | 2.16 | 4 (19%)  |
| 80  | G7M  | Bv    | 46   | 80   | 23,26,27     | 1.62 | 3 (13%)  | 34,39,42    | 1.89 | 6 (17%)  |
| 46  | PSU  | S2    | 36   | 46   | 18,21,22     | 1.52 | 4 (22%)  | 21,30,33    | 2.24 | 3 (14%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L5    | 1849 | 3    | 18,21,22     | 1.75 | 4 (22%)  | 21,30,33    | 2.14 | 5 (23%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | A2M  | L5    | 3804 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 1612 | 84,3 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4966 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | OMC  | S2    | 621  | 46   | -       | 4/9/27/28  | 0/2/2/2 |
| 46  | PSU  | S2    | 1625 | 46   | -       | 2/7/25/26  | 0/2/2/2 |
| 46  | OMC  | S2    | 1391 | 46   | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 1768 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 34   | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3694 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 105  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | 4AC  | S2    | 1337 | 46   | -       | 1/11/29/30 | 0/2/2/2 |
| 3   | PSU  | L5    | 4331 | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 406  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | 2MG  | L5    | 1504 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | A2M  | S2    | 1678 | 46   | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 3848 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4549 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 4593 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 4493 | 84,3 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4323 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 2802 | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 46  | A2M  | S2    | 484  | 46   | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 1177 | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4390 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 4362 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 3697 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | OMG  | S2    | 1328 | 46   | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4522 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 3846 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4401 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 1731 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4373 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 3878 | 3    | -       | 1/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 3   | PSU  | L5    | 3743 | 3     | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | UR3  | L5    | 4500 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | A2M  | S2    | 27   | 46,84 | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 109  | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | OMU  | S2    | 121  | 46    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L5    | 2350 | 84,3  | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 1521 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 1664 | 3     | -       | 2/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1643 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 2352 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMU  | L5    | 4590 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L5    | 3723 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | UY1  | L5    | 3797 | 84,3  | -       | 7/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4427 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1081 | 46    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4266 | 3     | -       | 2/7/25/26  | 0/2/2/2 |
| 46  | 6MZ  | S2    | 1832 | 46    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 1045 | 46    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 389  | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 3771 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | OMU  | S2    | 172  | 46    | -       | 2/9/27/28  | 0/2/2/2 |
| 46  | MA6  | S2    | 1851 | 46    | -       | 2/11/29/30 | 0/3/3/3 |
| 3   | OMG  | L5    | 2863 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 801  | 46    | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4269 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 80  | H2U  | Bv    | 47   | 80    | -       | 1/7/38/39  | 0/2/2/2 |
| 3   | PSU  | L5    | 3709 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1174 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L5    | 4197 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 1670 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L5    | 4468 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 1569 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4598 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | OMU  | S2    | 1326 | 46    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4263 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L5    | 3904 | 3     | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L5    | 1303 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 3787 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L5    | 2774 | 84,3  | -       | 4/9/27/28  | 0/3/3/3 |
| 46  | A2M  | S2    | 159  | 46    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 3   | PSU  | L5    | 4975 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | A2M  | S2    | 99   | 46    | -       | 2/9/27/28  | 0/3/3/3 |
| 46  | OMU  | S2    | 116  | 46    | -       | 3/9/27/28  | 0/2/2/2 |
| 46  | OMG  | S2    | 509  | 46,84 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 4506 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L5    | 2411 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 4588 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 80  | UY4  | Bv    | 37   | 80    | -       | 3/23/50/51 | 0/3/3/3 |
| 3   | OMG  | L5    | 4469 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 3809 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 3764 | 3     | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 2409 | 84,3  | -       | 0/9/27/28  | 0/2/2/2 |
| 80  | 1MA  | Bv    | 58   | 80    | -       | 2/7/25/26  | 0/3/3/3 |
| 3   | 6MZ  | L5    | 4190 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 815  | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 1511 | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 2388 | 84,3  | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 3832 | 84,3  | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1692 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1445 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 80  | PSU  | Bv    | 28   | 80    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 4426 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 46  | MA6  | S2    | 1850 | 46    | -       | 2/11/29/30 | 0/3/3/3 |
| 3   | PSU  | L5    | 2402 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4491 | 84,3  | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 863  | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1244 | 46    | -       | 2/7/25/26  | 0/2/2/2 |
| 81  | MEQ  | j     | 185  | 81    | -       | 0/8/9/11   | -       |
| 3   | PSU  | L5    | 3618 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 2495 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 80  | PSU  | Bv    | 27   | 80    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 1523 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | A2M  | S2    | 166  | 46    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | OMG  | S2    | 436  | 46    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 3741 | 3     | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | 5MC  | L5    | 3761 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | G7M  | S2    | 1639 | 46,80 | -       | 0/7/25/26  | 0/3/3/3 |
| 46  | B8N  | S2    | 1248 | 46    | 1/1/7/7 | 1/16/34/35 | 0/2/2/2 |
| 46  | PSU  | S2    | 1238 | 46    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1367 | 46    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 3   | PSU  | L5    | 3747 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 4607 | 3     | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 3899 | 84,3  | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4606 | 3     | -       | 3/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L5    | 1858 | 84,3  | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 3616 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L5    | 1327 | 3     | -       | 0/9/27/28 | 0/2/2/2 |
| 46  | OMC  | S2    | 462  | 46    | -       | 0/9/27/28 | 0/2/2/2 |
| 46  | OMU  | S2    | 1804 | 46    | -       | 2/9/27/28 | 0/2/2/2 |
| 81  | UXY  | j     | 63   | 81    | -       | 3/8/9/11  | -       |
| 3   | OMC  | L5    | 3680 | 3     | -       | 4/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L5    | 4643 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | A2M  | S2    | 468  | 46    | -       | 1/9/27/28 | 0/3/3/3 |
| 46  | OMC  | S2    | 174  | 46    | -       | 1/9/27/28 | 0/2/2/2 |
| 46  | PSU  | S2    | 814  | 46    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L5    | 3820 | 3     | -       | 2/9/27/28 | 0/2/2/2 |
| 80  | H2U  | Bv    | 16   | 80    | -       | 2/7/38/39 | 0/2/2/2 |
| 41  | MLZ  | Lm    | 98   | 41    | -       | 1/7/8/10  | -       |
| 3   | PSU  | L5    | 1847 | 3     | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4441 | 3     | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 1779 | 3     | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 2619 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 3606 | 3     | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 3830 | 3     | -       | 2/7/25/26 | 0/2/2/2 |
| 3   | 1MA  | L5    | 1309 | 84,3  | -       | 0/7/25/26 | 0/3/3/3 |
| 3   | OMG  | L5    | 2351 | 3     | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 1769 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4659 | 3     | -       | 0/7/25/26 | 0/2/2/2 |
| 5   | OMG  | L8    | 75   | 5     | -       | 0/9/27/28 | 0/3/3/3 |
| 80  | 2MG  | Bv    | 10   | 80    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMU  | L5    | 2824 | 3     | -       | 0/9/27/28 | 0/2/2/2 |
| 46  | A2M  | S2    | 668  | 46,84 | -       | 4/9/27/28 | 0/3/3/3 |
| 46  | OMU  | S2    | 1288 | 46    | -       | 0/9/27/28 | 0/2/2/2 |
| 6   | MLZ  | LC    | 333  | 6     | -       | 4/7/8/10  | -       |
| 3   | OMG  | L5    | 364  | 3     | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L5    | 2791 | 3     | -       | 0/9/27/28 | 0/2/2/2 |
| 80  | PSU  | Bv    | 55   | 80    | -       | 1/7/25/26 | 0/2/2/2 |
| 5   | PSU  | L8    | 55   | 5     | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L5    | 3866 | 3     | -       | 1/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 46  | A2M  | S2    | 576  | 46   | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 3823 | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 80  | M2G  | Bv    | 26   | 80   | -       | 0/11/29/30 | 0/3/3/3 |
| 46  | PSU  | S2    | 649  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | OMC  | S2    | 1703 | 46   | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L5    | 4464 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 4340 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 572  | 46   | -       | 1/7/25/26  | 0/2/2/2 |
| 46  | A2M  | S2    | 590  | 46   | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 1313 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 4166 | 80,3 | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 609  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 1004 | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4282 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | A2M  | S2    | 512  | 46   | -       | 2/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 119  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 3703 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | OMC  | S2    | 517  | 46   | -       | 1/9/27/28  | 0/2/2/2 |
| 46  | OMG  | S2    | 601  | 46   | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 686  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | PSU  | S2    | 822  | 46   | -       | 2/7/25/26  | 0/2/2/2 |
| 46  | OMU  | S2    | 428  | 46   | -       | 6/9/27/28  | 0/2/2/2 |
| 46  | PSU  | S2    | 1347 | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 2848 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 73  | IAS  | SO    | 138  | 73   | -       | 3/7/7/8    | -       |
| 3   | OMU  | L5    | 4276 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4546 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4412 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | OMG  | S2    | 1490 | 46   | -       | 3/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 93   | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4502 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 4541 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 46  | PSU  | S2    | 218  | 46   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 1509 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 2338 | 3    | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 3737 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 46  | OMG  | S2    | 683  | 46   | -       | 2/9/27/28  | 0/3/3/3 |
| 46  | 4AC  | S2    | 1842 | 46   | -       | 2/11/29/30 | 0/2/2/2 |
| 46  | OMU  | S2    | 1442 | 46   | -       | 2/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 80  | 1MG  | Bv    | 9    | 80   | -       | 2/7/25/26 | 0/3/3/3 |
| 46  | PSU  | S2    | 1046 | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | A2M  | S2    | 1031 | 46   | -       | 0/9/27/28 | 0/3/3/3 |
| 5   | PSU  | L8    | 69   | 5    | -       | 1/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4470 | 3    | -       | 3/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 3749 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | A2M  | L5    | 3739 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | 5MC  | L5    | 4417 | 3    | -       | 3/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 3713 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4937 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | PSU  | S2    | 866  | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 3674 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4393 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | OMG  | S2    | 644  | 46   | -       | 3/9/27/28 | 0/3/3/3 |
| 46  | PSU  | S2    | 1136 | 46   | -       | 2/7/25/26 | 0/2/2/2 |
| 46  | PSU  | S2    | 1232 | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | PSU  | S2    | 966  | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 46  | A2M  | S2    | 1383 | 46   | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L5    | 2811 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 46  | OMG  | S2    | 867  | 46   | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L5    | 391  | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L5    | 4198 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 46  | PSU  | S2    | 651  | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 80  | G7M  | Bv    | 46   | 80   | -       | 3/7/25/26 | 0/3/3/3 |
| 46  | PSU  | S2    | 36   | 46   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 1849 | 3    | -       | 2/7/25/26 | 0/2/2/2 |

All (722) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 80  | Bv    | 46   | G7M  | C5-N7   | -5.29 | 1.33        | 1.39     |
| 80  | Bv    | 37   | UY4  | C04-C02 | 5.17  | 1.60        | 1.52     |
| 46  | S2    | 1639 | G7M  | C5-N7   | -5.04 | 1.33        | 1.39     |
| 3   | L5    | 3904 | OMU  | C4-N3   | -4.73 | 1.30        | 1.38     |
| 3   | L5    | 3616 | PSU  | C4-N3   | -4.67 | 1.30        | 1.38     |
| 3   | L5    | 3674 | PSU  | C4-N3   | -4.54 | 1.30        | 1.38     |
| 3   | L5    | 3618 | PSU  | C4-N3   | -4.48 | 1.30        | 1.38     |
| 3   | L5    | 4491 | PSU  | C4-N3   | -4.47 | 1.30        | 1.38     |
| 3   | L5    | 1303 | OMG  | C6-N1   | -4.38 | 1.30        | 1.38     |
| 3   | L5    | 1523 | PSU  | C4-N3   | -4.36 | 1.30        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L5    | 4522 | PSU  | C4-N3 | -4.28 | 1.30        | 1.38     |
| 3   | L5    | 4362 | OMG  | C6-N1 | -4.26 | 1.30        | 1.38     |
| 80  | Bv    | 37   | UY4  | C5-C4 | 4.22  | 1.46        | 1.39     |
| 3   | L5    | 4590 | OMU  | C4-N3 | -4.21 | 1.31        | 1.38     |
| 3   | L5    | 1670 | PSU  | C2-N1 | -4.19 | 1.31        | 1.36     |
| 46  | S2    | 1248 | B8N  | C4-N3 | -4.18 | 1.32        | 1.40     |
| 46  | S2    | 1832 | 6MZ  | C5-C4 | 4.12  | 1.46        | 1.39     |
| 3   | L5    | 4464 | OMG  | C6-N1 | -4.12 | 1.31        | 1.38     |
| 3   | L5    | 1670 | PSU  | C4-N3 | -4.12 | 1.31        | 1.38     |
| 3   | L5    | 3899 | PSU  | C4-N3 | -4.10 | 1.31        | 1.38     |
| 46  | S2    | 1851 | MA6  | C5-C4 | 4.08  | 1.46        | 1.39     |
| 3   | L5    | 3606 | OMG  | C6-N1 | -4.07 | 1.31        | 1.38     |
| 3   | L5    | 4607 | OMG  | C6-N1 | -4.03 | 1.31        | 1.38     |
| 3   | L5    | 3832 | PSU  | C4-N3 | -4.02 | 1.31        | 1.38     |
| 3   | L5    | 4323 | PSU  | C4-N3 | -4.02 | 1.31        | 1.38     |
| 3   | L5    | 3618 | PSU  | C2-N3 | -4.01 | 1.30        | 1.37     |
| 3   | L5    | 4643 | PSU  | C4-N3 | -4.00 | 1.31        | 1.38     |
| 3   | L5    | 4659 | PSU  | C4-N3 | -3.99 | 1.31        | 1.38     |
| 3   | L5    | 1509 | OMG  | C6-N1 | -3.98 | 1.31        | 1.38     |
| 3   | L5    | 3616 | PSU  | C2-N3 | -3.97 | 1.30        | 1.37     |
| 3   | L5    | 4276 | OMU  | C4-N3 | -3.97 | 1.31        | 1.38     |
| 3   | L5    | 364  | OMG  | C6-N1 | -3.97 | 1.31        | 1.38     |
| 3   | L5    | 3830 | PSU  | C4-N3 | -3.97 | 1.31        | 1.38     |
| 3   | L5    | 4966 | PSU  | C4-N3 | -3.95 | 1.31        | 1.38     |
| 3   | L5    | 1523 | PSU  | C2-N1 | -3.95 | 1.31        | 1.36     |
| 3   | L5    | 4263 | PSU  | C4-N3 | -3.94 | 1.31        | 1.38     |
| 46  | S2    | 1850 | MA6  | C5-C4 | 3.92  | 1.46        | 1.39     |
| 3   | L5    | 3618 | PSU  | C2-N1 | -3.87 | 1.31        | 1.36     |
| 3   | L5    | 1849 | PSU  | C4-N3 | -3.86 | 1.31        | 1.38     |
| 3   | L5    | 1313 | A2M  | C5-N7 | -3.86 | 1.32        | 1.39     |
| 3   | L5    | 4331 | PSU  | C4-N3 | -3.82 | 1.31        | 1.38     |
| 3   | L5    | 4598 | PSU  | C4-N3 | -3.82 | 1.31        | 1.38     |
| 3   | L5    | 4373 | PSU  | C4-N3 | -3.82 | 1.31        | 1.38     |
| 46  | S2    | 1081 | PSU  | C4-N3 | -3.81 | 1.31        | 1.38     |
| 3   | L5    | 1664 | PSU  | C4-N3 | -3.81 | 1.31        | 1.38     |
| 3   | L5    | 4393 | PSU  | C4-N3 | -3.79 | 1.31        | 1.38     |
| 3   | L5    | 1769 | PSU  | C4-N3 | -3.79 | 1.31        | 1.38     |
| 3   | L5    | 3616 | PSU  | C2-N1 | -3.78 | 1.31        | 1.36     |
| 3   | L5    | 4197 | OMU  | C4-N3 | -3.77 | 1.32        | 1.38     |
| 3   | L5    | 1569 | PSU  | C4-N3 | -3.77 | 1.31        | 1.38     |
| 3   | L5    | 1779 | PSU  | C4-N3 | -3.76 | 1.31        | 1.38     |
| 46  | S2    | 1692 | PSU  | C4-N3 | -3.76 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L5    | 1309 | 1MA  | C5-N7 | -3.74 | 1.31        | 1.39     |
| 3   | L5    | 4590 | OMU  | C2-N3 | -3.74 | 1.31        | 1.38     |
| 3   | L5    | 1523 | PSU  | C2-N3 | -3.73 | 1.31        | 1.37     |
| 3   | L5    | 3904 | OMU  | C2-N3 | -3.73 | 1.31        | 1.38     |
| 3   | L5    | 4282 | PSU  | C4-N3 | -3.73 | 1.31        | 1.38     |
| 3   | L5    | 4468 | OMU  | C4-N3 | -3.72 | 1.32        | 1.38     |
| 3   | L5    | 4593 | OMG  | C6-N1 | -3.72 | 1.31        | 1.38     |
| 3   | L5    | 4598 | PSU  | C2-N1 | -3.72 | 1.31        | 1.36     |
| 3   | L5    | 4427 | PSU  | C4-N3 | -3.72 | 1.31        | 1.38     |
| 3   | L5    | 4659 | PSU  | C2-N1 | -3.71 | 1.31        | 1.36     |
| 3   | L5    | 4269 | PSU  | C4-N3 | -3.71 | 1.31        | 1.38     |
| 3   | L5    | 4401 | PSU  | C4-N3 | -3.70 | 1.31        | 1.38     |
| 3   | L5    | 4502 | PSU  | C4-N3 | -3.70 | 1.31        | 1.38     |
| 46  | S2    | 406  | PSU  | C4-N3 | -3.69 | 1.31        | 1.38     |
| 3   | L5    | 4340 | OMG  | C6-N1 | -3.69 | 1.32        | 1.38     |
| 3   | L5    | 2351 | OMG  | C6-N1 | -3.68 | 1.32        | 1.38     |
| 3   | L5    | 4166 | OMG  | C6-N1 | -3.67 | 1.32        | 1.38     |
| 3   | L5    | 4975 | PSU  | C4-N3 | -3.66 | 1.32        | 1.38     |
| 3   | L5    | 4937 | PSU  | C4-N3 | -3.66 | 1.32        | 1.38     |
| 3   | L5    | 3899 | PSU  | C2-N3 | -3.65 | 1.31        | 1.37     |
| 3   | L5    | 4331 | PSU  | C2-N3 | -3.65 | 1.31        | 1.37     |
| 80  | Bv    | 37   | UY4  | C6-N1 | 3.65  | 1.40        | 1.35     |
| 3   | L5    | 4468 | OMU  | C2-N3 | -3.65 | 1.31        | 1.38     |
| 3   | L5    | 2619 | PSU  | C4-N3 | -3.64 | 1.32        | 1.38     |
| 3   | L5    | 4441 | PSU  | C4-N3 | -3.63 | 1.32        | 1.38     |
| 3   | L5    | 1731 | PSU  | C4-N3 | -3.62 | 1.32        | 1.38     |
| 3   | L5    | 3737 | PSU  | C4-N3 | -3.61 | 1.32        | 1.38     |
| 3   | L5    | 1504 | 2MG  | C6-N1 | -3.61 | 1.32        | 1.38     |
| 3   | L5    | 1670 | PSU  | C2-N3 | -3.60 | 1.31        | 1.37     |
| 3   | L5    | 3832 | PSU  | C2-N3 | -3.60 | 1.31        | 1.37     |
| 3   | L5    | 4331 | PSU  | C2-N1 | -3.59 | 1.32        | 1.36     |
| 46  | S2    | 1174 | PSU  | C4-N3 | -3.58 | 1.32        | 1.38     |
| 46  | S2    | 1248 | B8N  | C2-N3 | -3.57 | 1.32        | 1.38     |
| 3   | L5    | 2402 | PSU  | C4-N3 | -3.57 | 1.32        | 1.38     |
| 3   | L5    | 4643 | PSU  | C2-N1 | -3.57 | 1.32        | 1.36     |
| 3   | L5    | 3747 | PSU  | C4-N3 | -3.56 | 1.32        | 1.38     |
| 3   | L5    | 4491 | PSU  | C2-N3 | -3.56 | 1.31        | 1.37     |
| 3   | L5    | 2495 | PSU  | C4-N3 | -3.55 | 1.32        | 1.38     |
| 46  | S2    | 651  | PSU  | C4-N3 | -3.53 | 1.32        | 1.38     |
| 3   | L5    | 4549 | PSU  | C4-N3 | -3.53 | 1.32        | 1.38     |
| 46  | S2    | 686  | PSU  | C4-N3 | -3.53 | 1.32        | 1.38     |
| 3   | L5    | 4549 | PSU  | C2-N3 | -3.53 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L5    | 4412 | PSU  | C4-N3 | -3.52 | 1.32        | 1.38     |
| 3   | L5    | 4643 | PSU  | C2-N3 | -3.52 | 1.31        | 1.37     |
| 3   | L5    | 3749 | PSU  | C4-N3 | -3.52 | 1.32        | 1.38     |
| 3   | L5    | 2863 | OMG  | C6-N1 | -3.51 | 1.32        | 1.38     |
| 5   | L8    | 55   | PSU  | C4-N3 | -3.51 | 1.32        | 1.38     |
| 3   | L5    | 3723 | OMG  | C6-N1 | -3.51 | 1.32        | 1.38     |
| 3   | L5    | 4269 | PSU  | C2-N1 | -3.50 | 1.32        | 1.36     |
| 3   | L5    | 3743 | PSU  | C4-N3 | -3.49 | 1.32        | 1.38     |
| 46  | S2    | 601  | OMG  | C6-N1 | -3.49 | 1.32        | 1.38     |
| 3   | L5    | 3797 | UY1  | C4-N3 | -3.48 | 1.32        | 1.38     |
| 3   | L5    | 1612 | OMG  | C6-N1 | -3.48 | 1.32        | 1.38     |
| 3   | L5    | 4417 | 5MC  | C6-N1 | -3.48 | 1.32        | 1.38     |
| 3   | L5    | 1847 | PSU  | C2-N1 | -3.47 | 1.32        | 1.36     |
| 3   | L5    | 3674 | PSU  | C2-N3 | -3.47 | 1.31        | 1.37     |
| 3   | L5    | 1731 | PSU  | C2-N1 | -3.47 | 1.32        | 1.36     |
| 3   | L5    | 4469 | OMG  | C6-N1 | -3.47 | 1.32        | 1.38     |
| 3   | L5    | 3823 | PSU  | C4-N3 | -3.47 | 1.32        | 1.38     |
| 3   | L5    | 4263 | PSU  | C2-N3 | -3.46 | 1.31        | 1.37     |
| 3   | L5    | 1779 | PSU  | C2-N3 | -3.45 | 1.31        | 1.37     |
| 3   | L5    | 4190 | 6MZ  | C5-C4 | 3.45  | 1.45        | 1.39     |
| 3   | L5    | 2824 | OMU  | C4-N3 | -3.44 | 1.32        | 1.38     |
| 46  | S2    | 109  | PSU  | C4-N3 | -3.44 | 1.32        | 1.38     |
| 3   | L5    | 3823 | PSU  | C2-N1 | -3.42 | 1.32        | 1.36     |
| 3   | L5    | 3830 | PSU  | C2-N1 | -3.42 | 1.32        | 1.36     |
| 3   | L5    | 4588 | OMG  | C6-N1 | -3.42 | 1.32        | 1.38     |
| 46  | S2    | 1004 | PSU  | C4-N3 | -3.42 | 1.32        | 1.38     |
| 3   | L5    | 1509 | OMG  | C5-N7 | -3.42 | 1.32        | 1.39     |
| 3   | L5    | 4522 | PSU  | C2-N1 | -3.42 | 1.32        | 1.36     |
| 3   | L5    | 1313 | A2M  | C8-N9 | -3.42 | 1.31        | 1.37     |
| 5   | L8    | 69   | PSU  | C4-N3 | -3.41 | 1.32        | 1.38     |
| 3   | L5    | 4966 | PSU  | C2-N3 | -3.41 | 1.31        | 1.37     |
| 3   | L5    | 4190 | 6MZ  | C5-N7 | -3.41 | 1.32        | 1.39     |
| 3   | L5    | 3878 | OMG  | C6-N1 | -3.40 | 1.32        | 1.38     |
| 46  | S2    | 1177 | PSU  | C4-N3 | -3.40 | 1.32        | 1.38     |
| 46  | S2    | 1232 | PSU  | C4-N3 | -3.40 | 1.32        | 1.38     |
| 46  | S2    | 1490 | OMG  | C6-N1 | -3.39 | 1.32        | 1.38     |
| 46  | S2    | 1136 | PSU  | C4-N3 | -3.39 | 1.32        | 1.38     |
| 3   | L5    | 3832 | PSU  | C2-N1 | -3.38 | 1.32        | 1.36     |
| 46  | S2    | 649  | PSU  | C4-N3 | -3.38 | 1.32        | 1.38     |
| 3   | L5    | 4546 | PSU  | C4-N3 | -3.37 | 1.32        | 1.38     |
| 3   | L5    | 3904 | OMU  | C5-C4 | -3.37 | 1.36        | 1.43     |
| 3   | L5    | 4323 | PSU  | C2-N3 | -3.37 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L5    | 1670 | PSU  | C6-N1 | -3.37 | 1.30        | 1.36     |
| 46  | S2    | 1238 | PSU  | C4-N3 | -3.37 | 1.32        | 1.38     |
| 3   | L5    | 4502 | PSU  | C2-N3 | -3.36 | 1.31        | 1.37     |
| 3   | L5    | 1768 | PSU  | C4-N3 | -3.36 | 1.32        | 1.38     |
| 3   | L5    | 4470 | PSU  | C4-N3 | -3.35 | 1.32        | 1.38     |
| 3   | L5    | 4412 | PSU  | C2-N1 | -3.35 | 1.32        | 1.36     |
| 46  | S2    | 815  | PSU  | C4-N3 | -3.34 | 1.32        | 1.38     |
| 3   | L5    | 4441 | PSU  | C2-N1 | -3.33 | 1.32        | 1.36     |
| 3   | L5    | 4427 | PSU  | C2-N3 | -3.31 | 1.32        | 1.37     |
| 3   | L5    | 2411 | OMG  | C6-N1 | -3.31 | 1.32        | 1.38     |
| 3   | L5    | 3761 | 5MC  | C6-N1 | -3.30 | 1.32        | 1.38     |
| 3   | L5    | 1847 | PSU  | C4-N3 | -3.30 | 1.32        | 1.38     |
| 3   | L5    | 4606 | PSU  | C4-N3 | -3.30 | 1.32        | 1.38     |
| 46  | S2    | 1326 | OMU  | C4-N3 | -3.30 | 1.33        | 1.38     |
| 3   | L5    | 1849 | PSU  | C2-N3 | -3.29 | 1.32        | 1.37     |
| 46  | S2    | 966  | PSU  | C4-N3 | -3.29 | 1.32        | 1.38     |
| 46  | S2    | 1045 | PSU  | C4-N3 | -3.29 | 1.32        | 1.38     |
| 80  | Bv    | 9    | 1MG  | C5-C4 | 3.29  | 1.47        | 1.38     |
| 3   | L5    | 4266 | PSU  | C4-N3 | -3.29 | 1.32        | 1.38     |
| 3   | L5    | 3674 | PSU  | C2-N1 | -3.29 | 1.32        | 1.36     |
| 46  | S2    | 121  | OMU  | C4-N3 | -3.28 | 1.33        | 1.38     |
| 3   | L5    | 4464 | OMG  | C5-N7 | -3.28 | 1.32        | 1.39     |
| 3   | L5    | 3694 | PSU  | C4-N3 | -3.28 | 1.32        | 1.38     |
| 46  | S2    | 801  | PSU  | C4-N3 | -3.27 | 1.32        | 1.38     |
| 3   | L5    | 1847 | PSU  | C2-N3 | -3.27 | 1.32        | 1.37     |
| 3   | L5    | 1504 | 2MG  | C5-N7 | -3.27 | 1.32        | 1.39     |
| 46  | S2    | 863  | PSU  | C4-N3 | -3.27 | 1.32        | 1.38     |
| 3   | L5    | 2619 | PSU  | C2-N3 | -3.26 | 1.32        | 1.37     |
| 3   | L5    | 4659 | PSU  | C2-N3 | -3.26 | 1.32        | 1.37     |
| 3   | L5    | 4373 | PSU  | C2-N3 | -3.25 | 1.32        | 1.37     |
| 3   | L5    | 3899 | PSU  | C2-N1 | -3.25 | 1.32        | 1.36     |
| 3   | L5    | 3741 | PSU  | C4-N3 | -3.25 | 1.32        | 1.38     |
| 3   | L5    | 4522 | PSU  | C2-N3 | -3.25 | 1.32        | 1.37     |
| 46  | S2    | 1643 | PSU  | C4-N3 | -3.25 | 1.32        | 1.38     |
| 3   | L5    | 1731 | PSU  | C2-N3 | -3.25 | 1.32        | 1.37     |
| 3   | L5    | 3737 | PSU  | C2-N3 | -3.24 | 1.32        | 1.37     |
| 46  | S2    | 36   | PSU  | C4-N3 | -3.24 | 1.32        | 1.38     |
| 3   | L5    | 3830 | PSU  | C2-N3 | -3.24 | 1.32        | 1.37     |
| 3   | L5    | 4276 | OMU  | C2-N3 | -3.24 | 1.32        | 1.38     |
| 46  | S2    | 105  | PSU  | C4-N3 | -3.24 | 1.32        | 1.38     |
| 3   | L5    | 3709 | PSU  | C4-N3 | -3.23 | 1.32        | 1.38     |
| 80  | Bv    | 58   | 1MA  | C6-N6 | 3.23  | 1.35        | 1.28     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 46  | S2    | 814  | PSU  | C4-N3 | -3.23 | 1.32        | 1.38     |
| 46  | S2    | 119  | PSU  | C4-N3 | -3.23 | 1.32        | 1.38     |
| 3   | L5    | 2824 | OMU  | C5-C4 | -3.22 | 1.36        | 1.43     |
| 80  | Bv    | 55   | PSU  | C6-C5 | 3.21  | 1.38        | 1.35     |
| 3   | L5    | 4282 | PSU  | C2-N3 | -3.21 | 1.32        | 1.37     |
| 3   | L5    | 1303 | OMG  | C5-N7 | -3.21 | 1.32        | 1.39     |
| 46  | S2    | 683  | OMG  | C6-N1 | -3.20 | 1.32        | 1.38     |
| 5   | L8    | 75   | OMG  | C6-N1 | -3.20 | 1.32        | 1.38     |
| 3   | L5    | 4546 | PSU  | C2-N1 | -3.20 | 1.32        | 1.36     |
| 46  | S2    | 218  | PSU  | C4-N3 | -3.20 | 1.32        | 1.38     |
| 80  | Bv    | 58   | 1MA  | C5-C4 | 3.19  | 1.47        | 1.38     |
| 3   | L5    | 4590 | OMU  | C5-C4 | -3.19 | 1.36        | 1.43     |
| 3   | L5    | 3771 | OMG  | C6-N1 | -3.19 | 1.32        | 1.38     |
| 3   | L5    | 3723 | OMG  | C5-N7 | -3.18 | 1.32        | 1.39     |
| 3   | L5    | 1569 | PSU  | C2-N1 | -3.18 | 1.32        | 1.36     |
| 46  | S2    | 1046 | PSU  | C4-N3 | -3.17 | 1.32        | 1.38     |
| 3   | L5    | 3771 | OMG  | C5-N7 | -3.17 | 1.32        | 1.39     |
| 80  | Bv    | 46   | G7M  | C5-C4 | 3.16  | 1.46        | 1.38     |
| 80  | Bv    | 27   | PSU  | C6-C5 | 3.16  | 1.38        | 1.35     |
| 46  | S2    | 1367 | PSU  | C4-N3 | -3.16 | 1.32        | 1.38     |
| 46  | S2    | 1081 | PSU  | C2-N3 | -3.16 | 1.32        | 1.37     |
| 46  | S2    | 1442 | OMU  | C4-N3 | -3.16 | 1.33        | 1.38     |
| 46  | S2    | 1347 | PSU  | C4-N3 | -3.15 | 1.32        | 1.38     |
| 3   | L5    | 1569 | PSU  | C2-N3 | -3.15 | 1.32        | 1.37     |
| 3   | L5    | 4276 | OMU  | C5-C4 | -3.15 | 1.36        | 1.43     |
| 46  | S2    | 34   | PSU  | C4-N3 | -3.15 | 1.33        | 1.38     |
| 46  | S2    | 1850 | MA6  | C8-N9 | -3.13 | 1.32        | 1.37     |
| 46  | S2    | 644  | OMG  | C6-N1 | -3.13 | 1.33        | 1.38     |
| 3   | L5    | 4269 | PSU  | C2-N3 | -3.13 | 1.32        | 1.37     |
| 3   | L5    | 2495 | PSU  | C2-N1 | -3.13 | 1.32        | 1.36     |
| 3   | L5    | 4263 | PSU  | C2-N1 | -3.12 | 1.32        | 1.36     |
| 3   | L5    | 4323 | PSU  | C2-N1 | -3.12 | 1.32        | 1.36     |
| 3   | L5    | 3713 | PSU  | C4-N3 | -3.12 | 1.33        | 1.38     |
| 46  | S2    | 866  | PSU  | C4-N3 | -3.11 | 1.33        | 1.38     |
| 3   | L5    | 1769 | PSU  | C2-N3 | -3.11 | 1.32        | 1.37     |
| 3   | L5    | 4502 | PSU  | C2-N1 | -3.11 | 1.32        | 1.36     |
| 3   | L5    | 3747 | PSU  | C2-N3 | -3.10 | 1.32        | 1.37     |
| 3   | L5    | 1313 | A2M  | C4-N9 | -3.10 | 1.31        | 1.37     |
| 3   | L5    | 364  | OMG  | C5-N7 | -3.09 | 1.32        | 1.39     |
| 46  | S2    | 436  | OMG  | C6-N1 | -3.09 | 1.33        | 1.38     |
| 46  | S2    | 1328 | OMG  | C6-N1 | -3.08 | 1.33        | 1.38     |
| 3   | L5    | 3747 | PSU  | C2-N1 | -3.08 | 1.32        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | S2    | 572  | PSU  | C4-N3   | -3.08 | 1.33        | 1.38     |
| 3   | L5    | 2411 | OMG  | C4-N9   | -3.07 | 1.30        | 1.38     |
| 46  | S2    | 1692 | PSU  | C2-N3   | -3.07 | 1.32        | 1.37     |
| 3   | L5    | 4966 | PSU  | C2-N1   | -3.07 | 1.32        | 1.36     |
| 80  | Bv    | 26   | M2G  | C5-C4   | 3.07  | 1.47        | 1.38     |
| 80  | Bv    | 37   | UY4  | C09-N6  | 3.07  | 1.44        | 1.37     |
| 46  | S2    | 1174 | PSU  | C2-N1   | -3.07 | 1.32        | 1.36     |
| 3   | L5    | 2411 | OMG  | C5-N7   | -3.06 | 1.32        | 1.39     |
| 46  | S2    | 609  | PSU  | C4-N3   | -3.06 | 1.33        | 1.38     |
| 3   | L5    | 4606 | PSU  | C2-N3   | -3.06 | 1.32        | 1.37     |
| 3   | L5    | 4198 | OMG  | C6-N1   | -3.06 | 1.33        | 1.38     |
| 46  | S2    | 1136 | PSU  | C2-N3   | -3.06 | 1.32        | 1.37     |
| 46  | S2    | 866  | PSU  | C6-C5   | 3.06  | 1.38        | 1.35     |
| 46  | S2    | 1445 | PSU  | C4-N3   | -3.05 | 1.33        | 1.38     |
| 3   | L5    | 2495 | PSU  | C2-N3   | -3.04 | 1.32        | 1.37     |
| 80  | Bv    | 10   | 2MG  | C5-C4   | 3.04  | 1.47        | 1.38     |
| 46  | S2    | 121  | OMU  | C2-N3   | -3.04 | 1.32        | 1.38     |
| 46  | S2    | 172  | OMU  | C4-N3   | -3.04 | 1.33        | 1.38     |
| 3   | L5    | 4607 | OMG  | C5-N7   | -3.03 | 1.33        | 1.39     |
| 3   | L5    | 2402 | PSU  | C2-N3   | -3.03 | 1.32        | 1.37     |
| 46  | S2    | 822  | PSU  | C4-N3   | -3.03 | 1.33        | 1.38     |
| 46  | S2    | 1337 | 4AC  | C4-N4   | -3.03 | 1.35        | 1.39     |
| 3   | L5    | 3743 | PSU  | C2-N3   | -3.03 | 1.32        | 1.37     |
| 3   | L5    | 4598 | PSU  | C2-N3   | -3.02 | 1.32        | 1.37     |
| 3   | L5    | 4937 | PSU  | C2-N3   | -3.02 | 1.32        | 1.37     |
| 46  | S2    | 509  | OMG  | C6-N1   | -3.02 | 1.33        | 1.38     |
| 46  | S2    | 1046 | PSU  | C2-N1   | -3.02 | 1.32        | 1.36     |
| 3   | L5    | 2824 | OMU  | C2-N3   | -3.02 | 1.32        | 1.38     |
| 46  | S2    | 1232 | PSU  | C6-C5   | 3.02  | 1.38        | 1.35     |
| 3   | L5    | 4549 | PSU  | C2-N1   | -3.01 | 1.32        | 1.36     |
| 3   | L5    | 4401 | PSU  | C2-N1   | -3.01 | 1.32        | 1.36     |
| 3   | L5    | 4197 | OMU  | C2-N3   | -3.01 | 1.32        | 1.38     |
| 3   | L5    | 1664 | PSU  | C2-N3   | -3.00 | 1.32        | 1.37     |
| 46  | S2    | 1177 | PSU  | C2-N1   | -3.00 | 1.32        | 1.36     |
| 3   | L5    | 3761 | 5MC  | C5-C4   | 2.99  | 1.46        | 1.44     |
| 3   | L5    | 1664 | PSU  | O4'-C1' | -2.99 | 1.39        | 1.43     |
| 3   | L5    | 4401 | PSU  | C2-N3   | -2.99 | 1.32        | 1.37     |
| 3   | L5    | 1612 | OMG  | C5-N7   | -2.98 | 1.33        | 1.39     |
| 46  | S2    | 105  | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 3   | L5    | 1309 | 1MA  | C4-N9   | -2.97 | 1.30        | 1.38     |
| 3   | L5    | 3820 | OMC  | C5-C4   | -2.97 | 1.36        | 1.42     |
| 46  | S2    | 93   | PSU  | C4-N3   | -2.97 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 46  | S2    | 1288 | OMU  | C4-N3 | -2.96 | 1.33        | 1.38     |
| 46  | S2    | 572  | PSU  | C6-C5 | 2.96  | 1.38        | 1.35     |
| 3   | L5    | 4598 | PSU  | C6-N1 | -2.96 | 1.31        | 1.36     |
| 3   | L5    | 4975 | PSU  | C2-N1 | -2.96 | 1.32        | 1.36     |
| 3   | L5    | 4412 | PSU  | C2-N3 | -2.96 | 1.32        | 1.37     |
| 3   | L5    | 4427 | PSU  | C2-N1 | -2.95 | 1.32        | 1.36     |
| 80  | Bv    | 28   | PSU  | C4-N3 | -2.94 | 1.33        | 1.38     |
| 3   | L5    | 4975 | PSU  | C6-C5 | 2.93  | 1.38        | 1.35     |
| 3   | L5    | 4468 | OMU  | C5-C4 | -2.93 | 1.37        | 1.43     |
| 46  | S2    | 1832 | 6MZ  | C4-N9 | -2.92 | 1.31        | 1.37     |
| 3   | L5    | 1849 | PSU  | C2-N1 | -2.92 | 1.32        | 1.36     |
| 3   | L5    | 4190 | 6MZ  | C4-N9 | -2.92 | 1.31        | 1.37     |
| 46  | S2    | 1625 | PSU  | C4-N3 | -2.90 | 1.33        | 1.38     |
| 46  | S2    | 867  | OMG  | C6-N1 | -2.90 | 1.33        | 1.38     |
| 3   | L5    | 3878 | OMG  | C5-N7 | -2.90 | 1.33        | 1.39     |
| 46  | S2    | 1804 | OMU  | C4-N3 | -2.90 | 1.33        | 1.38     |
| 3   | L5    | 4198 | OMG  | C5-N7 | -2.89 | 1.33        | 1.39     |
| 46  | S2    | 649  | PSU  | C2-N3 | -2.88 | 1.32        | 1.37     |
| 3   | L5    | 1664 | PSU  | C2-N1 | -2.88 | 1.32        | 1.36     |
| 46  | S2    | 1244 | PSU  | C4-N3 | -2.87 | 1.33        | 1.38     |
| 3   | L5    | 2863 | OMG  | C5-N7 | -2.87 | 1.33        | 1.39     |
| 3   | L5    | 4340 | OMG  | C5-N7 | -2.87 | 1.33        | 1.39     |
| 3   | L5    | 4166 | OMG  | C5-N7 | -2.87 | 1.33        | 1.39     |
| 46  | S2    | 406  | PSU  | C2-N3 | -2.87 | 1.32        | 1.37     |
| 46  | S2    | 601  | OMG  | C5-N7 | -2.87 | 1.33        | 1.39     |
| 3   | L5    | 2338 | OMC  | C5-C4 | -2.87 | 1.36        | 1.42     |
| 5   | L8    | 69   | PSU  | C2-N3 | -2.87 | 1.32        | 1.37     |
| 46  | S2    | 1177 | PSU  | C2-N3 | -2.86 | 1.32        | 1.37     |
| 80  | Bv    | 28   | PSU  | C6-C5 | 2.86  | 1.38        | 1.35     |
| 3   | L5    | 3743 | PSU  | C2-N1 | -2.86 | 1.32        | 1.36     |
| 3   | L5    | 3694 | PSU  | C2-N3 | -2.86 | 1.32        | 1.37     |
| 46  | S2    | 686  | PSU  | C2-N3 | -2.86 | 1.32        | 1.37     |
| 46  | S2    | 109  | PSU  | C2-N3 | -2.84 | 1.32        | 1.37     |
| 3   | L5    | 4197 | OMU  | C5-C4 | -2.84 | 1.37        | 1.43     |
| 46  | S2    | 649  | PSU  | C6-C5 | 2.84  | 1.38        | 1.35     |
| 3   | L5    | 4266 | PSU  | C2-N3 | -2.84 | 1.32        | 1.37     |
| 3   | L5    | 3797 | UY1  | C2-N3 | -2.84 | 1.32        | 1.37     |
| 3   | L5    | 4362 | OMG  | C5-N7 | -2.84 | 1.33        | 1.39     |
| 3   | L5    | 1313 | A2M  | C5-C4 | 2.84  | 1.44        | 1.39     |
| 3   | L5    | 3823 | PSU  | C2-N3 | -2.83 | 1.32        | 1.37     |
| 3   | L5    | 4166 | OMG  | C4-N9 | -2.83 | 1.30        | 1.38     |
| 3   | L5    | 2619 | PSU  | C2-N1 | -2.83 | 1.33        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | L5    | 4606 | PSU  | C2-N1   | -2.82 | 1.33        | 1.36     |
| 46  | S2    | 863  | PSU  | C2-N1   | -2.82 | 1.33        | 1.36     |
| 46  | S2    | 1639 | G7M  | C6-N1   | -2.82 | 1.33        | 1.38     |
| 3   | L5    | 3741 | PSU  | C6-C5   | 2.82  | 1.38        | 1.35     |
| 80  | Bv    | 37   | UY4  | C5-N7   | -2.82 | 1.33        | 1.39     |
| 3   | L5    | 1768 | PSU  | C2-N1   | -2.81 | 1.33        | 1.36     |
| 5   | L8    | 55   | PSU  | C2-N1   | -2.81 | 1.33        | 1.36     |
| 46  | S2    | 1842 | 4AC  | C6-N1   | -2.81 | 1.31        | 1.38     |
| 46  | S2    | 863  | PSU  | C6-C5   | 2.81  | 1.38        | 1.35     |
| 3   | L5    | 4441 | PSU  | C2-N3   | -2.81 | 1.32        | 1.37     |
| 46  | S2    | 1326 | OMU  | C2-N3   | -2.80 | 1.33        | 1.38     |
| 3   | L5    | 4282 | PSU  | C2-N1   | -2.80 | 1.33        | 1.36     |
| 3   | L5    | 1768 | PSU  | C2-N3   | -2.80 | 1.32        | 1.37     |
| 46  | S2    | 1238 | PSU  | C2-N1   | -2.79 | 1.33        | 1.36     |
| 3   | L5    | 4491 | PSU  | O4'-C1' | -2.79 | 1.40        | 1.43     |
| 46  | S2    | 116  | OMU  | C5-C4   | -2.79 | 1.37        | 1.43     |
| 3   | L5    | 4373 | PSU  | C2-N1   | -2.79 | 1.33        | 1.36     |
| 3   | L5    | 1769 | PSU  | C2-N1   | -2.79 | 1.33        | 1.36     |
| 3   | L5    | 3606 | OMG  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 3   | L5    | 4469 | OMG  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 46  | S2    | 1842 | 4AC  | C4-N4   | -2.78 | 1.35        | 1.39     |
| 46  | S2    | 1232 | PSU  | C2-N3   | -2.78 | 1.32        | 1.37     |
| 3   | L5    | 3723 | OMG  | C4-N9   | -2.78 | 1.31        | 1.38     |
| 46  | S2    | 1851 | MA6  | C5-N7   | -2.78 | 1.34        | 1.39     |
| 3   | L5    | 4500 | UR3  | C5-C4   | -2.78 | 1.36        | 1.43     |
| 3   | L5    | 3749 | PSU  | C2-N3   | -2.78 | 1.32        | 1.37     |
| 46  | S2    | 1639 | G7M  | C5-C4   | 2.78  | 1.45        | 1.38     |
| 46  | S2    | 814  | PSU  | C2-N3   | -2.77 | 1.32        | 1.37     |
| 3   | L5    | 3823 | PSU  | C6-N1   | -2.77 | 1.31        | 1.36     |
| 46  | S2    | 428  | OMU  | C4-N3   | -2.76 | 1.33        | 1.38     |
| 46  | S2    | 822  | PSU  | C6-C5   | 2.76  | 1.38        | 1.35     |
| 3   | L5    | 4546 | PSU  | C2-N3   | -2.75 | 1.32        | 1.37     |
| 46  | S2    | 1328 | OMG  | C5-C4   | 2.75  | 1.46        | 1.38     |
| 3   | L5    | 3737 | PSU  | C2-N1   | -2.75 | 1.33        | 1.36     |
| 46  | S2    | 172  | OMU  | C2-N3   | -2.75 | 1.33        | 1.38     |
| 46  | S2    | 1851 | MA6  | C8-N9   | -2.75 | 1.32        | 1.37     |
| 46  | S2    | 1490 | OMG  | C5-N7   | -2.74 | 1.33        | 1.39     |
| 3   | L5    | 2791 | OMC  | C5-C4   | -2.74 | 1.36        | 1.42     |
| 3   | L5    | 4393 | PSU  | C2-N3   | -2.74 | 1.33        | 1.37     |
| 46  | S2    | 1445 | PSU  | C6-C5   | 2.74  | 1.38        | 1.35     |
| 46  | S2    | 867  | OMG  | C5-C4   | 2.74  | 1.46        | 1.38     |
| 46  | S2    | 649  | PSU  | C2-N1   | -2.74 | 1.33        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | L5    | 2402 | PSU  | C2-N1 | -2.73 | 1.33        | 1.36     |
| 46  | S2    | 509  | OMG  | C5-C4 | 2.73  | 1.46        | 1.38     |
| 46  | S2    | 93   | PSU  | C2-N3 | -2.73 | 1.33        | 1.37     |
| 46  | S2    | 1177 | PSU  | C6-C5 | 2.73  | 1.38        | 1.35     |
| 80  | Bv    | 26   | M2G  | C2-N2 | 2.73  | 1.40        | 1.35     |
| 46  | S2    | 644  | OMG  | C5-C4 | 2.73  | 1.46        | 1.38     |
| 46  | S2    | 966  | PSU  | C6-C5 | 2.73  | 1.38        | 1.35     |
| 3   | L5    | 3616 | PSU  | C6-N1 | -2.73 | 1.31        | 1.36     |
| 46  | S2    | 644  | OMG  | C5-N7 | -2.72 | 1.33        | 1.39     |
| 5   | L8    | 75   | OMG  | C5-N7 | -2.72 | 1.33        | 1.39     |
| 3   | L5    | 4975 | PSU  | C2-N3 | -2.72 | 1.33        | 1.37     |
| 3   | L5    | 4393 | PSU  | C6-C5 | 2.72  | 1.38        | 1.35     |
| 46  | S2    | 1045 | PSU  | C2-N3 | -2.72 | 1.33        | 1.37     |
| 46  | S2    | 683  | OMG  | C5-N7 | -2.72 | 1.33        | 1.39     |
| 46  | S2    | 218  | PSU  | C6-C5 | 2.71  | 1.38        | 1.35     |
| 46  | S2    | 1692 | PSU  | C2-N1 | -2.71 | 1.33        | 1.36     |
| 46  | S2    | 609  | PSU  | C6-C5 | 2.71  | 1.38        | 1.35     |
| 46  | S2    | 116  | OMU  | C4-N3 | -2.71 | 1.34        | 1.38     |
| 3   | L5    | 2409 | OMC  | C5-C4 | -2.71 | 1.36        | 1.42     |
| 46  | S2    | 119  | PSU  | C2-N3 | -2.71 | 1.33        | 1.37     |
| 3   | L5    | 1779 | PSU  | C2-N1 | -2.71 | 1.33        | 1.36     |
| 80  | Bv    | 27   | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 46  | S2    | 1004 | PSU  | C2-N1 | -2.70 | 1.33        | 1.36     |
| 5   | L8    | 55   | PSU  | C2-N3 | -2.70 | 1.33        | 1.37     |
| 3   | L5    | 3709 | PSU  | C2-N3 | -2.70 | 1.33        | 1.37     |
| 46  | S2    | 34   | PSU  | C6-C5 | 2.69  | 1.38        | 1.35     |
| 46  | S2    | 509  | OMG  | C5-N7 | -2.69 | 1.33        | 1.39     |
| 3   | L5    | 4266 | PSU  | C6-C5 | 2.69  | 1.38        | 1.35     |
| 46  | S2    | 1046 | PSU  | C2-N3 | -2.69 | 1.33        | 1.37     |
| 46  | S2    | 1625 | PSU  | C6-C5 | 2.69  | 1.38        | 1.35     |
| 46  | S2    | 218  | PSU  | C2-N3 | -2.69 | 1.33        | 1.37     |
| 46  | S2    | 601  | OMG  | C4-N9 | -2.69 | 1.31        | 1.38     |
| 46  | S2    | 1442 | OMU  | C5-C4 | -2.67 | 1.37        | 1.43     |
| 5   | L8    | 75   | OMG  | C4-N9 | -2.67 | 1.31        | 1.38     |
| 80  | Bv    | 55   | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 46  | S2    | 1442 | OMU  | C2-N3 | -2.67 | 1.33        | 1.38     |
| 3   | L5    | 1303 | OMG  | C2-N1 | -2.66 | 1.31        | 1.37     |
| 3   | L5    | 4470 | PSU  | C2-N1 | -2.66 | 1.33        | 1.36     |
| 3   | L5    | 1327 | OMC  | C5-C4 | -2.66 | 1.36        | 1.42     |
| 46  | S2    | 683  | OMG  | C5-C4 | 2.66  | 1.46        | 1.38     |
| 46  | S2    | 651  | PSU  | C6-C5 | 2.65  | 1.38        | 1.35     |
| 46  | S2    | 1851 | MA6  | C4-N9 | -2.65 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | L5    | 2351 | OMG  | C5-N7   | -2.65 | 1.33        | 1.39     |
| 3   | L5    | 3848 | OMC  | C5-C4   | -2.65 | 1.36        | 1.42     |
| 3   | L5    | 4937 | PSU  | C2-N1   | -2.65 | 1.33        | 1.36     |
| 3   | L5    | 3749 | PSU  | C2-N1   | -2.65 | 1.33        | 1.36     |
| 3   | L5    | 4390 | PSU  | C4-N3   | -2.64 | 1.33        | 1.38     |
| 46  | S2    | 1045 | PSU  | C2-N1   | -2.64 | 1.33        | 1.36     |
| 46  | S2    | 1832 | 6MZ  | C8-N9   | -2.64 | 1.33        | 1.37     |
| 3   | L5    | 4522 | PSU  | C6-N1   | -2.64 | 1.32        | 1.36     |
| 46  | S2    | 1850 | MA6  | C5-N7   | -2.64 | 1.34        | 1.39     |
| 46  | S2    | 815  | PSU  | C2-N3   | -2.64 | 1.33        | 1.37     |
| 3   | L5    | 3797 | UY1  | O4'-C1' | -2.64 | 1.40        | 1.43     |
| 3   | L5    | 3694 | PSU  | C2-N1   | -2.64 | 1.33        | 1.36     |
| 46  | S2    | 105  | PSU  | C2-N3   | -2.64 | 1.33        | 1.37     |
| 46  | S2    | 116  | OMU  | C2-N3   | -2.64 | 1.33        | 1.38     |
| 3   | L5    | 4966 | PSU  | C6-C5   | 2.63  | 1.38        | 1.35     |
| 3   | L5    | 4643 | PSU  | C6-N1   | -2.63 | 1.32        | 1.36     |
| 46  | S2    | 1832 | 6MZ  | C5-C6   | 2.63  | 1.48        | 1.41     |
| 3   | L5    | 4470 | PSU  | C2-N3   | -2.63 | 1.33        | 1.37     |
| 46  | S2    | 36   | PSU  | C6-C5   | 2.63  | 1.38        | 1.35     |
| 46  | S2    | 1851 | MA6  | C5-C6   | 2.63  | 1.48        | 1.41     |
| 46  | S2    | 801  | PSU  | C2-N3   | -2.62 | 1.33        | 1.37     |
| 3   | L5    | 4426 | OMC  | C5-C4   | -2.62 | 1.36        | 1.42     |
| 3   | L5    | 4607 | OMG  | C4-N9   | -2.62 | 1.31        | 1.38     |
| 46  | S2    | 1174 | PSU  | C2-N3   | -2.62 | 1.33        | 1.37     |
| 3   | L5    | 4266 | PSU  | C2-N1   | -2.62 | 1.33        | 1.36     |
| 46  | S2    | 801  | PSU  | C6-C5   | 2.61  | 1.38        | 1.35     |
| 3   | L5    | 364  | OMG  | C4-N9   | -2.61 | 1.31        | 1.38     |
| 46  | S2    | 406  | PSU  | C2-N1   | -2.60 | 1.33        | 1.36     |
| 3   | L5    | 2791 | OMC  | C6-N1   | -2.60 | 1.31        | 1.38     |
| 46  | S2    | 815  | PSU  | C6-C5   | 2.60  | 1.38        | 1.35     |
| 46  | S2    | 601  | OMG  | C5-C4   | 2.60  | 1.45        | 1.38     |
| 3   | L5    | 4588 | OMG  | C4-N9   | -2.60 | 1.31        | 1.38     |
| 3   | L5    | 1847 | PSU  | C6-C5   | 2.59  | 1.38        | 1.35     |
| 46  | S2    | 1804 | OMU  | C5-C4   | -2.59 | 1.38        | 1.43     |
| 80  | Bv    | 47   | H2U  | C2-N3   | -2.59 | 1.33        | 1.38     |
| 3   | L5    | 4606 | PSU  | O4'-C1' | -2.58 | 1.40        | 1.43     |
| 80  | Bv    | 16   | H2U  | C2-N3   | -2.58 | 1.33        | 1.38     |
| 46  | S2    | 966  | PSU  | C2-N3   | -2.58 | 1.33        | 1.37     |
| 46  | S2    | 1232 | PSU  | C2-N1   | -2.57 | 1.33        | 1.36     |
| 3   | L5    | 4588 | OMG  | C5-N7   | -2.57 | 1.33        | 1.39     |
| 3   | L5    | 4491 | PSU  | C2-N1   | -2.57 | 1.33        | 1.36     |
| 3   | L5    | 3878 | OMG  | C4-N9   | -2.57 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | L5    | 3606 | OMG  | C4-N9   | -2.57 | 1.31        | 1.38     |
| 46  | S2    | 119  | PSU  | C6-C5   | 2.57  | 1.38        | 1.35     |
| 5   | L8    | 69   | PSU  | C6-N1   | -2.57 | 1.32        | 1.36     |
| 46  | S2    | 1004 | PSU  | C2-N3   | -2.57 | 1.33        | 1.37     |
| 46  | S2    | 1804 | OMU  | C2-N3   | -2.57 | 1.33        | 1.38     |
| 3   | L5    | 4412 | PSU  | O4'-C1' | -2.56 | 1.40        | 1.43     |
| 46  | S2    | 34   | PSU  | C2-N3   | -2.56 | 1.33        | 1.37     |
| 46  | S2    | 428  | OMU  | C2-N3   | -2.56 | 1.33        | 1.38     |
| 46  | S2    | 1288 | OMU  | C2-N3   | -2.56 | 1.33        | 1.38     |
| 46  | S2    | 1367 | PSU  | C6-C5   | 2.55  | 1.38        | 1.35     |
| 46  | S2    | 1081 | PSU  | C2-N1   | -2.55 | 1.33        | 1.36     |
| 3   | L5    | 3680 | OMC  | C6-N1   | -2.55 | 1.32        | 1.38     |
| 3   | L5    | 4393 | PSU  | C2-N1   | -2.55 | 1.33        | 1.36     |
| 3   | L5    | 4522 | PSU  | C6-C5   | 2.54  | 1.38        | 1.35     |
| 46  | S2    | 814  | PSU  | C6-C5   | 2.54  | 1.38        | 1.35     |
| 3   | L5    | 364  | OMG  | C8-N9   | -2.54 | 1.31        | 1.37     |
| 46  | S2    | 1328 | OMG  | C5-N7   | -2.54 | 1.34        | 1.39     |
| 46  | S2    | 1643 | PSU  | C2-N3   | -2.54 | 1.33        | 1.37     |
| 3   | L5    | 3820 | OMC  | C6-N1   | -2.54 | 1.32        | 1.38     |
| 46  | S2    | 822  | PSU  | C2-N1   | -2.53 | 1.33        | 1.36     |
| 3   | L5    | 1523 | PSU  | C6-N1   | -2.53 | 1.32        | 1.36     |
| 46  | S2    | 1136 | PSU  | C2-N1   | -2.53 | 1.33        | 1.36     |
| 3   | L5    | 3713 | PSU  | C2-N3   | -2.53 | 1.33        | 1.37     |
| 3   | L5    | 4362 | OMG  | C4-N9   | -2.53 | 1.31        | 1.38     |
| 46  | S2    | 93   | PSU  | C2-N1   | -2.53 | 1.33        | 1.36     |
| 3   | L5    | 3771 | OMG  | C4-N9   | -2.52 | 1.31        | 1.38     |
| 3   | L5    | 4469 | OMG  | C4-N9   | -2.52 | 1.31        | 1.38     |
| 46  | S2    | 1832 | 6MZ  | C5-N7   | -2.52 | 1.34        | 1.39     |
| 3   | L5    | 3787 | OMC  | C6-N1   | -2.52 | 1.32        | 1.38     |
| 46  | S2    | 1643 | PSU  | C2-N1   | -2.52 | 1.33        | 1.36     |
| 3   | L5    | 3797 | UY1  | C2-N1   | -2.51 | 1.33        | 1.36     |
| 46  | S2    | 109  | PSU  | C2-N1   | -2.50 | 1.33        | 1.36     |
| 46  | S2    | 36   | PSU  | C2-N3   | -2.50 | 1.33        | 1.37     |
| 46  | S2    | 651  | PSU  | C2-N3   | -2.50 | 1.33        | 1.37     |
| 46  | S2    | 1850 | MA6  | C5-C6   | 2.50  | 1.47        | 1.41     |
| 3   | L5    | 4276 | OMU  | C6-N1   | -2.49 | 1.32        | 1.38     |
| 3   | L5    | 4426 | OMC  | C6-N1   | -2.49 | 1.32        | 1.38     |
| 3   | L5    | 4506 | OMC  | C6-N1   | -2.48 | 1.32        | 1.38     |
| 3   | L5    | 4323 | PSU  | O4'-C1' | -2.48 | 1.40        | 1.43     |
| 46  | S2    | 1244 | PSU  | C2-N1   | -2.48 | 1.33        | 1.36     |
| 46  | S2    | 814  | PSU  | C2-N1   | -2.48 | 1.33        | 1.36     |
| 3   | L5    | 4441 | PSU  | C6-N1   | -2.47 | 1.32        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | S2    | 36   | PSU  | C2-N1   | -2.47 | 1.33        | 1.36     |
| 80  | Bv    | 9    | 1MG  | C2-N1   | 2.47  | 1.41        | 1.37     |
| 46  | S2    | 1850 | MA6  | C4-N9   | -2.47 | 1.32        | 1.37     |
| 46  | S2    | 1625 | PSU  | C2-N3   | -2.46 | 1.33        | 1.37     |
| 3   | L5    | 4390 | PSU  | C2-N1   | -2.46 | 1.33        | 1.36     |
| 3   | L5    | 2848 | OMC  | C6-N1   | -2.46 | 1.32        | 1.38     |
| 46  | S2    | 815  | PSU  | C2-N1   | -2.45 | 1.33        | 1.36     |
| 46  | S2    | 436  | OMG  | C5-C4   | 2.45  | 1.45        | 1.38     |
| 3   | L5    | 4659 | PSU  | C6-N1   | -2.44 | 1.32        | 1.36     |
| 80  | Bv    | 26   | M2G  | C6-N1   | -2.43 | 1.34        | 1.38     |
| 3   | L5    | 3618 | PSU  | C6-N1   | -2.43 | 1.32        | 1.36     |
| 3   | L5    | 3899 | PSU  | C6-N1   | -2.43 | 1.32        | 1.36     |
| 3   | L5    | 4323 | PSU  | C6-N1   | -2.43 | 1.32        | 1.36     |
| 3   | L5    | 4269 | PSU  | C6-N1   | -2.43 | 1.32        | 1.36     |
| 46  | S2    | 1238 | PSU  | C6-C5   | 2.42  | 1.38        | 1.35     |
| 3   | L5    | 4198 | OMG  | C4-N9   | -2.42 | 1.31        | 1.38     |
| 3   | L5    | 1509 | OMG  | C4-N9   | -2.42 | 1.31        | 1.38     |
| 46  | S2    | 1367 | PSU  | C2-N1   | -2.42 | 1.33        | 1.36     |
| 46  | S2    | 801  | PSU  | C2-N1   | -2.42 | 1.33        | 1.36     |
| 3   | L5    | 1849 | PSU  | C6-C5   | 2.42  | 1.38        | 1.35     |
| 46  | S2    | 1244 | PSU  | C2-N3   | -2.42 | 1.33        | 1.37     |
| 46  | S2    | 686  | PSU  | C2-N1   | -2.41 | 1.33        | 1.36     |
| 46  | S2    | 1347 | PSU  | C2-N3   | -2.41 | 1.33        | 1.37     |
| 80  | Bv    | 10   | 2MG  | C6-N1   | -2.41 | 1.34        | 1.38     |
| 46  | S2    | 1004 | PSU  | C6-C5   | 2.41  | 1.38        | 1.35     |
| 46  | S2    | 621  | OMC  | C6-N1   | -2.41 | 1.32        | 1.38     |
| 46  | S2    | 609  | PSU  | C2-N1   | -2.41 | 1.33        | 1.36     |
| 46  | S2    | 863  | PSU  | C2-N3   | -2.40 | 1.33        | 1.37     |
| 46  | S2    | 436  | OMG  | C5-N7   | -2.40 | 1.34        | 1.39     |
| 3   | L5    | 4362 | OMG  | C2-N1   | -2.40 | 1.31        | 1.37     |
| 46  | S2    | 406  | PSU  | C6-C5   | 2.40  | 1.37        | 1.35     |
| 3   | L5    | 4441 | PSU  | C6-C5   | 2.40  | 1.37        | 1.35     |
| 3   | L5    | 3741 | PSU  | C2-N3   | -2.40 | 1.33        | 1.37     |
| 80  | Bv    | 47   | H2U  | C4-N3   | -2.39 | 1.33        | 1.37     |
| 3   | L5    | 4401 | PSU  | C6-N1   | -2.39 | 1.32        | 1.36     |
| 3   | L5    | 1612 | OMG  | C4-N9   | -2.39 | 1.32        | 1.38     |
| 3   | L5    | 4470 | PSU  | O4'-C1' | -2.39 | 1.40        | 1.43     |
| 3   | L5    | 1569 | PSU  | C6-N1   | -2.39 | 1.32        | 1.36     |
| 3   | L5    | 2351 | OMG  | C4-N9   | -2.39 | 1.32        | 1.38     |
| 3   | L5    | 3618 | PSU  | O4'-C1' | -2.39 | 1.40        | 1.43     |
| 46  | S2    | 867  | OMG  | C5-N7   | -2.39 | 1.34        | 1.39     |
| 5   | L8    | 69   | PSU  | C2-N1   | -2.38 | 1.33        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | S2    | 1347 | PSU  | C6-C5   | 2.38  | 1.37        | 1.35     |
| 80  | Bv    | 46   | G7M  | C6-N1   | -2.38 | 1.34        | 1.38     |
| 3   | L5    | 2863 | OMG  | C4-N9   | -2.38 | 1.32        | 1.38     |
| 46  | S2    | 1238 | PSU  | C2-N3   | -2.37 | 1.33        | 1.37     |
| 3   | L5    | 4607 | OMG  | C5-C4   | 2.37  | 1.45        | 1.38     |
| 46  | S2    | 105  | PSU  | C2-N1   | -2.37 | 1.33        | 1.36     |
| 3   | L5    | 3797 | UY1  | C6-N1   | -2.36 | 1.32        | 1.36     |
| 46  | S2    | 1046 | PSU  | C6-C5   | 2.36  | 1.37        | 1.35     |
| 3   | L5    | 1303 | OMG  | C4-N9   | -2.36 | 1.32        | 1.38     |
| 46  | S2    | 1639 | G7M  | C4-N9   | -2.36 | 1.32        | 1.38     |
| 46  | S2    | 1490 | OMG  | C5-C4   | 2.36  | 1.45        | 1.38     |
| 3   | L5    | 2352 | OMC  | C5-C4   | -2.36 | 1.37        | 1.42     |
| 3   | L5    | 4469 | OMG  | C5-C4   | 2.36  | 1.45        | 1.38     |
| 80  | Bv    | 58   | 1MA  | C2-N3   | 2.36  | 1.34        | 1.30     |
| 3   | L5    | 1847 | PSU  | C6-N1   | -2.36 | 1.32        | 1.36     |
| 3   | L5    | 3904 | OMU  | C6-N1   | -2.35 | 1.32        | 1.38     |
| 3   | L5    | 3787 | OMC  | C5-C4   | -2.35 | 1.37        | 1.42     |
| 46  | S2    | 428  | OMU  | C5-C4   | -2.35 | 1.38        | 1.43     |
| 3   | L5    | 1504 | 2MG  | C2-N1   | -2.35 | 1.33        | 1.36     |
| 46  | S2    | 1367 | PSU  | C2-N3   | -2.35 | 1.33        | 1.37     |
| 80  | Bv    | 16   | H2U  | C4-N3   | -2.34 | 1.33        | 1.37     |
| 3   | L5    | 4502 | PSU  | C6-N1   | -2.34 | 1.32        | 1.36     |
| 5   | L8    | 75   | OMG  | C5-C4   | 2.34  | 1.45        | 1.38     |
| 3   | L5    | 2848 | OMC  | C5-C4   | -2.34 | 1.37        | 1.42     |
| 3   | L5    | 3674 | PSU  | C6-N1   | -2.33 | 1.32        | 1.36     |
| 3   | L5    | 4593 | OMG  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 3   | L5    | 1309 | 1MA  | C8-N9   | -2.33 | 1.32        | 1.37     |
| 3   | L5    | 3878 | OMG  | C8-N9   | -2.33 | 1.32        | 1.37     |
| 46  | S2    | 1625 | PSU  | C2-N1   | -2.33 | 1.33        | 1.36     |
| 3   | L5    | 4593 | OMG  | C5-C4   | 2.33  | 1.45        | 1.38     |
| 3   | L5    | 4282 | PSU  | C6-N1   | -2.33 | 1.32        | 1.36     |
| 46  | S2    | 93   | PSU  | C6-C5   | 2.32  | 1.37        | 1.35     |
| 3   | L5    | 2409 | OMC  | C6-N1   | -2.32 | 1.32        | 1.38     |
| 3   | L5    | 364  | OMG  | C2-N1   | -2.32 | 1.32        | 1.37     |
| 3   | L5    | 2811 | OMC  | C5-C4   | -2.32 | 1.37        | 1.42     |
| 46  | S2    | 1244 | PSU  | C6-C5   | 2.31  | 1.37        | 1.35     |
| 46  | S2    | 1445 | PSU  | C2-N3   | -2.31 | 1.33        | 1.37     |
| 3   | L5    | 3830 | PSU  | O4'-C1' | -2.31 | 1.40        | 1.43     |
| 3   | L5    | 2402 | PSU  | O4'-C1' | -2.31 | 1.40        | 1.43     |
| 46  | S2    | 1692 | PSU  | C6-C5   | 2.31  | 1.37        | 1.35     |
| 3   | L5    | 4340 | OMG  | C5-C4   | 2.31  | 1.45        | 1.38     |
| 3   | L5    | 4427 | PSU  | C6-N1   | -2.30 | 1.32        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | S2    | 1347 | PSU  | C2-N1   | -2.30 | 1.33        | 1.36     |
| 46  | S2    | 572  | PSU  | C2-N3   | -2.30 | 1.33        | 1.37     |
| 46  | S2    | 1337 | 4AC  | C7-N4   | -2.30 | 1.32        | 1.37     |
| 46  | S2    | 609  | PSU  | C2-N3   | -2.29 | 1.33        | 1.37     |
| 46  | S2    | 172  | OMU  | C6-N1   | -2.29 | 1.32        | 1.38     |
| 3   | L5    | 4491 | PSU  | C6-N1   | -2.29 | 1.32        | 1.36     |
| 3   | L5    | 2338 | OMC  | C6-N1   | -2.29 | 1.32        | 1.38     |
| 3   | L5    | 3899 | PSU  | C6-C5   | 2.29  | 1.37        | 1.35     |
| 3   | L5    | 1303 | OMG  | C8-N9   | -2.29 | 1.32        | 1.37     |
| 3   | L5    | 3823 | PSU  | C6-C5   | 2.29  | 1.37        | 1.35     |
| 46  | S2    | 1046 | PSU  | O4'-C1' | -2.29 | 1.40        | 1.43     |
| 46  | S2    | 121  | OMU  | C5-C4   | -2.28 | 1.38        | 1.43     |
| 3   | L5    | 4190 | 6MZ  | C8-N9   | -2.28 | 1.33        | 1.37     |
| 3   | L5    | 4464 | OMG  | C5-C4   | 2.28  | 1.45        | 1.38     |
| 3   | L5    | 4506 | OMC  | C5-C4   | -2.28 | 1.37        | 1.42     |
| 80  | Bv    | 37   | UY4  | C5-C6   | 2.28  | 1.47        | 1.41     |
| 46  | S2    | 1643 | PSU  | C6-C5   | 2.28  | 1.37        | 1.35     |
| 3   | L5    | 3866 | OMC  | C5-C4   | -2.28 | 1.37        | 1.42     |
| 3   | L5    | 1509 | OMG  | C5-C4   | 2.28  | 1.44        | 1.38     |
| 5   | L8    | 69   | PSU  | O4'-C1' | -2.27 | 1.40        | 1.43     |
| 3   | L5    | 2811 | OMC  | C6-N1   | -2.27 | 1.32        | 1.38     |
| 3   | L5    | 3723 | OMG  | C5-C4   | 2.27  | 1.44        | 1.38     |
| 46  | S2    | 863  | PSU  | C6-N1   | -2.27 | 1.32        | 1.36     |
| 3   | L5    | 4401 | PSU  | C6-C5   | 2.26  | 1.37        | 1.35     |
| 46  | S2    | 1703 | OMC  | C5-C4   | -2.26 | 1.37        | 1.42     |
| 3   | L5    | 3741 | PSU  | O4'-C1' | -2.25 | 1.40        | 1.43     |
| 3   | L5    | 4546 | PSU  | C6-N1   | -2.25 | 1.32        | 1.36     |
| 46  | S2    | 1081 | PSU  | C6-C5   | 2.25  | 1.37        | 1.35     |
| 46  | S2    | 866  | PSU  | C2-N3   | -2.25 | 1.33        | 1.37     |
| 3   | L5    | 4390 | PSU  | C2-N3   | -2.24 | 1.33        | 1.37     |
| 3   | L5    | 4373 | PSU  | O4'-C1' | -2.24 | 1.40        | 1.43     |
| 3   | L5    | 2411 | OMG  | C5-C4   | 2.23  | 1.44        | 1.38     |
| 3   | L5    | 2619 | PSU  | C6-N1   | -2.23 | 1.32        | 1.36     |
| 3   | L5    | 3741 | PSU  | C2-N1   | -2.23 | 1.33        | 1.36     |
| 46  | S2    | 406  | PSU  | O4'-C1' | -2.23 | 1.40        | 1.43     |
| 46  | S2    | 172  | OMU  | C5-C4   | -2.23 | 1.38        | 1.43     |
| 3   | L5    | 1327 | OMC  | C6-N1   | -2.23 | 1.32        | 1.38     |
| 3   | L5    | 4502 | PSU  | C6-C5   | 2.23  | 1.37        | 1.35     |
| 3   | L5    | 2863 | OMG  | C2-N1   | -2.22 | 1.32        | 1.37     |
| 3   | L5    | 1768 | PSU  | C6-N1   | -2.22 | 1.32        | 1.36     |
| 3   | L5    | 4263 | PSU  | C6-N1   | -2.21 | 1.32        | 1.36     |
| 3   | L5    | 1612 | OMG  | C5-C4   | 2.21  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 46  | S2    | 1081 | PSU  | O4'-C1' | -2.21 | 1.40        | 1.43     |
| 46  | S2    | 218  | PSU  | C2-N1   | -2.21 | 1.33        | 1.36     |
| 3   | L5    | 3606 | OMG  | C2-N1   | -2.20 | 1.32        | 1.37     |
| 3   | L5    | 4470 | PSU  | C6-N1   | -2.20 | 1.32        | 1.36     |
| 46  | S2    | 621  | OMC  | C5-C4   | -2.20 | 1.37        | 1.42     |
| 3   | L5    | 2824 | OMU  | C6-N1   | -2.20 | 1.32        | 1.38     |
| 46  | S2    | 1643 | PSU  | O4'-C1' | -2.20 | 1.40        | 1.43     |
| 3   | L5    | 2495 | PSU  | C6-N1   | -2.19 | 1.32        | 1.36     |
| 46  | S2    | 822  | PSU  | C2-N3   | -2.19 | 1.33        | 1.37     |
| 46  | S2    | 1174 | PSU  | C6-N1   | -2.19 | 1.32        | 1.36     |
| 3   | L5    | 3709 | PSU  | C2-N1   | -2.19 | 1.33        | 1.36     |
| 3   | L5    | 4197 | OMU  | C6-N1   | -2.19 | 1.32        | 1.38     |
| 3   | L5    | 4427 | PSU  | O4'-C1' | -2.19 | 1.40        | 1.43     |
| 3   | L5    | 3713 | PSU  | O4'-C1' | -2.19 | 1.40        | 1.43     |
| 3   | L5    | 4588 | OMG  | C5-C4   | 2.18  | 1.44        | 1.38     |
| 3   | L5    | 1309 | 1MA  | C6-N6   | 2.18  | 1.33        | 1.28     |
| 3   | L5    | 4549 | PSU  | C6-C5   | 2.18  | 1.37        | 1.35     |
| 3   | L5    | 3832 | PSU  | C6-N1   | -2.18 | 1.32        | 1.36     |
| 46  | S2    | 866  | PSU  | C2-N1   | -2.18 | 1.33        | 1.36     |
| 46  | S2    | 109  | PSU  | C6-C5   | 2.18  | 1.37        | 1.35     |
| 46  | S2    | 686  | PSU  | C6-C5   | 2.17  | 1.37        | 1.35     |
| 3   | L5    | 1309 | 1MA  | C5-C4   | 2.17  | 1.44        | 1.38     |
| 3   | L5    | 2863 | OMG  | C5-C4   | 2.17  | 1.44        | 1.38     |
| 3   | L5    | 1504 | 2MG  | C8-N9   | -2.17 | 1.32        | 1.37     |
| 3   | L5    | 3737 | PSU  | C6-C5   | 2.17  | 1.37        | 1.35     |
| 3   | L5    | 2619 | PSU  | O4'-C1' | -2.17 | 1.40        | 1.43     |
| 3   | L5    | 3694 | PSU  | C6-C5   | 2.17  | 1.37        | 1.35     |
| 46  | S2    | 1804 | OMU  | C2-N1   | 2.16  | 1.41        | 1.38     |
| 3   | L5    | 4464 | OMG  | C4-N9   | -2.16 | 1.32        | 1.38     |
| 3   | L5    | 1664 | PSU  | C6-N1   | -2.16 | 1.32        | 1.36     |
| 3   | L5    | 3680 | OMC  | C5-C4   | -2.15 | 1.37        | 1.42     |
| 46  | S2    | 822  | PSU  | O4'-C1' | -2.15 | 1.40        | 1.43     |
| 3   | L5    | 4502 | PSU  | O4'-C1' | -2.15 | 1.40        | 1.43     |
| 80  | Bv    | 28   | PSU  | C2-N3   | -2.15 | 1.33        | 1.37     |
| 3   | L5    | 3747 | PSU  | C6-N1   | -2.15 | 1.32        | 1.36     |
| 80  | Bv    | 37   | UY4  | C6-N6   | -2.14 | 1.34        | 1.39     |
| 3   | L5    | 1769 | PSU  | C6-N1   | -2.14 | 1.32        | 1.36     |
| 3   | L5    | 3743 | PSU  | C6-C5   | 2.14  | 1.37        | 1.35     |
| 3   | L5    | 2351 | OMG  | C5-C4   | 2.14  | 1.44        | 1.38     |
| 3   | L5    | 4340 | OMG  | C4-N9   | -2.13 | 1.32        | 1.38     |
| 3   | L5    | 4263 | PSU  | C6-C5   | 2.13  | 1.37        | 1.35     |
| 3   | L5    | 1313 | A2M  | C2'-C1' | -2.13 | 1.47        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | L5    | 1769 | PSU  | C6-C5   | 2.13  | 1.37        | 1.35     |
| 3   | L5    | 2352 | OMC  | C6-N1   | -2.13 | 1.33        | 1.38     |
| 3   | L5    | 3830 | PSU  | C6-N1   | -2.13 | 1.32        | 1.36     |
| 3   | L5    | 4198 | OMG  | C5-C4   | 2.13  | 1.44        | 1.38     |
| 46  | S2    | 1703 | OMC  | C6-N1   | -2.13 | 1.33        | 1.38     |
| 46  | S2    | 572  | PSU  | O4'-C1' | -2.13 | 1.40        | 1.43     |
| 3   | L5    | 1731 | PSU  | C6-N1   | -2.13 | 1.32        | 1.36     |
| 3   | L5    | 4464 | OMG  | C2-N1   | -2.13 | 1.32        | 1.37     |
| 46  | S2    | 119  | PSU  | C2-N1   | -2.13 | 1.33        | 1.36     |
| 3   | L5    | 4331 | PSU  | C6-N1   | -2.12 | 1.32        | 1.36     |
| 3   | L5    | 1569 | PSU  | C6-C5   | 2.12  | 1.37        | 1.35     |
| 80  | Bv    | 9    | 1MG  | C5-N7   | -2.12 | 1.34        | 1.39     |
| 46  | S2    | 966  | PSU  | C2-N1   | -2.12 | 1.33        | 1.36     |
| 3   | L5    | 3713 | PSU  | C6-C5   | 2.12  | 1.37        | 1.35     |
| 3   | L5    | 4966 | PSU  | O4'-C1' | -2.12 | 1.40        | 1.43     |
| 3   | L5    | 3709 | PSU  | C6-C5   | 2.12  | 1.37        | 1.35     |
| 80  | Bv    | 10   | 2MG  | C2-N3   | 2.12  | 1.36        | 1.32     |
| 46  | S2    | 1288 | OMU  | C2-N1   | 2.12  | 1.41        | 1.38     |
| 46  | S2    | 1248 | B8N  | C6-C5   | 2.11  | 1.38        | 1.35     |
| 3   | L5    | 1779 | PSU  | C6-N1   | -2.11 | 1.32        | 1.36     |
| 46  | S2    | 1174 | PSU  | C6-C5   | 2.11  | 1.37        | 1.35     |
| 3   | L5    | 4362 | OMG  | C5-C4   | 2.11  | 1.44        | 1.38     |
| 3   | L5    | 4362 | OMG  | C8-N9   | -2.11 | 1.32        | 1.37     |
| 80  | Bv    | 26   | M2G  | C5-N7   | -2.10 | 1.34        | 1.39     |
| 3   | L5    | 4470 | PSU  | C6-C5   | 2.10  | 1.37        | 1.35     |
| 3   | L5    | 4937 | PSU  | C6-N1   | -2.10 | 1.32        | 1.36     |
| 80  | Bv    | 10   | 2MG  | C5-N7   | -2.10 | 1.34        | 1.39     |
| 46  | S2    | 1442 | OMU  | C6-N1   | -2.10 | 1.33        | 1.38     |
| 3   | L5    | 4549 | PSU  | C6-N1   | -2.10 | 1.32        | 1.36     |
| 46  | S2    | 1288 | OMU  | C5-C4   | -2.10 | 1.39        | 1.43     |
| 3   | L5    | 1523 | PSU  | O4'-C1' | -2.10 | 1.40        | 1.43     |
| 3   | L5    | 3713 | PSU  | C2-N1   | -2.10 | 1.33        | 1.36     |
| 46  | S2    | 34   | PSU  | C2-N1   | -2.10 | 1.33        | 1.36     |
| 3   | L5    | 1504 | 2MG  | C4-N9   | -2.10 | 1.32        | 1.38     |
| 3   | L5    | 3674 | PSU  | O4'-C1' | -2.10 | 1.40        | 1.43     |
| 3   | L5    | 4607 | OMG  | C2-N1   | -2.10 | 1.32        | 1.37     |
| 3   | L5    | 4373 | PSU  | C6-N1   | -2.09 | 1.32        | 1.36     |
| 46  | S2    | 651  | PSU  | C2-N1   | -2.08 | 1.33        | 1.36     |
| 3   | L5    | 3606 | OMG  | C5-C4   | 2.08  | 1.44        | 1.38     |
| 46  | S2    | 1445 | PSU  | C2-N1   | -2.08 | 1.33        | 1.36     |
| 3   | L5    | 3747 | PSU  | C6-C5   | 2.08  | 1.37        | 1.35     |
| 3   | L5    | 1509 | OMG  | C2-N1   | -2.08 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | L5    | 4412 | PSU  | C6-N1   | -2.08 | 1.32        | 1.36     |
| 80  | Bv    | 58   | 1MA  | C5-N7   | -2.08 | 1.34        | 1.39     |
| 73  | SO    | 138  | IAS  | CB-CG   | 2.07  | 1.55        | 1.50     |
| 3   | L5    | 3749 | PSU  | C6-N1   | -2.07 | 1.32        | 1.36     |
| 3   | L5    | 4937 | PSU  | C6-C5   | 2.07  | 1.37        | 1.35     |
| 46  | S2    | 1490 | OMG  | C2-N1   | -2.07 | 1.32        | 1.37     |
| 46  | S2    | 1004 | PSU  | C6-N1   | -2.07 | 1.32        | 1.36     |
| 3   | L5    | 4263 | PSU  | O4'-C1' | -2.07 | 1.41        | 1.43     |
| 3   | L5    | 4468 | OMU  | C6-N1   | -2.07 | 1.33        | 1.38     |
| 80  | Bv    | 37   | UY4  | C4-N9   | -2.06 | 1.33        | 1.37     |
| 3   | L5    | 4588 | OMG  | C8-N9   | -2.06 | 1.32        | 1.37     |
| 3   | L5    | 1309 | 1MA  | C2-N1   | -2.06 | 1.31        | 1.35     |
| 3   | L5    | 4598 | PSU  | O4'-C1' | -2.06 | 1.41        | 1.43     |
| 3   | L5    | 3616 | PSU  | O4'-C1' | -2.06 | 1.41        | 1.43     |
| 3   | L5    | 4659 | PSU  | O4'-C1' | -2.05 | 1.41        | 1.43     |
| 46  | S2    | 174  | OMC  | C6-N1   | -2.05 | 1.33        | 1.38     |
| 3   | L5    | 1303 | OMG  | C5-C4   | 2.04  | 1.44        | 1.38     |
| 5   | L8    | 55   | PSU  | C6-N1   | -2.04 | 1.33        | 1.36     |
| 3   | L5    | 4331 | PSU  | O4'-C1' | -2.03 | 1.41        | 1.43     |
| 3   | L5    | 4643 | PSU  | O4'-C1' | -2.03 | 1.41        | 1.43     |
| 5   | L8    | 55   | PSU  | C6-C5   | 2.03  | 1.37        | 1.35     |
| 3   | L5    | 1504 | 2MG  | C5-C4   | 2.03  | 1.44        | 1.38     |
| 3   | L5    | 4198 | OMG  | C8-N9   | -2.03 | 1.33        | 1.37     |
| 46  | S2    | 644  | OMG  | C4-N9   | -2.02 | 1.32        | 1.38     |
| 46  | S2    | 1326 | OMU  | C6-N1   | -2.02 | 1.33        | 1.38     |
| 46  | S2    | 1326 | OMU  | C5-C4   | -2.02 | 1.39        | 1.43     |
| 46  | S2    | 517  | OMC  | C5-C4   | -2.02 | 1.38        | 1.42     |
| 46  | S2    | 1692 | PSU  | C6-N1   | -2.02 | 1.33        | 1.36     |
| 3   | L5    | 4340 | OMG  | C2-N1   | -2.02 | 1.32        | 1.37     |
| 46  | S2    | 1248 | B8N  | O4'-C1' | -2.01 | 1.41        | 1.43     |
| 46  | S2    | 436  | OMG  | C4-N9   | -2.01 | 1.32        | 1.38     |
| 46  | S2    | 686  | PSU  | C6-N1   | -2.01 | 1.33        | 1.36     |
| 3   | L5    | 4546 | PSU  | O4'-C1' | -2.01 | 1.41        | 1.43     |
| 3   | L5    | 4340 | OMG  | C8-N9   | -2.01 | 1.33        | 1.37     |
| 46  | S2    | 1842 | 4AC  | C5-C4   | -2.01 | 1.36        | 1.41     |
| 3   | L5    | 4166 | OMG  | C2-N1   | -2.01 | 1.32        | 1.37     |
| 3   | L5    | 1509 | OMG  | C8-N9   | -2.01 | 1.33        | 1.37     |
| 46  | S2    | 119  | PSU  | O4'-C1' | -2.00 | 1.41        | 1.43     |
| 46  | S2    | 1490 | OMG  | C4-N9   | -2.00 | 1.33        | 1.38     |
| 3   | L5    | 1768 | PSU  | O4'-C1' | -2.00 | 1.41        | 1.43     |

All (894) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 46  | S2    | 1842 | 4AC  | CM7-C7-N4 | 11.26 | 133.45      | 115.27   |
| 46  | S2    | 1337 | 4AC  | N4-C4-N3  | 9.21  | 128.82      | 113.87   |
| 3   | L5    | 3899 | PSU  | N1-C2-N3  | 7.90  | 123.50      | 115.17   |
| 3   | L5    | 4522 | PSU  | N1-C2-N3  | 7.89  | 123.49      | 115.17   |
| 3   | L5    | 1769 | PSU  | N1-C2-N3  | 7.77  | 123.36      | 115.17   |
| 3   | L5    | 4323 | PSU  | N1-C2-N3  | 7.75  | 123.34      | 115.17   |
| 3   | L5    | 3616 | PSU  | N1-C2-N3  | 7.68  | 123.27      | 115.17   |
| 3   | L5    | 4441 | PSU  | N1-C2-N3  | 7.61  | 123.20      | 115.17   |
| 3   | L5    | 2402 | PSU  | N1-C2-N3  | 7.59  | 123.18      | 115.17   |
| 3   | L5    | 3741 | PSU  | N1-C2-N3  | 7.57  | 123.16      | 115.17   |
| 3   | L5    | 4598 | PSU  | N1-C2-N3  | 7.56  | 123.14      | 115.17   |
| 5   | L8    | 69   | PSU  | N1-C2-N3  | 7.56  | 123.14      | 115.17   |
| 3   | L5    | 3823 | PSU  | N1-C2-N3  | 7.53  | 123.11      | 115.17   |
| 3   | L5    | 1504 | 2MG  | C2-N3-C4  | 7.51  | 121.40      | 112.00   |
| 46  | S2    | 1842 | 4AC  | O7-C7-N4  | -7.49 | 110.11      | 121.90   |
| 3   | L5    | 3618 | PSU  | N1-C2-N3  | 7.48  | 123.06      | 115.17   |
| 3   | L5    | 4659 | PSU  | N1-C2-N3  | 7.43  | 123.00      | 115.17   |
| 3   | L5    | 4282 | PSU  | N1-C2-N3  | 7.42  | 123.00      | 115.17   |
| 3   | L5    | 4427 | PSU  | N1-C2-N3  | 7.42  | 123.00      | 115.17   |
| 3   | L5    | 4491 | PSU  | N1-C2-N3  | 7.36  | 122.93      | 115.17   |
| 3   | L5    | 4975 | PSU  | N1-C2-N3  | 7.35  | 122.92      | 115.17   |
| 46  | S2    | 1692 | PSU  | N1-C2-N3  | 7.30  | 122.87      | 115.17   |
| 3   | L5    | 1664 | PSU  | N1-C2-N3  | 7.29  | 122.85      | 115.17   |
| 3   | L5    | 4549 | PSU  | N1-C2-N3  | 7.27  | 122.84      | 115.17   |
| 3   | L5    | 4470 | PSU  | N1-C2-N3  | 7.24  | 122.81      | 115.17   |
| 3   | L5    | 2619 | PSU  | N1-C2-N3  | 7.23  | 122.79      | 115.17   |
| 3   | L5    | 1731 | PSU  | N1-C2-N3  | 7.22  | 122.78      | 115.17   |
| 3   | L5    | 4401 | PSU  | N1-C2-N3  | 7.21  | 122.78      | 115.17   |
| 46  | S2    | 686  | PSU  | N1-C2-N3  | 7.19  | 122.75      | 115.17   |
| 80  | Bv    | 10   | 2MG  | C2-N3-C4  | 7.19  | 120.99      | 112.00   |
| 46  | S2    | 1174 | PSU  | N1-C2-N3  | 7.18  | 122.75      | 115.17   |
| 46  | S2    | 406  | PSU  | N1-C2-N3  | 7.11  | 122.67      | 115.17   |
| 46  | S2    | 966  | PSU  | N1-C2-N3  | 7.09  | 122.64      | 115.17   |
| 46  | S2    | 1004 | PSU  | N1-C2-N3  | 7.05  | 122.61      | 115.17   |
| 46  | S2    | 1045 | PSU  | N1-C2-N3  | 7.03  | 122.58      | 115.17   |
| 46  | S2    | 36   | PSU  | N1-C2-N3  | 7.02  | 122.57      | 115.17   |
| 3   | L5    | 3830 | PSU  | N1-C2-N3  | 7.00  | 122.56      | 115.17   |
| 3   | L5    | 4263 | PSU  | N1-C2-N3  | 6.97  | 122.52      | 115.17   |
| 3   | L5    | 2863 | OMG  | C5-C4-N3  | -6.96 | 117.31      | 128.39   |
| 3   | L5    | 2351 | OMG  | C5-C4-N3  | -6.96 | 117.32      | 128.39   |
| 3   | L5    | 3713 | PSU  | N1-C2-N3  | 6.95  | 122.50      | 115.17   |
| 3   | L5    | 1670 | PSU  | N1-C2-N3  | 6.95  | 122.50      | 115.17   |
| 46  | S2    | 105  | PSU  | N1-C2-N3  | 6.94  | 122.49      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 46  | S2    | 1081 | PSU  | N1-C2-N3 | 6.94  | 122.49      | 115.17   |
| 5   | L8    | 55   | PSU  | N1-C2-N3 | 6.92  | 122.47      | 115.17   |
| 46  | S2    | 1232 | PSU  | N1-C2-N3 | 6.92  | 122.47      | 115.17   |
| 46  | S2    | 34   | PSU  | N1-C2-N3 | 6.90  | 122.45      | 115.17   |
| 3   | L5    | 3674 | PSU  | N1-C2-N3 | 6.89  | 122.44      | 115.17   |
| 3   | L5    | 1847 | PSU  | N1-C2-N3 | 6.88  | 122.43      | 115.17   |
| 46  | S2    | 815  | PSU  | N1-C2-N3 | 6.85  | 122.39      | 115.17   |
| 46  | S2    | 1367 | PSU  | N1-C2-N3 | 6.84  | 122.38      | 115.17   |
| 3   | L5    | 1569 | PSU  | N1-C2-N3 | 6.83  | 122.38      | 115.17   |
| 3   | L5    | 4412 | PSU  | N1-C2-N3 | 6.81  | 122.35      | 115.17   |
| 46  | S2    | 651  | PSU  | N1-C2-N3 | 6.81  | 122.35      | 115.17   |
| 46  | S2    | 822  | PSU  | N1-C2-N3 | 6.80  | 122.34      | 115.17   |
| 3   | L5    | 4546 | PSU  | N1-C2-N3 | 6.79  | 122.33      | 115.17   |
| 46  | S2    | 609  | PSU  | N1-C2-N3 | 6.78  | 122.32      | 115.17   |
| 3   | L5    | 4464 | OMG  | C5-C4-N3 | -6.77 | 117.61      | 128.39   |
| 3   | L5    | 1523 | PSU  | N1-C2-N3 | 6.74  | 122.28      | 115.17   |
| 46  | S2    | 649  | PSU  | N1-C2-N3 | 6.74  | 122.28      | 115.17   |
| 3   | L5    | 4166 | OMG  | C5-C4-N3 | -6.73 | 117.67      | 128.39   |
| 46  | S2    | 109  | PSU  | N1-C2-N3 | 6.70  | 122.24      | 115.17   |
| 46  | S2    | 572  | PSU  | N1-C2-N3 | 6.70  | 122.24      | 115.17   |
| 3   | L5    | 1504 | 2MG  | C5-C4-N3 | -6.70 | 117.73      | 128.39   |
| 46  | S2    | 1337 | 4AC  | C5-C4-N4 | -6.70 | 111.66      | 122.94   |
| 3   | L5    | 3737 | PSU  | N1-C2-N3 | 6.69  | 122.23      | 115.17   |
| 3   | L5    | 3747 | PSU  | N1-C2-N3 | 6.68  | 122.22      | 115.17   |
| 46  | S2    | 218  | PSU  | N1-C2-N3 | 6.67  | 122.20      | 115.17   |
| 3   | L5    | 1768 | PSU  | N1-C2-N3 | 6.66  | 122.20      | 115.17   |
| 3   | L5    | 1849 | PSU  | N1-C2-N3 | 6.66  | 122.19      | 115.17   |
| 3   | L5    | 4266 | PSU  | N1-C2-N3 | 6.66  | 122.19      | 115.17   |
| 3   | L5    | 3749 | PSU  | N1-C2-N3 | 6.65  | 122.19      | 115.17   |
| 46  | S2    | 814  | PSU  | N1-C2-N3 | 6.63  | 122.16      | 115.17   |
| 46  | S2    | 863  | PSU  | N1-C2-N3 | 6.63  | 122.16      | 115.17   |
| 3   | L5    | 3832 | PSU  | N1-C2-N3 | 6.62  | 122.15      | 115.17   |
| 46  | S2    | 1490 | OMG  | C5-C4-N3 | -6.62 | 117.85      | 128.39   |
| 3   | L5    | 4643 | PSU  | N1-C2-N3 | 6.62  | 122.15      | 115.17   |
| 3   | L5    | 4937 | PSU  | N1-C2-N3 | 6.62  | 122.15      | 115.17   |
| 46  | S2    | 436  | OMG  | C5-C4-N3 | -6.60 | 117.89      | 128.39   |
| 46  | S2    | 683  | OMG  | C5-C4-N3 | -6.60 | 117.89      | 128.39   |
| 3   | L5    | 2495 | PSU  | N1-C2-N3 | 6.59  | 122.12      | 115.17   |
| 46  | S2    | 1238 | PSU  | N1-C2-N3 | 6.56  | 122.09      | 115.17   |
| 46  | S2    | 866  | PSU  | N1-C2-N3 | 6.55  | 122.08      | 115.17   |
| 46  | S2    | 1136 | PSU  | N1-C2-N3 | 6.54  | 122.07      | 115.17   |
| 3   | L5    | 3709 | PSU  | N1-C2-N3 | 6.52  | 122.04      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L5    | 1303 | OMG  | C5-C4-N3 | -6.51 | 118.03      | 128.39   |
| 3   | L5    | 3743 | PSU  | N1-C2-N3 | 6.50  | 122.03      | 115.17   |
| 3   | L5    | 4373 | PSU  | N1-C2-N3 | 6.50  | 122.02      | 115.17   |
| 80  | Bv    | 28   | PSU  | N1-C2-N3 | 6.49  | 122.01      | 115.17   |
| 46  | S2    | 801  | PSU  | N1-C2-N3 | 6.48  | 122.01      | 115.17   |
| 3   | L5    | 4362 | OMG  | C5-C4-N3 | -6.48 | 118.08      | 128.39   |
| 80  | Bv    | 27   | PSU  | N1-C2-N3 | 6.48  | 122.00      | 115.17   |
| 46  | S2    | 119  | PSU  | N1-C2-N3 | 6.47  | 122.00      | 115.17   |
| 3   | L5    | 4502 | PSU  | N1-C2-N3 | 6.47  | 122.00      | 115.17   |
| 3   | L5    | 3694 | PSU  | N1-C2-N3 | 6.46  | 121.98      | 115.17   |
| 46  | S2    | 1244 | PSU  | N1-C2-N3 | 6.45  | 121.97      | 115.17   |
| 3   | L5    | 4593 | OMG  | C5-C4-N3 | -6.45 | 118.13      | 128.39   |
| 3   | L5    | 4340 | OMG  | C5-C4-N3 | -6.45 | 118.13      | 128.39   |
| 46  | S2    | 1328 | OMG  | C5-C4-N3 | -6.44 | 118.13      | 128.39   |
| 46  | S2    | 1347 | PSU  | N1-C2-N3 | 6.44  | 121.96      | 115.17   |
| 3   | L5    | 1509 | OMG  | C5-C4-N3 | -6.44 | 118.15      | 128.39   |
| 3   | L5    | 4966 | PSU  | N1-C2-N3 | 6.37  | 121.89      | 115.17   |
| 80  | Bv    | 55   | PSU  | N1-C2-N3 | 6.37  | 121.88      | 115.17   |
| 46  | S2    | 509  | OMG  | C5-C4-N3 | -6.36 | 118.26      | 128.39   |
| 3   | L5    | 4331 | PSU  | N1-C2-N3 | 6.35  | 121.86      | 115.17   |
| 3   | L5    | 4607 | OMG  | C5-C4-N3 | -6.34 | 118.30      | 128.39   |
| 3   | L5    | 1612 | OMG  | C5-C4-N3 | -6.34 | 118.30      | 128.39   |
| 46  | S2    | 644  | OMG  | C5-C4-N3 | -6.33 | 118.32      | 128.39   |
| 46  | S2    | 1643 | PSU  | N1-C2-N3 | 6.31  | 121.83      | 115.17   |
| 80  | Bv    | 26   | M2G  | C5-C4-N3 | -6.25 | 118.44      | 128.39   |
| 46  | S2    | 1445 | PSU  | N1-C2-N3 | 6.23  | 121.75      | 115.17   |
| 3   | L5    | 4393 | PSU  | N1-C2-N3 | 6.21  | 121.72      | 115.17   |
| 46  | S2    | 1625 | PSU  | N1-C2-N3 | 6.20  | 121.71      | 115.17   |
| 3   | L5    | 364  | OMG  | C5-C4-N3 | -6.20 | 118.53      | 128.39   |
| 80  | Bv    | 10   | 2MG  | C5-C4-N3 | -6.19 | 118.54      | 128.39   |
| 3   | L5    | 3878 | OMG  | C5-C4-N3 | -6.17 | 118.57      | 128.39   |
| 3   | L5    | 4390 | PSU  | N1-C2-N3 | 6.14  | 121.64      | 115.17   |
| 3   | L5    | 4469 | OMG  | C5-C4-N3 | -6.13 | 118.64      | 128.39   |
| 46  | S2    | 1046 | PSU  | N1-C2-N3 | 6.11  | 121.61      | 115.17   |
| 3   | L5    | 4269 | PSU  | N1-C2-N3 | 6.07  | 121.57      | 115.17   |
| 3   | L5    | 3797 | UY1  | N1-C2-N3 | 6.01  | 121.51      | 115.17   |
| 3   | L5    | 3771 | OMG  | C5-C4-N3 | -6.00 | 118.84      | 128.39   |
| 46  | S2    | 93   | PSU  | N1-C2-N3 | 6.00  | 121.50      | 115.17   |
| 3   | L5    | 4588 | OMG  | C5-C4-N3 | -5.99 | 118.86      | 128.39   |
| 5   | L8    | 75   | OMG  | C5-C4-N3 | -5.95 | 118.92      | 128.39   |
| 3   | L5    | 1779 | PSU  | N1-C2-N3 | 5.94  | 121.43      | 115.17   |
| 46  | S2    | 1177 | PSU  | N1-C2-N3 | 5.89  | 121.38      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 46  | S2    | 867  | OMG  | C5-C4-N3   | -5.88 | 119.03      | 128.39   |
| 3   | L5    | 3723 | OMG  | C5-C4-N3   | -5.85 | 119.08      | 128.39   |
| 3   | L5    | 364  | OMG  | N9-C4-N3   | 5.85  | 137.65      | 125.95   |
| 3   | L5    | 4606 | PSU  | N1-C2-N3   | 5.77  | 121.25      | 115.17   |
| 3   | L5    | 4417 | 5MC  | C5-C6-N1   | -5.75 | 117.07      | 123.31   |
| 3   | L5    | 1313 | A2M  | C5-C4-N3   | -5.68 | 118.89      | 126.72   |
| 3   | L5    | 2351 | OMG  | C2-N3-C4   | 5.67  | 122.07      | 112.30   |
| 46  | S2    | 1490 | OMG  | C2-N3-C4   | 5.67  | 122.07      | 112.30   |
| 46  | S2    | 1851 | MA6  | C5-C4-N3   | -5.65 | 118.94      | 126.72   |
| 3   | L5    | 3606 | OMG  | C5-C4-N3   | -5.61 | 119.46      | 128.39   |
| 80  | Bv    | 46   | G7M  | N9-C4-N3   | 5.58  | 137.11      | 125.95   |
| 80  | Bv    | 46   | G7M  | C5-C4-N3   | -5.57 | 117.63      | 128.15   |
| 3   | L5    | 4198 | OMG  | C5-C4-N3   | -5.56 | 119.54      | 128.39   |
| 3   | L5    | 2824 | OMU  | C4-N3-C2   | -5.55 | 119.72      | 126.61   |
| 3   | L5    | 4190 | 6MZ  | C5-C4-N3   | -5.55 | 119.08      | 126.72   |
| 3   | L5    | 1504 | 2MG  | N9-C4-N3   | 5.51  | 136.98      | 125.95   |
| 3   | L5    | 1664 | PSU  | C4-N3-C2   | -5.51 | 118.78      | 126.37   |
| 46  | S2    | 1326 | OMU  | C4-N3-C2   | -5.51 | 119.78      | 126.61   |
| 80  | Bv    | 58   | 1MA  | C5-C4-N3   | -5.49 | 119.19      | 127.27   |
| 80  | Bv    | 37   | UY4  | C5-C4-N3   | -5.43 | 119.24      | 126.72   |
| 46  | S2    | 172  | OMU  | C4-N3-C2   | -5.39 | 119.92      | 126.61   |
| 3   | L5    | 4500 | UR3  | C4-N3-C2   | -5.39 | 120.25      | 124.58   |
| 3   | L5    | 3878 | OMG  | C2-N3-C4   | 5.35  | 121.52      | 112.30   |
| 3   | L5    | 3771 | OMG  | C2-N3-C4   | 5.35  | 121.51      | 112.30   |
| 80  | Bv    | 9    | 1MG  | C5-C4-N3   | -5.34 | 119.90      | 128.39   |
| 3   | L5    | 2863 | OMG  | C2-N3-C4   | 5.33  | 121.49      | 112.30   |
| 46  | S2    | 436  | OMG  | C2-N3-C4   | 5.31  | 121.44      | 112.30   |
| 3   | L5    | 4362 | OMG  | C2-N3-C4   | 5.28  | 121.40      | 112.30   |
| 46  | S2    | 601  | OMG  | C5-C4-N3   | -5.26 | 120.02      | 128.39   |
| 46  | S2    | 1490 | OMG  | N9-C4-N3   | 5.23  | 136.42      | 125.95   |
| 46  | S2    | 1850 | MA6  | C5-C4-N3   | -5.22 | 119.53      | 126.72   |
| 3   | L5    | 2411 | OMG  | C5-C4-N3   | -5.22 | 120.08      | 128.39   |
| 3   | L5    | 4588 | OMG  | C2-N3-C4   | 5.20  | 121.26      | 112.30   |
| 3   | L5    | 1509 | OMG  | N9-C4-N3   | 5.20  | 136.34      | 125.95   |
| 3   | L5    | 4593 | OMG  | N9-C4-N3   | 5.20  | 136.34      | 125.95   |
| 3   | L5    | 4166 | OMG  | C2-N3-C4   | 5.16  | 121.19      | 112.30   |
| 3   | L5    | 4197 | OMU  | C4-N3-C2   | -5.16 | 120.20      | 126.61   |
| 3   | L5    | 4593 | OMG  | C2-N3-C4   | 5.16  | 121.19      | 112.30   |
| 3   | L5    | 1612 | OMG  | N9-C4-N3   | 5.15  | 136.25      | 125.95   |
| 3   | L5    | 4464 | OMG  | N9-C4-N3   | 5.15  | 136.24      | 125.95   |
| 80  | Bv    | 37   | UY4  | N6-C09-N08 | 5.14  | 120.83      | 113.77   |
| 46  | S2    | 509  | OMG  | N9-C4-N3   | 5.13  | 136.21      | 125.95   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L5    | 2402 | PSU  | C4-N3-C2 | -5.13 | 119.31      | 126.37   |
| 46  | S2    | 1832 | 6MZ  | C6-C5-N7 | 5.13  | 138.02      | 132.43   |
| 3   | L5    | 1509 | OMG  | C2-N3-C4 | 5.12  | 121.12      | 112.30   |
| 3   | L5    | 1612 | OMG  | C2-N3-C4 | 5.11  | 121.10      | 112.30   |
| 3   | L5    | 4549 | PSU  | C4-N3-C2 | -5.08 | 119.37      | 126.37   |
| 5   | L8    | 69   | PSU  | C4-N3-C2 | -5.08 | 119.38      | 126.37   |
| 3   | L5    | 4598 | PSU  | O2-C2-N1 | -5.07 | 117.56      | 122.79   |
| 3   | L5    | 1303 | OMG  | C2-N3-C4 | 5.06  | 121.01      | 112.30   |
| 3   | L5    | 364  | OMG  | C2-N3-C4 | 5.05  | 121.00      | 112.30   |
| 46  | S2    | 683  | OMG  | N9-C4-N3 | 5.05  | 136.04      | 125.95   |
| 3   | L5    | 4468 | OMU  | C4-N3-C2 | -5.03 | 120.36      | 126.61   |
| 3   | L5    | 3823 | PSU  | O2-C2-N1 | -5.02 | 117.61      | 122.79   |
| 3   | L5    | 4323 | PSU  | C4-N3-C2 | -5.02 | 119.45      | 126.37   |
| 5   | L8    | 75   | OMG  | C2-N3-C4 | 5.01  | 120.93      | 112.30   |
| 3   | L5    | 4197 | OMU  | N3-C2-N1 | 5.01  | 121.41      | 114.89   |
| 46  | S2    | 436  | OMG  | N9-C4-N3 | 5.00  | 135.96      | 125.95   |
| 3   | L5    | 4198 | OMG  | C2-N3-C4 | 5.00  | 120.91      | 112.30   |
| 3   | L5    | 3899 | PSU  | C4-N3-C2 | -4.98 | 119.51      | 126.37   |
| 3   | L5    | 1309 | 1MA  | C5-C4-N3 | -4.97 | 119.95      | 127.27   |
| 46  | S2    | 1639 | G7M  | N9-C4-N3 | 4.96  | 135.87      | 125.95   |
| 46  | S2    | 1328 | OMG  | C2-N3-C4 | 4.96  | 120.84      | 112.30   |
| 3   | L5    | 4469 | OMG  | C2-N3-C4 | 4.95  | 120.83      | 112.30   |
| 3   | L5    | 4427 | PSU  | C4-N3-C2 | -4.94 | 119.56      | 126.37   |
| 46  | S2    | 1851 | MA6  | C4-C5-N7 | -4.94 | 104.93      | 110.58   |
| 3   | L5    | 2351 | OMG  | N9-C4-N3 | 4.93  | 135.80      | 125.95   |
| 46  | S2    | 1442 | OMU  | C4-N3-C2 | -4.93 | 120.50      | 126.61   |
| 3   | L5    | 3823 | PSU  | C4-N3-C2 | -4.92 | 119.59      | 126.37   |
| 46  | S2    | 1832 | 6MZ  | C5-C4-N3 | -4.92 | 119.95      | 126.72   |
| 46  | S2    | 1639 | G7M  | C5-C4-N3 | -4.90 | 118.89      | 128.15   |
| 46  | S2    | 683  | OMG  | C2-N3-C4 | 4.89  | 120.72      | 112.30   |
| 3   | L5    | 3674 | PSU  | C4-N3-C2 | -4.87 | 119.66      | 126.37   |
| 3   | L5    | 4464 | OMG  | C2-N3-C4 | 4.86  | 120.67      | 112.30   |
| 46  | S2    | 428  | OMU  | C4-N3-C2 | -4.85 | 120.59      | 126.61   |
| 46  | S2    | 121  | OMU  | C4-N3-C2 | -4.85 | 120.59      | 126.61   |
| 3   | L5    | 4276 | OMU  | C4-N3-C2 | -4.84 | 120.60      | 126.61   |
| 3   | L5    | 2619 | PSU  | C4-N3-C2 | -4.84 | 119.71      | 126.37   |
| 3   | L5    | 4491 | PSU  | C4-N3-C2 | -4.83 | 119.72      | 126.37   |
| 46  | S2    | 1328 | OMG  | N9-C4-N3 | 4.81  | 135.57      | 125.95   |
| 3   | L5    | 2824 | OMU  | N3-C2-N1 | 4.81  | 121.15      | 114.89   |
| 3   | L5    | 1303 | OMG  | N9-C4-N3 | 4.80  | 135.56      | 125.95   |
| 46  | S2    | 1045 | PSU  | C4-N3-C2 | -4.79 | 119.78      | 126.37   |
| 3   | L5    | 3723 | OMG  | C2-N3-C4 | 4.78  | 120.53      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 46  | S2    | 121  | OMU  | N3-C2-N1 | 4.78  | 121.11      | 114.89   |
| 3   | L5    | 4412 | PSU  | C4-N3-C2 | -4.77 | 119.80      | 126.37   |
| 3   | L5    | 2863 | OMG  | N9-C4-N3 | 4.77  | 135.49      | 125.95   |
| 3   | L5    | 4340 | OMG  | C2-N3-C4 | 4.77  | 120.51      | 112.30   |
| 46  | S2    | 644  | OMG  | C2-N3-C4 | 4.76  | 120.51      | 112.30   |
| 80  | Bv    | 46   | G7M  | C2-N3-C4 | 4.76  | 120.50      | 112.30   |
| 3   | L5    | 3904 | OMU  | C5-C4-N3 | 4.75  | 121.46      | 114.80   |
| 46  | S2    | 867  | OMG  | C2-N3-C4 | 4.75  | 120.48      | 112.30   |
| 3   | L5    | 3741 | PSU  | C4-N3-C2 | -4.75 | 119.83      | 126.37   |
| 3   | L5    | 4522 | PSU  | C4-N3-C2 | -4.73 | 119.85      | 126.37   |
| 3   | L5    | 3713 | PSU  | C4-N3-C2 | -4.73 | 119.86      | 126.37   |
| 3   | L5    | 4470 | PSU  | C4-N3-C2 | -4.73 | 119.86      | 126.37   |
| 3   | L5    | 3904 | OMU  | C4-N3-C2 | -4.73 | 120.74      | 126.61   |
| 46  | S2    | 572  | PSU  | C4-N3-C2 | -4.73 | 119.86      | 126.37   |
| 3   | L5    | 3761 | 5MC  | O2-C2-N3 | -4.71 | 114.90      | 122.33   |
| 46  | S2    | 644  | OMG  | N9-C4-N3 | 4.71  | 135.36      | 125.95   |
| 3   | L5    | 2411 | OMG  | C2-N3-C4 | 4.70  | 120.40      | 112.30   |
| 46  | S2    | 509  | OMG  | C2-N3-C4 | 4.70  | 120.40      | 112.30   |
| 3   | L5    | 2338 | OMC  | O2-C2-N3 | -4.70 | 114.92      | 122.33   |
| 3   | L5    | 3709 | PSU  | C4-N3-C2 | -4.69 | 119.91      | 126.37   |
| 5   | L8    | 55   | PSU  | C4-N3-C2 | -4.69 | 119.91      | 126.37   |
| 46  | S2    | 1288 | OMU  | C4-N3-C2 | -4.68 | 120.80      | 126.61   |
| 46  | S2    | 1248 | B8N  | N3-C2-N1 | 4.68  | 122.43      | 116.72   |
| 80  | Bv    | 26   | M2G  | C2-N3-C4 | 4.67  | 121.15      | 112.51   |
| 3   | L5    | 3618 | PSU  | C4-N3-C2 | -4.67 | 119.94      | 126.37   |
| 3   | L5    | 4468 | OMU  | C5-C4-N3 | 4.67  | 121.34      | 114.80   |
| 3   | L5    | 1768 | PSU  | O2-C2-N1 | -4.66 | 117.98      | 122.79   |
| 3   | L5    | 4282 | PSU  | C4-N3-C2 | -4.66 | 119.95      | 126.37   |
| 3   | L5    | 1769 | PSU  | C4-N3-C2 | -4.66 | 119.96      | 126.37   |
| 3   | L5    | 3878 | OMG  | N9-C4-N3 | 4.65  | 135.25      | 125.95   |
| 3   | L5    | 4340 | OMG  | N9-C4-N3 | 4.65  | 135.24      | 125.95   |
| 46  | S2    | 1174 | PSU  | C4-N3-C2 | -4.64 | 119.98      | 126.37   |
| 46  | S2    | 686  | PSU  | C4-N3-C2 | -4.63 | 119.99      | 126.37   |
| 3   | L5    | 4546 | PSU  | C4-N3-C2 | -4.63 | 119.99      | 126.37   |
| 3   | L5    | 1309 | 1MA  | C2-N3-C4 | 4.63  | 121.61      | 112.53   |
| 3   | L5    | 3771 | OMG  | N9-C4-N3 | 4.63  | 135.21      | 125.95   |
| 46  | S2    | 1850 | MA6  | C4-C5-N7 | -4.60 | 105.32      | 110.58   |
| 80  | Bv    | 58   | 1MA  | C2-N3-C4 | 4.60  | 121.55      | 112.53   |
| 46  | S2    | 1850 | MA6  | C2-N1-C6 | 4.59  | 123.04      | 111.83   |
| 46  | S2    | 1081 | PSU  | C4-N3-C2 | -4.59 | 120.05      | 126.37   |
| 46  | S2    | 621  | OMC  | O2-C2-N3 | -4.59 | 115.10      | 122.33   |
| 3   | L5    | 3616 | PSU  | C4-N3-C2 | -4.58 | 120.06      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 46  | S2    | 1639 | G7M  | C2-N3-C4  | 4.58  | 120.19      | 112.30   |
| 46  | S2    | 109  | PSU  | C4-N3-C2  | -4.58 | 120.07      | 126.37   |
| 3   | L5    | 4546 | PSU  | O2-C2-N1  | -4.57 | 118.08      | 122.79   |
| 3   | L5    | 1523 | PSU  | O2-C2-N1  | -4.56 | 118.08      | 122.79   |
| 46  | S2    | 1326 | OMU  | N3-C2-N1  | 4.56  | 120.83      | 114.89   |
| 3   | L5    | 1731 | PSU  | C4-N3-C2  | -4.56 | 120.09      | 126.37   |
| 46  | S2    | 406  | PSU  | C4-N3-C2  | -4.56 | 120.09      | 126.37   |
| 80  | Bv    | 10   | 2MG  | N9-C4-N3  | 4.55  | 135.06      | 125.95   |
| 80  | Bv    | 26   | M2G  | N9-C4-N3  | 4.55  | 135.05      | 125.95   |
| 3   | L5    | 4500 | UR3  | C1'-N1-C2 | 4.54  | 124.47      | 117.04   |
| 46  | S2    | 867  | OMG  | N9-C4-N3  | 4.52  | 135.00      | 125.95   |
| 3   | L5    | 4470 | PSU  | O2-C2-N1  | -4.52 | 118.13      | 122.79   |
| 46  | S2    | 1136 | PSU  | C4-N3-C2  | -4.51 | 120.16      | 126.37   |
| 3   | L5    | 4469 | OMG  | N9-C4-N3  | 4.51  | 134.96      | 125.95   |
| 3   | L5    | 1731 | PSU  | O2-C2-N1  | -4.50 | 118.15      | 122.79   |
| 3   | L5    | 2402 | PSU  | O2-C2-N1  | -4.50 | 118.15      | 122.79   |
| 3   | L5    | 1313 | A2M  | N3-C4-N9  | 4.50  | 134.81      | 127.17   |
| 46  | S2    | 1851 | MA6  | C2-N1-C6  | 4.49  | 122.80      | 111.83   |
| 3   | L5    | 1847 | PSU  | O2-C2-N1  | -4.49 | 118.16      | 122.79   |
| 46  | S2    | 1804 | OMU  | C4-N3-C2  | -4.49 | 121.04      | 126.61   |
| 3   | L5    | 4266 | PSU  | C4-N3-C2  | -4.48 | 120.20      | 126.37   |
| 46  | S2    | 651  | PSU  | C4-N3-C2  | -4.47 | 120.21      | 126.37   |
| 46  | S2    | 218  | PSU  | C4-N3-C2  | -4.47 | 120.22      | 126.37   |
| 46  | S2    | 1692 | PSU  | C4-N3-C2  | -4.47 | 120.22      | 126.37   |
| 46  | S2    | 601  | OMG  | C2-N3-C4  | 4.46  | 119.98      | 112.30   |
| 5   | L8    | 75   | OMG  | N9-C4-N3  | 4.44  | 134.83      | 125.95   |
| 3   | L5    | 4468 | OMU  | N3-C2-N1  | 4.44  | 120.67      | 114.89   |
| 3   | L5    | 4975 | PSU  | C4-N3-C2  | -4.43 | 120.26      | 126.37   |
| 3   | L5    | 4607 | OMG  | C2-N3-C4  | 4.42  | 119.92      | 112.30   |
| 46  | S2    | 34   | PSU  | C4-N3-C2  | -4.42 | 120.28      | 126.37   |
| 3   | L5    | 2824 | OMU  | C5-C4-N3  | 4.41  | 120.98      | 114.80   |
| 46  | S2    | 966  | PSU  | C4-N3-C2  | -4.40 | 120.31      | 126.37   |
| 80  | Bv    | 37   | UY4  | N3-C4-N9  | 4.40  | 134.65      | 127.17   |
| 46  | S2    | 36   | PSU  | C4-N3-C2  | -4.39 | 120.32      | 126.37   |
| 3   | L5    | 4166 | OMG  | N9-C4-N3  | 4.37  | 134.70      | 125.95   |
| 3   | L5    | 1768 | PSU  | C4-N3-C2  | -4.37 | 120.35      | 126.37   |
| 3   | L5    | 1849 | PSU  | C4-N3-C2  | -4.37 | 120.35      | 126.37   |
| 3   | L5    | 4362 | OMG  | N9-C4-N3  | 4.36  | 134.68      | 125.95   |
| 5   | L8    | 55   | PSU  | O2-C2-N1  | -4.35 | 118.30      | 122.79   |
| 46  | S2    | 1326 | OMU  | C5-C4-N3  | 4.35  | 120.89      | 114.80   |
| 46  | S2    | 1851 | MA6  | N3-C4-N9  | 4.35  | 134.56      | 127.17   |
| 46  | S2    | 1004 | PSU  | C4-N3-C2  | -4.34 | 120.39      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | L5    | 4590 | OMU  | N3-C2-N1 | 4.34  | 120.55      | 114.89   |
| 46  | S2    | 172  | OMU  | N3-C2-N1 | 4.34  | 120.54      | 114.89   |
| 3   | L5    | 3723 | OMG  | N9-C4-N3 | 4.33  | 134.61      | 125.95   |
| 80  | Bv    | 9    | 1MG  | C2-N3-C4 | 4.33  | 121.71      | 111.98   |
| 46  | S2    | 1804 | OMU  | C5-C4-N3 | 4.33  | 120.86      | 114.80   |
| 3   | L5    | 4373 | PSU  | C4-N3-C2 | -4.31 | 120.44      | 126.37   |
| 3   | L5    | 3904 | OMU  | N3-C2-N1 | 4.31  | 120.50      | 114.89   |
| 3   | L5    | 4263 | PSU  | C4-N3-C2 | -4.31 | 120.44      | 126.37   |
| 3   | L5    | 4606 | PSU  | C4-N3-C2 | -4.30 | 120.45      | 126.37   |
| 46  | S2    | 866  | PSU  | C4-N3-C2 | -4.30 | 120.45      | 126.37   |
| 46  | S2    | 1367 | PSU  | C4-N3-C2 | -4.29 | 120.45      | 126.37   |
| 3   | L5    | 4441 | PSU  | O2-C2-N1 | -4.29 | 118.36      | 122.79   |
| 3   | L5    | 4276 | OMU  | C5-C4-N3 | 4.29  | 120.80      | 114.80   |
| 3   | L5    | 3797 | UY1  | C4-N3-C2 | -4.29 | 120.47      | 126.37   |
| 3   | L5    | 3747 | PSU  | O2-C2-N1 | -4.28 | 118.38      | 122.79   |
| 46  | S2    | 1832 | 6MZ  | C9-N6-C6 | 4.27  | 126.81      | 122.85   |
| 5   | L8    | 69   | PSU  | O2-C2-N1 | -4.27 | 118.39      | 122.79   |
| 80  | Bv    | 55   | PSU  | C4-N3-C2 | -4.26 | 120.50      | 126.37   |
| 80  | Bv    | 28   | PSU  | C4-N3-C2 | -4.25 | 120.52      | 126.37   |
| 3   | L5    | 4588 | OMG  | N9-C4-N3 | 4.25  | 134.45      | 125.95   |
| 46  | S2    | 1174 | PSU  | O2-C2-N1 | -4.25 | 118.41      | 122.79   |
| 3   | L5    | 3749 | PSU  | C4-N3-C2 | -4.25 | 120.52      | 126.37   |
| 46  | S2    | 814  | PSU  | C4-N3-C2 | -4.24 | 120.54      | 126.37   |
| 46  | S2    | 1442 | OMU  | N3-C2-N1 | 4.23  | 120.40      | 114.89   |
| 3   | L5    | 4401 | PSU  | O2-C2-N1 | -4.23 | 118.43      | 122.79   |
| 3   | L5    | 4598 | PSU  | C4-N3-C2 | -4.22 | 120.55      | 126.37   |
| 3   | L5    | 3606 | OMG  | C2-N3-C4 | 4.22  | 119.57      | 112.30   |
| 46  | S2    | 1288 | OMU  | C5-C4-N3 | 4.22  | 120.71      | 114.80   |
| 46  | S2    | 1643 | PSU  | C4-N3-C2 | -4.22 | 120.56      | 126.37   |
| 3   | L5    | 4966 | PSU  | C4-N3-C2 | -4.22 | 120.56      | 126.37   |
| 46  | S2    | 801  | PSU  | C4-N3-C2 | -4.21 | 120.56      | 126.37   |
| 46  | S2    | 119  | PSU  | C4-N3-C2 | -4.21 | 120.57      | 126.37   |
| 3   | L5    | 4331 | PSU  | C4-N3-C2 | -4.21 | 120.57      | 126.37   |
| 80  | Bv    | 27   | PSU  | C4-N3-C2 | -4.21 | 120.57      | 126.37   |
| 46  | S2    | 36   | PSU  | O2-C2-N1 | -4.20 | 118.46      | 122.79   |
| 3   | L5    | 4659 | PSU  | C4-N3-C2 | -4.19 | 120.59      | 126.37   |
| 3   | L5    | 3694 | PSU  | C4-N3-C2 | -4.19 | 120.60      | 126.37   |
| 3   | L5    | 3606 | OMG  | N9-C4-N3 | 4.18  | 134.31      | 125.95   |
| 46  | S2    | 822  | PSU  | O2-C2-N1 | -4.17 | 118.48      | 122.79   |
| 46  | S2    | 116  | OMU  | C4-N3-C2 | -4.17 | 121.43      | 126.61   |
| 46  | S2    | 172  | OMU  | C5-C4-N3 | 4.17  | 120.64      | 114.80   |
| 46  | S2    | 609  | PSU  | C4-N3-C2 | -4.17 | 120.63      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 46  | S2    | 863  | PSU  | C4-N3-C2  | -4.16 | 120.64      | 126.37   |
| 46  | S2    | 428  | OMU  | C5-C4-N3  | 4.15  | 120.61      | 114.80   |
| 46  | S2    | 1046 | PSU  | C4-N3-C2  | -4.15 | 120.66      | 126.37   |
| 3   | L5    | 4500 | UR3  | C6-N1-C2  | -4.15 | 118.41      | 121.80   |
| 3   | L5    | 4417 | 5MC  | CM5-C5-C4 | -4.14 | 113.70      | 120.51   |
| 3   | L5    | 4198 | OMG  | N9-C4-N3  | 4.14  | 134.24      | 125.95   |
| 3   | L5    | 4276 | OMU  | N3-C2-N1  | 4.14  | 120.28      | 114.89   |
| 3   | L5    | 1779 | PSU  | C4-N3-C2  | -4.14 | 120.67      | 126.37   |
| 80  | Bv    | 9    | 1MG  | N9-C4-N3  | 4.13  | 134.22      | 125.95   |
| 46  | S2    | 1232 | PSU  | C4-N3-C2  | -4.13 | 120.68      | 126.37   |
| 46  | S2    | 1832 | 6MZ  | C4-C5-N7  | -4.13 | 105.86      | 110.58   |
| 46  | S2    | 93   | PSU  | C4-N3-C2  | -4.12 | 120.69      | 126.37   |
| 3   | L5    | 4441 | PSU  | C4-N3-C2  | -4.10 | 120.72      | 126.37   |
| 46  | S2    | 1347 | PSU  | C4-N3-C2  | -4.10 | 120.73      | 126.37   |
| 3   | L5    | 1569 | PSU  | O2-C2-N1  | -4.09 | 118.57      | 122.79   |
| 3   | L5    | 4190 | 6MZ  | C9-N6-C6  | -4.09 | 119.06      | 122.85   |
| 46  | S2    | 1337 | 4AC  | C1'-N1-C2 | 4.08  | 127.45      | 118.44   |
| 46  | S2    | 1004 | PSU  | O2-C2-N1  | -4.07 | 118.59      | 122.79   |
| 46  | S2    | 1850 | MA6  | N3-C4-N9  | 4.07  | 134.09      | 127.17   |
| 3   | L5    | 4390 | PSU  | C4-N3-C2  | -4.06 | 120.77      | 126.37   |
| 3   | L5    | 4269 | PSU  | C4-N3-C2  | -4.06 | 120.78      | 126.37   |
| 46  | S2    | 1238 | PSU  | C4-N3-C2  | -4.06 | 120.78      | 126.37   |
| 3   | L5    | 4401 | PSU  | C4-N3-C2  | -4.06 | 120.78      | 126.37   |
| 3   | L5    | 3820 | OMC  | O2-C2-N3  | -4.05 | 115.94      | 122.33   |
| 3   | L5    | 1569 | PSU  | C4-N3-C2  | -4.05 | 120.79      | 126.37   |
| 3   | L5    | 4607 | OMG  | N9-C4-N3  | 4.05  | 134.06      | 125.95   |
| 46  | S2    | 1244 | PSU  | C4-N3-C2  | -4.05 | 120.79      | 126.37   |
| 3   | L5    | 4412 | PSU  | O2-C2-N1  | -4.04 | 118.62      | 122.79   |
| 46  | S2    | 1445 | PSU  | C4-N3-C2  | -4.03 | 120.81      | 126.37   |
| 3   | L5    | 3832 | PSU  | C4-N3-C2  | -4.03 | 120.82      | 126.37   |
| 3   | L5    | 3741 | PSU  | O2-C2-N1  | -4.03 | 118.63      | 122.79   |
| 3   | L5    | 4323 | PSU  | O2-C2-N1  | -4.03 | 118.63      | 122.79   |
| 80  | Bv    | 37   | UY4  | C2-N3-C4  | 4.02  | 121.65      | 111.83   |
| 3   | L5    | 3709 | PSU  | O2-C2-N1  | -4.01 | 118.65      | 122.79   |
| 3   | L5    | 4975 | PSU  | O2-C2-N1  | -4.01 | 118.65      | 122.79   |
| 46  | S2    | 121  | OMU  | C5-C4-N3  | 4.00  | 120.41      | 114.80   |
| 3   | L5    | 3747 | PSU  | C4-N3-C2  | -4.00 | 120.86      | 126.37   |
| 46  | S2    | 105  | PSU  | C4-N3-C2  | -3.99 | 120.87      | 126.37   |
| 46  | S2    | 1625 | PSU  | C4-N3-C2  | -3.98 | 120.88      | 126.37   |
| 46  | S2    | 609  | PSU  | O2-C2-N1  | -3.98 | 118.69      | 122.79   |
| 46  | S2    | 428  | OMU  | N3-C2-N1  | 3.97  | 120.06      | 114.89   |
| 3   | L5    | 1670 | PSU  | C4-N3-C2  | -3.97 | 120.90      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 4197 | OMU  | C5-C4-N3    | 3.97  | 120.36      | 114.80   |
| 3   | L5    | 3737 | PSU  | C4-N3-C2    | -3.96 | 120.92      | 126.37   |
| 46  | S2    | 116  | OMU  | C5-C4-N3    | 3.96  | 120.34      | 114.80   |
| 3   | L5    | 1523 | PSU  | C4-N3-C2    | -3.96 | 120.92      | 126.37   |
| 3   | L5    | 2495 | PSU  | C4-N3-C2    | -3.96 | 120.92      | 126.37   |
| 46  | S2    | 1244 | PSU  | O2-C2-N1    | -3.95 | 118.71      | 122.79   |
| 46  | S2    | 1045 | PSU  | O2-C2-N1    | -3.95 | 118.71      | 122.79   |
| 46  | S2    | 1288 | OMU  | N3-C2-N1    | 3.95  | 120.03      | 114.89   |
| 3   | L5    | 4522 | PSU  | O2-C2-N1    | -3.94 | 118.72      | 122.79   |
| 46  | S2    | 815  | PSU  | C4-N3-C2    | -3.94 | 120.94      | 126.37   |
| 3   | L5    | 3743 | PSU  | O2-C2-N1    | -3.93 | 118.74      | 122.79   |
| 3   | L5    | 3830 | PSU  | C4-N3-C2    | -3.92 | 120.97      | 126.37   |
| 46  | S2    | 649  | PSU  | C4-N3-C2    | -3.91 | 120.98      | 126.37   |
| 3   | L5    | 4282 | PSU  | O2-C2-N1    | -3.91 | 118.76      | 122.79   |
| 3   | L5    | 1670 | PSU  | O2-C2-N1    | -3.91 | 118.76      | 122.79   |
| 46  | S2    | 1442 | OMU  | C5-C4-N3    | 3.90  | 120.27      | 114.80   |
| 3   | L5    | 4393 | PSU  | C4-N3-C2    | -3.90 | 120.99      | 126.37   |
| 46  | S2    | 1238 | PSU  | O2-C2-N1    | -3.90 | 118.76      | 122.79   |
| 3   | L5    | 1769 | PSU  | O2-C2-N1    | -3.90 | 118.77      | 122.79   |
| 3   | L5    | 3743 | PSU  | C4-N3-C2    | -3.89 | 121.01      | 126.37   |
| 46  | S2    | 1832 | 6MZ  | N3-C4-N9    | 3.88  | 133.77      | 127.17   |
| 46  | S2    | 822  | PSU  | C4-N3-C2    | -3.88 | 121.03      | 126.37   |
| 46  | S2    | 1851 | MA6  | C2-N3-C4    | 3.87  | 121.28      | 111.83   |
| 80  | Bv    | 28   | PSU  | O2-C2-N1    | -3.86 | 118.81      | 122.79   |
| 3   | L5    | 4502 | PSU  | C4-N3-C2    | -3.86 | 121.06      | 126.37   |
| 3   | L5    | 4643 | PSU  | C4-N3-C2    | -3.85 | 121.06      | 126.37   |
| 3   | L5    | 2824 | OMU  | O4-C4-C5    | -3.85 | 118.53      | 125.16   |
| 3   | L5    | 4643 | PSU  | O2-C2-N1    | -3.84 | 118.83      | 122.79   |
| 46  | S2    | 116  | OMU  | N3-C2-N1    | 3.84  | 119.88      | 114.89   |
| 46  | S2    | 1248 | B8N  | C4-N3-C2    | -3.83 | 120.91      | 125.62   |
| 3   | L5    | 1313 | A2M  | O3'-C3'-C2' | -3.82 | 100.50      | 111.19   |
| 46  | S2    | 686  | PSU  | O2-C2-N1    | -3.82 | 118.85      | 122.79   |
| 3   | L5    | 4198 | OMG  | C6-C5-N7    | 3.81  | 137.22      | 130.29   |
| 46  | S2    | 1347 | PSU  | O2-C2-N1    | -3.79 | 118.88      | 122.79   |
| 3   | L5    | 1847 | PSU  | C6-C5-C4    | -3.78 | 115.62      | 118.17   |
| 3   | L5    | 4427 | PSU  | C6-C5-C4    | -3.78 | 115.63      | 118.17   |
| 3   | L5    | 4937 | PSU  | C4-N3-C2    | -3.77 | 121.17      | 126.37   |
| 46  | S2    | 601  | OMG  | N9-C4-N3    | 3.77  | 133.50      | 125.95   |
| 3   | L5    | 4190 | 6MZ  | C6-C5-N7    | 3.77  | 136.54      | 132.43   |
| 3   | L5    | 1664 | PSU  | O2-C2-N1    | -3.77 | 118.90      | 122.79   |
| 46  | S2    | 1367 | PSU  | O2-C2-N1    | -3.76 | 118.91      | 122.79   |
| 3   | L5    | 4491 | PSU  | O2-C2-N1    | -3.76 | 118.92      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 4190 | 6MZ  | C2-N3-C4    | 3.75  | 121.00      | 111.83   |
| 3   | L5    | 4190 | 6MZ  | C4-C5-N7    | -3.75 | 106.29      | 110.58   |
| 46  | S2    | 1703 | OMC  | O2-C2-N3    | -3.75 | 116.42      | 122.33   |
| 3   | L5    | 4263 | PSU  | O2-C2-N1    | -3.74 | 118.93      | 122.79   |
| 46  | S2    | 1832 | 6MZ  | N1-C2-N3    | -3.74 | 122.92      | 128.58   |
| 46  | S2    | 1177 | PSU  | C4-N3-C2    | -3.73 | 121.23      | 126.37   |
| 46  | S2    | 863  | PSU  | O2-C2-N1    | -3.73 | 118.94      | 122.79   |
| 46  | S2    | 649  | PSU  | O2-C2-N1    | -3.71 | 118.96      | 122.79   |
| 80  | Bv    | 27   | PSU  | O2-C2-N1    | -3.70 | 118.97      | 122.79   |
| 3   | L5    | 4588 | OMG  | C6-C5-N7    | 3.70  | 137.01      | 130.29   |
| 80  | Bv    | 55   | PSU  | O2-C2-N1    | -3.69 | 118.98      | 122.79   |
| 3   | L5    | 1847 | PSU  | C4-N3-C2    | -3.69 | 121.29      | 126.37   |
| 3   | L5    | 4549 | PSU  | O2-C2-N1    | -3.67 | 119.00      | 122.79   |
| 46  | S2    | 1851 | MA6  | N1-C2-N3    | -3.66 | 123.04      | 128.58   |
| 3   | L5    | 4362 | OMG  | C6-C5-N7    | 3.65  | 136.94      | 130.29   |
| 46  | S2    | 1804 | OMU  | N3-C2-N1    | 3.65  | 119.64      | 114.89   |
| 46  | S2    | 1851 | MA6  | C5-N7-C8    | 3.63  | 109.16      | 103.45   |
| 46  | S2    | 406  | PSU  | O2-C2-N1    | -3.62 | 119.06      | 122.79   |
| 3   | L5    | 3749 | PSU  | O2-C2-N1    | -3.62 | 119.06      | 122.79   |
| 3   | L5    | 4190 | 6MZ  | N3-C4-N9    | 3.62  | 133.32      | 127.17   |
| 3   | L5    | 3694 | PSU  | O2-C2-N1    | -3.62 | 119.06      | 122.79   |
| 46  | S2    | 815  | PSU  | O2-C2-N1    | -3.62 | 119.06      | 122.79   |
| 46  | S2    | 1842 | 4AC  | C6-C5-C4    | 3.61  | 121.35      | 117.00   |
| 46  | S2    | 1832 | 6MZ  | C2-N3-C4    | 3.61  | 120.66      | 111.83   |
| 46  | S2    | 801  | PSU  | O2-C2-N1    | -3.61 | 119.06      | 122.79   |
| 3   | L5    | 3713 | PSU  | O2-C2-N1    | -3.60 | 119.08      | 122.79   |
| 3   | L5    | 4390 | PSU  | O2-C2-N1    | -3.59 | 119.08      | 122.79   |
| 3   | L5    | 1313 | A2M  | C4-C5-N7    | -3.59 | 106.48      | 110.58   |
| 3   | L5    | 4417 | 5MC  | O2-C2-N3    | -3.59 | 116.67      | 122.33   |
| 3   | L5    | 3771 | OMG  | CM2-O2'-C2' | -3.58 | 105.28      | 114.47   |
| 46  | S2    | 1232 | PSU  | O2-C2-N1    | -3.58 | 119.10      | 122.79   |
| 46  | S2    | 1625 | PSU  | O2-C2-N1    | -3.57 | 119.11      | 122.79   |
| 46  | S2    | 116  | OMU  | O4-C4-C5    | -3.56 | 119.02      | 125.16   |
| 3   | L5    | 4590 | OMU  | C5-C4-N3    | 3.55  | 119.78      | 114.80   |
| 46  | S2    | 1643 | PSU  | O2-C2-N1    | -3.55 | 119.13      | 122.79   |
| 46  | S2    | 814  | PSU  | O2-C2-N1    | -3.54 | 119.14      | 122.79   |
| 46  | S2    | 109  | PSU  | O2-C2-N1    | -3.54 | 119.14      | 122.79   |
| 3   | L5    | 4500 | UR3  | C5-C4-N3    | 3.53  | 119.69      | 115.04   |
| 3   | L5    | 1313 | A2M  | C2-N3-C4    | 3.53  | 120.45      | 111.83   |
| 3   | L5    | 2411 | OMG  | N9-C4-N3    | 3.52  | 132.99      | 125.95   |
| 46  | S2    | 1442 | OMU  | O4-C4-C5    | -3.51 | 119.10      | 125.16   |
| 46  | S2    | 1804 | OMU  | C1'-N1-C2   | 3.51  | 123.90      | 117.59   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | L5    | 4331 | PSU  | C6-C5-C4  | -3.50 | 115.81      | 118.17   |
| 3   | L5    | 2338 | OMC  | O2-C2-N1  | 3.46  | 125.68      | 118.90   |
| 46  | S2    | 1804 | OMU  | O4-C4-C5  | -3.44 | 119.23      | 125.16   |
| 46  | S2    | 572  | PSU  | O2-C2-N1  | -3.43 | 119.25      | 122.79   |
| 3   | L5    | 3832 | PSU  | O2-C2-N1  | -3.42 | 119.26      | 122.79   |
| 46  | S2    | 966  | PSU  | O2-C2-N1  | -3.42 | 119.26      | 122.79   |
| 46  | S2    | 93   | PSU  | C6-C5-C4  | -3.41 | 115.87      | 118.17   |
| 46  | S2    | 428  | OMU  | O4-C4-C5  | -3.41 | 119.28      | 125.16   |
| 3   | L5    | 4607 | OMG  | C6-C5-N7  | 3.41  | 136.49      | 130.29   |
| 80  | Bv    | 58   | 1MA  | N9-C4-N3  | 3.40  | 134.65      | 126.90   |
| 3   | L5    | 1313 | A2M  | N3-C2-N1  | -3.40 | 123.44      | 128.58   |
| 3   | L5    | 4966 | PSU  | C6-C5-C4  | -3.40 | 115.88      | 118.17   |
| 3   | L5    | 2495 | PSU  | O2-C2-N1  | -3.38 | 119.30      | 122.79   |
| 46  | S2    | 1851 | MA6  | C4-N9-C8  | 3.37  | 109.28      | 105.74   |
| 46  | S2    | 1692 | PSU  | O2-C2-N1  | -3.36 | 119.32      | 122.79   |
| 46  | S2    | 34   | PSU  | O2-C2-N1  | -3.36 | 119.32      | 122.79   |
| 46  | S2    | 1850 | MA6  | N1-C2-N3  | -3.36 | 123.50      | 128.58   |
| 46  | S2    | 651  | PSU  | O2-C2-N1  | -3.35 | 119.33      | 122.79   |
| 80  | Bv    | 37   | UY4  | N3-C2-N1  | -3.34 | 123.52      | 128.58   |
| 46  | S2    | 1850 | MA6  | C2-N3-C4  | 3.34  | 119.99      | 111.83   |
| 46  | S2    | 1832 | 6MZ  | C4-N9-C8  | 3.32  | 109.23      | 105.74   |
| 3   | L5    | 2619 | PSU  | O2-C2-N1  | -3.31 | 119.38      | 122.79   |
| 3   | L5    | 4190 | 6MZ  | N1-C2-N3  | -3.30 | 123.58      | 128.58   |
| 80  | Bv    | 26   | M2G  | C6-C5-N7  | 3.30  | 136.29      | 130.29   |
| 3   | L5    | 4500 | UR3  | O2-C2-N3  | -3.29 | 116.78      | 121.33   |
| 3   | L5    | 2409 | OMC  | O2-C2-N3  | -3.29 | 117.14      | 122.33   |
| 46  | S2    | 601  | OMG  | C6-C5-N7  | 3.28  | 136.26      | 130.29   |
| 3   | L5    | 4266 | PSU  | O2-C2-N1  | -3.27 | 119.41      | 122.79   |
| 3   | L5    | 2411 | OMG  | C6-C5-N7  | 3.27  | 136.24      | 130.29   |
| 3   | L5    | 1504 | 2MG  | C2-N1-C6  | -3.25 | 120.62      | 124.55   |
| 3   | L5    | 4393 | PSU  | O2-C2-N1  | -3.24 | 119.45      | 122.79   |
| 46  | S2    | 866  | PSU  | O2-C2-N1  | -3.24 | 119.45      | 122.79   |
| 3   | L5    | 3904 | OMU  | O2-C2-N3  | -3.23 | 115.53      | 121.49   |
| 46  | S2    | 621  | OMC  | C1'-N1-C2 | 3.23  | 125.57      | 118.44   |
| 46  | S2    | 462  | OMC  | O2-C2-N3  | -3.22 | 117.25      | 122.33   |
| 3   | L5    | 4659 | PSU  | O2-C2-N1  | -3.22 | 119.47      | 122.79   |
| 3   | L5    | 3830 | PSU  | O2-C2-N1  | -3.19 | 119.50      | 122.79   |
| 46  | S2    | 1046 | PSU  | O2-C2-N1  | -3.19 | 119.50      | 122.79   |
| 80  | Bv    | 10   | 2MG  | C6-C5-N7  | 3.18  | 136.08      | 130.29   |
| 46  | S2    | 436  | OMG  | C6-C5-N7  | 3.18  | 136.07      | 130.29   |
| 46  | S2    | 1391 | OMC  | O2-C2-N3  | -3.18 | 117.32      | 122.33   |
| 46  | S2    | 1490 | OMG  | C6-C5-N7  | 3.18  | 136.07      | 130.29   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | S2    | 1445 | PSU  | O2-C2-N1    | -3.17 | 119.52      | 122.79   |
| 3   | L5    | 1509 | OMG  | CM2-O2'-C2' | -3.17 | 106.33      | 114.47   |
| 46  | S2    | 1850 | MA6  | C5-N7-C8    | 3.17  | 108.44      | 103.45   |
| 3   | L5    | 2351 | OMG  | C6-C5-N7    | 3.17  | 136.05      | 130.29   |
| 46  | S2    | 1850 | MA6  | C4-N9-C8    | 3.16  | 109.06      | 105.74   |
| 3   | L5    | 4590 | OMU  | C4-N3-C2    | -3.16 | 122.69      | 126.61   |
| 3   | L5    | 1303 | OMG  | C6-C5-N7    | 3.16  | 136.03      | 130.29   |
| 46  | S2    | 1842 | 4AC  | O7-C7-CM7   | -3.16 | 116.44      | 122.05   |
| 46  | S2    | 218  | PSU  | O2-C2-N1    | -3.15 | 119.53      | 122.79   |
| 3   | L5    | 3606 | OMG  | C6-C5-N7    | 3.15  | 136.02      | 130.29   |
| 3   | L5    | 4417 | 5MC  | N1-C2-N3    | 3.14  | 124.25      | 118.80   |
| 3   | L5    | 4607 | OMG  | C4-C5-N7    | -3.14 | 105.70      | 110.67   |
| 3   | L5    | 4966 | PSU  | O2-C2-N1    | -3.13 | 119.56      | 122.79   |
| 3   | L5    | 3761 | 5MC  | C1'-N1-C6   | -3.13 | 116.00      | 121.15   |
| 80  | Bv    | 55   | PSU  | C3'-C2'-C1' | 3.12  | 105.37      | 101.69   |
| 3   | L5    | 3771 | OMG  | C6-C5-N7    | 3.12  | 135.97      | 130.29   |
| 46  | S2    | 93   | PSU  | O2-C2-N1    | -3.12 | 119.57      | 122.79   |
| 3   | L5    | 4593 | OMG  | C6-C5-N7    | 3.11  | 135.96      | 130.29   |
| 5   | L8    | 75   | OMG  | C6-C5-N7    | 3.11  | 135.94      | 130.29   |
| 3   | L5    | 4427 | PSU  | O2-C2-N1    | -3.10 | 119.59      | 122.79   |
| 3   | L5    | 4276 | OMU  | O4-C4-C5    | -3.09 | 119.84      | 125.16   |
| 3   | L5    | 3674 | PSU  | C5-C6-N1    | -3.08 | 117.86      | 122.14   |
| 3   | L5    | 4937 | PSU  | O2-C2-N1    | -3.08 | 119.61      | 122.79   |
| 46  | S2    | 105  | PSU  | O2-C2-N1    | -3.08 | 119.61      | 122.79   |
| 3   | L5    | 4340 | OMG  | C6-C5-N7    | 3.07  | 135.88      | 130.29   |
| 46  | S2    | 1248 | B8N  | C1'-C5-C4   | 3.06  | 122.25      | 117.61   |
| 3   | L5    | 3616 | PSU  | O2-C2-N1    | -3.05 | 119.64      | 122.79   |
| 3   | L5    | 3761 | 5MC  | C5-C4-N3    | -3.05 | 118.63      | 121.75   |
| 3   | L5    | 4468 | OMU  | O4-C4-C5    | -3.05 | 119.90      | 125.16   |
| 3   | L5    | 4590 | OMU  | C6-N1-C2    | -3.04 | 117.29      | 121.00   |
| 3   | L5    | 4417 | 5MC  | C5-C4-N3    | -3.04 | 118.64      | 121.75   |
| 46  | S2    | 1177 | PSU  | O2-C2-N1    | -3.04 | 119.66      | 122.79   |
| 80  | Bv    | 37   | UY4  | C4-C5-N7    | -3.03 | 107.12      | 110.58   |
| 3   | L5    | 3904 | OMU  | C1'-N1-C2   | 3.03  | 123.03      | 117.59   |
| 3   | L5    | 1523 | PSU  | C6-C5-C4    | -3.02 | 116.14      | 118.17   |
| 46  | S2    | 172  | OMU  | O4-C4-C5    | -3.01 | 119.98      | 125.16   |
| 3   | L5    | 3866 | OMC  | O2-C2-N3    | -3.00 | 117.61      | 122.33   |
| 3   | L5    | 364  | OMG  | CM2-O2'-C2' | -2.99 | 106.79      | 114.47   |
| 3   | L5    | 3899 | PSU  | O2-C2-N1    | -2.99 | 119.71      | 122.79   |
| 3   | L5    | 4506 | OMC  | O2-C2-N3    | -2.98 | 117.62      | 122.33   |
| 3   | L5    | 4197 | OMU  | O4-C4-C5    | -2.98 | 120.03      | 125.16   |
| 3   | L5    | 3878 | OMG  | C6-C5-N7    | 2.97  | 135.69      | 130.29   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 1664 | PSU  | C5-C6-N1    | -2.96 | 118.03      | 122.14   |
| 3   | L5    | 1509 | OMG  | C2'-C1'-N9  | -2.96 | 108.62      | 114.24   |
| 3   | L5    | 1849 | PSU  | O2-C2-N1    | -2.95 | 119.74      | 122.79   |
| 3   | L5    | 4469 | OMG  | C6-C5-N7    | 2.95  | 135.65      | 130.29   |
| 3   | L5    | 2863 | OMG  | C6-C5-N7    | 2.94  | 135.64      | 130.29   |
| 3   | L5    | 1313 | A2M  | C2'-C1'-N9  | -2.94 | 108.92      | 113.75   |
| 46  | S2    | 867  | OMG  | C6-C5-N7    | 2.94  | 135.63      | 130.29   |
| 3   | L5    | 2351 | OMG  | O6-C6-C5    | -2.93 | 118.79      | 126.53   |
| 3   | L5    | 3771 | OMG  | O6-C6-C5    | -2.93 | 118.79      | 126.53   |
| 3   | L5    | 3723 | OMG  | C6-C5-N7    | 2.93  | 135.62      | 130.29   |
| 3   | L5    | 3848 | OMC  | O2-C2-N3    | -2.93 | 117.72      | 122.33   |
| 46  | S2    | 119  | PSU  | O2-C2-N1    | -2.93 | 119.77      | 122.79   |
| 80  | Bv    | 37   | UY4  | C2'-C1'-N9  | -2.92 | 106.05      | 113.30   |
| 80  | Bv    | 37   | UY4  | C6-C5-N7    | 2.92  | 135.61      | 132.43   |
| 3   | L5    | 3737 | PSU  | O2-C2-N1    | -2.92 | 119.78      | 122.79   |
| 80  | Bv    | 47   | H2U  | O4'-C1'-N1  | 2.91  | 113.27      | 109.30   |
| 46  | S2    | 1328 | OMG  | C6-C5-N7    | 2.90  | 135.56      | 130.29   |
| 46  | S2    | 174  | OMC  | O2-C2-N3    | -2.89 | 117.78      | 122.33   |
| 46  | S2    | 172  | OMU  | O2-C2-N1    | -2.89 | 119.04      | 122.80   |
| 3   | L5    | 1309 | 1MA  | N9-C4-N3    | 2.88  | 133.46      | 126.90   |
| 3   | L5    | 4166 | OMG  | C6-C5-N7    | 2.88  | 135.53      | 130.29   |
| 46  | S2    | 1288 | OMU  | O4-C4-C5    | -2.88 | 120.20      | 125.16   |
| 3   | L5    | 3899 | PSU  | O2-C2-N3    | -2.87 | 116.76      | 121.86   |
| 46  | S2    | 1842 | 4AC  | C5-C4-N3    | -2.87 | 118.11      | 122.60   |
| 3   | L5    | 1612 | OMG  | C6-C5-N7    | 2.87  | 135.51      | 130.29   |
| 80  | Bv    | 16   | H2U  | O4'-C1'-N1  | 2.87  | 113.20      | 109.30   |
| 3   | L5    | 2774 | A2M  | CM'-O2'-C2' | -2.86 | 107.13      | 114.47   |
| 3   | L5    | 3761 | 5MC  | C5-C6-N1    | -2.86 | 120.21      | 123.31   |
| 3   | L5    | 4426 | OMC  | O2-C2-N3    | -2.86 | 117.82      | 122.33   |
| 3   | L5    | 3904 | OMU  | O4-C4-C5    | -2.86 | 120.23      | 125.16   |
| 46  | S2    | 1136 | PSU  | O2-C2-N1    | -2.86 | 119.84      | 122.79   |
| 3   | L5    | 1309 | 1MA  | N1-C2-N3    | -2.85 | 122.61      | 126.00   |
| 46  | S2    | 1490 | OMG  | C5-C6-N1    | 2.84  | 120.49      | 113.25   |
| 46  | S2    | 121  | OMU  | O4-C4-C5    | -2.84 | 120.26      | 125.16   |
| 3   | L5    | 3674 | PSU  | O2-C2-N1    | -2.84 | 119.86      | 122.79   |
| 46  | S2    | 1177 | PSU  | C6-C5-C4    | -2.83 | 116.26      | 118.17   |
| 80  | Bv    | 46   | G7M  | O4'-C1'-N9  | 2.83  | 114.76      | 108.36   |
| 3   | L5    | 2338 | OMC  | C1'-N1-C2   | 2.82  | 124.67      | 118.44   |
| 3   | L5    | 1313 | A2M  | C4-N9-C8    | 2.82  | 108.70      | 105.74   |
| 3   | L5    | 4331 | PSU  | O2-C2-N1    | -2.81 | 119.89      | 122.79   |
| 3   | L5    | 3823 | PSU  | C6-C5-C4    | -2.81 | 116.28      | 118.17   |
| 46  | S2    | 1851 | MA6  | C6-C5-N7    | 2.80  | 137.91      | 133.43   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 46  | S2    | 1490 | OMG  | O6-C6-C5   | -2.80 | 119.14      | 126.53   |
| 3   | L5    | 3618 | PSU  | O2-C2-N1   | -2.80 | 119.90      | 122.79   |
| 3   | L5    | 1504 | 2MG  | O6-C6-C5   | -2.78 | 119.19      | 126.53   |
| 3   | L5    | 2411 | OMG  | O6-C6-C5   | -2.78 | 119.19      | 126.53   |
| 3   | L5    | 4417 | 5MC  | C1'-N1-C6  | 2.77  | 125.72      | 121.15   |
| 46  | S2    | 1842 | 4AC  | N4-C4-N3   | 2.76  | 118.35      | 113.87   |
| 3   | L5    | 2402 | PSU  | C5-C6-N1   | -2.76 | 118.31      | 122.14   |
| 3   | L5    | 364  | OMG  | C8-N9-C4   | 2.76  | 111.19      | 106.03   |
| 46  | S2    | 1326 | OMU  | O4-C4-C5   | -2.75 | 120.42      | 125.16   |
| 46  | S2    | 436  | OMG  | C4-C5-N7   | -2.75 | 106.32      | 110.67   |
| 3   | L5    | 1509 | OMG  | C6-C5-N7   | 2.74  | 135.28      | 130.29   |
| 3   | L5    | 4166 | OMG  | C2-N1-C6   | -2.74 | 120.14      | 125.11   |
| 3   | L5    | 3618 | PSU  | O2-C2-N3   | -2.74 | 117.00      | 121.86   |
| 3   | L5    | 2351 | OMG  | C4-C5-N7   | -2.73 | 106.34      | 110.67   |
| 3   | L5    | 3713 | PSU  | C5-C6-N1   | -2.73 | 118.35      | 122.14   |
| 3   | L5    | 3723 | OMG  | O6-C6-C5   | -2.72 | 119.35      | 126.53   |
| 46  | S2    | 1832 | 6MZ  | C5-N7-C8   | 2.71  | 107.72      | 103.45   |
| 3   | L5    | 4269 | PSU  | O2-C2-N1   | -2.71 | 119.99      | 122.79   |
| 3   | L5    | 4340 | OMG  | C4-C5-N7   | -2.71 | 106.37      | 110.67   |
| 46  | S2    | 1136 | PSU  | C6-C5-C4   | -2.71 | 116.34      | 118.17   |
| 3   | L5    | 3743 | PSU  | C6-C5-C4   | -2.70 | 116.35      | 118.17   |
| 3   | L5    | 3761 | 5MC  | O2-C2-N1   | 2.70  | 124.19      | 118.90   |
| 3   | L5    | 4362 | OMG  | C4-C5-N7   | -2.70 | 106.39      | 110.67   |
| 3   | L5    | 3616 | PSU  | O2-C2-N3   | -2.70 | 117.06      | 121.86   |
| 80  | Bv    | 26   | M2G  | C4-C5-N7   | -2.70 | 106.40      | 110.67   |
| 46  | S2    | 644  | OMG  | C6-C5-N7   | 2.69  | 135.19      | 130.29   |
| 80  | Bv    | 46   | G7M  | O6-C6-C5   | -2.69 | 122.01      | 128.01   |
| 46  | S2    | 1851 | MA6  | N9-C8-N7   | -2.69 | 110.13      | 113.94   |
| 3   | L5    | 3787 | OMC  | O2-C2-N3   | -2.68 | 118.10      | 122.33   |
| 3   | L5    | 2863 | OMG  | C4-C5-N7   | -2.68 | 106.42      | 110.67   |
| 46  | S2    | 1046 | PSU  | C6-C5-C4   | -2.68 | 116.37      | 118.17   |
| 3   | L5    | 4198 | OMG  | C4-C5-N7   | -2.68 | 106.43      | 110.67   |
| 3   | L5    | 1313 | A2M  | C5-N7-C8   | 2.67  | 107.64      | 103.45   |
| 46  | S2    | 1081 | PSU  | O2-C2-N1   | -2.67 | 120.04      | 122.79   |
| 80  | Bv    | 26   | M2G  | C2'-C1'-N9 | -2.66 | 105.84      | 113.25   |
| 3   | L5    | 4468 | OMU  | O2-C2-N1   | -2.66 | 119.34      | 122.80   |
| 3   | L5    | 364  | OMG  | C6-C5-N7   | 2.66  | 135.12      | 130.29   |
| 46  | S2    | 686  | PSU  | C5-C6-N1   | -2.65 | 118.46      | 122.14   |
| 46  | S2    | 1081 | PSU  | C6-C5-C4   | -2.65 | 116.39      | 118.17   |
| 3   | L5    | 3797 | UY1  | O2-C2-N1   | -2.64 | 120.06      | 122.79   |
| 3   | L5    | 1303 | OMG  | C4-C5-N7   | -2.64 | 106.48      | 110.67   |
| 46  | S2    | 116  | OMU  | C1'-N1-C2  | 2.64  | 122.33      | 117.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | S2    | 572  | PSU  | C5-C6-N1    | -2.64 | 118.48      | 122.14   |
| 3   | L5    | 4606 | PSU  | O2-C2-N1    | -2.63 | 120.08      | 122.79   |
| 46  | S2    | 621  | OMC  | C1'-N1-C6   | -2.62 | 115.19      | 120.78   |
| 3   | L5    | 3899 | PSU  | C6-C5-C4    | -2.62 | 116.41      | 118.17   |
| 3   | L5    | 1509 | OMG  | O6-C6-C5    | -2.61 | 119.64      | 126.53   |
| 3   | L5    | 3820 | OMC  | CM2-O2'-C2' | -2.61 | 107.77      | 114.47   |
| 46  | S2    | 1326 | OMU  | CM2-O2'-C2' | -2.61 | 107.79      | 114.47   |
| 3   | L5    | 1779 | PSU  | O2-C2-N3    | -2.60 | 117.23      | 121.86   |
| 3   | L5    | 4166 | OMG  | C4-C5-N7    | -2.60 | 106.55      | 110.67   |
| 3   | L5    | 4393 | PSU  | C6-C5-C4    | -2.60 | 116.42      | 118.17   |
| 46  | S2    | 1337 | 4AC  | C6-N1-C2    | -2.60 | 116.08      | 120.46   |
| 80  | Bv    | 9    | 1MG  | C6-C5-N7    | 2.59  | 135.11      | 129.36   |
| 80  | Bv    | 10   | 2MG  | C4-C5-N7    | -2.59 | 106.57      | 110.67   |
| 80  | Bv    | 58   | 1MA  | C4-C5-N7    | -2.58 | 106.59      | 110.67   |
| 3   | L5    | 4588 | OMG  | C4-C5-N7    | -2.57 | 106.60      | 110.67   |
| 46  | S2    | 1842 | 4AC  | C1'-N1-C2   | 2.56  | 124.09      | 118.44   |
| 3   | L5    | 4323 | PSU  | C5-C6-N1    | -2.56 | 118.59      | 122.14   |
| 3   | L5    | 4491 | PSU  | O4'-C1'-C2' | 2.56  | 108.69      | 105.15   |
| 3   | L5    | 364  | OMG  | O6-C6-C5    | -2.55 | 119.79      | 126.53   |
| 46  | S2    | 509  | OMG  | C6-C5-N7    | 2.55  | 134.94      | 130.29   |
| 3   | L5    | 4659 | PSU  | C6-N1-C2    | -2.55 | 120.32      | 122.69   |
| 3   | L5    | 1504 | 2MG  | CM2-N2-C2   | -2.55 | 118.17      | 123.65   |
| 80  | Bv    | 47   | H2U  | C5-C6-N1    | -2.54 | 103.83      | 111.52   |
| 3   | L5    | 3761 | 5MC  | C1'-N1-C2   | 2.54  | 124.05      | 118.44   |
| 3   | L5    | 2802 | A2M  | C4-N9-C1'   | 2.54  | 132.57      | 126.63   |
| 80  | Bv    | 16   | H2U  | C5-C6-N1    | -2.53 | 103.85      | 111.52   |
| 46  | S2    | 1850 | MA6  | C6-C5-N7    | 2.53  | 137.48      | 133.43   |
| 46  | S2    | 1337 | 4AC  | O2-C2-N3    | -2.53 | 118.34      | 122.33   |
| 46  | S2    | 621  | OMC  | O2-C2-N1    | 2.53  | 123.86      | 118.90   |
| 3   | L5    | 4491 | PSU  | C5-C6-N1    | -2.53 | 118.63      | 122.14   |
| 80  | Bv    | 47   | H2U  | C3'-C2'-C1' | 2.52  | 106.23      | 101.46   |
| 3   | L5    | 2802 | A2M  | C1'-N9-C8   | -2.52 | 121.50      | 127.09   |
| 3   | L5    | 2811 | OMC  | O2-C2-N3    | -2.52 | 118.36      | 122.33   |
| 46  | S2    | 1639 | G7M  | CN7-N7-C5   | 2.51  | 129.93      | 126.80   |
| 3   | L5    | 4427 | PSU  | O2-C2-N3    | -2.50 | 117.41      | 121.86   |
| 80  | Bv    | 9    | 1MG  | C4-C5-N7    | -2.50 | 106.70      | 110.67   |
| 3   | L5    | 364  | OMG  | C5-C6-N1    | 2.49  | 119.60      | 113.25   |
| 3   | L5    | 4588 | OMG  | O6-C6-C5    | -2.48 | 119.98      | 126.53   |
| 3   | L5    | 4441 | PSU  | C6-N1-C2    | -2.48 | 120.39      | 122.69   |
| 46  | S2    | 1328 | OMG  | C4-C5-N7    | -2.48 | 106.74      | 110.67   |
| 46  | S2    | 1081 | PSU  | O2-C2-N3    | -2.47 | 117.47      | 121.86   |
| 3   | L5    | 1504 | 2MG  | C6-C5-N7    | 2.47  | 134.78      | 130.29   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 2863 | OMG  | O6-C6-C5    | -2.46 | 120.03      | 126.53   |
| 3   | L5    | 4549 | PSU  | C6-C5-C4    | -2.46 | 116.51      | 118.17   |
| 3   | L5    | 4502 | PSU  | O2-C2-N1    | -2.45 | 120.26      | 122.79   |
| 3   | L5    | 4659 | PSU  | O2-C2-N3    | -2.45 | 117.51      | 121.86   |
| 3   | L5    | 3747 | PSU  | C6-C5-C4    | -2.45 | 116.52      | 118.17   |
| 3   | L5    | 3904 | OMU  | CM2-O2'-C2' | -2.44 | 108.20      | 114.47   |
| 3   | L5    | 4464 | OMG  | C6-C5-N7    | 2.44  | 134.74      | 130.29   |
| 46  | S2    | 651  | PSU  | C5-C6-N1    | -2.44 | 118.75      | 122.14   |
| 3   | L5    | 364  | OMG  | C2'-C1'-N9  | -2.44 | 109.61      | 114.24   |
| 3   | L5    | 3618 | PSU  | C5-C6-N1    | -2.44 | 118.76      | 122.14   |
| 3   | L5    | 1858 | A2M  | C2'-C1'-N9  | -2.43 | 109.75      | 113.75   |
| 3   | L5    | 4373 | PSU  | O2-C2-N3    | -2.43 | 117.55      | 121.86   |
| 3   | L5    | 1309 | 1MA  | C6-C5-N7    | 2.43  | 136.45      | 132.16   |
| 3   | L5    | 4659 | PSU  | C6-C5-C4    | -2.42 | 116.54      | 118.17   |
| 80  | Bv    | 37   | UY4  | C4-N9-C8    | 2.42  | 108.28      | 105.74   |
| 3   | L5    | 4166 | OMG  | O6-C6-C5    | -2.42 | 120.14      | 126.53   |
| 46  | S2    | 683  | OMG  | C6-C5-N7    | 2.40  | 134.65      | 130.29   |
| 3   | L5    | 2619 | PSU  | C5-C6-N1    | -2.39 | 118.82      | 122.14   |
| 3   | L5    | 4276 | OMU  | C1'-N1-C2   | 2.39  | 121.89      | 117.59   |
| 46  | S2    | 116  | OMU  | C6-N1-C2    | -2.39 | 118.09      | 121.00   |
| 46  | S2    | 668  | A2M  | C1'-N9-C8   | 2.39  | 132.39      | 127.09   |
| 3   | L5    | 2351 | OMG  | C2-N1-C6    | -2.38 | 120.79      | 125.11   |
| 46  | S2    | 1832 | 6MZ  | C2-N1-C6    | 2.38  | 123.13      | 115.24   |
| 46  | S2    | 1703 | OMC  | C1'-N1-C2   | 2.38  | 123.70      | 118.44   |
| 3   | L5    | 4412 | PSU  | C6-C5-C4    | -2.38 | 116.57      | 118.17   |
| 3   | L5    | 3878 | OMG  | O6-C6-C5    | -2.38 | 120.26      | 126.53   |
| 46  | S2    | 863  | PSU  | C6-C5-C4    | -2.38 | 116.57      | 118.17   |
| 3   | L5    | 3904 | OMU  | C6-N1-C2    | -2.37 | 118.11      | 121.00   |
| 3   | L5    | 4266 | PSU  | C6-C5-C4    | -2.37 | 116.58      | 118.17   |
| 3   | L5    | 3674 | PSU  | O2-C2-N3    | -2.36 | 117.66      | 121.86   |
| 46  | S2    | 1337 | 4AC  | O7-C7-CM7   | -2.36 | 117.85      | 122.05   |
| 46  | S2    | 966  | PSU  | C5-C6-N1    | -2.36 | 118.87      | 122.14   |
| 3   | L5    | 4598 | PSU  | C6-N1-C2    | -2.35 | 120.51      | 122.69   |
| 3   | L5    | 4590 | OMU  | O4-C4-C5    | -2.35 | 121.11      | 125.16   |
| 3   | L5    | 4588 | OMG  | C2-N1-C6    | -2.35 | 120.85      | 125.11   |
| 3   | L5    | 1779 | PSU  | C5-C6-N1    | -2.35 | 118.88      | 122.14   |
| 3   | L5    | 3616 | PSU  | C5-C6-N1    | -2.35 | 118.88      | 122.14   |
| 46  | S2    | 1337 | 4AC  | C6-C5-C4    | 2.35  | 119.83      | 117.00   |
| 46  | S2    | 406  | PSU  | C5-C6-N1    | -2.34 | 118.89      | 122.14   |
| 3   | L5    | 2863 | OMG  | C2-N1-C6    | -2.34 | 120.86      | 125.11   |
| 3   | L5    | 4593 | OMG  | C4-C5-N7    | -2.34 | 106.96      | 110.67   |
| 46  | S2    | 1692 | PSU  | C5-C6-N1    | -2.34 | 118.89      | 122.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 2495 | PSU  | C6-C5-C4    | -2.33 | 116.60      | 118.17   |
| 3   | L5    | 1309 | 1MA  | C4-C5-N7    | -2.33 | 106.97      | 110.67   |
| 3   | L5    | 4190 | 6MZ  | C5-N7-C8    | 2.33  | 107.11      | 103.45   |
| 80  | Bv    | 28   | PSU  | C5-C6-N1    | -2.32 | 118.92      | 122.14   |
| 3   | L5    | 4607 | OMG  | CM2-O2'-C2' | -2.32 | 108.52      | 114.47   |
| 3   | L5    | 4340 | OMG  | O6-C6-C5    | -2.32 | 120.41      | 126.53   |
| 46  | S2    | 644  | OMG  | C4-C5-N7    | -2.32 | 106.99      | 110.67   |
| 3   | L5    | 4502 | PSU  | O2-C2-N3    | -2.32 | 117.74      | 121.86   |
| 3   | L5    | 4522 | PSU  | O2-C2-N3    | -2.32 | 117.74      | 121.86   |
| 46  | S2    | 509  | OMG  | C4-C5-N7    | -2.32 | 107.00      | 110.67   |
| 46  | S2    | 683  | OMG  | O6-C6-C5    | -2.32 | 120.41      | 126.53   |
| 3   | L5    | 3709 | PSU  | C5-C6-N1    | -2.31 | 118.93      | 122.14   |
| 3   | L5    | 4373 | PSU  | O2-C2-N1    | -2.31 | 120.40      | 122.79   |
| 46  | S2    | 1639 | G7M  | C5-C6-N1    | 2.31  | 116.61      | 111.84   |
| 3   | L5    | 4607 | OMG  | C2-N1-C6    | -2.31 | 120.92      | 125.11   |
| 3   | L5    | 4606 | PSU  | C5-C6-N1    | -2.31 | 118.94      | 122.14   |
| 3   | L5    | 3820 | OMC  | C1'-N1-C2   | 2.31  | 123.53      | 118.44   |
| 46  | S2    | 649  | PSU  | C6-C5-C4    | -2.31 | 116.62      | 118.17   |
| 46  | S2    | 1490 | OMG  | C2-N1-C6    | -2.30 | 120.93      | 125.11   |
| 46  | S2    | 119  | PSU  | C5-C6-N1    | -2.30 | 118.95      | 122.14   |
| 46  | S2    | 1248 | B8N  | O2-C2-N3    | -2.30 | 118.89      | 121.98   |
| 3   | L5    | 4588 | OMG  | C5-C6-N1    | 2.29  | 119.09      | 113.25   |
| 46  | S2    | 866  | PSU  | C5-C6-N1    | -2.29 | 118.96      | 122.14   |
| 3   | L5    | 1569 | PSU  | C6-C5-C4    | -2.29 | 116.63      | 118.17   |
| 3   | L5    | 1504 | 2MG  | C5-C6-N1    | 2.29  | 119.09      | 113.25   |
| 3   | L5    | 389  | A2M  | CM'-O2'-C2' | -2.29 | 108.59      | 114.47   |
| 80  | Bv    | 10   | 2MG  | N1-C2-N2    | 2.29  | 118.90      | 116.56   |
| 46  | S2    | 601  | OMG  | C4-C5-N7    | -2.29 | 107.04      | 110.67   |
| 46  | S2    | 428  | OMU  | O2-C2-N1    | -2.29 | 119.82      | 122.80   |
| 46  | S2    | 867  | OMG  | O6-C6-C5    | -2.29 | 120.50      | 126.53   |
| 46  | S2    | 1692 | PSU  | O2-C2-N3    | -2.28 | 117.80      | 121.86   |
| 3   | L5    | 4590 | OMU  | C1'-N1-C6   | 2.28  | 125.66      | 120.78   |
| 46  | S2    | 1045 | PSU  | C5-C6-N1    | -2.28 | 118.97      | 122.14   |
| 80  | Bv    | 16   | H2U  | C3'-C2'-C1' | 2.28  | 105.77      | 101.46   |
| 3   | L5    | 3820 | OMC  | O2-C2-N1    | 2.28  | 123.36      | 118.90   |
| 3   | L5    | 4282 | PSU  | C5-C6-N1    | -2.28 | 118.98      | 122.14   |
| 80  | Bv    | 37   | UY4  | C5-N7-C8    | 2.27  | 107.02      | 103.45   |
| 3   | L5    | 2351 | OMG  | C5-C6-N1    | 2.27  | 119.03      | 113.25   |
| 3   | L5    | 2619 | PSU  | O2-C2-N3    | -2.27 | 117.83      | 121.86   |
| 3   | L5    | 4469 | OMG  | C4-C5-N7    | -2.27 | 107.08      | 110.67   |
| 3   | L5    | 4198 | OMG  | O6-C6-C5    | -2.27 | 120.55      | 126.53   |
| 80  | Bv    | 37   | UY4  | O29-C09-N6  | -2.26 | 119.62      | 123.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 4417 | 5MC  | N4-C4-N3    | 2.26  | 122.60      | 118.51   |
| 3   | L5    | 3832 | PSU  | C5-C6-N1    | -2.26 | 119.00      | 122.14   |
| 46  | S2    | 644  | OMG  | O6-C6-C5    | -2.26 | 120.57      | 126.53   |
| 3   | L5    | 1769 | PSU  | O2-C2-N3    | -2.25 | 117.87      | 121.86   |
| 46  | S2    | 572  | PSU  | O4'-C1'-C2' | 2.24  | 108.25      | 105.15   |
| 46  | S2    | 668  | A2M  | C4-N9-C1'   | -2.24 | 121.39      | 126.63   |
| 3   | L5    | 3830 | PSU  | C6-N1-C2    | -2.24 | 120.61      | 122.69   |
| 3   | L5    | 4340 | OMG  | CM2-O2'-C2' | -2.24 | 108.72      | 114.47   |
| 3   | L5    | 4493 | A2M  | CM'-O2'-C2' | -2.24 | 108.72      | 114.47   |
| 46  | S2    | 218  | PSU  | C5-C6-N1    | -2.24 | 119.03      | 122.14   |
| 46  | S2    | 105  | PSU  | O2-C2-N3    | -2.24 | 117.89      | 121.86   |
| 3   | L5    | 4197 | OMU  | O2-C2-N1    | -2.23 | 119.89      | 122.80   |
| 3   | L5    | 4362 | OMG  | C5-C6-N1    | 2.23  | 118.93      | 113.25   |
| 3   | L5    | 1849 | PSU  | C5-C6-N1    | -2.23 | 119.05      | 122.14   |
| 46  | S2    | 1174 | PSU  | C6-C5-C4    | -2.22 | 116.67      | 118.17   |
| 3   | L5    | 1509 | OMG  | C5-C6-N1    | 2.22  | 118.90      | 113.25   |
| 3   | L5    | 3830 | PSU  | C6-C5-C4    | -2.21 | 116.68      | 118.17   |
| 3   | L5    | 4522 | PSU  | C6-C5-C4    | -2.21 | 116.68      | 118.17   |
| 80  | Bv    | 55   | PSU  | C5-C6-N1    | -2.21 | 119.08      | 122.14   |
| 3   | L5    | 3830 | PSU  | O2-C2-N3    | -2.21 | 117.94      | 121.86   |
| 80  | Bv    | 58   | 1MA  | C6-C5-N7    | 2.21  | 136.06      | 132.16   |
| 3   | L5    | 4502 | PSU  | C6-C5-C4    | -2.20 | 116.69      | 118.17   |
| 3   | L5    | 3694 | PSU  | C5-C6-N1    | -2.20 | 119.09      | 122.14   |
| 46  | S2    | 814  | PSU  | C6-C5-C4    | -2.20 | 116.69      | 118.17   |
| 46  | S2    | 1850 | MA6  | N9-C8-N7    | -2.20 | 110.82      | 113.94   |
| 46  | S2    | 867  | OMG  | C4-C5-N7    | -2.20 | 107.19      | 110.67   |
| 3   | L5    | 1612 | OMG  | C5-C6-N1    | 2.19  | 118.84      | 113.25   |
| 3   | L5    | 4593 | OMG  | C5-C6-N1    | 2.19  | 118.84      | 113.25   |
| 3   | L5    | 4401 | PSU  | C5-C6-N1    | -2.19 | 119.10      | 122.14   |
| 46  | S2    | 1244 | PSU  | C6-C5-C4    | -2.19 | 116.70      | 118.17   |
| 3   | L5    | 1612 | OMG  | O6-C6-C5    | -2.19 | 120.75      | 126.53   |
| 5   | L8    | 69   | PSU  | C5-C6-N1    | -2.19 | 119.11      | 122.14   |
| 3   | L5    | 3878 | OMG  | C5-C6-N1    | 2.19  | 118.82      | 113.25   |
| 46  | S2    | 822  | PSU  | O4'-C1'-C2' | 2.18  | 108.17      | 105.15   |
| 3   | L5    | 3737 | PSU  | O2-C2-N3    | -2.18 | 117.99      | 121.86   |
| 3   | L5    | 4362 | OMG  | O6-C6-C5    | -2.17 | 120.80      | 126.53   |
| 3   | L5    | 3771 | OMG  | C4-C5-N7    | -2.17 | 107.23      | 110.67   |
| 3   | L5    | 3878 | OMG  | C2-N1-C6    | -2.17 | 121.18      | 125.11   |
| 46  | S2    | 109  | PSU  | C5-C6-N1    | -2.17 | 119.13      | 122.14   |
| 46  | S2    | 1326 | OMU  | C5-C6-N1    | -2.16 | 118.32      | 121.84   |
| 3   | L5    | 3606 | OMG  | C4-C5-N7    | -2.16 | 107.24      | 110.67   |
| 3   | L5    | 4323 | PSU  | O2-C2-N3    | -2.16 | 118.02      | 121.86   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 1612 | OMG  | C4-C5-N7    | -2.16 | 107.25      | 110.67   |
| 5   | L8    | 75   | OMG  | O6-C6-C5    | -2.16 | 120.83      | 126.53   |
| 3   | L5    | 2402 | PSU  | O4'-C1'-C2' | 2.16  | 108.14      | 105.15   |
| 5   | L8    | 75   | OMG  | C4-C5-N7    | -2.16 | 107.25      | 110.67   |
| 80  | Bv    | 46   | G7M  | C5-C6-N1    | 2.15  | 116.29      | 111.84   |
| 80  | Bv    | 26   | M2G  | O6-C6-C5    | -2.15 | 120.85      | 126.53   |
| 46  | S2    | 517  | OMC  | O2-C2-N3    | -2.15 | 118.94      | 122.33   |
| 46  | S2    | 1326 | OMU  | O2-C2-N1    | -2.15 | 120.00      | 122.80   |
| 46  | S2    | 436  | OMG  | C8-N7-C5    | 2.15  | 108.09      | 104.26   |
| 3   | L5    | 4198 | OMG  | C8-N7-C5    | 2.15  | 108.09      | 104.26   |
| 3   | L5    | 1313 | A2M  | N9-C8-N7    | -2.15 | 110.89      | 113.94   |
| 3   | L5    | 4390 | PSU  | O4'-C1'-C2' | 2.15  | 108.12      | 105.15   |
| 3   | L5    | 1849 | PSU  | O2-C2-N3    | -2.14 | 118.06      | 121.86   |
| 3   | L5    | 3741 | PSU  | C5-C6-N1    | -2.14 | 119.17      | 122.14   |
| 3   | L5    | 4464 | OMG  | C2-N1-C6    | -2.14 | 121.23      | 125.11   |
| 80  | Bv    | 10   | 2MG  | O6-C6-C5    | -2.14 | 120.89      | 126.53   |
| 46  | S2    | 1832 | 6MZ  | N9-C8-N7    | -2.14 | 110.91      | 113.94   |
| 3   | L5    | 3723 | OMG  | C5-C6-N1    | 2.14  | 118.69      | 113.25   |
| 3   | L5    | 3878 | OMG  | C4-C5-N7    | -2.13 | 107.30      | 110.67   |
| 3   | L5    | 3846 | A2M  | C1'-N9-C8   | -2.13 | 122.38      | 127.09   |
| 3   | L5    | 4166 | OMG  | C5-C6-N1    | 2.13  | 118.66      | 113.25   |
| 46  | S2    | 1136 | PSU  | O2-C2-N3    | -2.12 | 118.09      | 121.86   |
| 46  | S2    | 966  | PSU  | O2-C2-N3    | -2.12 | 118.09      | 121.86   |
| 3   | L5    | 2411 | OMG  | C5-C6-N1    | 2.12  | 118.65      | 113.25   |
| 5   | L8    | 55   | PSU  | C5-C6-N1    | -2.12 | 119.20      | 122.14   |
| 3   | L5    | 3787 | OMC  | C6-C5-C4    | 2.12  | 121.00      | 117.53   |
| 3   | L5    | 3771 | OMG  | C5-C6-N1    | 2.12  | 118.64      | 113.25   |
| 3   | L5    | 4464 | OMG  | O6-C6-C5    | -2.12 | 120.95      | 126.53   |
| 80  | Bv    | 27   | PSU  | C5-C6-N1    | -2.12 | 119.20      | 122.14   |
| 46  | S2    | 683  | OMG  | C2-N1-C6    | -2.11 | 121.28      | 125.11   |
| 3   | L5    | 4197 | OMU  | C1'-N1-C2   | 2.11  | 121.38      | 117.59   |
| 46  | S2    | 509  | OMG  | O6-C6-C5    | -2.11 | 120.97      | 126.53   |
| 5   | L8    | 75   | OMG  | C5-C6-N1    | 2.10  | 118.61      | 113.25   |
| 3   | L5    | 4491 | PSU  | O2-C2-N3    | -2.10 | 118.12      | 121.86   |
| 3   | L5    | 4276 | OMU  | O2-C2-N3    | -2.10 | 117.61      | 121.49   |
| 3   | L5    | 4464 | OMG  | C4-C5-N7    | -2.10 | 107.34      | 110.67   |
| 3   | L5    | 3846 | A2M  | C4-N9-C1'   | 2.10  | 131.54      | 126.63   |
| 46  | S2    | 1804 | OMU  | O2-C2-N3    | -2.10 | 117.62      | 121.49   |
| 3   | L5    | 2791 | OMC  | C1'-N1-C2   | 2.09  | 123.06      | 118.44   |
| 3   | L5    | 3771 | OMG  | C2-N1-C6    | -2.09 | 121.32      | 125.11   |
| 3   | L5    | 4549 | PSU  | O2-C2-N3    | -2.09 | 118.15      | 121.86   |
| 3   | L5    | 1612 | OMG  | C2-N1-C6    | -2.09 | 121.33      | 125.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L5    | 4549 | PSU  | C5-C6-N1    | -2.09 | 119.25      | 122.14   |
| 3   | L5    | 1847 | PSU  | C6-N1-C2    | -2.08 | 120.76      | 122.69   |
| 81  | j     | 63   | UXY  | C07-C06-C04 | -2.08 | 109.09      | 113.47   |
| 46  | S2    | 462  | OMC  | O2-C2-N1    | 2.08  | 122.97      | 118.90   |
| 3   | L5    | 4464 | OMG  | C5-C6-N1    | 2.07  | 118.52      | 113.25   |
| 46  | S2    | 34   | PSU  | C5-C6-N1    | -2.07 | 119.27      | 122.14   |
| 3   | L5    | 4500 | UR3  | C3U-N3-C2   | 2.07  | 120.94      | 117.33   |
| 80  | Bv    | 10   | 2MG  | C2'-C1'-N9  | -2.07 | 107.49      | 113.25   |
| 3   | L5    | 4269 | PSU  | C5-C6-N1    | -2.07 | 119.27      | 122.14   |
| 46  | S2    | 1445 | PSU  | C5-C6-N1    | -2.06 | 119.28      | 122.14   |
| 46  | S2    | 1643 | PSU  | C6-C5-C4    | -2.06 | 116.78      | 118.17   |
| 3   | L5    | 1504 | 2MG  | C1'-N9-C8   | -2.06 | 120.88      | 126.73   |
| 46  | S2    | 683  | OMG  | C4-C5-N7    | -2.06 | 107.41      | 110.67   |
| 46  | S2    | 1337 | 4AC  | CM7-C7-N4   | 2.06  | 118.59      | 115.27   |
| 3   | L5    | 4282 | PSU  | O2-C2-N3    | -2.06 | 118.20      | 121.86   |
| 3   | L5    | 3741 | PSU  | O2-C2-N3    | -2.06 | 118.21      | 121.86   |
| 3   | L5    | 4607 | OMG  | C8-N7-C5    | 2.06  | 107.92      | 104.26   |
| 3   | L5    | 1664 | PSU  | O4'-C1'-C2' | 2.05  | 107.99      | 105.15   |
| 46  | S2    | 436  | OMG  | C2-N1-C6    | -2.05 | 121.39      | 125.11   |
| 3   | L5    | 4340 | OMG  | C5-C6-N1    | 2.05  | 118.47      | 113.25   |
| 3   | L5    | 4469 | OMG  | O6-C6-C5    | -2.05 | 121.12      | 126.53   |
| 46  | S2    | 590  | A2M  | C4-N9-C1'   | 2.05  | 131.42      | 126.63   |
| 46  | S2    | 1248 | B8N  | C31-N3-C4   | 2.05  | 120.08      | 117.18   |
| 46  | S2    | 119  | PSU  | O2-C2-N3    | -2.05 | 118.23      | 121.86   |
| 46  | S2    | 1248 | B8N  | C32-C33-C34 | -2.04 | 105.03      | 110.45   |
| 46  | S2    | 34   | PSU  | O2-C2-N3    | -2.04 | 118.23      | 121.86   |
| 80  | Bv    | 10   | 2MG  | C2-N1-C6    | -2.04 | 122.08      | 124.55   |
| 3   | L5    | 2863 | OMG  | C5-C6-N1    | 2.04  | 118.45      | 113.25   |
| 80  | Bv    | 37   | UY4  | O03-C02-C04 | 2.04  | 121.22      | 114.15   |
| 3   | L5    | 4937 | PSU  | O2-C2-N3    | -2.04 | 118.24      | 121.86   |
| 3   | L5    | 1664 | PSU  | O2-C2-N3    | -2.04 | 118.24      | 121.86   |
| 3   | L5    | 3723 | OMG  | C4-C5-N7    | -2.04 | 107.44      | 110.67   |
| 3   | L5    | 4331 | PSU  | O2-C2-N3    | -2.03 | 118.25      | 121.86   |
| 3   | L5    | 1327 | OMC  | O2-C2-N3    | -2.03 | 119.12      | 122.33   |
| 3   | L5    | 4263 | PSU  | C5-C6-N1    | -2.03 | 119.32      | 122.14   |
| 46  | S2    | 1347 | PSU  | C5-C6-N1    | -2.03 | 119.32      | 122.14   |
| 46  | S2    | 621  | OMC  | CM2-O2'-C2' | -2.03 | 109.27      | 114.47   |
| 46  | S2    | 218  | PSU  | O2-C2-N3    | -2.03 | 118.26      | 121.86   |
| 3   | L5    | 3797 | UY1  | C5-C6-N1    | -2.02 | 119.33      | 122.14   |
| 46  | S2    | 1328 | OMG  | O6-C6-C5    | -2.02 | 121.19      | 126.53   |
| 3   | L5    | 4166 | OMG  | CM2-O2'-C2' | -2.02 | 109.28      | 114.47   |
| 46  | S2    | 1337 | 4AC  | C1'-N1-C6   | -2.02 | 116.46      | 120.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | S2    | 406  | PSU  | O2-C2-N3    | -2.02 | 118.28      | 121.86   |
| 46  | S2    | 686  | PSU  | O4'-C1'-C2' | 2.02  | 107.94      | 105.15   |
| 46  | S2    | 436  | OMG  | C5-C6-N1    | 2.02  | 118.39      | 113.25   |
| 3   | L5    | 2409 | OMC  | C1'-N1-C2   | 2.02  | 122.89      | 118.44   |
| 46  | S2    | 801  | PSU  | C5-C6-N1    | -2.01 | 119.35      | 122.14   |
| 3   | L5    | 3606 | OMG  | C2'-C1'-N9  | -2.01 | 110.42      | 114.24   |
| 46  | S2    | 1625 | PSU  | C6-C5-C4    | -2.01 | 116.82      | 118.17   |
| 3   | L5    | 4937 | PSU  | C5-C6-N1    | -2.01 | 119.36      | 122.14   |
| 3   | L5    | 3606 | OMG  | C5-C6-N1    | 2.01  | 118.36      | 113.25   |
| 80  | Bv    | 37   | UY4  | O03-C02-O01 | -2.00 | 119.53      | 124.08   |
| 3   | L5    | 3713 | PSU  | O4'-C1'-C2' | 2.00  | 107.92      | 105.15   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 46  | S2    | 1248 | B8N  | C33  |

All (181) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | LC    | 333  | MLZ  | N-CA-CB-CG      |
| 6   | LC    | 333  | MLZ  | C-CA-CB-CG      |
| 6   | LC    | 333  | MLZ  | O-C-CA-CB       |
| 6   | LC    | 333  | MLZ  | CD-CE-NZ-CM     |
| 3   | L5    | 2351 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L5    | 2802 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L5    | 2802 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3680 | OMC  | C2'-C1'-N1-C6   |
| 3   | L5    | 3764 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L5    | 4390 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 4470 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 428  | OMU  | C2'-C1'-N1-C2   |
| 46  | S2    | 428  | OMU  | C2'-C1'-N1-C6   |
| 46  | S2    | 621  | OMC  | O4'-C1'-N1-C2   |
| 46  | S2    | 621  | OMC  | O4'-C1'-N1-C6   |
| 46  | S2    | 621  | OMC  | O4'-C4'-C5'-O5' |
| 46  | S2    | 644  | OMG  | O4'-C4'-C5'-O5' |
| 46  | S2    | 644  | OMG  | C3'-C4'-C5'-O5' |
| 46  | S2    | 683  | OMG  | O4'-C4'-C5'-O5' |
| 46  | S2    | 683  | OMG  | C3'-C4'-C5'-O5' |
| 46  | S2    | 822  | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1136 | PSU  | O4'-C1'-C5-C4   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 46  | S2    | 1136 | PSU  | O4'-C1'-C5-C6   |
| 46  | S2    | 1337 | 4AC  | N3-C4-N4-C7     |
| 46  | S2    | 1442 | OMU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1850 | MA6  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1850 | MA6  | C3'-C4'-C5'-O5' |
| 80  | Bv    | 58   | 1MA  | O4'-C4'-C5'-O5' |
| 81  | j     | 63   | UXY  | O-C-CA-C03      |
| 81  | j     | 63   | UXY  | O05-C04-C06-C07 |
| 3   | L5    | 1303 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L5    | 2351 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3764 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3846 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L5    | 3899 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3899 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 4470 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 4606 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 99   | A2M  | O4'-C4'-C5'-O5' |
| 46  | S2    | 116  | OMU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 116  | OMU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 172  | OMU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 822  | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1244 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1625 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1703 | OMC  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1804 | OMU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1804 | OMU  | O4'-C4'-C5'-O5' |
| 80  | Bv    | 28   | PSU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 1779 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 2411 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L5    | 2411 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3846 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L5    | 4606 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 172  | OMU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 428  | OMU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 428  | OMU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 668  | A2M  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1442 | OMU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1490 | OMG  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1625 | PSU  | O4'-C4'-C5'-O5' |
| 80  | Bv    | 28   | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 3680 | OMC  | C2'-C1'-N1-C2   |
| 3   | L5    | 3820 | OMC  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 46  | S2    | 590  | A2M  | C3'-C4'-C5'-O5' |
| 46  | S2    | 621  | OMC  | C3'-C4'-C5'-O5' |
| 46  | S2    | 668  | A2M  | C3'-C4'-C5'-O5' |
| 80  | Bv    | 58   | 1MA  | C3'-C4'-C5'-O5' |
| 81  | j     | 63   | UXY  | C03-C04-C06-C07 |
| 3   | L5    | 3743 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 4390 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 590  | A2M  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1490 | OMG  | O4'-C4'-C5'-O5' |
| 80  | Bv    | 37   | UY4  | C3'-C4'-C5'-O5' |
| 73  | SO    | 138  | IAS  | N-CA-CB-CG      |
| 3   | L5    | 1849 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 3797 | UY1  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3797 | UY1  | O4'-C4'-C5'-O5' |
| 3   | L5    | 4331 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1244 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1703 | OMC  | C3'-C4'-C5'-O5' |
| 3   | L5    | 1768 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3830 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 512  | A2M  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1045 | PSU  | O4'-C4'-C5'-O5' |
| 80  | Bv    | 37   | UY4  | O4'-C4'-C5'-O5' |
| 3   | L5    | 3739 | A2M  | O4'-C4'-C5'-O5' |
| 46  | S2    | 576  | A2M  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1045 | PSU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 1303 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3743 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 3820 | OMC  | O4'-C4'-C5'-O5' |
| 46  | S2    | 99   | A2M  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1081 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1842 | 4AC  | O7-C7-N4-C4     |
| 46  | S2    | 1842 | 4AC  | CM7-C7-N4-C4    |
| 3   | L5    | 2774 | A2M  | C2'-C1'-N9-C8   |
| 3   | L5    | 1779 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 644  | OMG  | C4'-C5'-O5'-P   |
| 3   | L5    | 3739 | A2M  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3878 | OMG  | C3'-C4'-C5'-O5' |
| 3   | L5    | 3904 | OMU  | C3'-C4'-C5'-O5' |
| 3   | L5    | 4266 | PSU  | C3'-C4'-C5'-O5' |
| 80  | Bv    | 46   | G7M  | O4'-C4'-C5'-O5' |
| 80  | Bv    | 9    | 1MG  | O4'-C4'-C5'-O5' |
| 73  | SO    | 138  | IAS  | C-CA-CB-CG      |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 46  | S2    | 1248 | B8N  | N3-C31-C32-C33  |
| 73  | SO    | 138  | IAS  | CA-CB-CG-OD1    |
| 3   | L5    | 4588 | OMG  | O4'-C4'-C5'-O5' |
| 46  | S2    | 468  | A2M  | O4'-C4'-C5'-O5' |
| 80  | Bv    | 46   | G7M  | C4'-C5'-O5'-P   |
| 3   | L5    | 4441 | PSU  | C3'-C4'-C5'-O5' |
| 80  | Bv    | 55   | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 4417 | 5MC  | O4'-C1'-N1-C6   |
| 3   | L5    | 2388 | A2M  | C3'-C2'-O2'-CM' |
| 3   | L5    | 3797 | UY1  | C1'-C2'-O2'-CM2 |
| 3   | L5    | 3797 | UY1  | C3'-C2'-O2'-CM2 |
| 46  | S2    | 174  | OMC  | C3'-C2'-O2'-CM2 |
| 3   | L5    | 364  | OMG  | C4'-C5'-O5'-P   |
| 3   | L5    | 4470 | PSU  | C4'-C5'-O5'-P   |
| 46  | S2    | 1490 | OMG  | C4'-C5'-O5'-P   |
| 46  | S2    | 1851 | MA6  | C4'-C5'-O5'-P   |
| 3   | L5    | 4417 | 5MC  | C2'-C1'-N1-C6   |
| 3   | L5    | 1664 | PSU  | O4'-C1'-C5-C4   |
| 3   | L5    | 3797 | UY1  | O4'-C1'-C5-C4   |
| 46  | S2    | 572  | PSU  | O4'-C1'-C5-C4   |
| 3   | L5    | 2774 | A2M  | C2'-C1'-N9-C4   |
| 3   | L5    | 3680 | OMC  | O4'-C1'-N1-C2   |
| 3   | L5    | 1768 | PSU  | O4'-C4'-C5'-O5' |
| 41  | Lm    | 98   | MLZ  | CA-CB-CG-CD     |
| 3   | L5    | 2802 | A2M  | C4'-C5'-O5'-P   |
| 46  | S2    | 576  | A2M  | O4'-C4'-C5'-O5' |
| 3   | L5    | 3680 | OMC  | O4'-C1'-N1-C6   |
| 3   | L5    | 3606 | OMG  | O4'-C4'-C5'-O5' |
| 46  | S2    | 512  | A2M  | O4'-C4'-C5'-O5' |
| 46  | S2    | 428  | OMU  | O4'-C1'-N1-C6   |
| 3   | L5    | 2802 | A2M  | C3'-C2'-O2'-CM' |
| 3   | L5    | 3904 | OMU  | C3'-C2'-O2'-CM2 |
| 46  | S2    | 436  | OMG  | C3'-C2'-O2'-CM2 |
| 46  | S2    | 668  | A2M  | C3'-C2'-O2'-CM' |
| 3   | L5    | 3797 | UY1  | C4'-C5'-O5'-P   |
| 46  | S2    | 576  | A2M  | C4'-C5'-O5'-P   |
| 46  | S2    | 590  | A2M  | C4'-C5'-O5'-P   |
| 3   | L5    | 1847 | PSU  | O4'-C4'-C5'-O5' |
| 5   | L8    | 69   | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 1081 | PSU  | C4'-C5'-O5'-P   |
| 80  | Bv    | 16   | H2U  | C4'-C5'-O5'-P   |
| 46  | S2    | 668  | A2M  | C2'-C1'-N9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 46  | S2    | 1391 | OMC  | C1'-C2'-O2'-CM2 |
| 3   | L5    | 3823 | PSU  | C4'-C5'-O5'-P   |
| 3   | L5    | 3866 | OMC  | C4'-C5'-O5'-P   |
| 3   | L5    | 3830 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 436  | OMG  | C3'-C4'-C5'-O5' |
| 3   | L5    | 1664 | PSU  | O4'-C1'-C5-C6   |
| 3   | L5    | 3797 | UY1  | O4'-C1'-C5-C6   |
| 3   | L5    | 4606 | PSU  | O4'-C1'-C5-C6   |
| 3   | L5    | 2338 | OMC  | C3'-C2'-O2'-CM2 |
| 3   | L5    | 2774 | A2M  | C3'-C2'-O2'-CM' |
| 46  | S2    | 116  | OMU  | C3'-C2'-O2'-CM2 |
| 46  | S2    | 517  | OMC  | C3'-C2'-O2'-CM2 |
| 46  | S2    | 1391 | OMC  | C3'-C2'-O2'-CM2 |
| 46  | S2    | 428  | OMU  | O4'-C1'-N1-C2   |
| 3   | L5    | 4417 | 5MC  | O4'-C1'-N1-C2   |
| 80  | Bv    | 9    | 1MG  | C2'-C1'-N9-C8   |
| 80  | Bv    | 46   | G7M  | C3'-C4'-C5'-O5' |
| 80  | Bv    | 37   | UY4  | C02-C04-C05-C07 |
| 3   | L5    | 3764 | A2M  | C2'-C1'-N9-C8   |
| 3   | L5    | 2774 | A2M  | O4'-C1'-N9-C8   |
| 3   | L5    | 1521 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L5    | 4266 | PSU  | O4'-C4'-C5'-O5' |
| 46  | S2    | 801  | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 3   | L5    | 2338 | OMC  | C2'-C1'-N1-C2   |
| 3   | L5    | 391  | A2M  | C3'-C2'-O2'-CM' |
| 3   | L5    | 2350 | A2M  | C3'-C2'-O2'-CM' |
| 3   | L5    | 3741 | PSU  | O4'-C4'-C5'-O5' |
| 3   | L5    | 1511 | A2M  | O4'-C1'-N9-C8   |
| 80  | Bv    | 16   | H2U  | O4'-C1'-N1-C6   |
| 80  | Bv    | 47   | H2U  | O4'-C1'-N1-C6   |
| 3   | L5    | 1849 | PSU  | C3'-C4'-C5'-O5' |
| 46  | S2    | 590  | A2M  | O4'-C1'-N9-C8   |

There are no ring outliers.

45 monomers are involved in 61 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 46  | S2    | 621  | OMC  | 1       | 0            |
| 46  | S2    | 1391 | OMC  | 1       | 0            |
| 3   | L5    | 4493 | A2M  | 1       | 0            |
| 3   | L5    | 3697 | A2M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L5    | 4500 | UR3  | 1       | 0            |
| 46  | S2    | 27   | A2M  | 1       | 0            |
| 3   | L5    | 3797 | UY1  | 1       | 0            |
| 46  | S2    | 172  | OMU  | 1       | 0            |
| 3   | L5    | 4269 | PSU  | 1       | 0            |
| 3   | L5    | 4263 | PSU  | 2       | 0            |
| 46  | S2    | 159  | A2M  | 1       | 0            |
| 46  | S2    | 116  | OMU  | 1       | 0            |
| 46  | S2    | 509  | OMG  | 1       | 0            |
| 3   | L5    | 2411 | OMG  | 1       | 0            |
| 80  | Bv    | 37   | UY4  | 1       | 0            |
| 80  | Bv    | 58   | 1MA  | 4       | 0            |
| 3   | L5    | 4190 | 6MZ  | 1       | 0            |
| 3   | L5    | 1511 | A2M  | 1       | 0            |
| 80  | Bv    | 28   | PSU  | 5       | 0            |
| 81  | j     | 185  | MEQ  | 6       | 0            |
| 80  | Bv    | 27   | PSU  | 5       | 0            |
| 46  | S2    | 436  | OMG  | 1       | 0            |
| 3   | L5    | 4606 | PSU  | 1       | 0            |
| 3   | L5    | 1858 | A2M  | 1       | 0            |
| 46  | S2    | 462  | OMC  | 1       | 0            |
| 81  | j     | 63   | UXY  | 1       | 0            |
| 46  | S2    | 814  | PSU  | 1       | 0            |
| 3   | L5    | 4441 | PSU  | 1       | 0            |
| 5   | L8    | 75   | OMG  | 1       | 0            |
| 80  | Bv    | 10   | 2MG  | 1       | 0            |
| 6   | LC    | 333  | MLZ  | 1       | 0            |
| 80  | Bv    | 26   | M2G  | 2       | 0            |
| 46  | S2    | 512  | A2M  | 1       | 0            |
| 46  | S2    | 601  | OMG  | 1       | 0            |
| 46  | S2    | 428  | OMU  | 1       | 0            |
| 73  | SO    | 138  | IAS  | 3       | 0            |
| 3   | L5    | 4412 | PSU  | 1       | 0            |
| 46  | S2    | 1490 | OMG  | 1       | 0            |
| 3   | L5    | 4502 | PSU  | 1       | 0            |
| 3   | L5    | 2338 | OMC  | 1       | 0            |
| 46  | S2    | 1031 | A2M  | 1       | 0            |
| 3   | L5    | 3749 | PSU  | 1       | 0            |
| 46  | S2    | 867  | OMG  | 1       | 0            |
| 3   | L5    | 391  | A2M  | 1       | 0            |
| 80  | Bv    | 46   | G7M  | 2       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 201 ligands modelled in this entry, 200 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 | $\# Z  > 2$ |
| 85  | MVM  | L5    | 5246 | -    | 35,35,35     | 0.83 | 0           | 44,49,49    | 1.35 | 5 (11%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 85  | MVM  | L5    | 5246 | -    | -       | 0/20/28/28 | 0/5/5/5 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 85  | L5    | 5246 | MVM  | C1-C9-N1   | -3.54 | 107.27      | 116.16   |
| 85  | L5    | 5246 | MVM  | C6-N1-C9   | 3.30  | 123.30      | 118.40   |
| 85  | L5    | 5246 | MVM  | N7-C22-N4  | 3.15  | 129.42      | 125.88   |
| 85  | L5    | 5246 | MVM  | C16-C15-N4 | -2.13 | 117.65      | 119.93   |
| 85  | L5    | 5246 | MVM  | C9-N1-C5   | -2.08 | 115.51      | 118.64   |

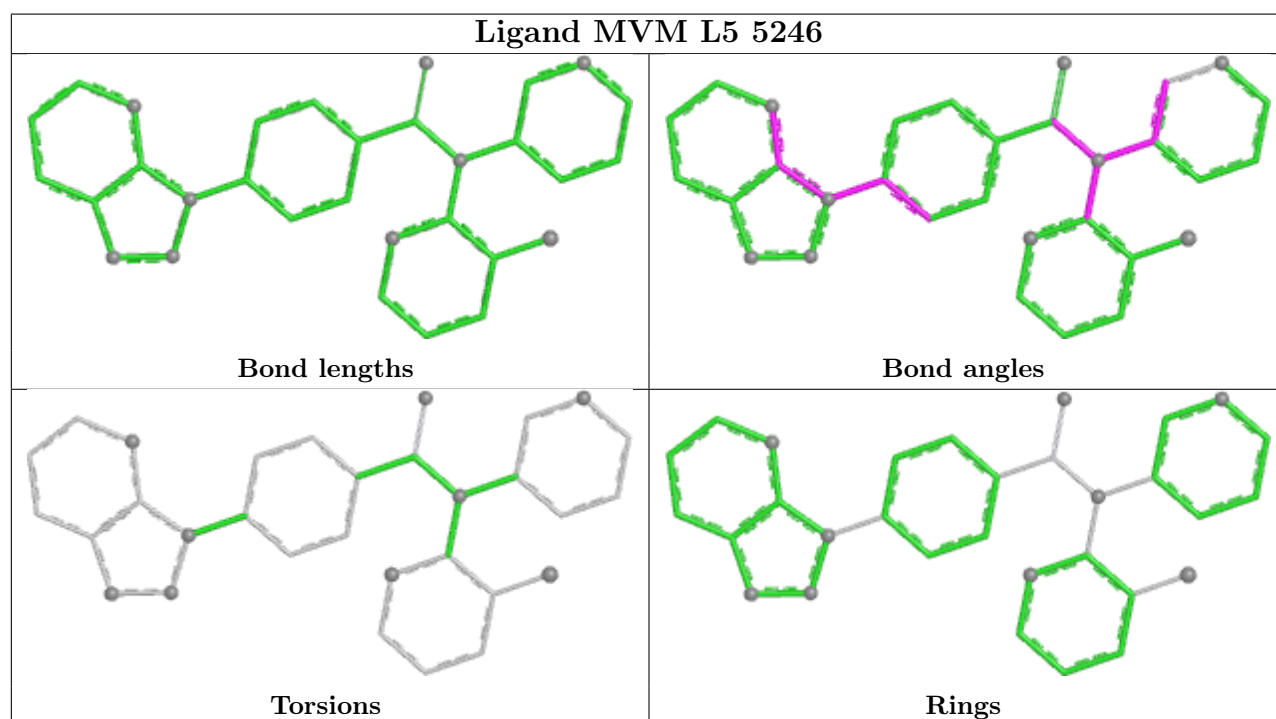
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | L5    | 22               |
| 46  | S2    | 13               |
| 81  | j     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | L5    | 482:G     | O3'    | 495:G     | P      | 26.99        |
| 1     | L5    | 173:G     | O3'    | 186:G     | P      | 24.85        |
| 1     | S2    | 689:U     | O3'    | 799:U     | P      | 24.17        |
| 1     | L5    | 250:G     | O3'    | 253:G     | P      | 24.06        |
| 1     | L5    | 646:C     | O3'    | 659:C     | P      | 21.79        |
| 1     | L5    | 2897:G    | O3'    | 3563:C    | P      | 20.78        |
| 1     | S2    | 834:C     | O3'    | 840:C     | P      | 18.34        |
| 1     | L5    | 4076:A    | O3'    | 4086:G    | P      | 17.74        |
| 1     | S2    | 130:G     | O3'    | 140:C     | P      | 17.44        |
| 1     | S2    | 536:A     | O3'    | 549:C     | P      | 17.41        |
| 1     | L5    | 4742:C    | O3'    | 4826:G    | P      | 17.30        |
| 1     | S2    | 323:C     | O3'    | 328:U     | P      | 16.97        |
| 1     | S2    | 880:G     | O3'    | 906:U     | P      | 16.72        |
| 1     | L5    | 1746:G    | O3'    | 1760:U    | P      | 16.64        |
| 1     | L5    | 976:U     | O3'    | 1051:G    | P      | 16.02        |
| 1     | L5    | 4114:C    | O3'    | 4117:G    | P      | 16.02        |
| 1     | L5    | 1389:C    | O3'    | 1402:G    | P      | 15.89        |
| 1     | L5    | 1237:C    | O3'    | 1247:G    | P      | 15.86        |
| 1     | L5    | 503:U     | O3'    | 637:G     | P      | 15.77        |
| 1     | L5    | 748:G     | O3'    | 893:C     | P      | 15.72        |
| 1     | S2    | 72:C      | O3'    | 76:U      | P      | 15.38        |
| 1     | L5    | 132:G     | O3'    | 134:G     | P      | 14.76        |
| 1     | L5    | 1207:G    | O3'    | 1221:G    | P      | 14.33        |
| 1     | S2    | 1114:U    | O3'    | 1120:U    | P      | 14.12        |
| 1     | S2    | 1751:C    | O3'    | 1784:G    | P      | 13.97        |
| 1     | L5    | 2100:G    | O3'    | 2236:C    | P      | 12.67        |
| 1     | S2    | 1417:C    | O3'    | 1421:A    | P      | 10.12        |
| 1     | L5    | 3927:C    | O3'    | 4044:U    | P      | 9.76         |
| 1     | L5    | 4700:C    | O3'    | 4703:A    | P      | 9.72         |
| 1     | S2    | 1551:U    | O3'    | 1558:C    | P      | 9.16         |
| 1     | S2    | 225:G     | O3'    | 287:U     | P      | 7.98         |
| 1     | L5    | 1696:C    | O3'    | 1701:C    | P      | 6.69         |
| 1     | L5    | 1087:U    | O3'    | 1155:G    | P      | 6.26         |
| 1     | L5    | 212:C     | O3'    | 217:C     | P      | 5.87         |
| 1     | S2    | 1432:U    | O3'    | 1438:A    | P      | 4.96         |
| 1     | j     | 330:ARG   | C      | 345:TYR   | N      | 4.65         |
| 1     | j     | 185:MEQ   | C      | 186:SER   | N      | 1.16         |

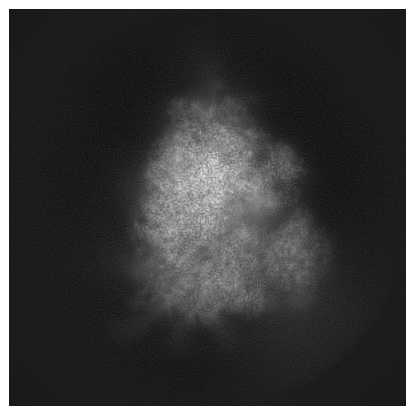
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22085. These allow visual inspection of the internal detail of the map and identification of artifacts.

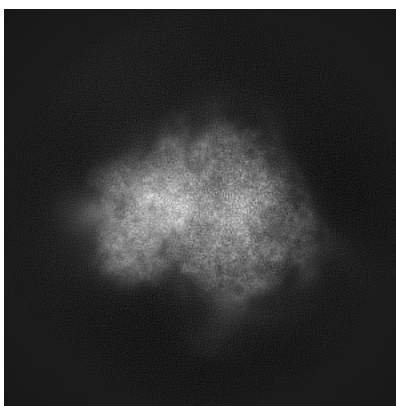
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

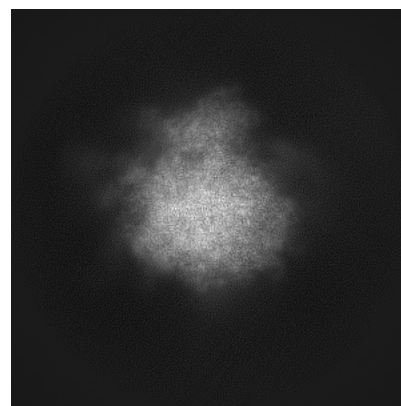
#### 6.1.1 Primary map



X

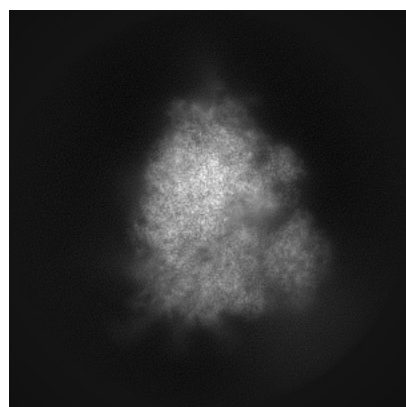


Y

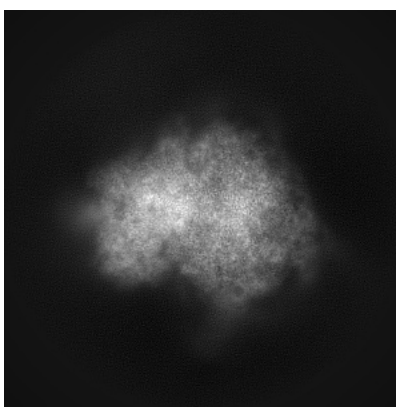


Z

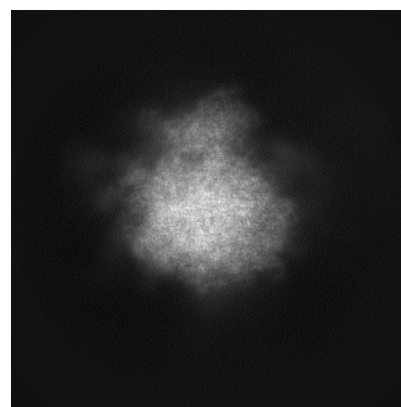
#### 6.1.2 Raw map



X



Y

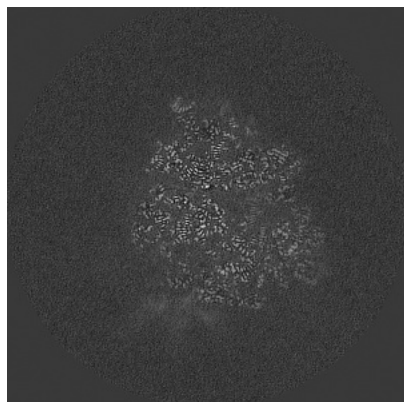


Z

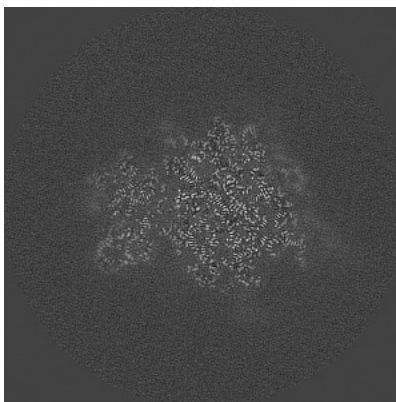
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

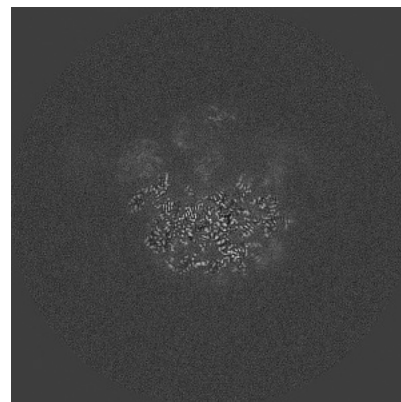
### 6.2.1 Primary map



X Index: 215

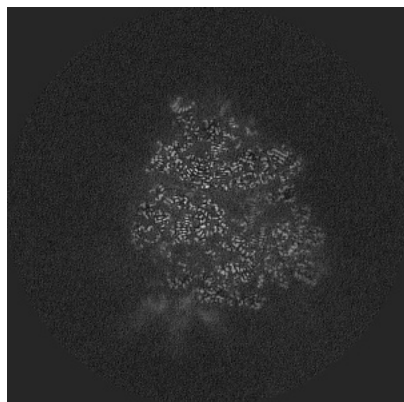


Y Index: 215

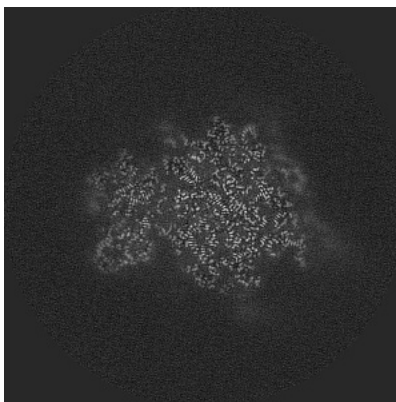


Z Index: 215

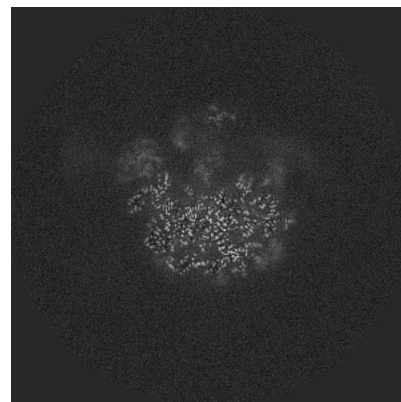
### 6.2.2 Raw map



X Index: 215



Y Index: 215

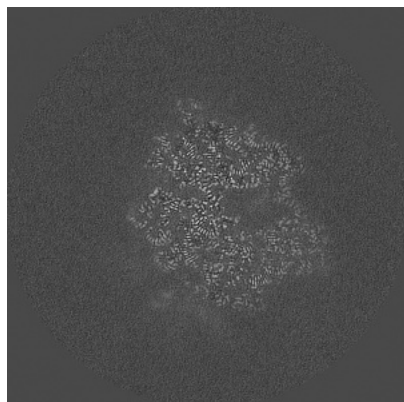


Z Index: 215

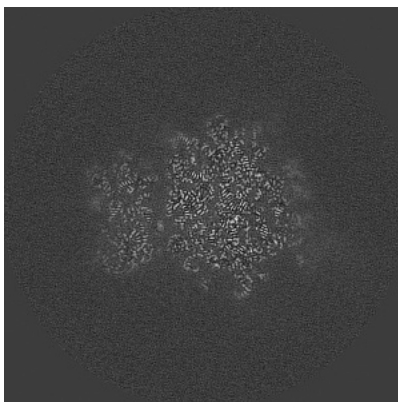
The images above show central slices of the map in three orthogonal directions.

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

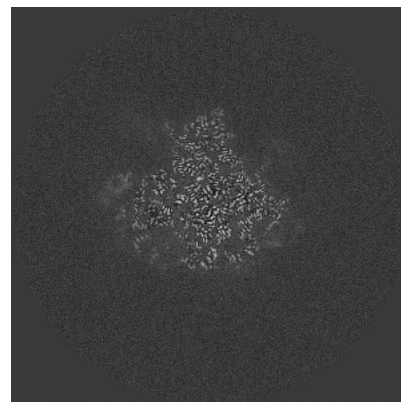
### 6.3.1 Primary map



X Index: 222

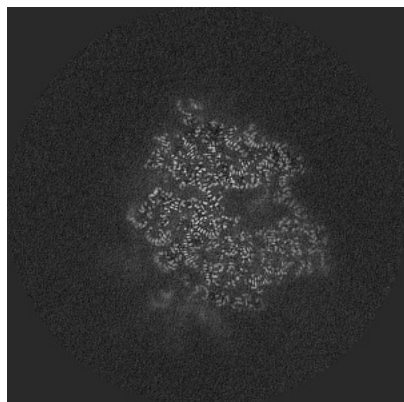


Y Index: 210

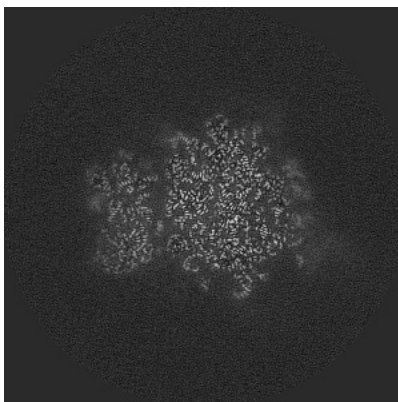


Z Index: 255

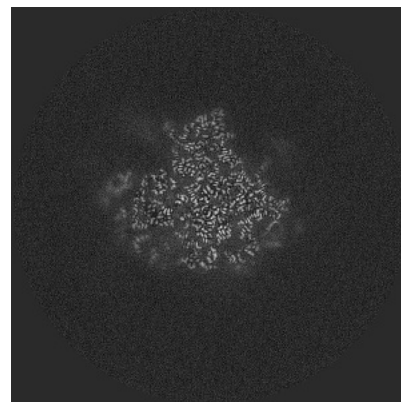
### 6.3.2 Raw map



X Index: 222



Y Index: 210

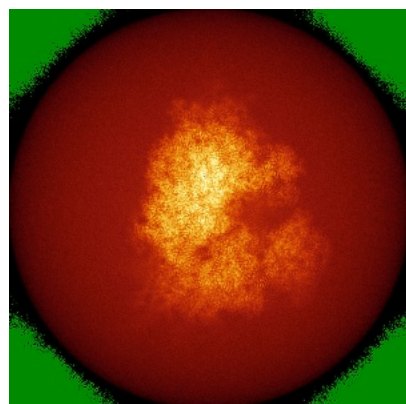


Z Index: 255

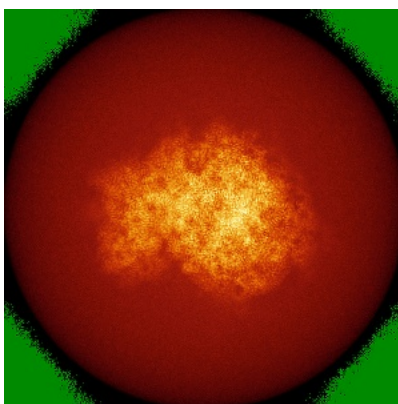
The images above show the largest variance slices of the map in three orthogonal directions.

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

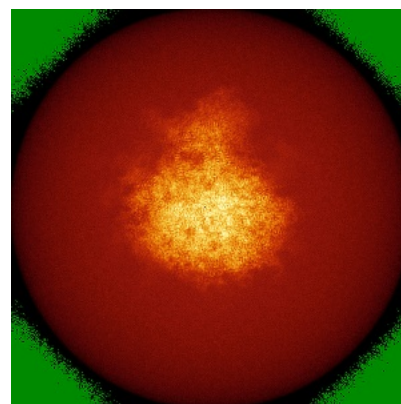
### 6.4.1 Primary map



X

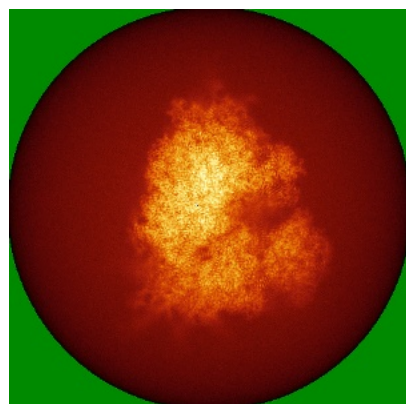


Y

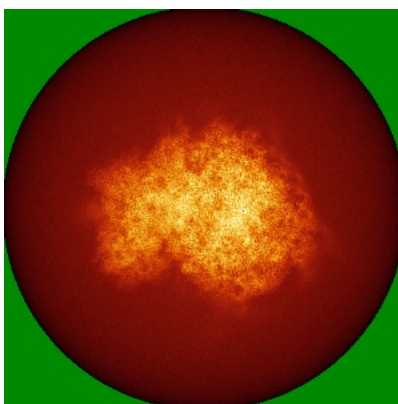


Z

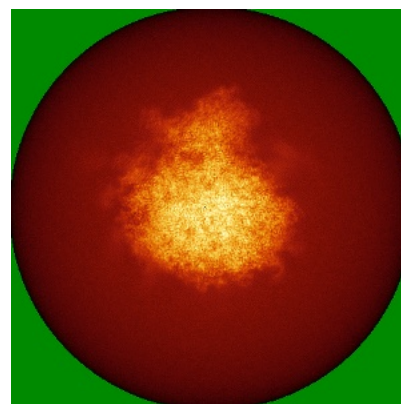
### 6.4.2 Raw map



X



Y



Z

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

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

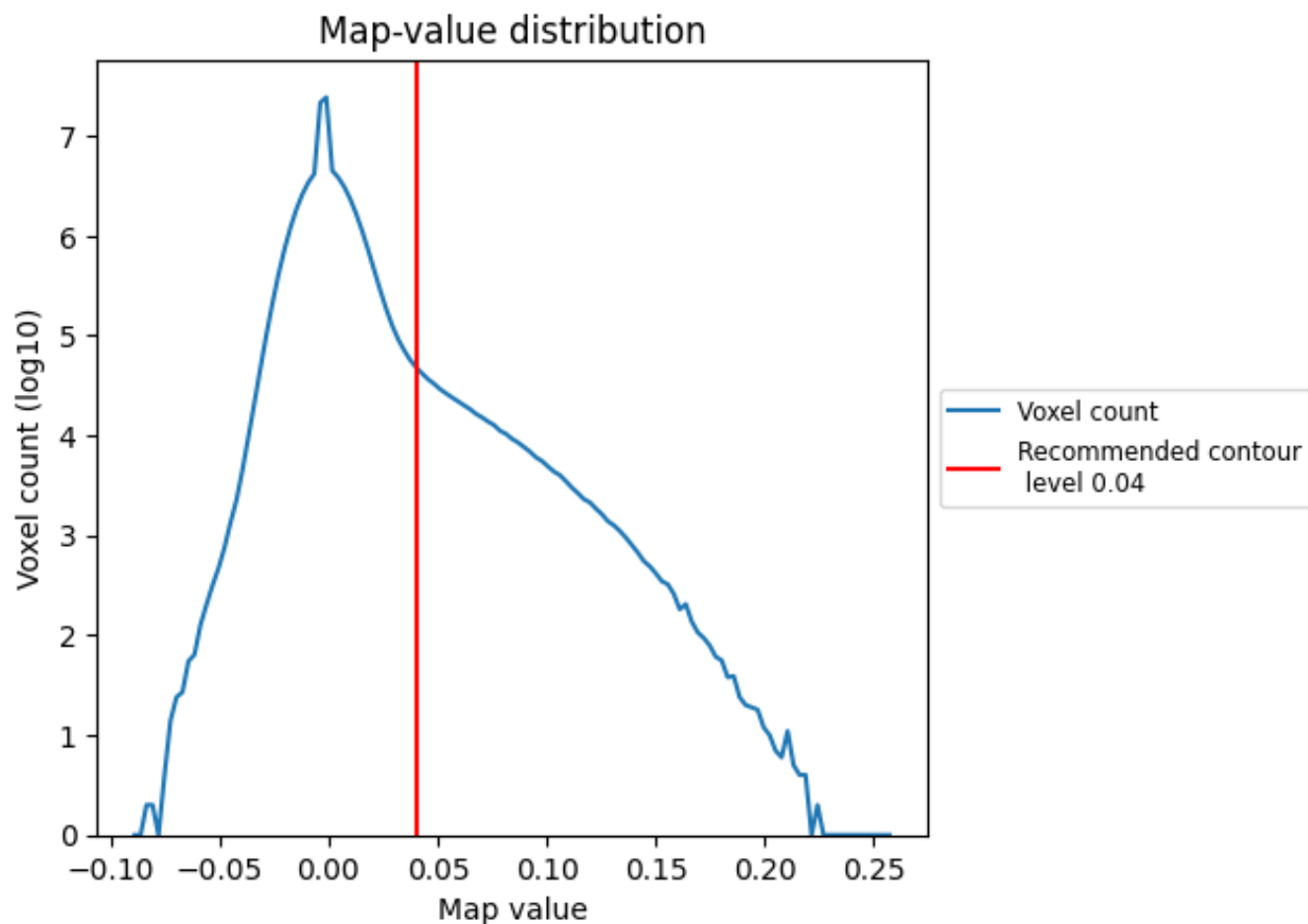
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

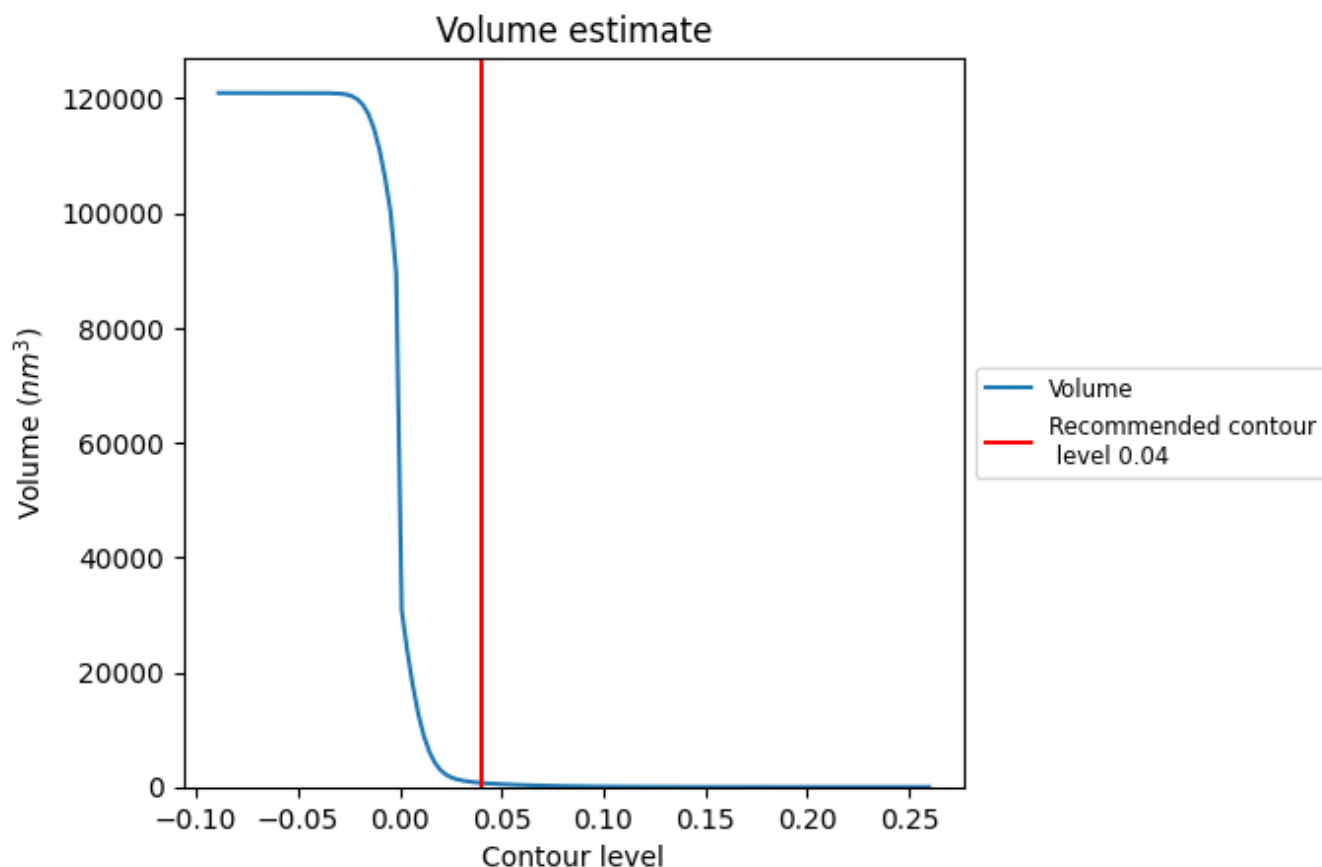
This section contains the results of statistical analysis of the map.

### 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.

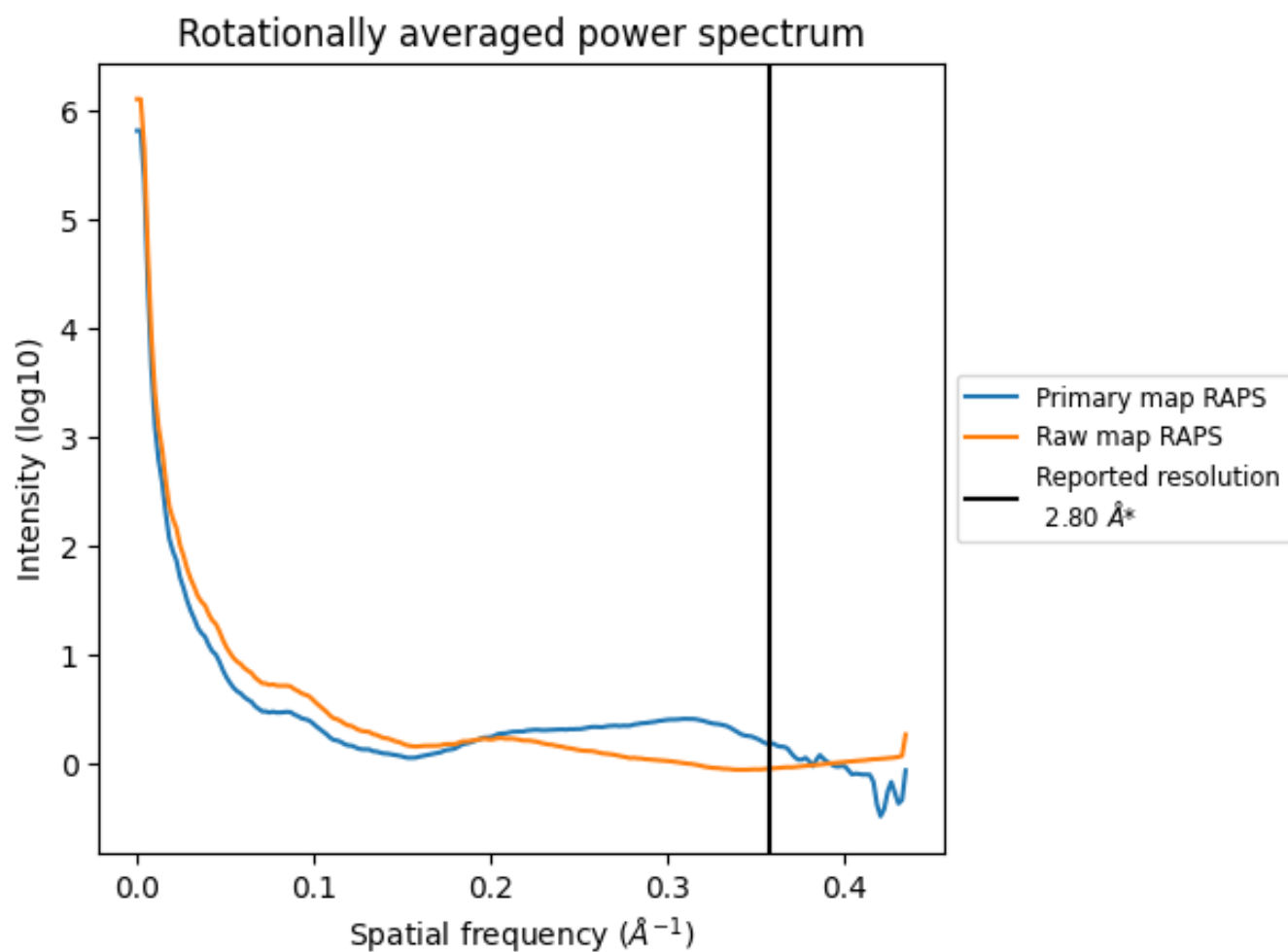
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709  $\text{nm}^3$ ; this corresponds to an approximate mass of 641 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 ⓘ

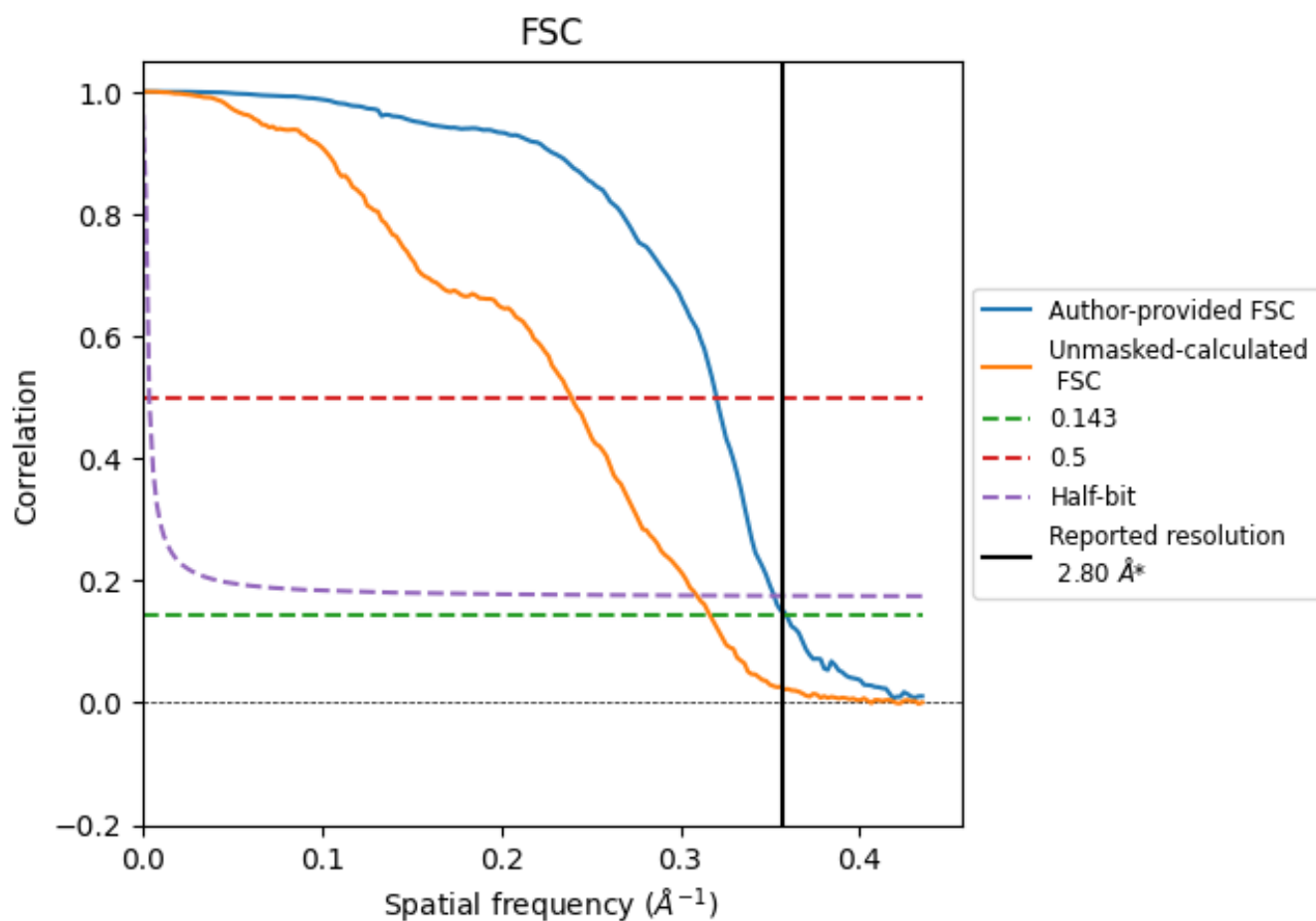


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates

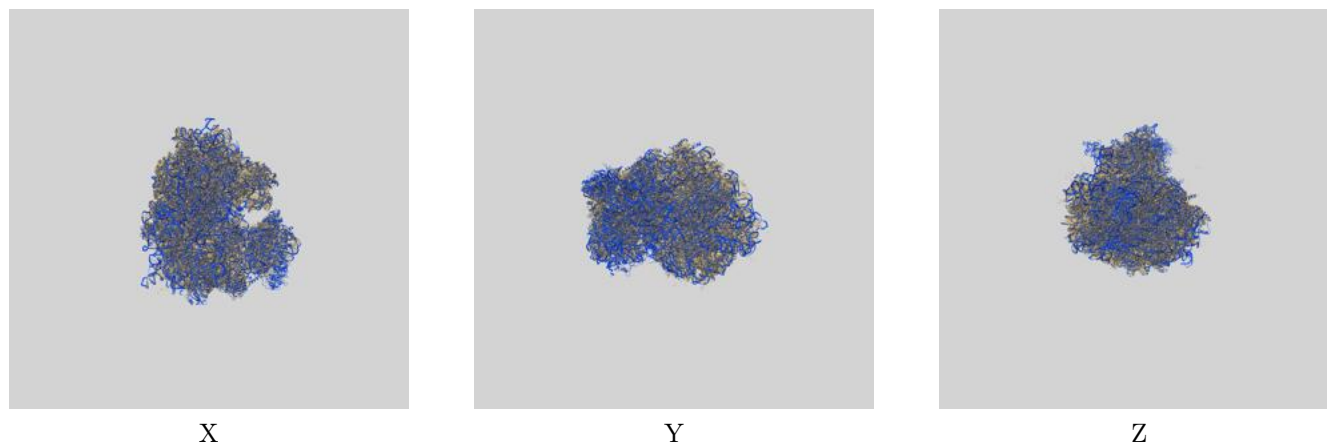
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.80                               | -    | -        |
| Author-provided FSC curve | 2.79                               | 3.12 | 2.84     |
| Unmasked-calculated*      | 3.16                               | 4.18 | 3.24     |

\*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 3.16 differs from the reported value 2.8 by more than 10 %

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

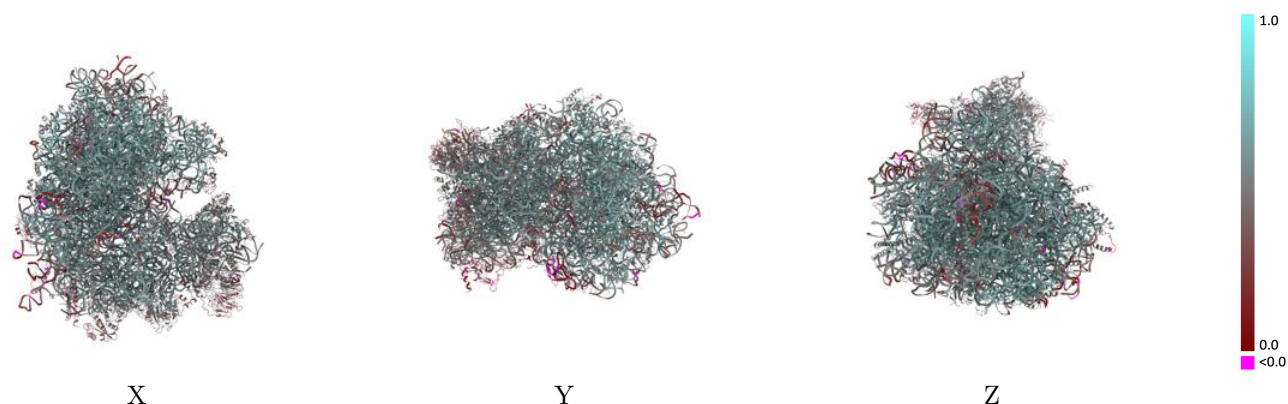
This section contains information regarding the fit between EMDB map EMD-22085 and PDB model 6XA1. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

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



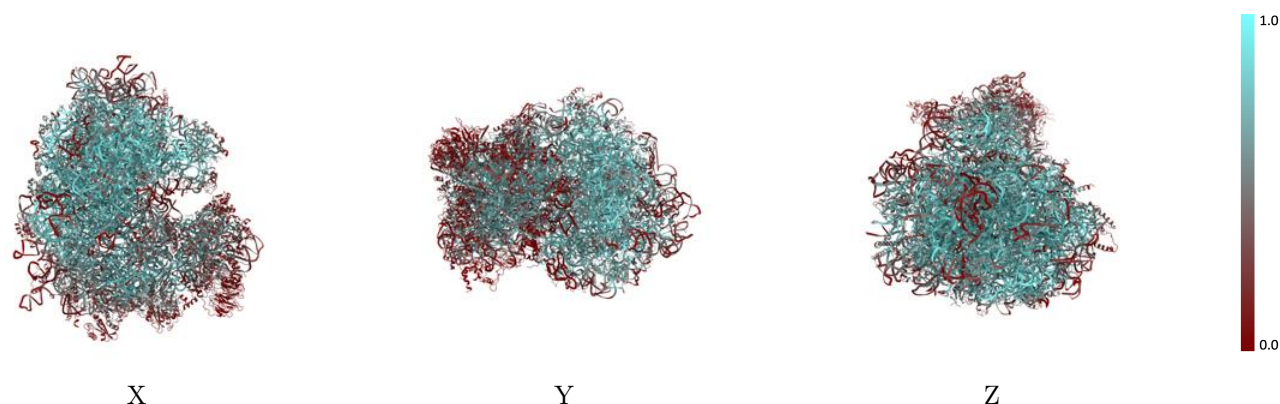
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



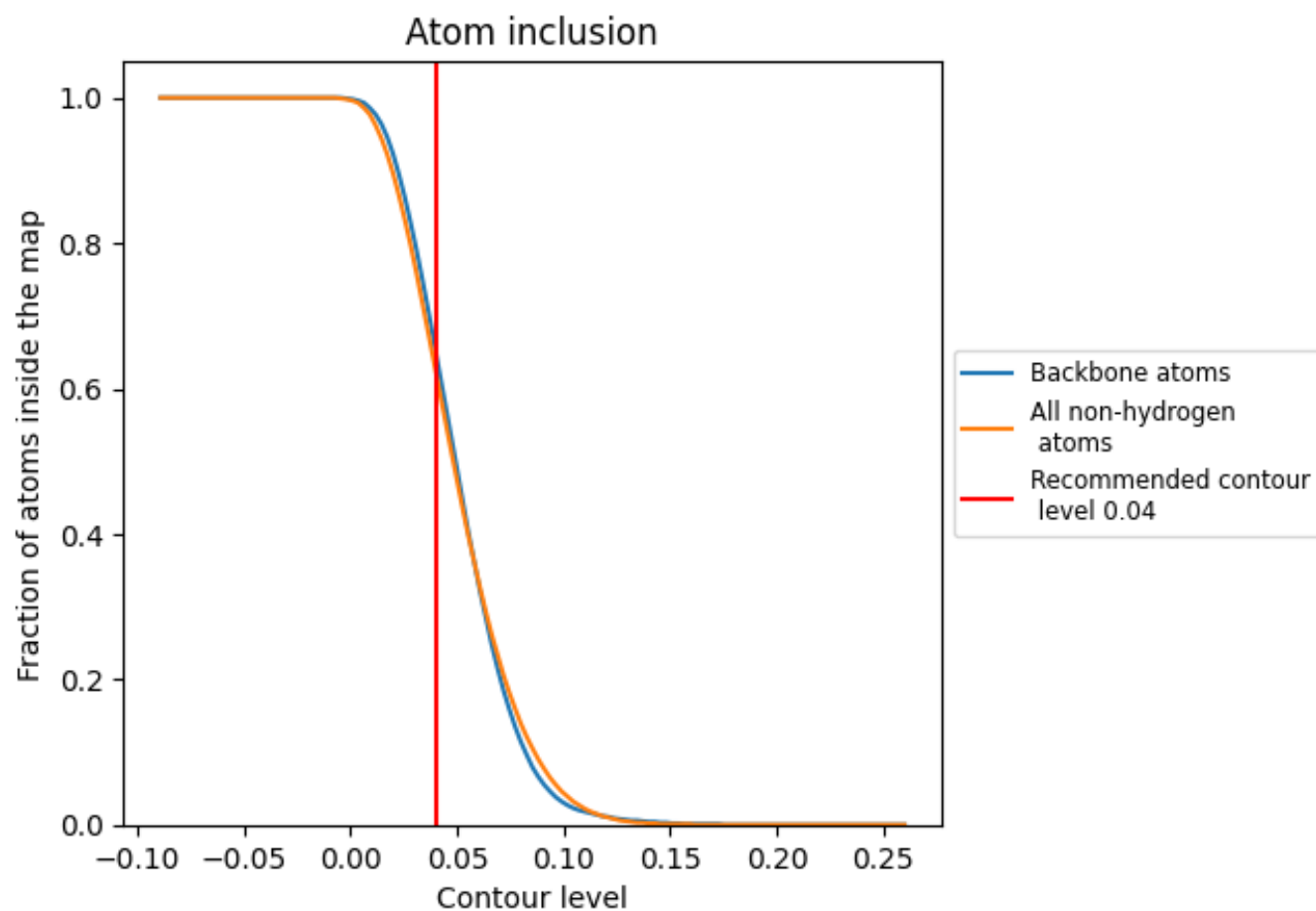
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6240   |  0.5350   |
| Bv    |  0.2910   |  0.4180   |
| L5    |  0.7530   |  0.5620   |
| L7    |  0.8360   |  0.6110   |
| L8    |  0.7940   |  0.5730   |
| LA    |  0.8070   |  0.6000   |
| LB    |  0.6830   |  0.5690   |
| LC    |  0.7420   |  0.6000   |
| LD    |  0.5550   |  0.5440   |
| LE    |  0.4890   |  0.4950   |
| LF    |  0.7550   |  0.5880   |
| LG    |  0.5150   |  0.4920   |
| LH    |  0.5370   |  0.5200   |
| LI    |  0.6450   |  0.5490   |
| LJ    |  0.4100  |  0.4390  |
| LL    |  0.6300 |  0.5520 |
| LM    |  0.6120 |  0.5480 |
| LN    |  0.8590 |  0.6190 |
| LO    |  0.7330 |  0.5730 |
| LP    |  0.7380 |  0.5870 |
| LQ    |  0.7760 |  0.6090 |
| LR    |  0.5960 |  0.4970 |
| LS    |  0.7360 |  0.5900 |
| LT    |  0.6650 |  0.5430 |
| LU    |  0.2970 |  0.4320 |
| LV    |  0.7030 |  0.5660 |
| LW    |  0.3300 |  0.3420 |
| LX    |  0.6140 |  0.5400 |
| LY    |  0.6460 |  0.5600 |
| LZ    |  0.5640 |  0.5300 |
| La    |  0.8010 |  0.6140 |
| Lb    |  0.5350 |  0.5060 |
| Lc    |  0.5860 |  0.5160 |
| Ld    |  0.6310 |  0.5330 |
| Le    |  0.7680 |  0.6030 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Lf    |  0.7920   |  0.5980   |
| Lg    |  0.6950   |  0.5600   |
| Lh    |  0.6000   |  0.5500   |
| Li    |  0.5830   |  0.5370   |
| Lj    |  0.8380   |  0.6010   |
| Lk    |  0.4090   |  0.4600   |
| Ll    |  0.7520   |  0.5630   |
| Lm    |  0.6550   |  0.5470   |
| Ln    |  0.7750   |  0.5660   |
| Lo    |  0.6370   |  0.5440   |
| Lp    |  0.6910   |  0.5640   |
| Lr    |  0.6990   |  0.5760   |
| NC    |  0.4180   |  0.5180   |
| S2    |  0.6580   |  0.5500   |
| SA    |  0.3770   |  0.4910   |
| SB    |  0.3680   |  0.5050   |
| SC    |  0.4780   |  0.5110   |
| SD    |  0.2190  |  0.4090  |
| SE    |  0.3620 |  0.4870 |
| SF    |  0.3380 |  0.4960 |
| SG    |  0.1820 |  0.3930 |
| SH    |  0.1890 |  0.3800 |
| SI    |  0.4680 |  0.5040 |
| SJ    |  0.3930 |  0.4920 |
| SK    |  0.1590 |  0.4240 |
| SL    |  0.5810 |  0.5350 |
| SM    |  0.0010 |  0.1650 |
| SN    |  0.5010 |  0.5230 |
| SO    |  0.4830 |  0.5300 |
| SP    |  0.2320 |  0.4310 |
| SQ    |  0.3280 |  0.4820 |
| SR    |  0.2120 |  0.4120 |
| SS    |  0.2500 |  0.4570 |
| ST    |  0.2730 |  0.4870 |
| SU    |  0.2330 |  0.3680 |
| SV    |  0.3480 |  0.4750 |
| SW    |  0.5670 |  0.5380 |
| SX    |  0.5870 |  0.5430 |
| SY    |  0.2360 |  0.4300 |
| SZ    |  0.1560 |  0.4540 |
| Sa    |  0.5560 |  0.5290 |
| Sb    |  0.3190 |  0.4510 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Sc    |  0.2130 |  0.4180 |
| Sd    |  0.4590 |  0.5040 |
| Se    |  0.3370 |  0.4500 |
| Sf    |  0.0120 |  0.2590 |
| Sg    |  0.0600 |  0.3550 |
| j     |  0.1570 |  0.4010 |
| k     |  0.4940 |  0.5190 |