



## Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 12:49 pm BST

PDB ID : 7O80 / pdb\_00007o80  
EMDB ID : EMD-12758  
Title : Rabbit 80S ribosome in complex with eRF1 and ABCE1 stalled at the STOP codon in the mutated SARS-CoV-2 slippery site  
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.  
Deposited on : 2021-04-14  
Resolution : 2.90 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:

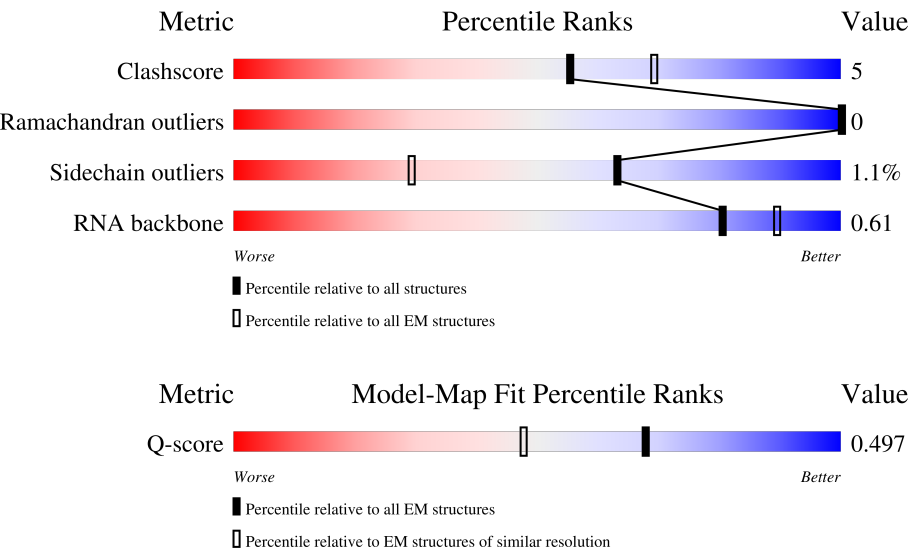
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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                       | 13054 ( 2.40 - 3.40 )                                    |

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   | A2    | 1870   |                  |
| 2   | AA    | 84     |                  |
| 3   | AB    | 69     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | AC    | 156    |                  |
| 5   | AD    | 133    |                  |
| 6   | AE    | 115    |                  |
| 7   | AF    | 317    |                  |
| 8   | AG    | 56     |                  |
| 9   | AH    | 217    |                  |
| 10  | AI    | 76     |                  |
| 11  | AT    | 86     |                  |
| 12  | AZ    | 295    |                  |
| 13  | Aa    | 264    |                  |
| 14  | Ab    | 293    |                  |
| 15  | Ac    | 281    |                  |
| 16  | Ad    | 263    |                  |
| 17  | Ae    | 204    |                  |
| 18  | Af    | 249    |                  |
| 19  | Ag    | 194    |                  |
| 20  | Ah    | 208    |                  |
| 21  | Ai    | 194    |                  |
| 22  | Aj    | 165    |                  |
| 23  | Ak    | 158    |                  |
| 24  | Al    | 132    |                  |
| 25  | Am    | 151    |                  |
| 26  | An    | 151    |                  |
| 27  | Ao    | 145    |                  |
| 28  | Ap    | 146    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | Aq    | 135    |                  |
| 30  | Ar    | 152    |                  |
| 31  | As    | 145    |                  |
| 32  | At    | 119    |                  |
| 33  | Au    | 83     |                  |
| 34  | Av    | 130    |                  |
| 35  | Aw    | 143    |                  |
| 36  | Ax    | 130    |                  |
| 37  | Ay    | 124    |                  |
| 38  | Az    | 25     |                  |
| 39  | B5    | 4808   |                  |
| 40  | B7    | 119    |                  |
| 41  | B8    | 158    |                  |
| 42  | BA    | 257    |                  |
| 43  | BB    | 403    |                  |
| 44  | BC    | 413    |                  |
| 45  | BD    | 297    |                  |
| 46  | BE    | 291    |                  |
| 47  | BF    | 247    |                  |
| 48  | BG    | 266    |                  |
| 49  | BH    | 192    |                  |
| 50  | BI    | 214    |                  |
| 51  | BJ    | 178    |                  |
| 52  | BK    | 1071   |                  |
| 53  | BL    | 211    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | BM    | 218    |                  |
| 55  | BN    | 204    |                  |
| 56  | BO    | 203    |                  |
| 57  | BP    | 184    |                  |
| 58  | BQ    | 188    |                  |
| 59  | BR    | 196    |                  |
| 60  | BS    | 176    |                  |
| 61  | BT    | 160    |                  |
| 62  | BU    | 128    |                  |
| 63  | BV    | 140    |                  |
| 64  | BW    | 157    |                  |
| 65  | BX    | 156    |                  |
| 66  | BY    | 145    |                  |
| 67  | BZ    | 136    |                  |
| 68  | Ba    | 148    |                  |
| 69  | Bb    | 245    |                  |
| 70  | Bc    | 115    |                  |
| 71  | Bd    | 125    |                  |
| 72  | Be    | 135    |                  |
| 73  | Bf    | 110    |                  |
| 74  | Bg    | 117    |                  |
| 75  | Bh    | 123    |                  |
| 76  | Bi    | 105    |                  |
| 77  | Bj    | 97     |                  |
| 78  | Bk    | 70     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 79  | Bl    | 51     |                  |
| 80  | Bm    | 128    |                  |
| 81  | Bo    | 106    |                  |
| 82  | Bp    | 92     |                  |
| 83  | Br    | 137    |                  |
| 84  | Bs    | 318    |                  |
| 85  | Bt    | 165    |                  |
| 86  | Bv    | 217    |                  |
| 87  | By    | 437    |                  |
| 88  | Bz    | 599    |                  |

## 2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 235677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A2    | 1770     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 37833 | 16911 | 6781 | 12371 | 1770 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference         |
|-------|---------|----------|--------|----------|-------------------|
| A2    | 1249    | B8N      | C      | conflict | GB GBCT01000564.1 |
| A2    | 1338    | 4AC      | C      | conflict | GB GBCT01000564.1 |
| A2    | 1843    | 4AC      | C      | conflict | GB GBCT01000564.1 |

- Molecule 2 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | AA    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 3 is a protein called Ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | AB    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 495   | 302 | 98 | 93 | 2 |         |       |

- Molecule 4 is a protein called Ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | AC    | 73       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 601   | 379 | 115 | 100 | 7 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 5   | AD    | 57       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 457   | 282 | 101 | 73 | 1 |         |       |

- Molecule 6 is a protein called Ribosomal protein eS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | AE    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 814   | 507 | 170 | 132 | 5 |         |       |

- Molecule 7 is a protein called RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | AF    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 8 is a protein called uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | AG    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 9   | AH    | 24       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 508   | 227 | 84 | 173 | 24 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| AH    | 3466    | U        | A      | conflict | GB NC_045512.2 |
| AH    | 3468    | A        | C      | conflict | GB NC_045512.2 |

- Molecule 10 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 10  | AI    | 76       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 939   | 393 | 11 | 459 | 76 |         |       |

- Molecule 11 is a RNA chain called P-site Leu-tRNA(Leu).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11  | AT    | 86       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1840  | 820 | 330 | 604 | 86 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein SA.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | AZ    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1743  | 1107 | 305 | 323 | 8 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | Aa    | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1815  | 1152 | 328 | 321 | 14 |         |       |

- Molecule 14 is a protein called Ribosomal protein uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | Ab    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1706  | 1105 | 292 | 300 | 9 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | Ac    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1751  | 1116 | 315 | 313 | 7 |         |       |

- Molecule 16 is a protein called Ribosomal protein eS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | Ad    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 17 is a protein called Ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Ae    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 943 | 286 | 273 | 7 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | Af    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | Ag    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1529  | 975 | 281 | 272 | 1 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | Ah    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Ah    | 47      | ARG      | GLY    | conflict | UNP G1TJW1 |

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | Ai    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 22 is a protein called Ribosomal protein eS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | Aj    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 530 | 143 | 131 | 6 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Ak    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1262  | 804 | 236 | 216 | 6 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Al    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 600 | 170 | 179 | 9 |         |       |

- Molecule 25 is a protein called uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Am    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | An    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 621 | 199 | 190 | 6 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Ao    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1091  | 694 | 205 | 185 | 7 |         |       |

- Molecule 28 is a protein called Ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | Ap    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 715 | 212 | 194 | 3 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | Aq    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 678 | 201 | 197 | 4 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Ar    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1200  | 753 | 242 | 204 | 1 |         |       |

- Molecule 31 is a protein called Ribosomal protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | As    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1113  | 698 | 214 | 198 | 3 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | At    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |

- Molecule 33 is a protein called Ribosomal protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Au    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 640   | 394 | 117 | 124 | 5 |         |       |

- Molecule 34 is a protein called Ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Av    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Aw    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1099  | 693 | 219 | 184 | 3 |         |       |

- Molecule 36 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Ax    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 642 | 199 | 169 | 5 |         |       |

- Molecule 37 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Ay    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 683   | 439 | 128 | 115 | 1 |         |       |

- Molecule 38 is a protein called 60s ribosomal protein l41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | Az    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 39 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 39  | B5    | 3764     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 80772 | 36003 | 14762 | 26243 | 3764 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference         |
|-------|---------|----------|--------|----------|-------------------|
| B5    | 3550    | UY1      | U      | conflict | GB GBCN01009604.1 |

- Molecule 40 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 40  | B7    | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2538  | 1131 | 451 | 837 | 119 |         |       |

- Molecule 41 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 41  | B8    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3319  | 1481 | 585 | 1097 | 156 |         |       |

- Molecule 42 is a protein called Ribosomal protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | BA    | 253      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1940  | 1214 | 396 | 324 | 6 |         |       |

- Molecule 43 is a protein called Ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | BB    | 398      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3206  | 2042 | 605 | 546 | 13 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | BC    | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2886  | 1814 | 577 | 481 | 14 |         |       |

- Molecule 45 is a protein called Ribosomal\_L18\_c domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 45  | BD    | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2398  | 1516 | 439 | 429 | 14 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BD    | 2       | AAC      | GLY    | conflict | UNP G1SYJ6 |

- Molecule 46 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | BE    | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1960  | 1258 | 378 | 321 | 3 |         |       |

- Molecule 47 is a protein called Ribosomal Protein uL30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | BF    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1886  | 1211 | 362 | 304 | 9 |         |       |

- Molecule 48 is a protein called Ribosomal protein eL8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | BG    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1877  | 1197 | 361 | 315 | 4 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | BH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 954 | 284 | 272 | 6 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | BI    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1717  | 1086 | 332 | 285 | 14 |         |       |

- Molecule 51 is a protein called Ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | BJ    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1362  | 861 | 254 | 241 | 6 |         |       |

- Molecule 52 is a protein called Replicase polyprotein 1ab.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52  | BK    | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 273   | 169 | 46 | 52 | 6 |         |       |

- Molecule 53 is a protein called Ribosomal protein eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | BL    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1702  | 1065 | 354 | 279 | 4 |         |       |

- Molecule 54 is a protein called Ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | BM    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1137  | 727 | 221 | 182 | 7 |         |       |

- Molecule 55 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | BN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 56 is a protein called Ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | BO    | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1630  | 1051 | 319 | 255 | 5 |         |       |

- Molecule 57 is a protein called uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | BP    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1289  | 809 | 249 | 222 | 9 |         |       |

- Molecule 58 is a protein called Ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | BQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1515  | 946 | 315 | 250 | 4 |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | BR    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 933 | 328 | 238 | 9 |         |       |

- Molecule 60 is a protein called Ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 60  | BS    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1457  | 924 | 288 | 234 | 11 |         |       |

- Molecule 61 is a protein called eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | BT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 62 is a protein called Ribosomal protein eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | BU    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 806   | 516 | 141 | 147 | 2 |         |       |

- Molecule 63 is a protein called Ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | BV    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 648 | 199 | 182 | 5 |         |       |

- Molecule 64 is a protein called eL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | BW    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 991   | 619 | 202 | 166 | 4 |         |       |

- Molecule 65 is a protein called uL23.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | BX    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 618 | 181 | 167 | 1 |         |       |

- Molecule 66 is a protein called Ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | BY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 67 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | BZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | Ba    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 734 | 239 | 186 | 4 |         |       |

- Molecule 69 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | Bb    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 881   | 548 | 196 | 134 | 3 |         |       |

- Molecule 70 is a protein called eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | Bc    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 836   | 530 | 148 | 151 | 7 |         |       |

- Molecule 71 is a protein called eL31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | Bd    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 72 is a protein called eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | Be    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1070  | 676 | 221 | 168 | 5 |         |       |

- Molecule 73 is a protein called eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | Bf    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 884   | 560 | 175 | 144 | 5 |         |       |

- Molecule 74 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Bg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 75 is a protein called uL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | Bh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 640 | 204 | 168 | 1 |         |       |

- Molecule 76 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | Bi    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 520 | 176 | 129 | 5 |         |       |

- Molecule 77 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Bj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 78 is a protein called eL38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 78  | Bk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Bk    | 24      | LYS      | ASN    | conflict | UNP G1U001 |

- Molecule 79 is a protein called eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 79  | Bl    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 447   | 286 | 96 | 64 | 1 |         |       |

- Molecule 80 is a protein called 60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | Bm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 432   | 269 | 90 | 67 | 6 |         |       |

- Molecule 81 is a protein called eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | Bo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 863   | 543 | 175 | 139 | 6 |         |       |

- Molecule 82 is a protein called eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | Bp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 83 is a protein called Ribosomal protein eL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | Br    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1014  | 629 | 209 | 170 | 6 |         |       |

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | Bs    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1507  | 959 | 263 | 276 | 9 |         |       |

- Molecule 85 is a protein called Ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 85  | Bt    | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1178  | 733 | 221 | 220 | 4 |         |       |

- Molecule 86 is a protein called Ribosomal protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 86  | Bv    | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1707  | 1092 | 308 | 299 | 8 |         |       |

- Molecule 87 is a protein called Eukaryotic peptide chain release factor subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 87  | By    | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2087 | 559 | 623 | 11 |         |       |

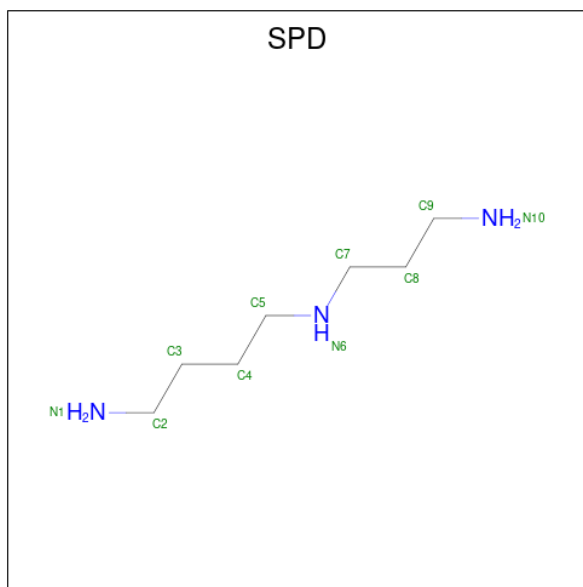
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| By    | 183     | ALA      | GLY    | engineered mutation | UNP P62497 |
| By    | 184     | ALA      | GLY    | engineered mutation | UNP P62497 |

- Molecule 88 is a protein called ATP binding cassette subfamily E member 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 88  | Bz    | 595      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4668  | 2982 | 801 | 854 | 31 |         |       |

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 89  | A2    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 90  | A2    | 102      | Total | Mg  | 0       |
|     |       |          | 102   | 102 |         |
| 90  | AH    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | AT    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 90  | B5    | 235      | Total | Mg  | 0       |
|     |       |          | 235   | 235 |         |
| 90  | B7    | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 90  | B8    | 6        | Total | Mg  | 0       |
|     |       |          | 6     | 6   |         |
| 90  | BI    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | BP    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | BR    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | BV    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 90  | Ba    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 91 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 91  | A2    | 76       | Total<br>76  | X<br>76  | 0       |
| 91  | AT    | 4        | Total<br>4   | X<br>4   | 0       |
| 91  | Ab    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | Ak    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | Ar    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | B5    | 244      | Total<br>244 | X<br>244 | 0       |
| 91  | B7    | 10       | Total<br>10  | X<br>10  | 0       |
| 91  | B8    | 16       | Total<br>16  | X<br>16  | 0       |
| 91  | BA    | 2        | Total<br>2   | X<br>2   | 0       |
| 91  | BB    | 3        | Total<br>3   | X<br>3   | 0       |
| 91  | BC    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | BH    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | BI    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | BL    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | BN    | 2        | Total<br>2   | X<br>2   | 0       |
| 91  | BP    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | BQ    | 2        | Total<br>2   | X<br>2   | 0       |
| 91  | BT    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | Bb    | 1        | Total<br>1   | X<br>1   | 0       |
| 91  | Be    | 2        | Total<br>2   | X<br>2   | 0       |
| 91  | Bf    | 1        | Total<br>1   | X<br>1   | 0       |

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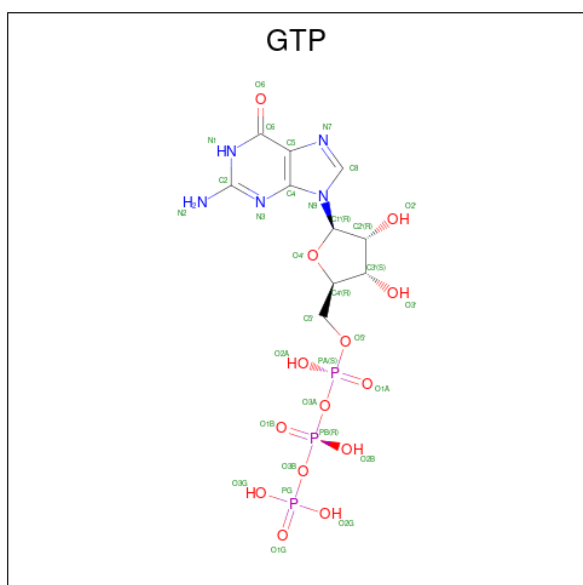
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| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 91  | Bg    | 1        | Total | X | 0       |
|     |       |          | 1     | 1 |         |
| 91  | Bo    | 1        | Total | X | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

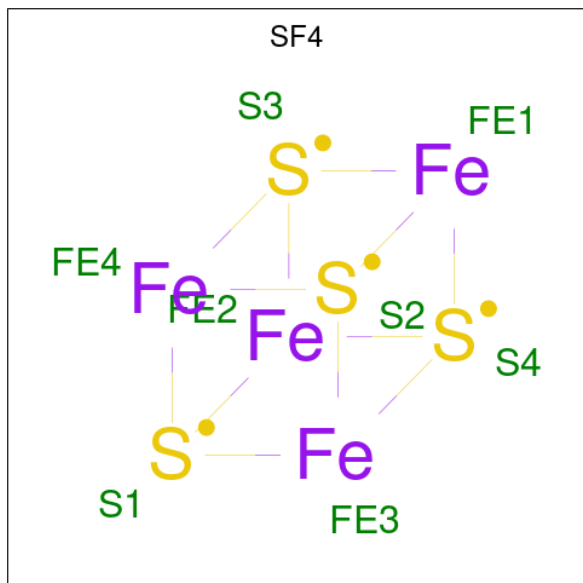
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 92  | AC    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | AE    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | AG    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | Bg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | Bj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | Bm    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | Bo    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 92  | Bp    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 93  | B7    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 94 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 94  | Bz    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 94  | Bz    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 95 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 95  | A2    | 473      | Total | O   | 0       |
|     |       |          | 473   | 473 |         |
| 95  | AH    | 10       | Total | O   | 0       |
|     |       |          | 10    | 10  |         |
| 95  | AT    | 12       | Total | O   | 0       |
|     |       |          | 12    | 12  |         |
| 95  | Aa    | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |
| 95  | Ab    | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |
| 95  | Ad    | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |
| 95  | Af    | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |

Continued on next page...



*Continued from previous page...*

| Mol | Chain | Residues | Atoms         |           | AltConf |
|-----|-------|----------|---------------|-----------|---------|
| 95  | Ak    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | Am    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | An    | 2        | Total<br>2    | O<br>2    | 0       |
| 95  | Ap    | 4        | Total<br>4    | O<br>4    | 0       |
| 95  | Ar    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | As    | 4        | Total<br>4    | O<br>4    | 0       |
| 95  | Aw    | 4        | Total<br>4    | O<br>4    | 0       |
| 95  | B5    | 1117     | Total<br>1117 | O<br>1117 | 0       |
| 95  | B7    | 17       | Total<br>17   | O<br>17   | 0       |
| 95  | B8    | 31       | Total<br>31   | O<br>31   | 0       |
| 95  | BA    | 5        | Total<br>5    | O<br>5    | 0       |
| 95  | BB    | 7        | Total<br>7    | O<br>7    | 0       |
| 95  | BC    | 3        | Total<br>3    | O<br>3    | 0       |
| 95  | BD    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | BF    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | BH    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | BI    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | BL    | 1        | Total<br>1    | O<br>1    | 0       |
| 95  | BN    | 2        | Total<br>2    | O<br>2    | 0       |
| 95  | BO    | 3        | Total<br>3    | O<br>3    | 0       |
| 95  | BP    | 3        | Total<br>3    | O<br>3    | 0       |

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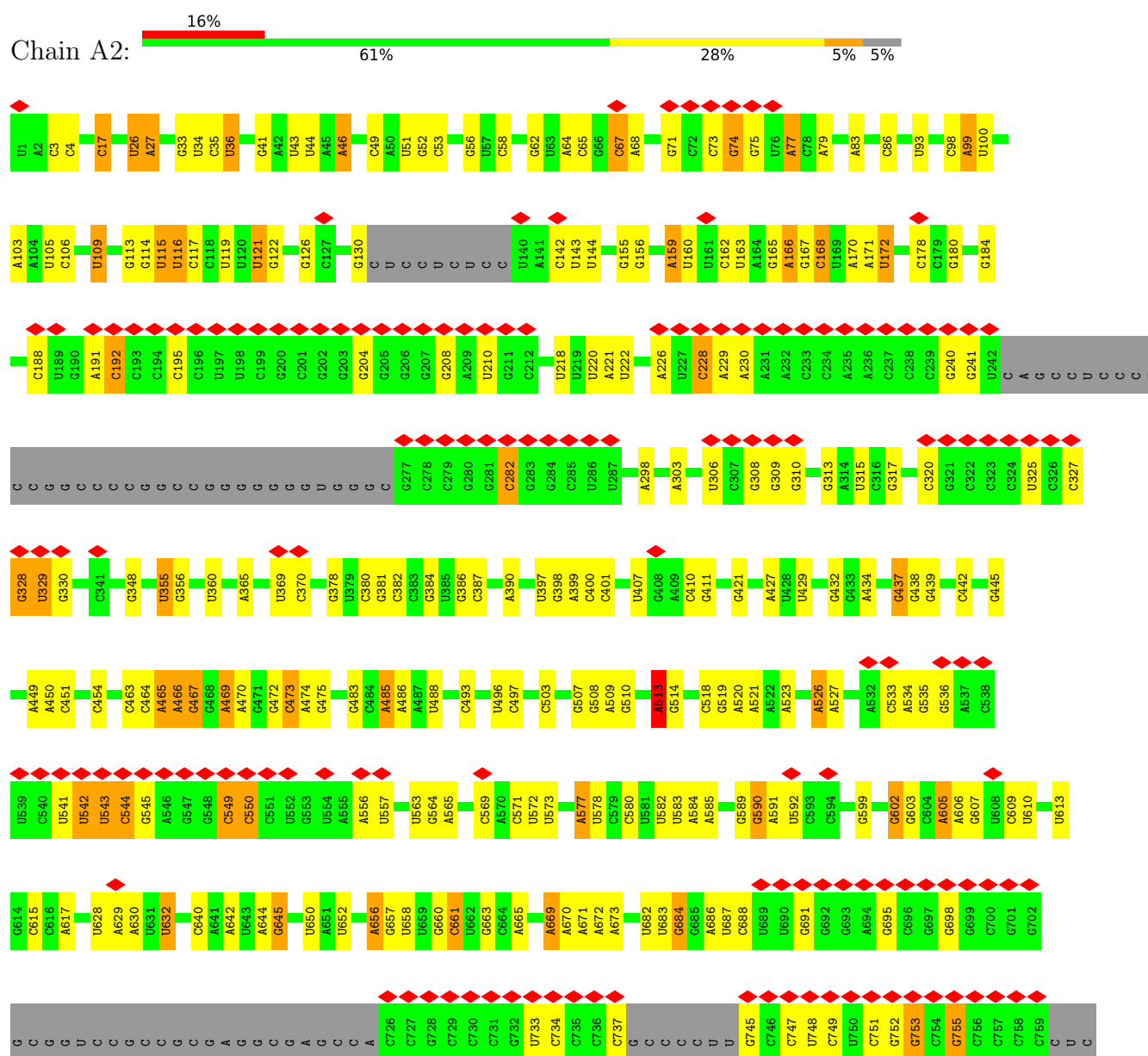
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 95  | BR    | 5        | Total<br>5 | O<br>5 | 0       |
| 95  | BV    | 4        | Total<br>4 | O<br>4 | 0       |
| 95  | BX    | 1        | Total<br>1 | O<br>1 | 0       |
| 95  | BY    | 1        | Total<br>1 | O<br>1 | 0       |
| 95  | Ba    | 7        | Total<br>7 | O<br>7 | 0       |
| 95  | Bb    | 1        | Total<br>1 | O<br>1 | 0       |
| 95  | Bd    | 1        | Total<br>1 | O<br>1 | 0       |
| 95  | Be    | 4        | Total<br>4 | O<br>4 | 0       |
| 95  | Bf    | 1        | Total<br>1 | O<br>1 | 0       |
| 95  | By    | 1        | Total<br>1 | O<br>1 | 0       |

### 3 Residue-property plots

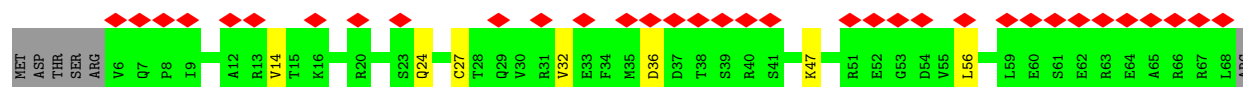
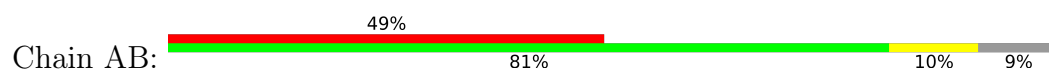
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 18S rRNA

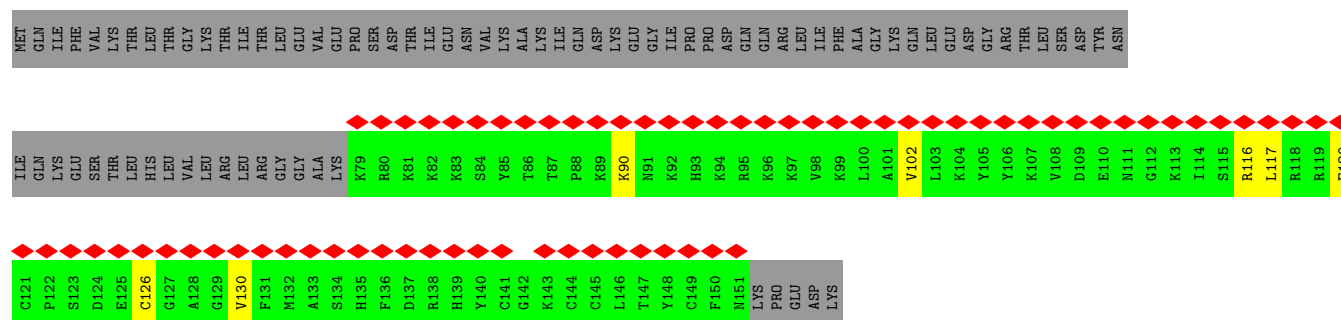




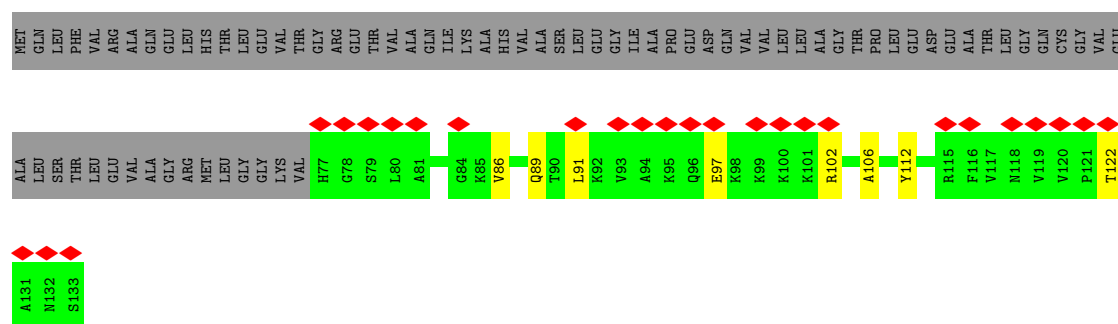
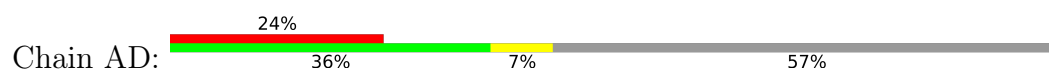
- Molecule 3: Ribosomal protein S28



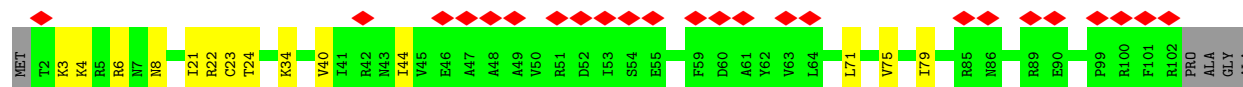
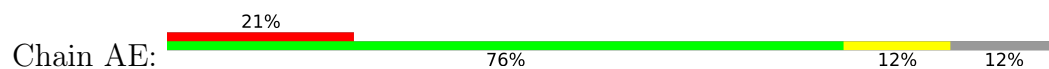
- Molecule 4: Ribosomal protein S27a



- Molecule 5: 40S ribosomal protein S30



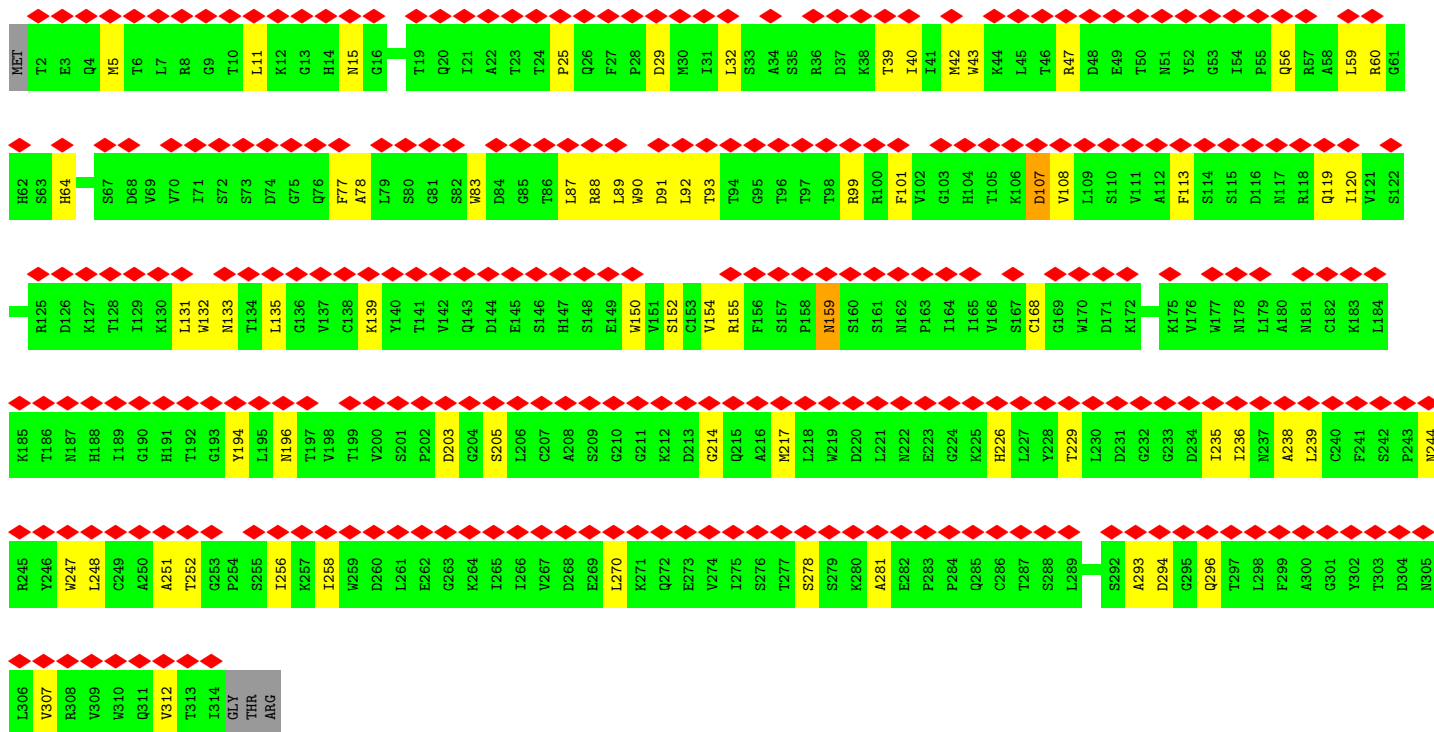
- Molecule 6: Ribosomal protein eS26



ALA  
PRO  
ARG  
E3  
PRO  
PRO  
LVS  
PRO  
MET

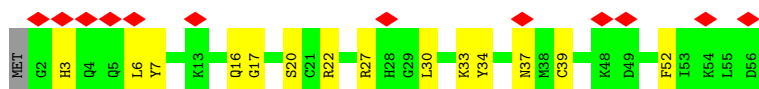
• Molecule 7: RACK1

Chain AF: 



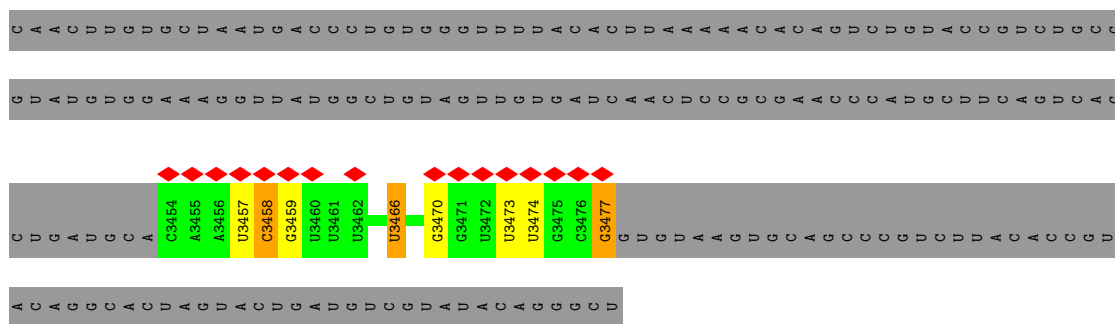
• Molecule 8: uS14

Chain AG: 



• Molecule 9: mRNA containing SARS-CoV-2 sequence

Chain AH: 



• Molecule 10: E-site tRNA

Chain AI:

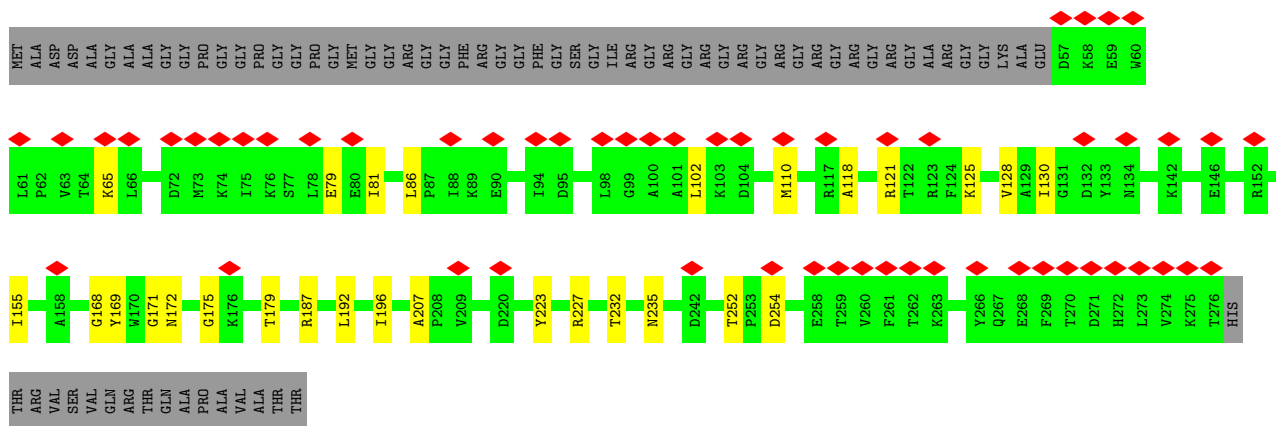
Chain AT:

Chain AZ:

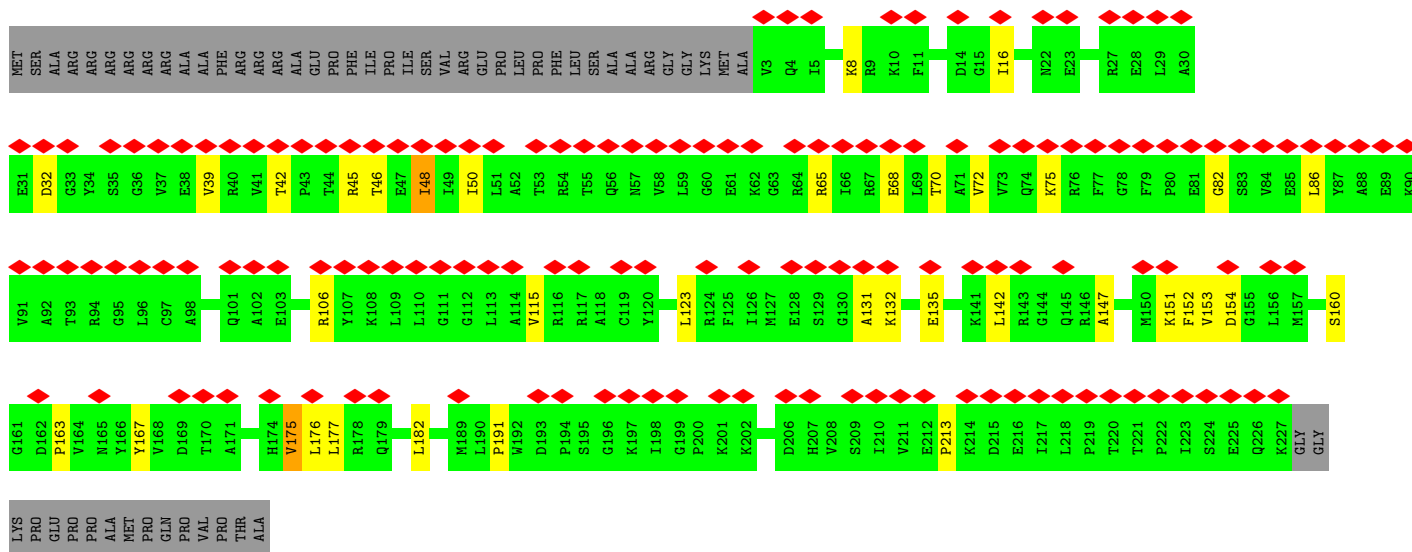
Chain Aa:



- Molecule 14: Ribosomal protein uS5

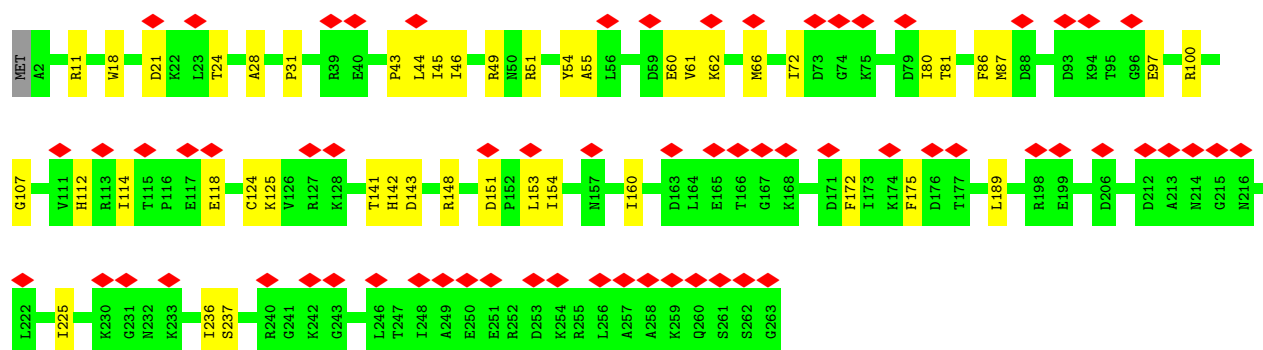
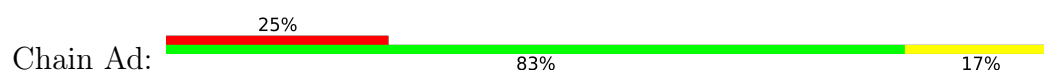


- Molecule 15: 40S ribosomal protein S3

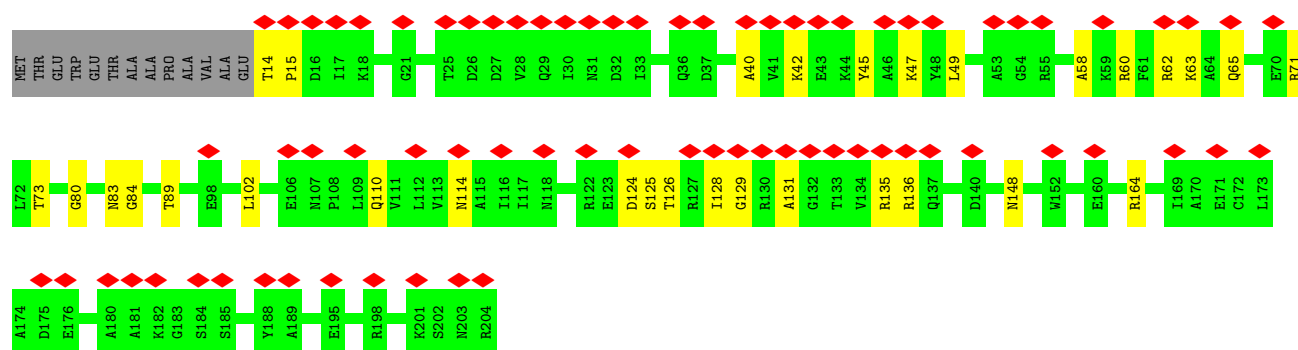
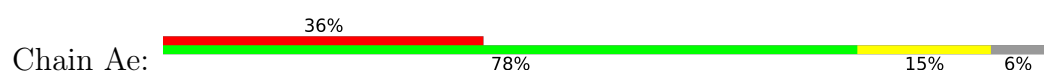


- Molecule 16: Ribosomal protein eS4

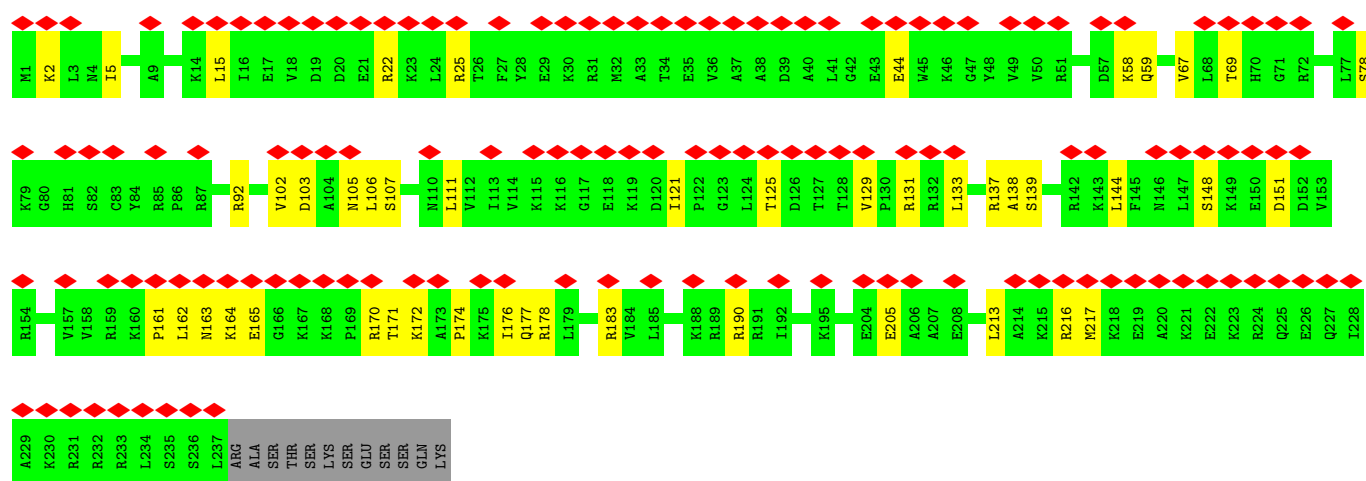
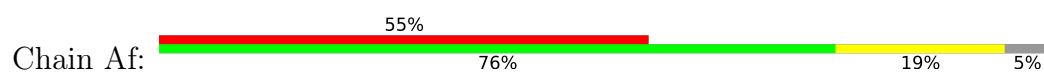




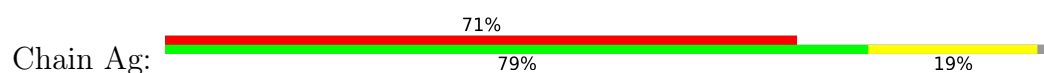
• Molecule 17: Ribosomal protein S5



• Molecule 18: 40S ribosomal protein S6

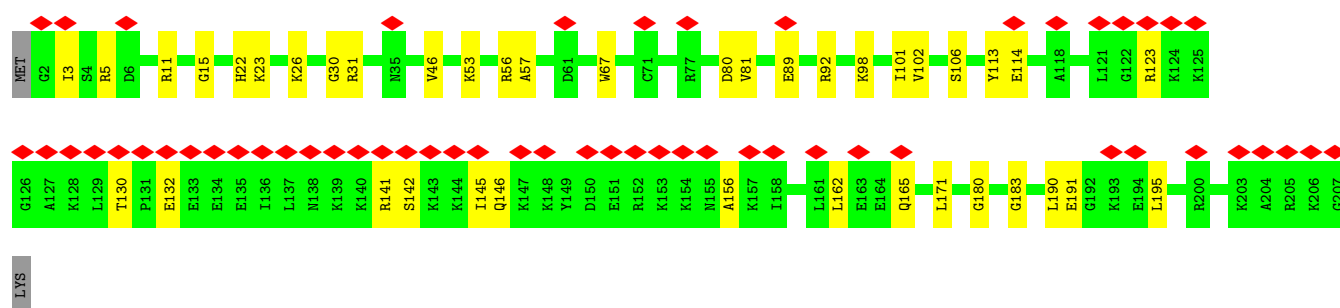
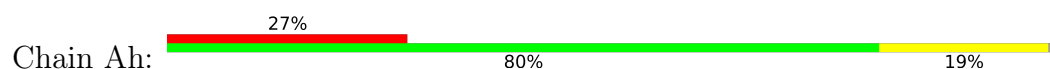


• Molecule 19: 40S ribosomal protein S7

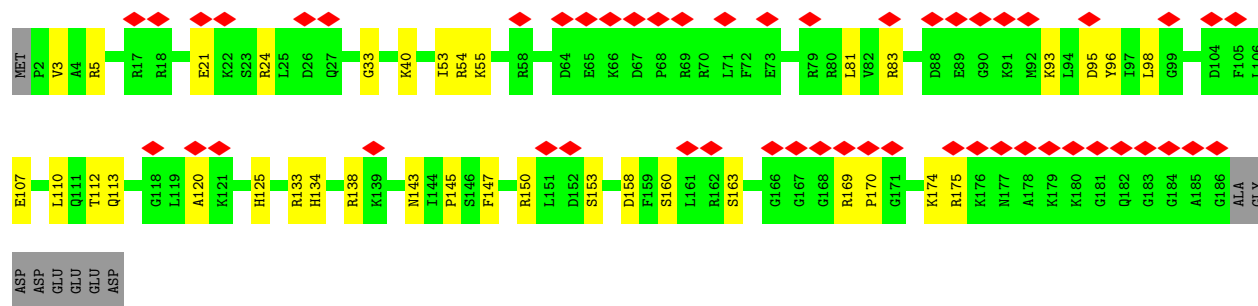
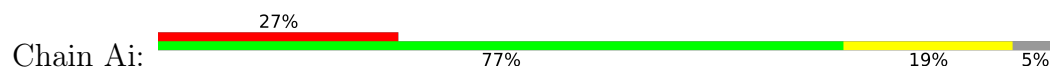




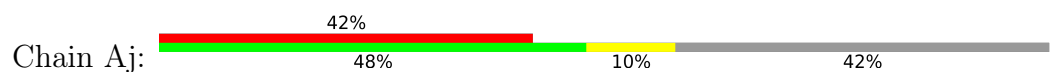
• Molecule 20: 40S ribosomal protein S8



• Molecule 21: Ribosomal protein S9 (Predicted)



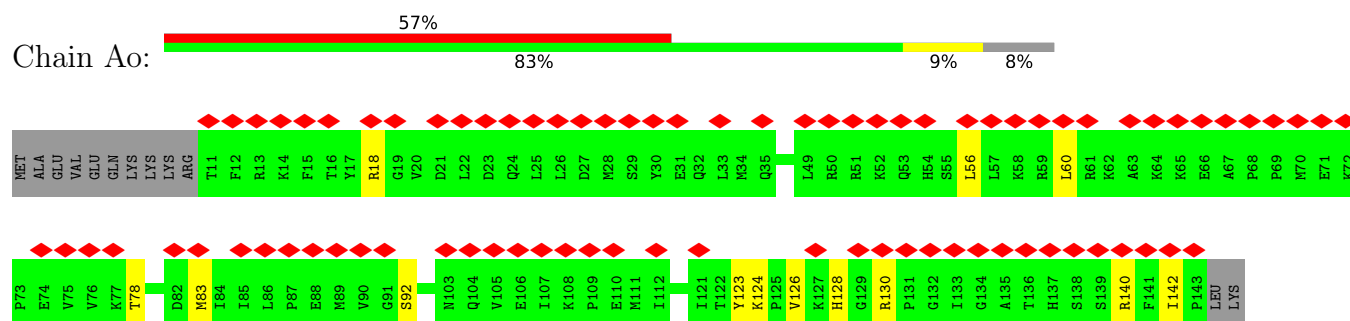
• Molecule 22: Ribosomal protein eS10





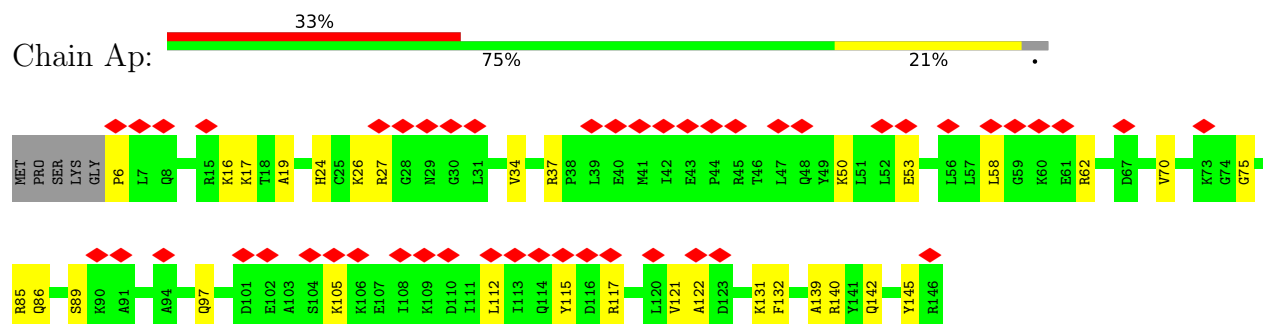
- Molecule 27: 40S ribosomal protein uS19

Chain Ao:



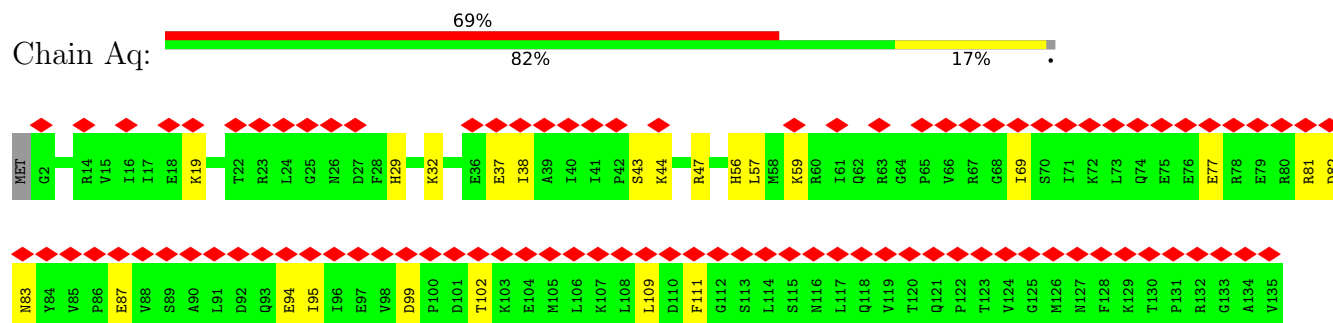
- Molecule 28: Ribosomal protein S16

Chain Ap:



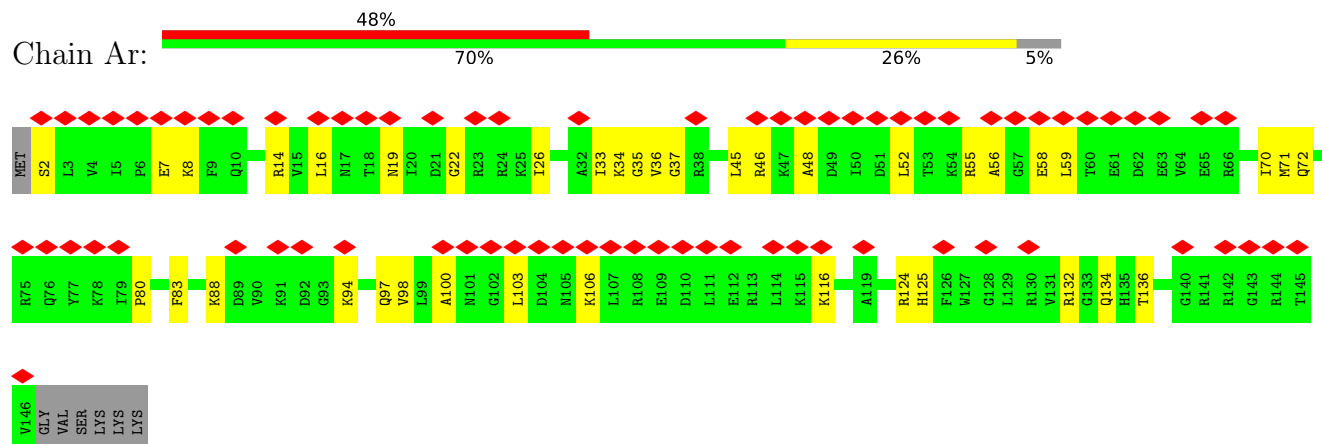
- Molecule 29: 40S ribosomal protein eS17

Chain Aq:



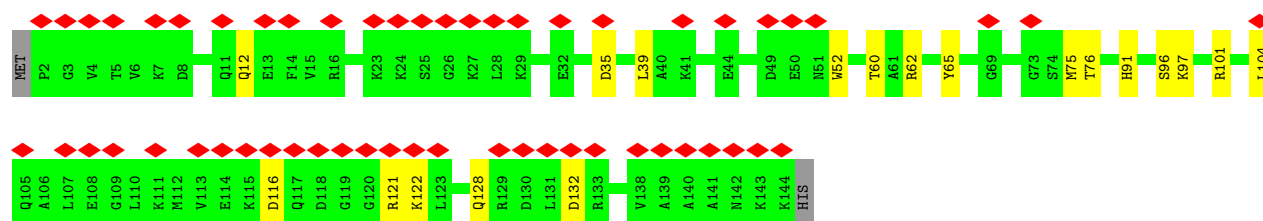
- Molecule 30: 40S ribosomal protein S18

Chain Ar:



- Molecule 31: Ribosomal protein eS19

Chain As: 



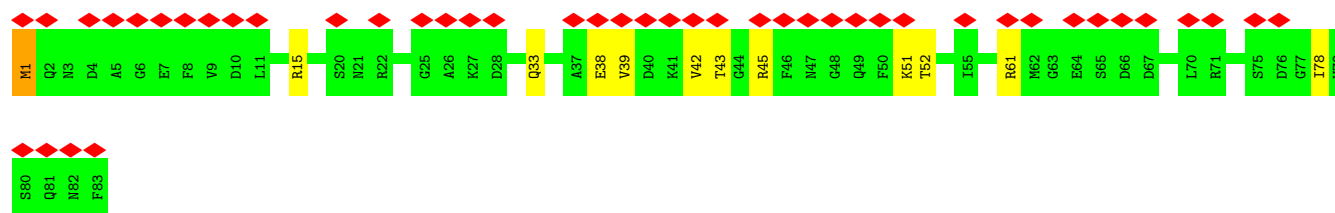
• Molecule 32: 40S ribosomal protein uS10

Chain At: 

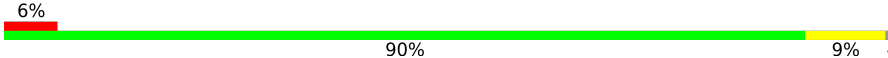


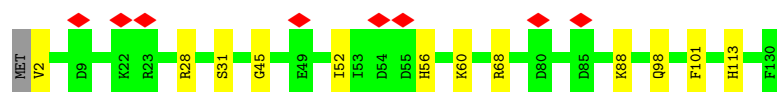
• Molecule 33: Ribosomal protein eS21

Chain Au: 



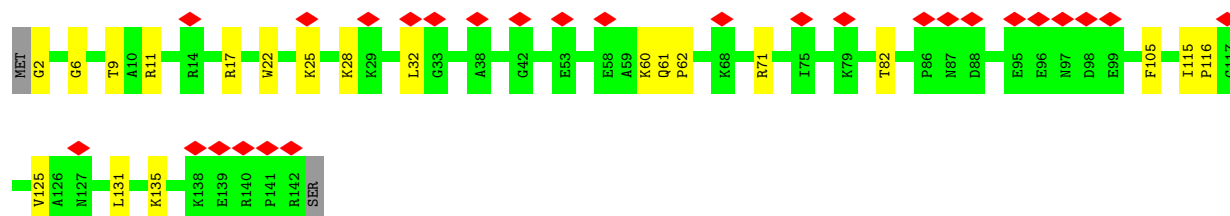
• Molecule 34: Ribosomal protein S15a

Chain Av: 

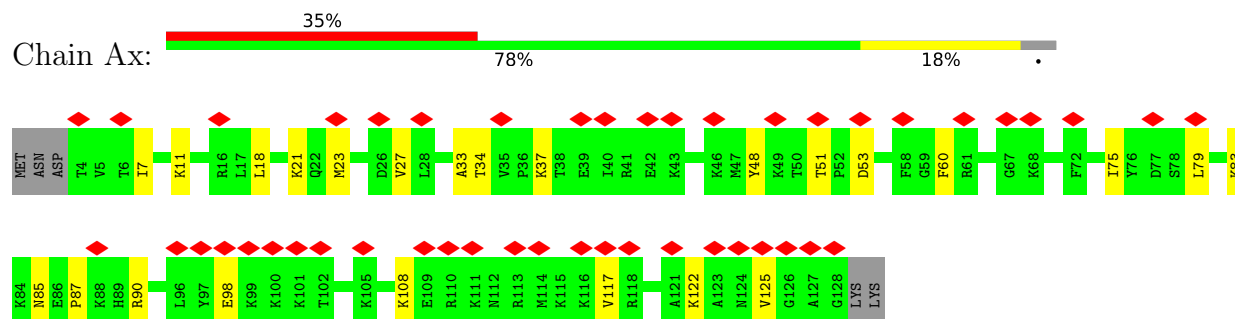


• Molecule 35: 40S ribosomal protein S23

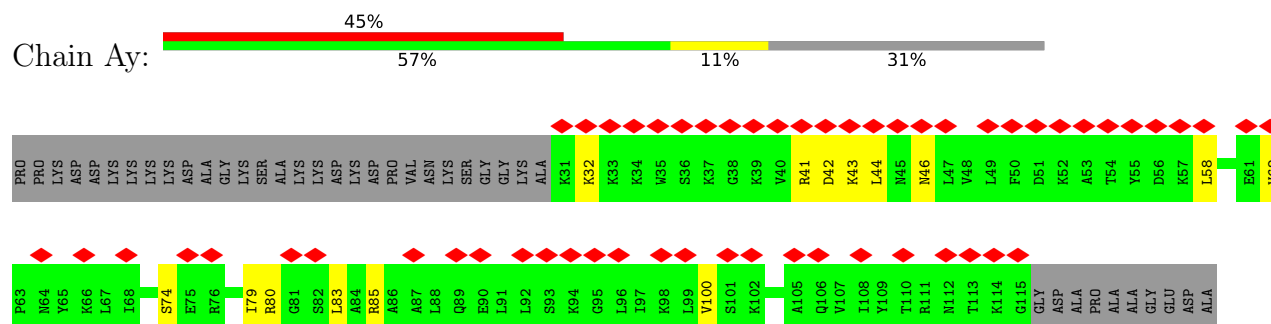
Chain Aw: 



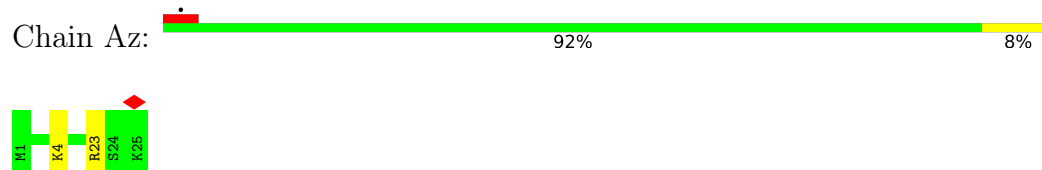
- Chain Ax:



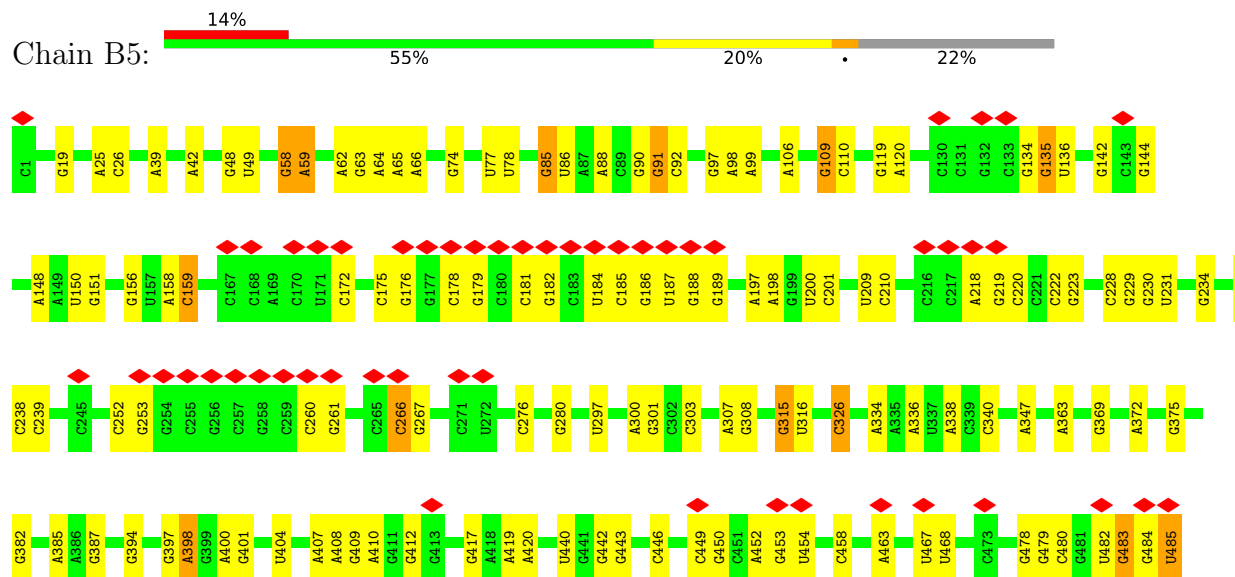
- Chain Ay:



- Chain Az:



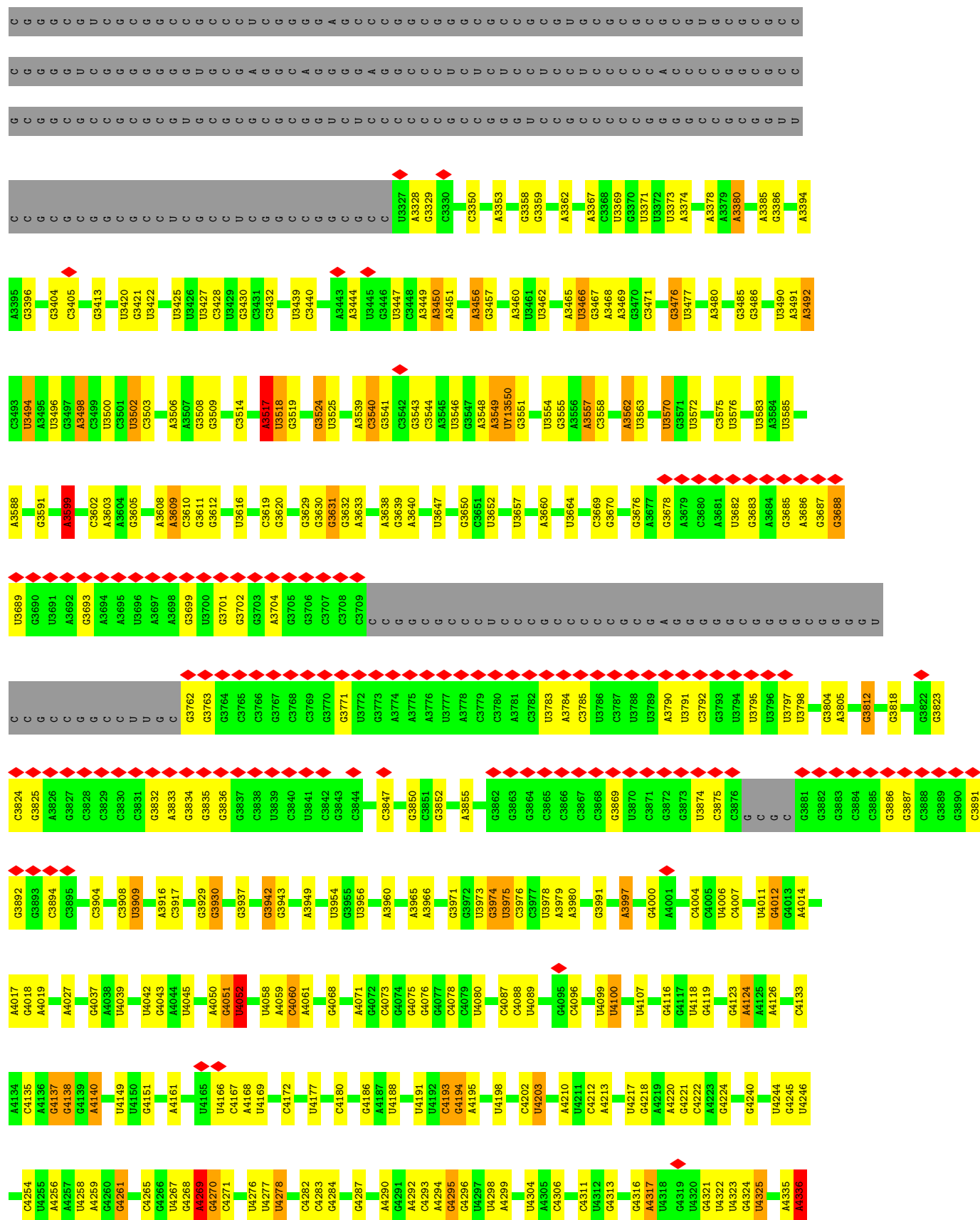
- Chain B5:

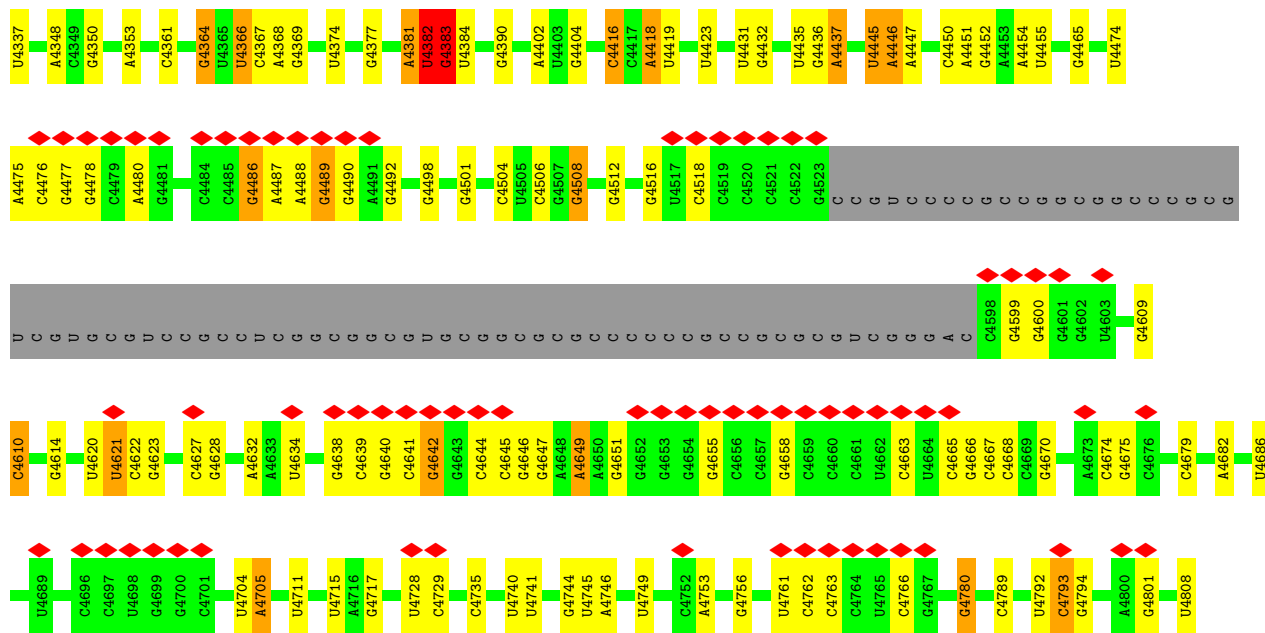




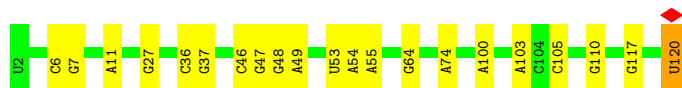
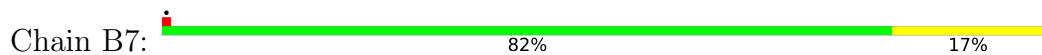








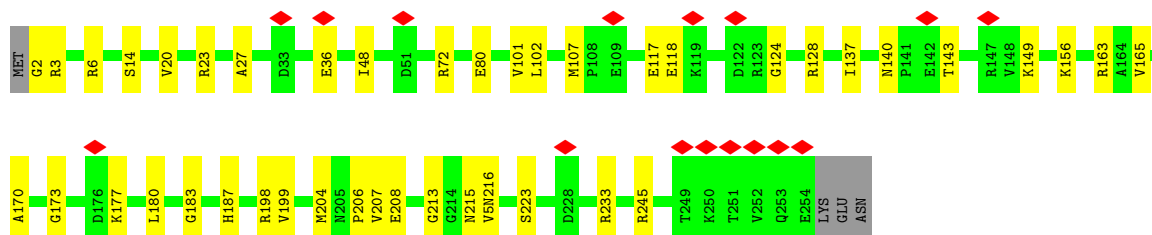
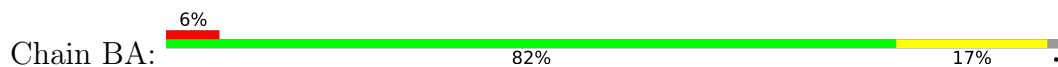
• Molecule 40: 5S rRNA



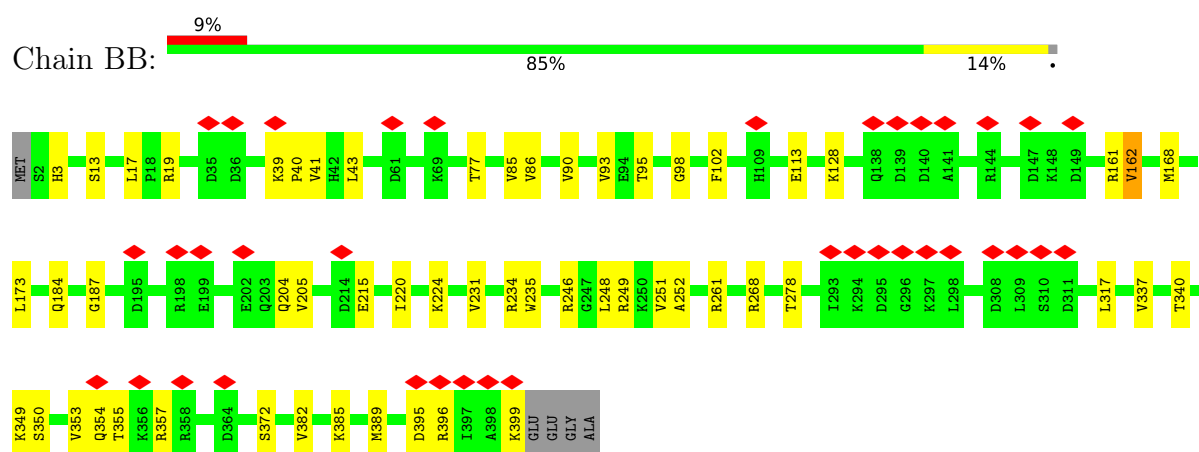
• Molecule 41: 5.8S rRNA



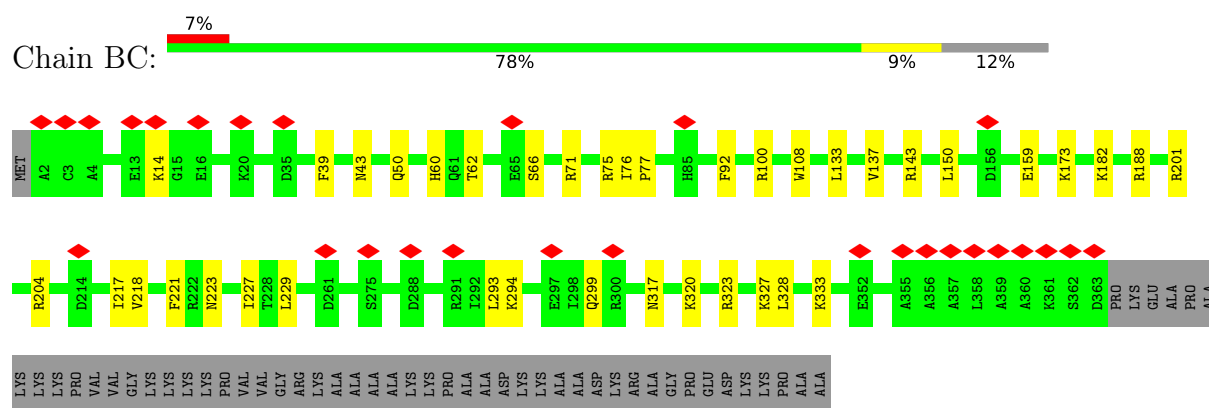
• Molecule 42: Ribosomal protein uL2



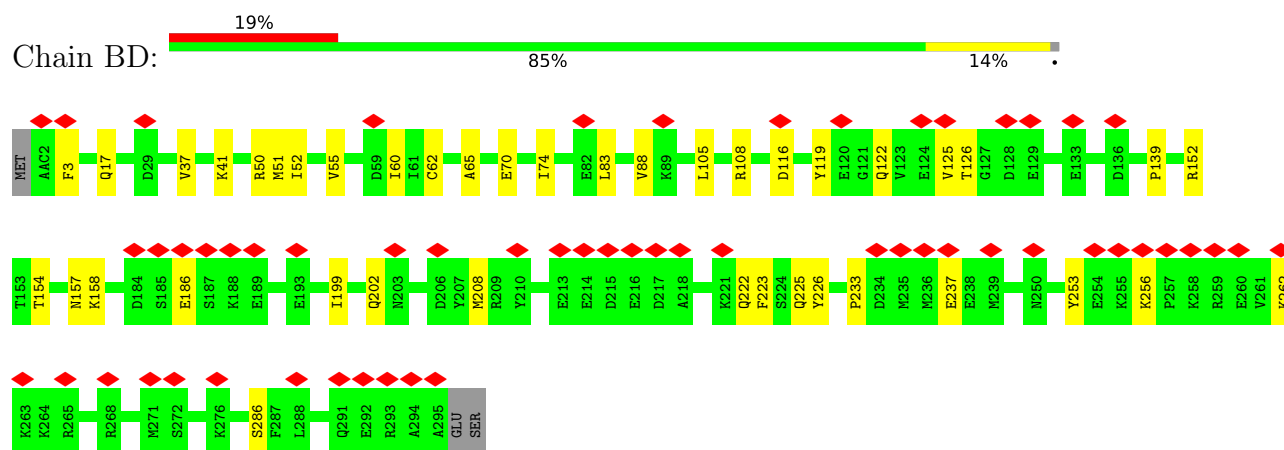
• Molecule 43: Ribosomal protein L3



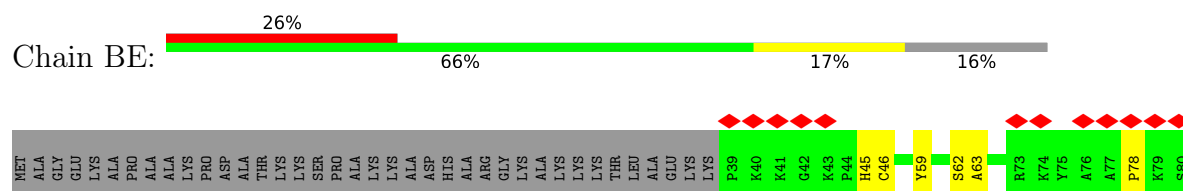
- Molecule 44: 60S ribosomal protein L4

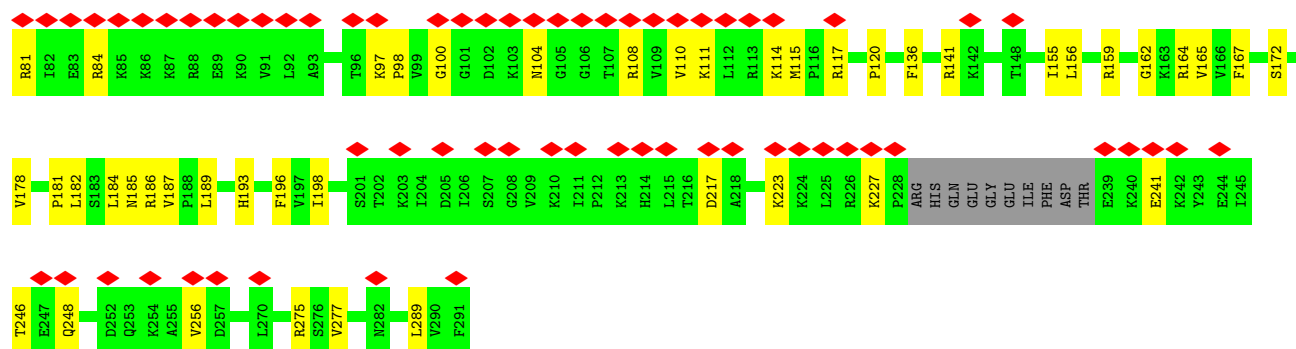


- Molecule 45: Ribosomal\_L18\_c domain-containing protein

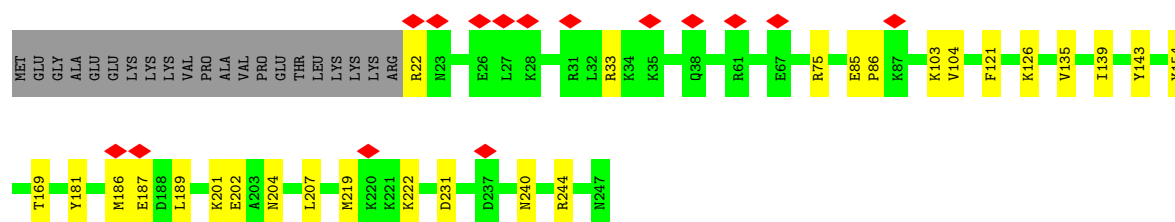
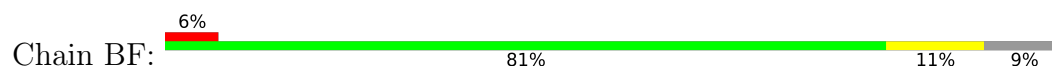


- Molecule 46: 60S ribosomal protein L6

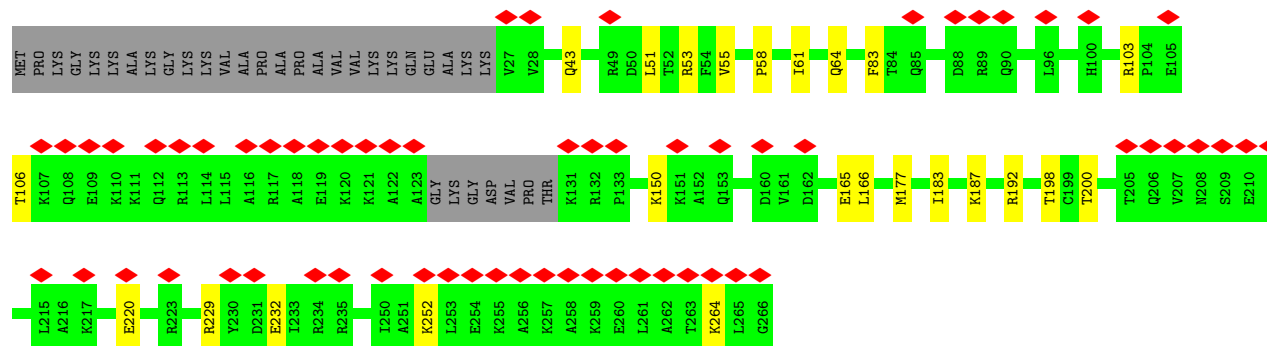
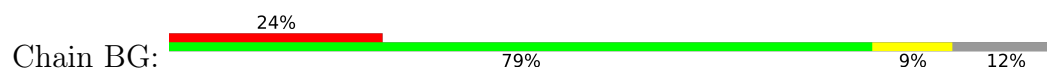




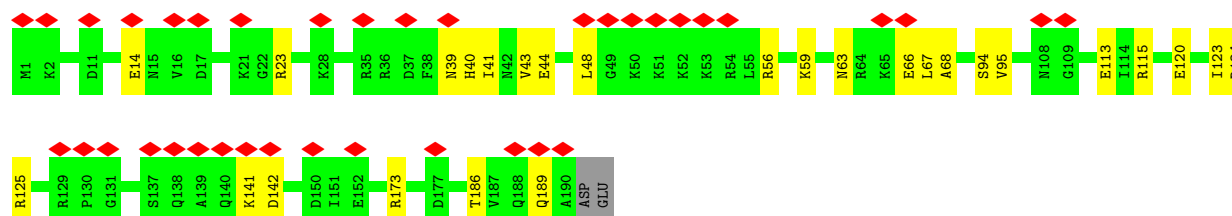
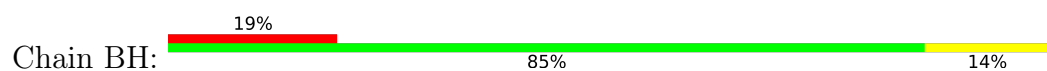
• Molecule 47: Ribosomal Protein uL30



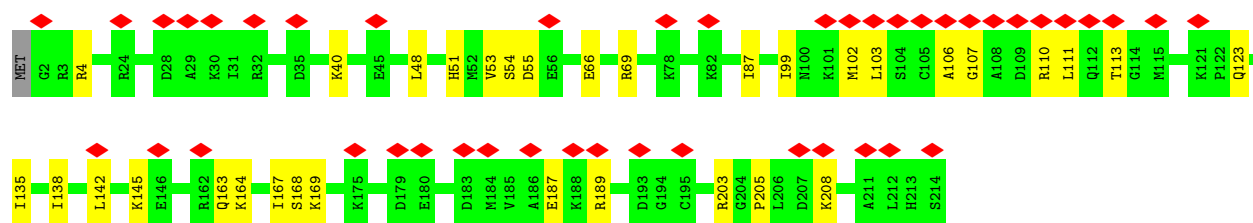
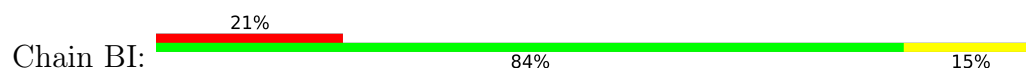
• Molecule 48: Ribosomal protein eL8



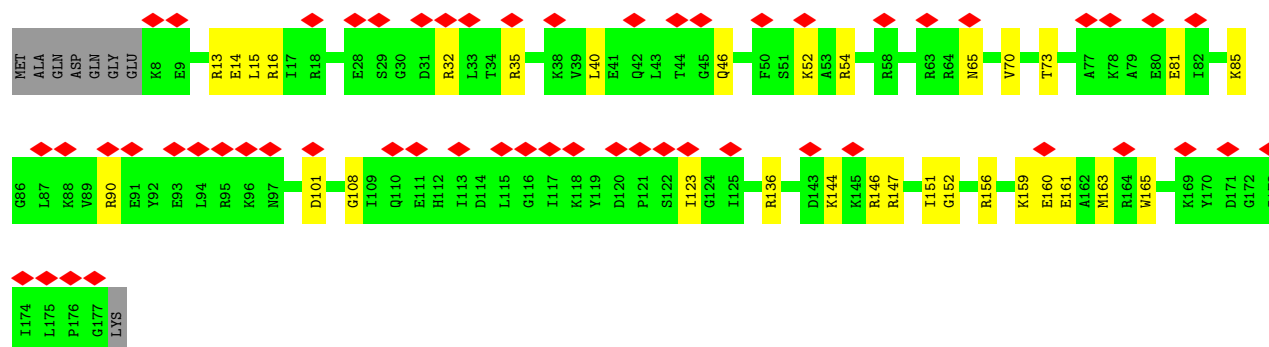
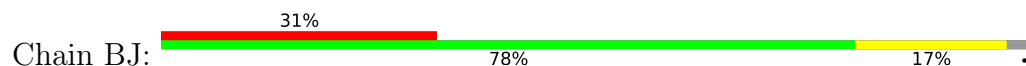
• Molecule 49: 60S ribosomal protein L9



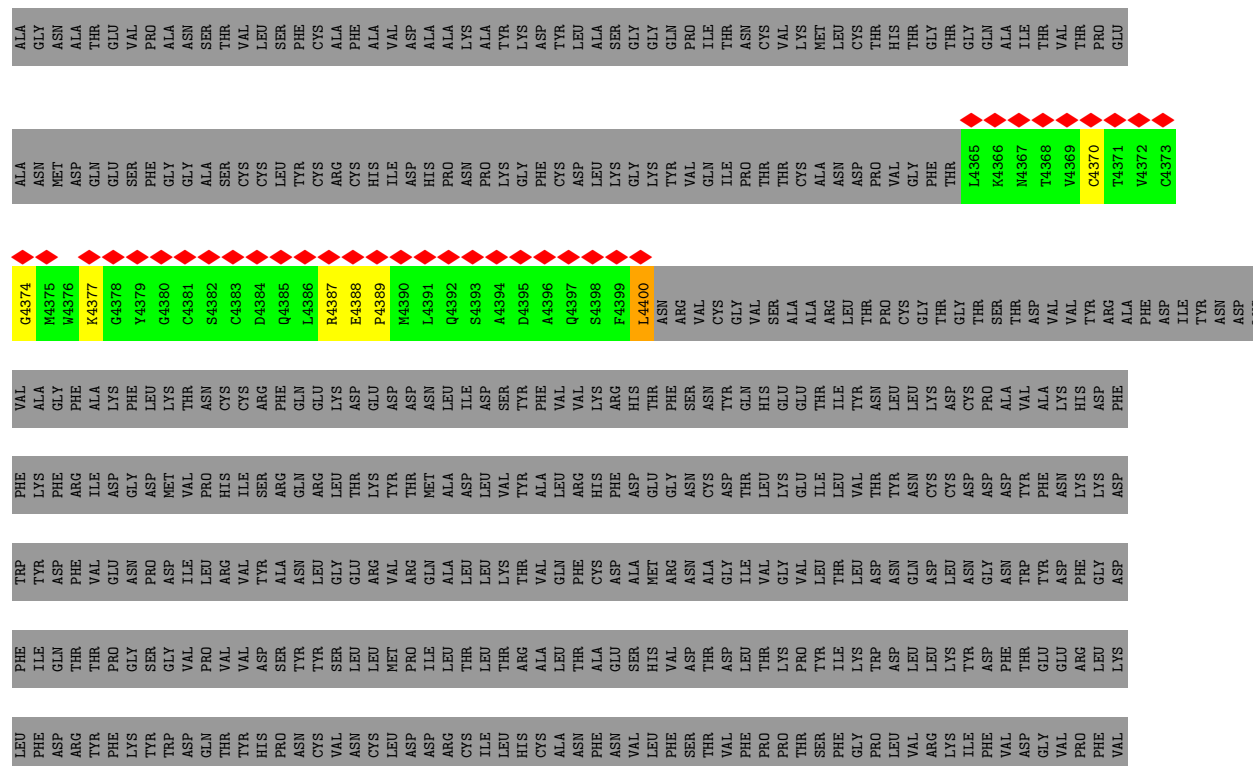
• Molecule 50: 60S ribosomal protein L10



• Molecule 51: Ribosomal protein L11

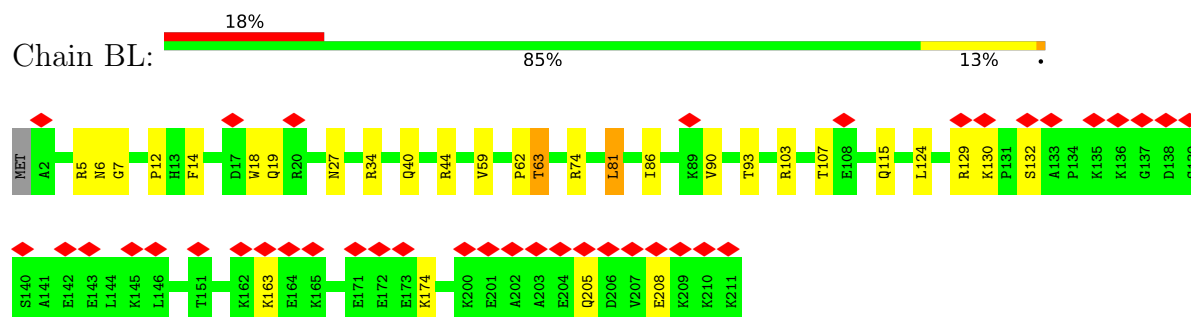


• Molecule 52: Replicase polypeptide 1ab

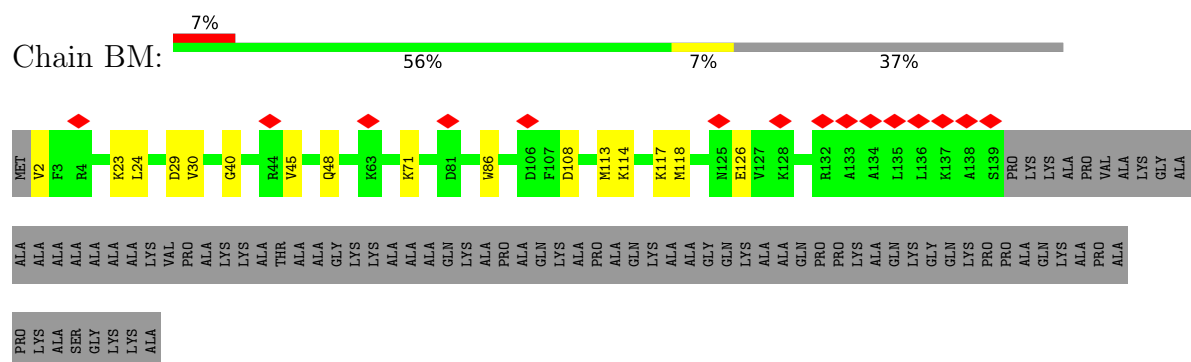


[illegible]

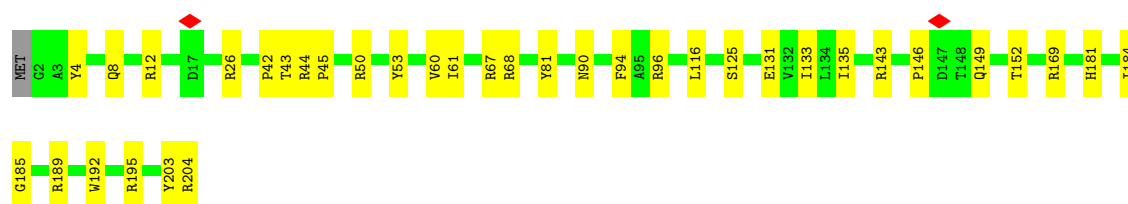
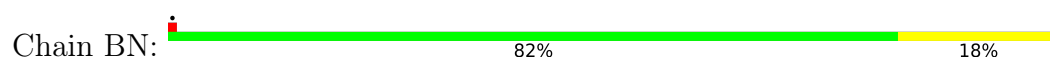
- Molecule 53: Ribosomal protein eL13



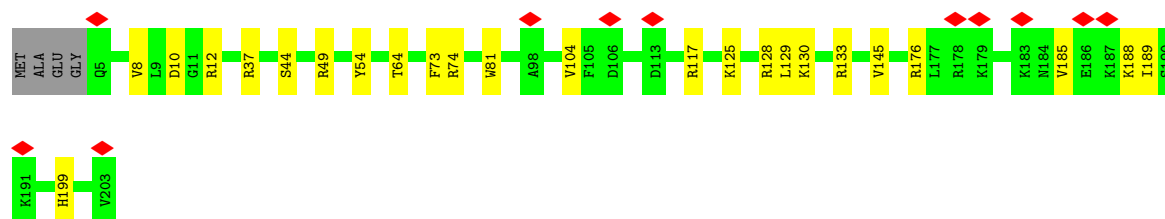
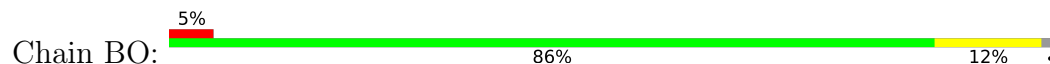
- Molecule 54: Ribosomal protein L14



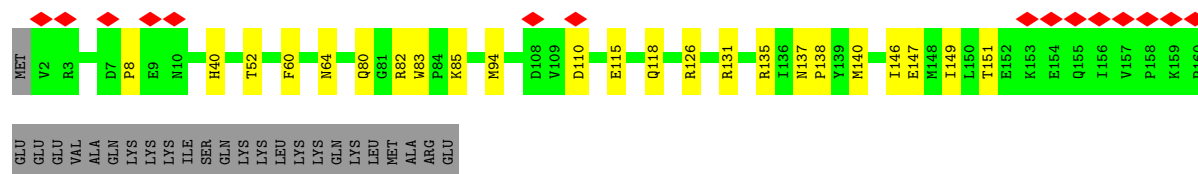
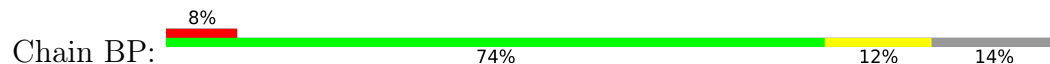
- Molecule 55: Ribosomal protein L15



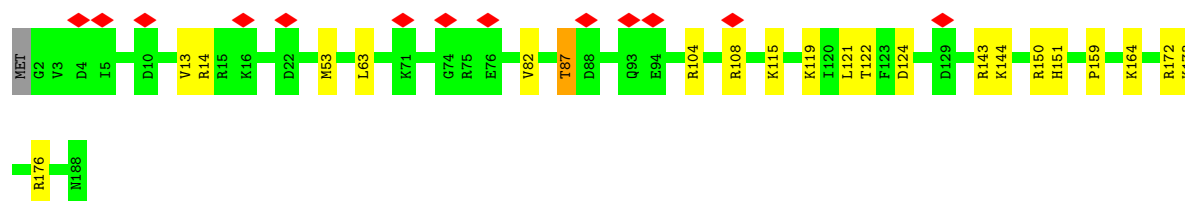
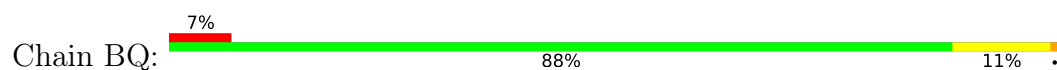
- Molecule 56: Ribosomal protein L13a



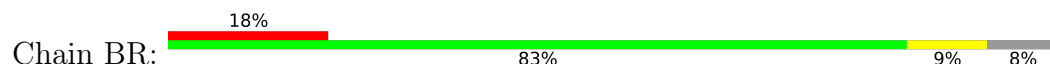
- Molecule 57: uL22

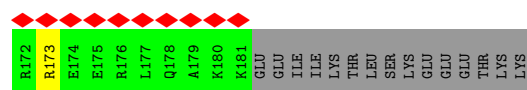


- Molecule 58: Ribosomal protein L18

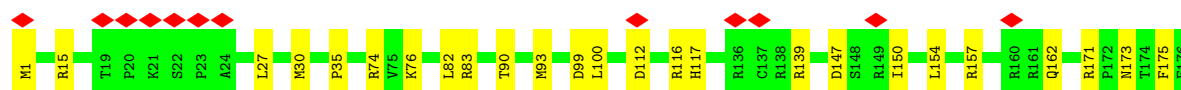
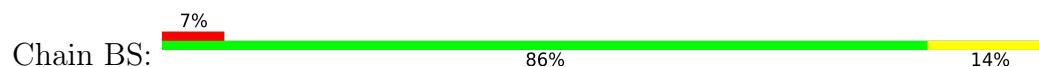


- Molecule 59: 60S ribosomal protein L19

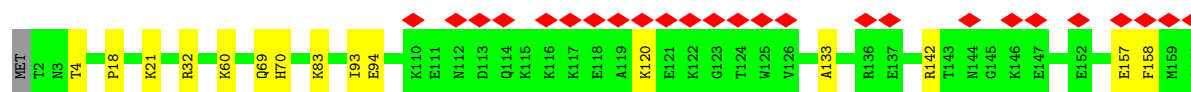




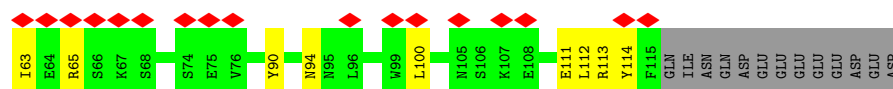
- Molecule 60: Ribosomal protein L18a



- Molecule 61: eL21



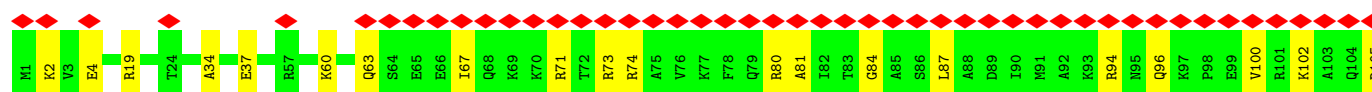
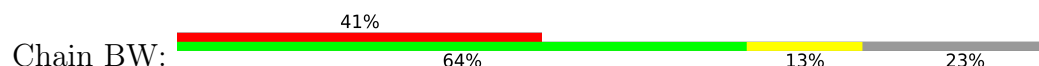
- Molecule 62: Ribosomal protein eL22



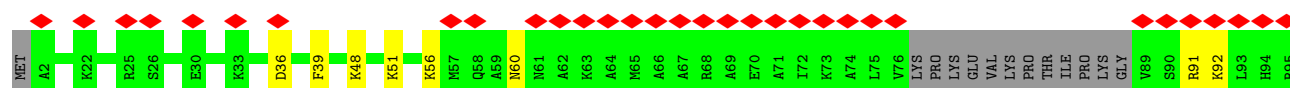
- Molecule 63: Ribosomal protein L23

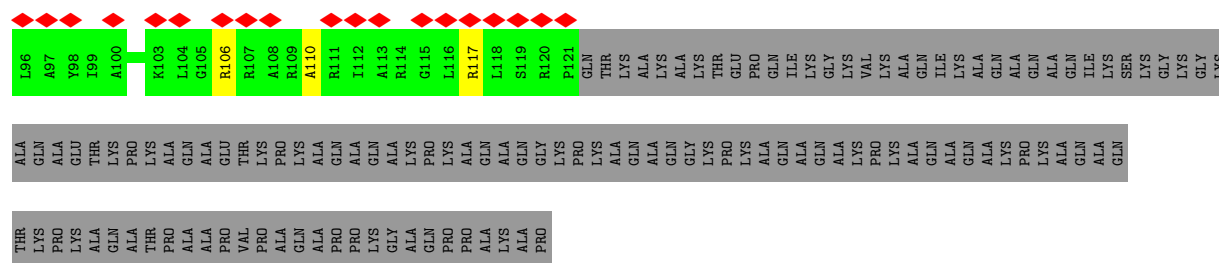


- Molecule 64: eL24

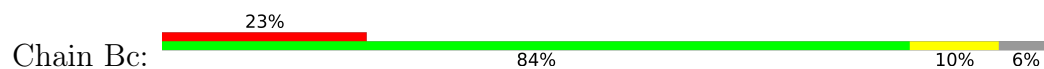




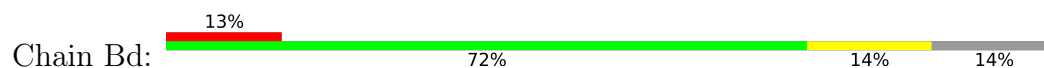




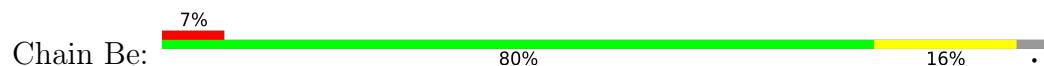
- Molecule 70: eL30



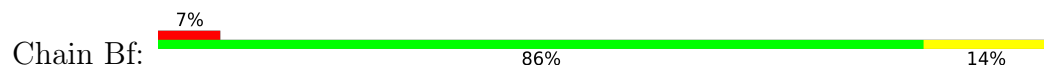
- Molecule 71: eL31



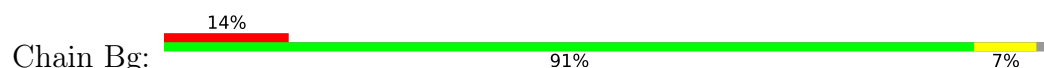
- Molecule 72: eL32



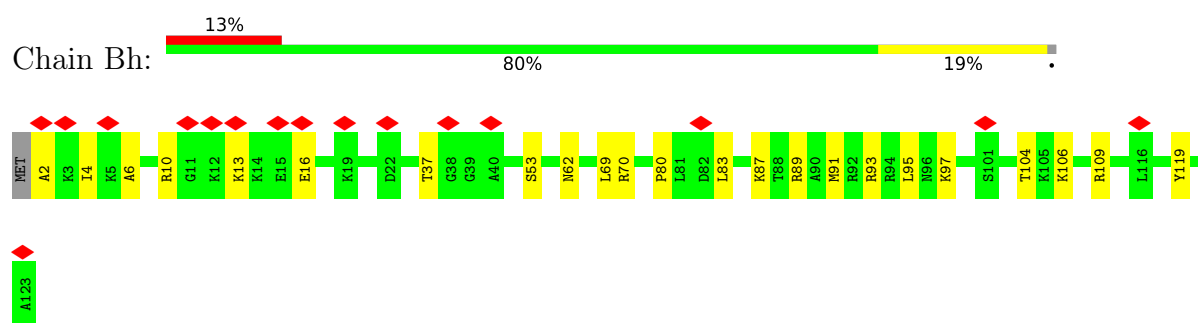
- Molecule 73: eL33



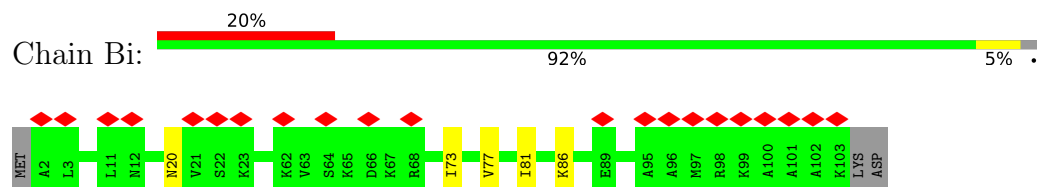
- Molecule 74: 60S ribosomal protein L34



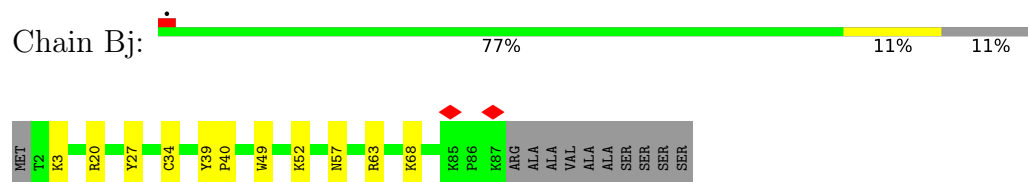
- Molecule 75: uL29



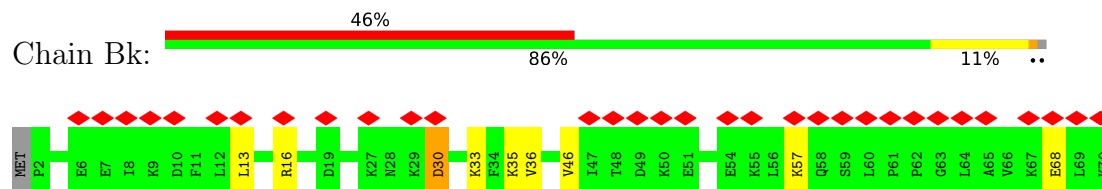
- Molecule 76: 60S ribosomal protein L36



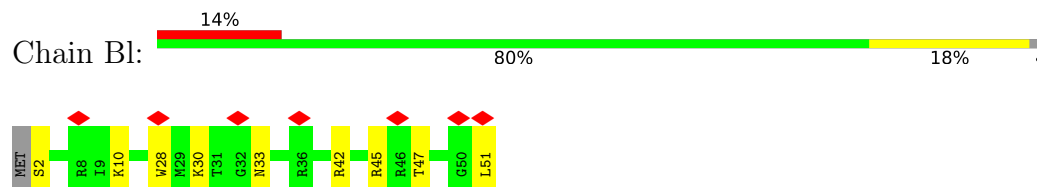
- Molecule 77: Ribosomal protein L37



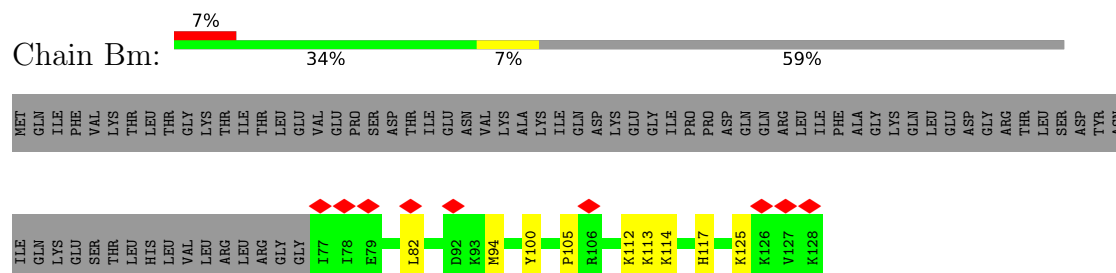
- Molecule 78: eL38



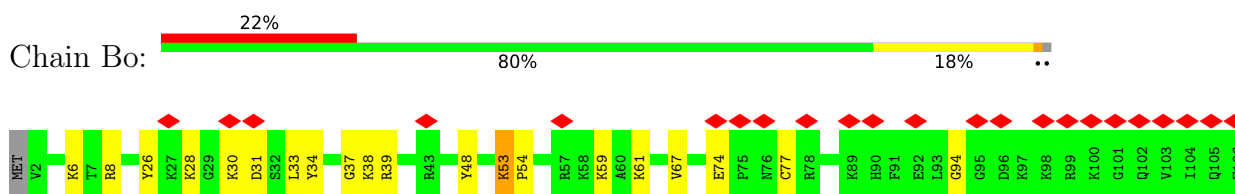
- Molecule 79: eL39



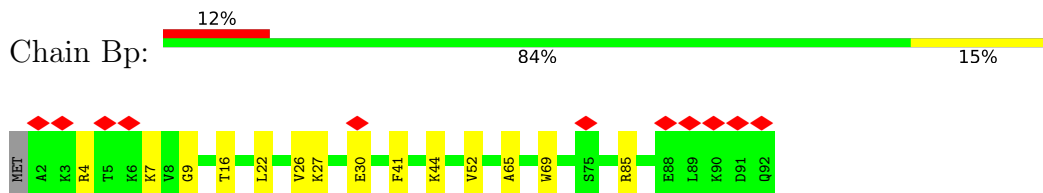
- Molecule 80: 60S ribosomal protein L40



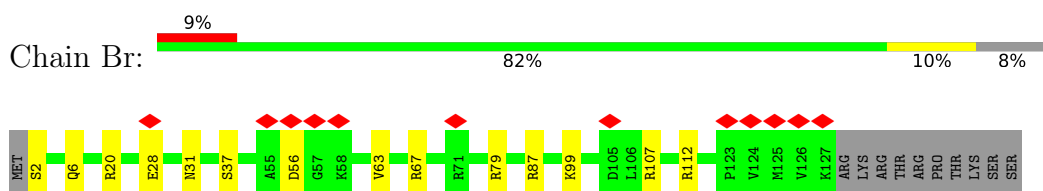
- Molecule 81: eL42



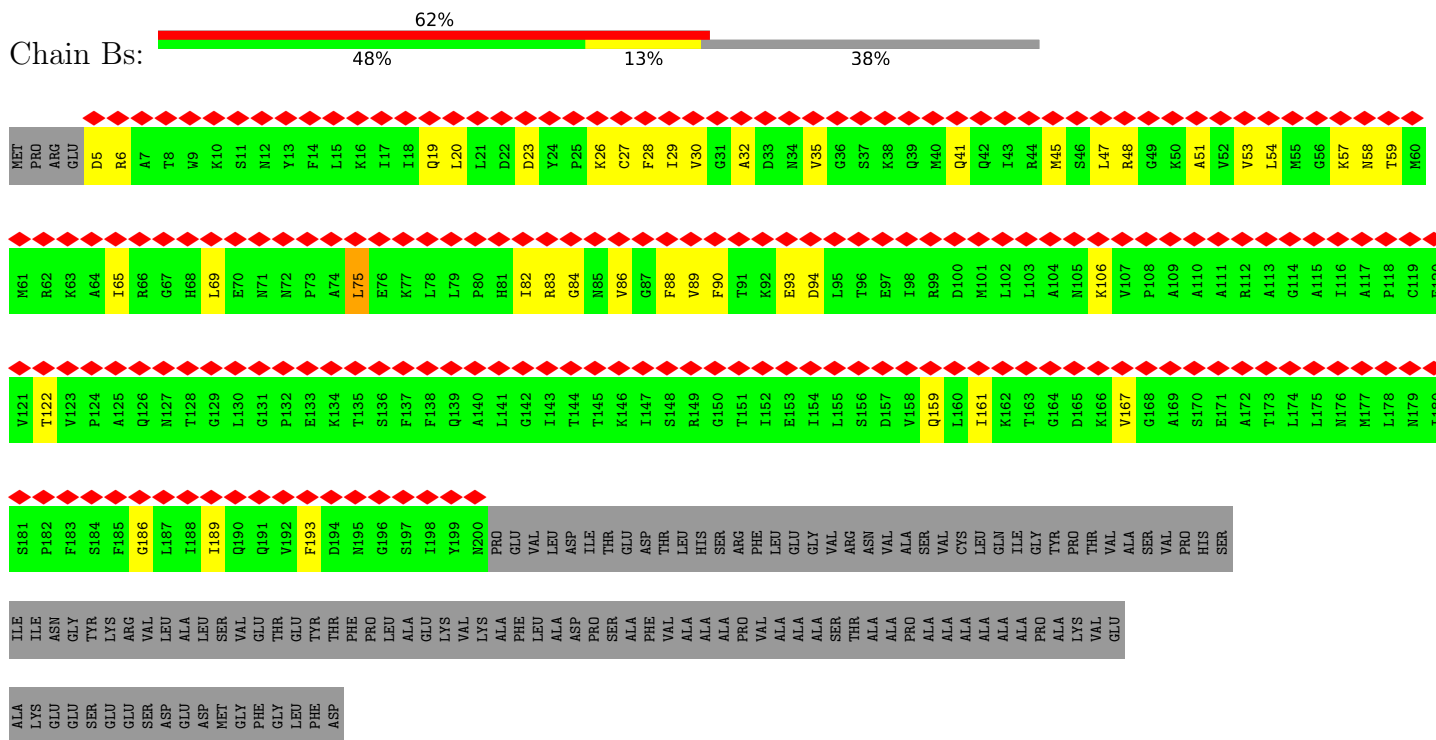
- Molecule 82: eL43



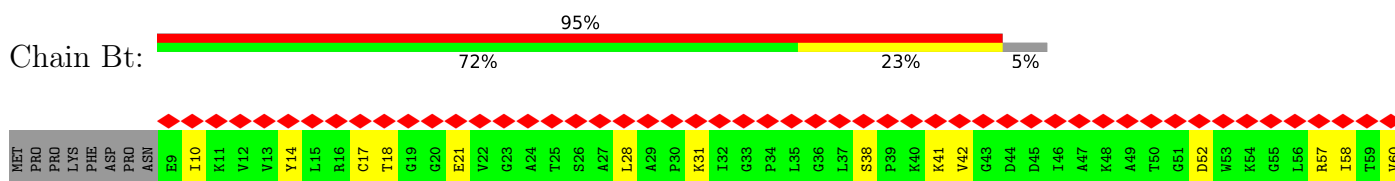
- Molecule 83: Ribosomal protein eL28



- Molecule 84: 60S acidic ribosomal protein P0

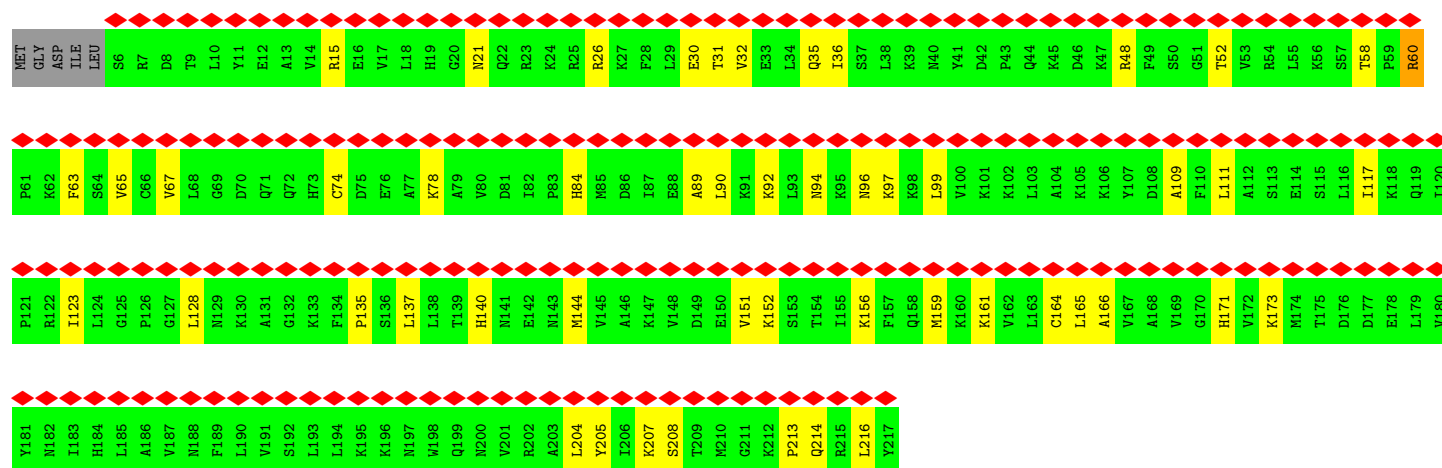
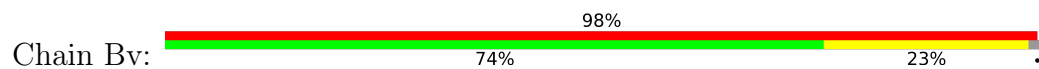


- Molecule 85: Ribosomal protein L12

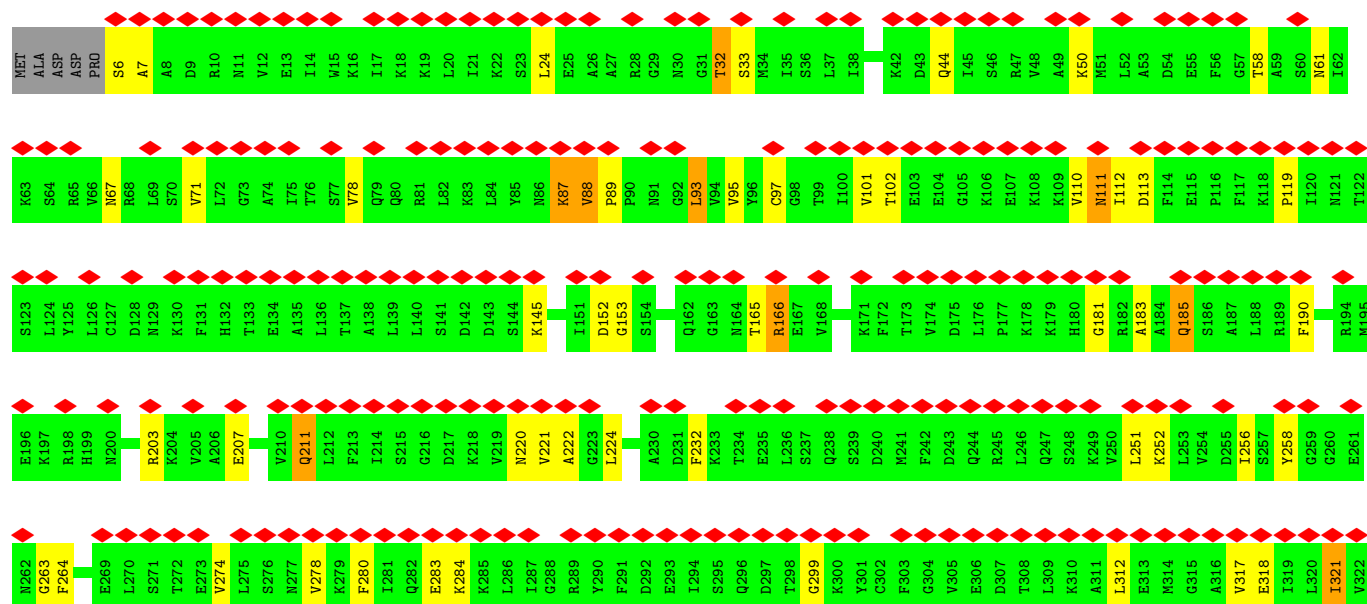
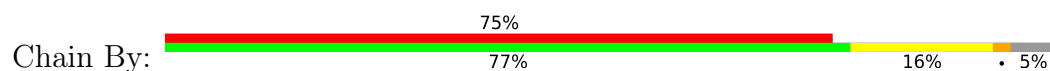


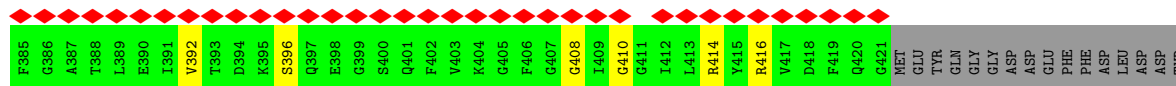
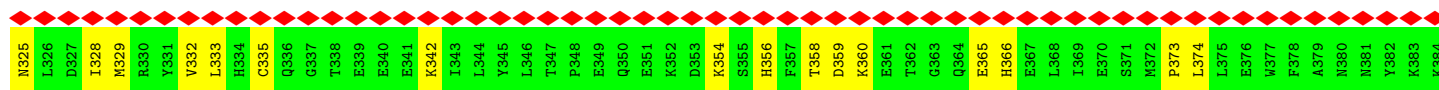


• Molecule 86: Ribosomal protein

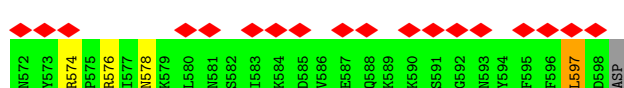
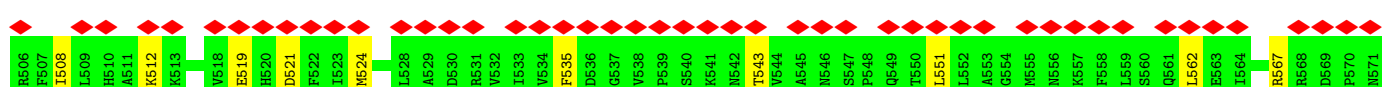
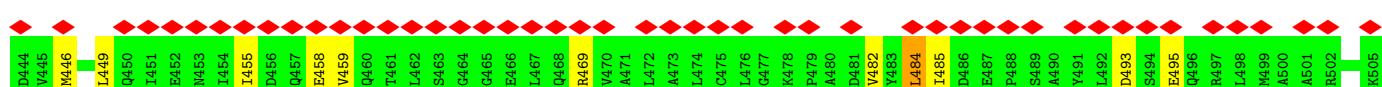
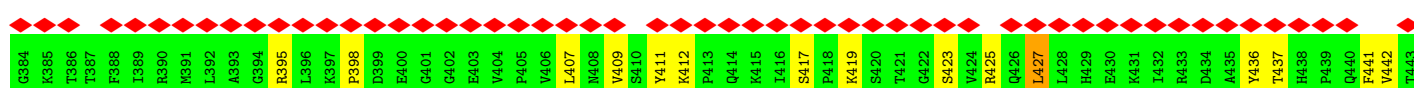
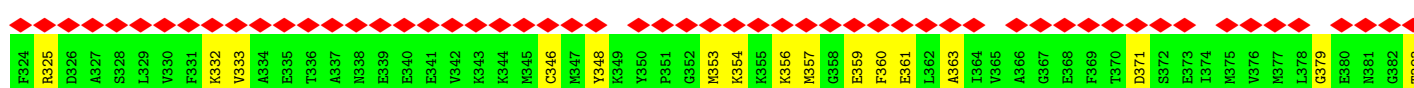
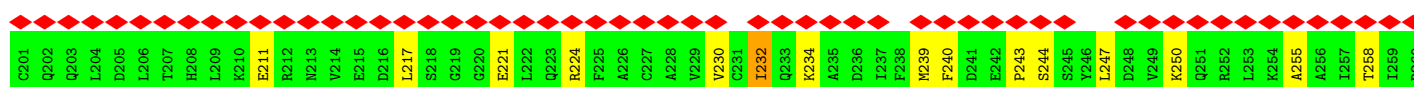
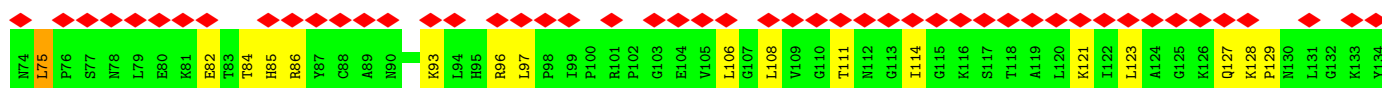
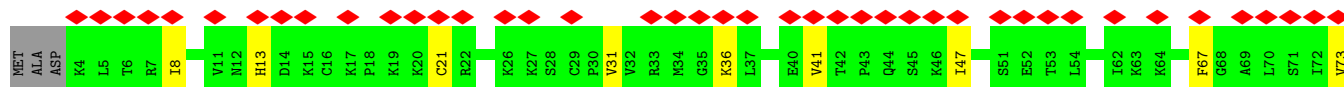
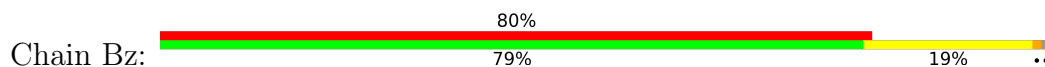


• Molecule 87: Eukaryotic peptide chain release factor subunit 1





• Molecule 88: ATP binding cassette subfamily E member 1



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 55057                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | 56604                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 4.379                                   | Depositor |
| Minimum map value                    | -1.818                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.131                                   | Depositor |
| Recommended contour level            | 0.7                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 593.6, 593.6, 593.6                     | wwPDB     |
| Map dimensions                       | 560, 560, 560                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HIC, PSU, AME, SPD, 5MC, OMC, NMM, MA6, UR3, 6MZ, GTP, SF4, SAC, A2M, M3L, UNX, HY3, G7M, 4AC, AAC, ZN, AYA, B8N, UY1, OMU, MG, 1MA, V5N, OMG, 5MU, MLZ

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   | A2    | 0.14         | 1/40342 (0.0%) | 0.14        | 0/62877 |
| 2   | AA    | 0.08         | 0/665          | 0.22        | 0/891   |
| 3   | AB    | 0.08         | 0/497          | 0.19        | 0/666   |
| 4   | AC    | 0.08         | 0/613          | 0.25        | 0/811   |
| 5   | AD    | 0.08         | 0/462          | 0.21        | 0/607   |
| 6   | AE    | 0.09         | 0/828          | 0.23        | 0/1109  |
| 7   | AF    | 0.08         | 0/2493         | 0.23        | 0/3394  |
| 8   | AG    | 0.08         | 0/470          | 0.22        | 0/623   |
| 9   | AH    | 0.06         | 0/566          | 0.11        | 0/879   |
| 10  | AI    | 0.09         | 0/68           | 0.17        | 0/103   |
| 11  | AT    | 0.07         | 0/2011         | 0.14        | 0/3133  |
| 12  | AZ    | 0.08         | 0/1771         | 0.21        | 0/2406  |
| 13  | Aa    | 0.08         | 0/1841         | 0.20        | 0/2459  |
| 14  | Ab    | 0.09         | 0/1742         | 0.23        | 0/2354  |
| 15  | Ac    | 0.08         | 0/1779         | 0.21        | 0/2395  |
| 16  | Ad    | 0.08         | 0/2118         | 0.22        | 0/2849  |
| 17  | Ae    | 0.08         | 0/1531         | 0.24        | 0/2059  |
| 18  | Af    | 0.08         | 0/1946         | 0.21        | 0/2590  |
| 19  | Ag    | 0.09         | 0/1552         | 0.23        | 0/2079  |
| 20  | Ah    | 0.08         | 0/1715         | 0.21        | 0/2287  |
| 21  | Ai    | 0.08         | 0/1550         | 0.21        | 0/2069  |
| 22  | Aj    | 0.08         | 0/834          | 0.25        | 0/1125  |
| 23  | Ak    | 0.09         | 0/1284         | 0.22        | 0/1717  |
| 24  | Al    | 0.08         | 0/968          | 0.22        | 0/1296  |
| 25  | Am    | 0.08         | 0/1232         | 0.21        | 0/1656  |
| 26  | An    | 0.09         | 0/1029         | 0.23        | 0/1380  |
| 27  | Ao    | 0.09         | 0/1114         | 0.20        | 0/1490  |
| 28  | Ap    | 0.09         | 0/1142         | 0.26        | 0/1528  |
| 29  | Aq    | 0.07         | 0/1094         | 0.20        | 0/1469  |
| 30  | Ar    | 0.07         | 0/1209         | 0.21        | 0/1620  |
| 31  | As    | 0.07         | 0/1119         | 0.18        | 0/1498  |



| Mol | Chain | Bond lengths |                | Bond angles |          |
|-----|-------|--------------|----------------|-------------|----------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5  |
| 32  | At    | 0.09         | 0/831          | 0.23        | 0/1115   |
| 33  | Au    | 0.08         | 0/636          | 0.21        | 0/852    |
| 34  | Av    | 0.10         | 0/1051         | 0.22        | 0/1406   |
| 35  | Aw    | 0.09         | 0/1107         | 0.22        | 0/1475   |
| 36  | Ax    | 0.07         | 0/1032         | 0.19        | 0/1371   |
| 37  | Ay    | 0.09         | 0/691          | 0.20        | 0/922    |
| 38  | Az    | 0.08         | 0/240          | 0.19        | 0/305    |
| 39  | B5    | 0.12         | 2/87403 (0.0%) | 0.15        | 0/136359 |
| 40  | B7    | 0.08         | 0/2835         | 0.12        | 0/4418   |
| 41  | B8    | 0.09         | 0/3635         | 0.13        | 0/5661   |
| 42  | BA    | 0.11         | 0/1965         | 0.25        | 0/2633   |
| 43  | BB    | 0.10         | 0/3261         | 0.23        | 0/4364   |
| 44  | BC    | 0.10         | 0/2932         | 0.22        | 0/3939   |
| 45  | BD    | 0.08         | 0/2437         | 0.20        | 0/3264   |
| 46  | BE    | 0.09         | 0/1998         | 0.23        | 0/2673   |
| 47  | BF    | 0.10         | 0/1922         | 0.24        | 0/2563   |
| 48  | BG    | 0.09         | 0/1908         | 0.21        | 0/2566   |
| 49  | BH    | 0.09         | 0/1535         | 0.22        | 0/2063   |
| 50  | BI    | 0.10         | 0/1756         | 0.23        | 0/2346   |
| 51  | BJ    | 0.08         | 0/1385         | 0.21        | 0/1852   |
| 52  | BK    | 0.11         | 0/277          | 0.27        | 0/372    |
| 53  | BL    | 0.10         | 0/1733         | 0.22        | 0/2316   |
| 54  | BM    | 0.09         | 0/1158         | 0.22        | 0/1547   |
| 55  | BN    | 0.10         | 0/1746         | 0.23        | 0/2338   |
| 56  | BO    | 0.09         | 0/1662         | 0.22        | 0/2222   |
| 57  | BP    | 0.10         | 0/1317         | 0.23        | 0/1768   |
| 58  | BQ    | 0.10         | 0/1539         | 0.24        | 0/2054   |
| 59  | BR    | 0.08         | 0/1524         | 0.19        | 0/2013   |
| 60  | BS    | 0.10         | 0/1497         | 0.22        | 0/2008   |
| 61  | BT    | 0.09         | 0/1326         | 0.20        | 0/1770   |
| 62  | BU    | 0.08         | 0/820          | 0.22        | 0/1100   |
| 63  | BV    | 0.10         | 0/1048         | 0.24        | 0/1402   |
| 64  | BW    | 0.08         | 0/1006         | 0.21        | 0/1334   |
| 65  | BX    | 0.08         | 0/984          | 0.21        | 0/1323   |
| 66  | BY    | 0.09         | 0/1132         | 0.24        | 0/1504   |
| 67  | BZ    | 0.08         | 0/1130         | 0.19        | 0/1507   |
| 68  | Ba    | 0.10         | 0/1179         | 0.25        | 0/1572   |
| 69  | Bb    | 0.09         | 0/884          | 0.22        | 0/1169   |
| 70  | Bc    | 0.08         | 0/847          | 0.20        | 0/1134   |
| 71  | Bd    | 0.10         | 0/903          | 0.21        | 0/1216   |
| 72  | Be    | 0.10         | 0/1088         | 0.25        | 0/1451   |
| 73  | Bf    | 0.11         | 0/903          | 0.24        | 0/1208   |
| 74  | Bg    | 0.09         | 0/916          | 0.25        | 0/1220   |

| Mol | Chain | Bond lengths |                 | Bond angles |          |
|-----|-------|--------------|-----------------|-------------|----------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5  |
| 75  | Bh    | 0.08         | 0/1021          | 0.18        | 0/1348   |
| 76  | Bi    | 0.08         | 0/841           | 0.23        | 0/1112   |
| 77  | Bj    | 0.11         | 0/720           | 0.27        | 0/952    |
| 78  | Bk    | 0.08         | 0/575           | 0.20        | 0/761    |
| 79  | Bl    | 0.09         | 0/459           | 0.21        | 0/608    |
| 80  | Bm    | 0.08         | 0/426           | 0.21        | 0/564    |
| 81  | Bo    | 0.09         | 0/866           | 0.20        | 0/1141   |
| 82  | Bp    | 0.10         | 0/718           | 0.24        | 0/953    |
| 83  | Br    | 0.09         | 0/1020          | 0.23        | 0/1366   |
| 84  | Bs    | 0.08         | 0/1530          | 0.22        | 0/2064   |
| 85  | Bt    | 0.09         | 0/1193          | 0.24        | 0/1609   |
| 86  | Bv    | 0.09         | 0/1735          | 0.25        | 0/2328   |
| 87  | By    | 0.09         | 0/3333          | 0.24        | 0/4483   |
| 88  | Bz    | 0.10         | 0/4755          | 0.26        | 0/6421   |
| All | All   | 0.11         | 3/243956 (0.0%) | 0.18        | 0/356824 |

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 |
|-----|-------|---------------------|---------------------|
| 81  | Bo    | 0                   | 1                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 39  | B5    | 4761 | U    | C4-O4 | 5.13 | 1.33        | 1.23     |
| 39  | B5    | 3456 | A2M  | O3'-P | 5.02 | 1.61        | 1.56     |
| 1   | A2    | 1032 | A2M  | O3'-P | 5.01 | 1.61        | 1.56     |

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 81  | Bo    | 53  | MLZ  | Mainchain |

## 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   | A2    | 37833 | 0        | 19168    | 335     | 0            |
| 2   | AA    | 651   | 0        | 672      | 9       | 0            |
| 3   | AB    | 495   | 0        | 523      | 5       | 0            |
| 4   | AC    | 601   | 0        | 621      | 6       | 0            |
| 5   | AD    | 457   | 0        | 502      | 7       | 0            |
| 6   | AE    | 814   | 0        | 863      | 9       | 0            |
| 7   | AF    | 2436  | 0        | 2393     | 38      | 0            |
| 8   | AG    | 459   | 0        | 448      | 11      | 0            |
| 9   | AH    | 508   | 0        | 255      | 4       | 0            |
| 10  | AI    | 939   | 0        | 618      | 5       | 0            |
| 11  | AT    | 1840  | 0        | 930      | 24      | 0            |
| 12  | AZ    | 1743  | 0        | 1748     | 31      | 0            |
| 13  | Aa    | 1815  | 0        | 1908     | 21      | 0            |
| 14  | Ab    | 1706  | 0        | 1796     | 19      | 0            |
| 15  | Ac    | 1751  | 0        | 1846     | 25      | 0            |
| 16  | Ad    | 2076  | 0        | 2177     | 31      | 0            |
| 17  | Ae    | 1509  | 0        | 1563     | 25      | 0            |
| 18  | Af    | 1923  | 0        | 2089     | 40      | 0            |
| 19  | Ag    | 1529  | 0        | 1627     | 23      | 0            |
| 20  | Ah    | 1686  | 0        | 1772     | 26      | 0            |
| 21  | Ai    | 1525  | 0        | 1640     | 24      | 0            |
| 22  | Aj    | 810   | 0        | 836      | 11      | 0            |
| 23  | Ak    | 1262  | 0        | 1335     | 11      | 0            |
| 24  | Al    | 958   | 0        | 993      | 15      | 0            |
| 25  | Am    | 1208  | 0        | 1294     | 17      | 0            |
| 26  | An    | 1016  | 0        | 1039     | 19      | 0            |
| 27  | Ao    | 1091  | 0        | 1138     | 12      | 0            |
| 28  | Ap    | 1124  | 0        | 1193     | 20      | 0            |
| 29  | Aq    | 1080  | 0        | 1135     | 16      | 0            |
| 30  | Ar    | 1200  | 0        | 1262     | 23      | 0            |
| 31  | As    | 1113  | 0        | 1145     | 17      | 0            |
| 32  | At    | 821   | 0        | 883      | 7       | 0            |
| 33  | Au    | 640   | 0        | 633      | 9       | 0            |
| 34  | Av    | 1034  | 0        | 1080     | 11      | 0            |
| 35  | Aw    | 1099  | 0        | 1162     | 13      | 0            |
| 36  | Ax    | 1015  | 0        | 1086     | 16      | 0            |
| 37  | Ay    | 683   | 0        | 761      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | Az    | 239   | 0        | 289      | 3       | 0            |
| 39  | B5    | 80772 | 0        | 40878    | 557     | 0            |
| 40  | B7    | 2538  | 0        | 1283     | 15      | 0            |
| 41  | B8    | 3319  | 0        | 1684     | 25      | 0            |
| 42  | BA    | 1940  | 0        | 2029     | 28      | 0            |
| 43  | BB    | 3206  | 0        | 3353     | 37      | 0            |
| 44  | BC    | 2886  | 0        | 3057     | 29      | 0            |
| 45  | BD    | 2398  | 0        | 2430     | 33      | 0            |
| 46  | BE    | 1960  | 0        | 2153     | 31      | 0            |
| 47  | BF    | 1886  | 0        | 2008     | 22      | 0            |
| 48  | BG    | 1877  | 0        | 2023     | 16      | 0            |
| 49  | BH    | 1516  | 0        | 1597     | 17      | 0            |
| 50  | BI    | 1717  | 0        | 1764     | 21      | 0            |
| 51  | BJ    | 1362  | 0        | 1399     | 20      | 0            |
| 52  | BK    | 273   | 0        | 265      | 5       | 0            |
| 53  | BL    | 1702  | 0        | 1820     | 22      | 0            |
| 54  | BM    | 1137  | 0        | 1211     | 12      | 0            |
| 55  | BN    | 1701  | 0        | 1749     | 31      | 0            |
| 56  | BO    | 1630  | 0        | 1778     | 18      | 0            |
| 57  | BP    | 1289  | 0        | 1329     | 16      | 0            |
| 58  | BQ    | 1515  | 0        | 1634     | 15      | 0            |
| 59  | BR    | 1508  | 0        | 1664     | 14      | 0            |
| 60  | BS    | 1457  | 0        | 1492     | 14      | 0            |
| 61  | BT    | 1298  | 0        | 1366     | 15      | 0            |
| 62  | BU    | 806   | 0        | 827      | 9       | 0            |
| 63  | BV    | 1034  | 0        | 1097     | 14      | 0            |
| 64  | BW    | 991   | 0        | 1048     | 17      | 0            |
| 65  | BX    | 967   | 0        | 1040     | 5       | 0            |
| 66  | BY    | 1115  | 0        | 1205     | 14      | 0            |
| 67  | BZ    | 1107  | 0        | 1182     | 15      | 0            |
| 68  | Ba    | 1163  | 0        | 1202     | 13      | 0            |
| 69  | Bb    | 881   | 0        | 957      | 9       | 0            |
| 70  | Bc    | 836   | 0        | 888      | 7       | 0            |
| 71  | Bd    | 888   | 0        | 930      | 9       | 0            |
| 72  | Be    | 1070  | 0        | 1165     | 17      | 0            |
| 73  | Bf    | 884   | 0        | 924      | 12      | 0            |
| 74  | Bg    | 906   | 0        | 998      | 6       | 0            |
| 75  | Bh    | 1013  | 0        | 1147     | 20      | 0            |
| 76  | Bi    | 830   | 0        | 916      | 3       | 0            |
| 77  | Bj    | 705   | 0        | 737      | 8       | 0            |
| 78  | Bk    | 569   | 0        | 637      | 6       | 0            |
| 79  | Bl    | 447   | 0        | 479      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 80  | Bm    | 432   | 0        | 470      | 8       | 0            |
| 81  | Bo    | 863   | 0        | 929      | 15      | 0            |
| 82  | Bp    | 708   | 0        | 756      | 13      | 0            |
| 83  | Br    | 1014  | 0        | 1083     | 11      | 0            |
| 84  | Bs    | 1507  | 0        | 1564     | 25      | 0            |
| 85  | Bt    | 1178  | 0        | 1235     | 24      | 0            |
| 86  | Bv    | 1707  | 0        | 1815     | 29      | 0            |
| 87  | By    | 3280  | 0        | 3326     | 45      | 0            |
| 88  | Bz    | 4668  | 0        | 4784     | 61      | 0            |
| 89  | A2    | 10    | 0        | 19       | 1       | 0            |
| 90  | A2    | 102   | 0        | 0        | 0       | 0            |
| 90  | AH    | 1     | 0        | 0        | 0       | 0            |
| 90  | AT    | 2     | 0        | 0        | 0       | 0            |
| 90  | B5    | 235   | 0        | 0        | 0       | 0            |
| 90  | B7    | 4     | 0        | 0        | 0       | 0            |
| 90  | B8    | 6     | 0        | 0        | 0       | 0            |
| 90  | BI    | 1     | 0        | 0        | 0       | 0            |
| 90  | BP    | 1     | 0        | 0        | 0       | 0            |
| 90  | BR    | 1     | 0        | 0        | 0       | 0            |
| 90  | BV    | 1     | 0        | 0        | 0       | 0            |
| 90  | Ba    | 1     | 0        | 0        | 0       | 0            |
| 91  | A2    | 76    | 0        | 0        | 0       | 0            |
| 91  | AT    | 4     | 0        | 0        | 0       | 0            |
| 91  | Ab    | 1     | 0        | 0        | 0       | 0            |
| 91  | Ak    | 1     | 0        | 0        | 0       | 0            |
| 91  | Ar    | 1     | 0        | 0        | 0       | 0            |
| 91  | B5    | 244   | 0        | 0        | 0       | 0            |
| 91  | B7    | 10    | 0        | 0        | 0       | 0            |
| 91  | B8    | 16    | 0        | 0        | 0       | 0            |
| 91  | BA    | 2     | 0        | 0        | 0       | 0            |
| 91  | BB    | 3     | 0        | 0        | 0       | 0            |
| 91  | BC    | 1     | 0        | 0        | 0       | 0            |
| 91  | BH    | 1     | 0        | 0        | 0       | 0            |
| 91  | BI    | 1     | 0        | 0        | 0       | 0            |
| 91  | BL    | 1     | 0        | 0        | 0       | 0            |
| 91  | BN    | 2     | 0        | 0        | 0       | 0            |
| 91  | BP    | 1     | 0        | 0        | 0       | 0            |
| 91  | BQ    | 2     | 0        | 0        | 0       | 0            |
| 91  | BT    | 1     | 0        | 0        | 0       | 0            |
| 91  | Bb    | 1     | 0        | 0        | 0       | 0            |
| 91  | Be    | 2     | 0        | 0        | 0       | 0            |
| 91  | Bf    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 91  | Bg    | 1     | 0        | 0        | 0       | 0            |
| 91  | Bo    | 1     | 0        | 0        | 0       | 0            |
| 92  | AC    | 1     | 0        | 0        | 0       | 0            |
| 92  | AE    | 1     | 0        | 0        | 0       | 0            |
| 92  | AG    | 1     | 0        | 0        | 0       | 0            |
| 92  | Bg    | 1     | 0        | 0        | 0       | 0            |
| 92  | Bj    | 1     | 0        | 0        | 0       | 0            |
| 92  | Bm    | 1     | 0        | 0        | 0       | 0            |
| 92  | Bo    | 1     | 0        | 0        | 0       | 0            |
| 92  | Bp    | 1     | 0        | 0        | 0       | 0            |
| 93  | B7    | 32    | 0        | 11       | 0       | 0            |
| 94  | Bz    | 16    | 0        | 0        | 0       | 0            |
| 95  | A2    | 473   | 0        | 0        | 8       | 0            |
| 95  | AH    | 10    | 0        | 0        | 0       | 0            |
| 95  | AT    | 12    | 0        | 0        | 1       | 0            |
| 95  | Aa    | 2     | 0        | 0        | 1       | 0            |
| 95  | Ab    | 1     | 0        | 0        | 0       | 0            |
| 95  | Ad    | 1     | 0        | 0        | 0       | 0            |
| 95  | Af    | 2     | 0        | 0        | 0       | 0            |
| 95  | Ak    | 1     | 0        | 0        | 0       | 0            |
| 95  | Am    | 1     | 0        | 0        | 0       | 0            |
| 95  | An    | 2     | 0        | 0        | 1       | 0            |
| 95  | Ap    | 4     | 0        | 0        | 1       | 0            |
| 95  | Ar    | 1     | 0        | 0        | 0       | 0            |
| 95  | As    | 4     | 0        | 0        | 0       | 0            |
| 95  | Aw    | 4     | 0        | 0        | 0       | 0            |
| 95  | B5    | 1117  | 0        | 0        | 17      | 0            |
| 95  | B7    | 17    | 0        | 0        | 0       | 0            |
| 95  | B8    | 31    | 0        | 0        | 0       | 0            |
| 95  | BA    | 5     | 0        | 0        | 0       | 0            |
| 95  | BB    | 7     | 0        | 0        | 0       | 0            |
| 95  | BC    | 3     | 0        | 0        | 1       | 0            |
| 95  | BD    | 1     | 0        | 0        | 0       | 0            |
| 95  | BF    | 1     | 0        | 0        | 0       | 0            |
| 95  | BH    | 1     | 0        | 0        | 0       | 0            |
| 95  | BI    | 1     | 0        | 0        | 0       | 0            |
| 95  | BL    | 1     | 0        | 0        | 0       | 0            |
| 95  | BN    | 2     | 0        | 0        | 0       | 0            |
| 95  | BO    | 3     | 0        | 0        | 0       | 0            |
| 95  | BP    | 3     | 0        | 0        | 0       | 0            |
| 95  | BR    | 5     | 0        | 0        | 1       | 0            |
| 95  | BV    | 4     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 95  | BX    | 1      | 0        | 0        | 0       | 0            |
| 95  | BY    | 1      | 0        | 0        | 0       | 0            |
| 95  | Ba    | 7      | 0        | 0        | 0       | 0            |
| 95  | Bb    | 1      | 0        | 0        | 0       | 0            |
| 95  | Bd    | 1      | 0        | 0        | 0       | 0            |
| 95  | Be    | 4      | 0        | 0        | 0       | 0            |
| 95  | Bf    | 1      | 0        | 0        | 1       | 0            |
| 95  | By    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 235677 | 0        | 175760   | 1886    | 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 5.

All (1886) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A2:1092:C:HO2'  | 34:Av:2:VAL:N      | 1.53                     | 1.06              |
| 41:B8:81:C:HO2'   | 75:Bh:2:ALA:N      | 1.77                     | 0.82              |
| 46:BE:227:LYS:HE2 | 46:BE:241:GLU:H    | 1.50                     | 0.77              |
| 87:By:318:GLU:HB2 | 87:By:414:ARG:HG3  | 1.68                     | 0.76              |
| 39:B5:3373:U:OP2  | 39:B5:3378:A:N6    | 2.19                     | 0.75              |
| 39:B5:4480:A:H61  | 39:B5:4704:U:H3    | 1.34                     | 0.75              |
| 49:BH:23:ARG:HE   | 49:BH:39:ASN:HA    | 1.51                     | 0.75              |
| 1:A2:1397:A:O2'   | 1:A2:1399:G:N7     | 2.20                     | 0.74              |
| 39:B5:3669:C:H1'  | 55:BN:125:SER:HB3  | 1.70                     | 0.74              |
| 7:AF:247:TRP:HB3  | 7:AF:258:ILE:HD11  | 1.69                     | 0.73              |
| 18:Af:161:PRO:HD3 | 64:BW:84:GLY:HA2   | 1.70                     | 0.73              |
| 1:A2:926:G:H1     | 1:A2:1018:U:H3     | 1.36                     | 0.72              |
| 39:B5:2106:A:OP1  | 83:Br:107:ARG:NH2  | 2.23                     | 0.72              |
| 39:B5:1415:C:H5'' | 58:BQ:144:LYS:HG2  | 1.72                     | 0.72              |
| 48:BG:58:PRO:HD2  | 48:BG:61:ILE:HD12  | 1.72                     | 0.72              |
| 87:By:252:LYS:HD2 | 87:By:274:VAL:HG21 | 1.72                     | 0.72              |
| 1:A2:869:G:OP2    | 1:A2:869:G:N2      | 2.22                     | 0.71              |
| 1:A2:929:G:H1     | 1:A2:1014:U:H3     | 1.37                     | 0.71              |
| 1:A2:1600:U:OP2   | 37:Ay:46:ASN:ND2   | 2.23                     | 0.71              |
| 1:A2:1605:G:P     | 95:A2:2103:HOH:O   | 2.46                     | 0.71              |
| 1:A2:1021:A:N7    | 25:Am:70:LYS:NZ    | 2.39                     | 0.70              |
| 19:Ag:143:ARG:HB2 | 19:Ag:155:LYS:HB2  | 1.73                     | 0.70              |
| 57:BP:126:ARG:HG3 | 57:BP:140:MET:HE1  | 1.73                     | 0.70              |
| 87:By:97:CYS:SG   | 87:By:111:ASN:ND2  | 2.65                     | 0.70              |
| 1:A2:1843:4AC:O7  | 38:Az:4:LYS:NZ     | 2.25                     | 0.69              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 71:Bd:64:ILE:HG23   | 71:Bd:68:LEU:HD23  | 1.74                     | 0.69              |
| 39:B5:1394:U:HO2'   | 47:BF:33:ARG:HE    | 1.40                     | 0.69              |
| 39:B5:3519:G:C8     | 95:B5:5434:HOH:O   | 2.44                     | 0.69              |
| 1:A2:1392:OMC:HM22  | 1:A2:1393:U:H5'    | 1.75                     | 0.69              |
| 39:B5:3555:G:N2     | 39:B5:3555:G:OP2   | 2.26                     | 0.69              |
| 39:B5:375:G:OP2     | 77:Bj:52:LYS:NZ    | 2.25                     | 0.69              |
| 19:Ag:34:SER:HA     | 19:Ag:37:LYS:HB2   | 1.74                     | 0.68              |
| 39:B5:4292:A:N7     | 42:BA:215:ASN:ND2  | 2.42                     | 0.68              |
| 1:A2:1131:G:N2      | 1:A2:1131:G:OP2    | 2.24                     | 0.68              |
| 39:B5:2143:A:N7     | 44:BC:143:ARG:NH1  | 2.40                     | 0.68              |
| 1:A2:1289:OMU:HN3   | 1:A2:1312:C:H42    | 1.40                     | 0.68              |
| 64:BW:81:ALA:HB2    | 64:BW:87:LEU:HB2   | 1.76                     | 0.67              |
| 1:A2:862:A:O2'      | 1:A2:863:A:N7      | 2.26                     | 0.67              |
| 13:Aa:28:LYS:HB3    | 13:Aa:48:LEU:HD11  | 1.74                     | 0.67              |
| 12:AZ:94:THR:HG23   | 12:AZ:186:ARG:HH12 | 1.59                     | 0.67              |
| 39:B5:2444:A:N6     | 39:B5:2587:A:OP2   | 2.27                     | 0.67              |
| 39:B5:4287:G:N2     | 39:B5:4290:A:OP2   | 2.27                     | 0.67              |
| 54:BM:40:GLY:HA3    | 54:BM:45:VAL:HB    | 1.77                     | 0.66              |
| 1:A2:1355:G:N2      | 1:A2:1358:A:OP2    | 2.24                     | 0.66              |
| 88:Bz:250:LYS:HB2   | 88:Bz:562:LEU:HD22 | 1.78                     | 0.66              |
| 1:A2:1491:OMG:HM22  | 1:A2:1492:G:H5'    | 1.76                     | 0.66              |
| 21:Ai:170:PRO:HB3   | 21:Ai:174:LYS:HE3  | 1.77                     | 0.66              |
| 39:B5:2302:G:N2     | 39:B5:2305:C:OP2   | 2.28                     | 0.66              |
| 84:Bs:28:PHE:HB2    | 84:Bs:89:VAL:HB    | 1.76                     | 0.66              |
| 39:B5:4004:C:OP2    | 51:BJ:54:ARG:NH1   | 2.28                     | 0.66              |
| 1:A2:577:A2M:HM'2   | 1:A2:578:U:H5'     | 1.77                     | 0.66              |
| 39:B5:2103:C:O2     | 83:Br:99:LYS:NZ    | 2.25                     | 0.66              |
| 39:B5:186:G:N2      | 39:B5:186:G:OP2    | 2.28                     | 0.66              |
| 7:AF:87:LEU:HB2     | 7:AF:101:PHE:HB2   | 1.78                     | 0.66              |
| 39:B5:2704:OMC:HM22 | 39:B5:2705:G:H5'   | 1.78                     | 0.65              |
| 39:B5:308:G:N2      | 39:B5:308:G:OP2    | 2.28                     | 0.65              |
| 63:BV:13:LYS:HB3    | 63:BV:128:LEU:HD11 | 1.77                     | 0.65              |
| 49:BH:113:GLU:HG2   | 49:BH:125:ARG:HG2  | 1.77                     | 0.65              |
| 24:Al:89:VAL:HG11   | 24:Al:109:VAL:HG11 | 1.79                     | 0.65              |
| 39:B5:1879:G:N2     | 39:B5:4180:C:OP1   | 2.29                     | 0.65              |
| 39:B5:4627:C:O2     | 39:B5:4670:G:N2    | 2.28                     | 0.65              |
| 1:A2:1285:A:H2'     | 24:Al:91:LEU:HD21  | 1.79                     | 0.65              |
| 1:A2:1551:G:H3'     | 1:A2:1580:A:H61    | 1.62                     | 0.65              |
| 39:B5:1260:OMG:HM22 | 39:B5:1261:U:H5'   | 1.79                     | 0.65              |
| 39:B5:3540:OMC:HM22 | 39:B5:3541:G:H5'   | 1.77                     | 0.65              |
| 39:B5:4679:C:OP1    | 46:BE:159:ARG:NH1  | 2.30                     | 0.65              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 58:BQ:119:LYS:HE3   | 58:BQ:121:LEU:HD21 | 1.79                     | 0.65              |
| 1:A2:513:A2M:HM'2   | 1:A2:514:G:H5'     | 1.79                     | 0.65              |
| 50:BI:53:VAL:HG11   | 61:BT:158:PHE:HZ   | 1.62                     | 0.65              |
| 86:Bv:74:CYS:SG     | 86:Bv:78:LYS:NZ    | 2.69                     | 0.65              |
| 68:Ba:72:THR:HG22   | 68:Ba:110:LYS:HB3  | 1.79                     | 0.64              |
| 1:A2:1598:C:OP2     | 37:Ay:85:ARG:NH2   | 2.31                     | 0.64              |
| 26:An:34:PHE:HB3    | 26:An:41:PHE:HB2   | 1.79                     | 0.64              |
| 39:B5:1810:A2M:HM'2 | 39:B5:1811:G:H5'   | 1.78                     | 0.64              |
| 42:BA:27:ALA:O      | 42:BA:128:ARG:NH1  | 2.30                     | 0.64              |
| 27:Ao:18:ARG:NH1    | 30:Ar:88:LYS:O     | 2.31                     | 0.64              |
| 39:B5:870:G:OP1     | 39:B5:2102:G:N2    | 2.30                     | 0.64              |
| 45:BD:83:LEU:HB3    | 45:BD:88:VAL:HB    | 1.80                     | 0.64              |
| 57:BP:138:PRO:HB3   | 57:BP:140:MET:HE3  | 1.79                     | 0.64              |
| 88:Bz:409:VAL:HG12  | 88:Bz:482:VAL:HB   | 1.80                     | 0.64              |
| 11:AT:10:G:O6       | 11:AT:45:G:N2      | 2.31                     | 0.64              |
| 39:B5:1227:G:N1     | 39:B5:2015:G:OP1   | 2.30                     | 0.64              |
| 39:B5:2161:G:N2     | 39:B5:2164:G:OP2   | 2.28                     | 0.64              |
| 85:Bt:38:SER:HB3    | 85:Bt:41:LYS:HG2   | 1.80                     | 0.64              |
| 28:Ap:132:PHE:O     | 28:Ap:140:ARG:NH2  | 2.29                     | 0.64              |
| 39:B5:4416:C:O2'    | 39:B5:4418:A:OP2   | 2.15                     | 0.63              |
| 39:B5:1391:C:O2'    | 69:Bb:106:ARG:NH2  | 2.31                     | 0.63              |
| 39:B5:4271:C:OP1    | 43:BB:246:ARG:NH1  | 2.31                     | 0.63              |
| 1:A2:437:OMG:HM22   | 1:A2:438:G:H5'     | 1.81                     | 0.63              |
| 1:A2:1143:G:OP1     | 14:Ab:187:ARG:NH1  | 2.31                     | 0.63              |
| 1:A2:1390:C:OP1     | 29:Aq:43:SER:OG    | 2.16                     | 0.63              |
| 1:A2:1416:C:O2'     | 31:As:132:ASP:OD2  | 2.17                     | 0.63              |
| 63:BV:69:LYS:HG2    | 63:BV:71:GLU:HG2   | 1.80                     | 0.63              |
| 25:Am:136:PRO:HG2   | 25:Am:139:TRP:HB2  | 1.79                     | 0.63              |
| 39:B5:3456:A2M:HM'2 | 39:B5:3457:G:H5'   | 1.81                     | 0.63              |
| 56:BO:81:TRP:HB2    | 56:BO:104:VAL:HG21 | 1.81                     | 0.63              |
| 62:BU:100:LEU:HD13  | 62:BU:112:LEU:HD23 | 1.80                     | 0.63              |
| 19:Ag:58:LYS:HB2    | 19:Ag:90:LYS:HG2   | 1.81                     | 0.63              |
| 20:Ah:101:ILE:HD12  | 20:Ah:190:LEU:HD11 | 1.81                     | 0.63              |
| 81:Bo:34:TYR:O      | 81:Bo:39:ARG:NH1   | 2.31                     | 0.63              |
| 39:B5:4018:G:OP2    | 39:B5:4018:G:N2    | 2.28                     | 0.62              |
| 39:B5:2194:OMC:HM22 | 39:B5:2195:U:H5'   | 1.80                     | 0.62              |
| 73:Bf:43:LEU:O      | 73:Bf:109:ARG:NH1  | 2.32                     | 0.62              |
| 88:Bz:310:ASN:OD1   | 88:Bz:574:ARG:NH1  | 2.31                     | 0.62              |
| 1:A2:1522:C:OP2     | 30:Ar:136:THR:OG1  | 2.16                     | 0.62              |
| 39:B5:1133:C:O2     | 39:B5:1207:G:N2    | 2.27                     | 0.62              |
| 39:B5:1879:G:H22    | 39:B5:4180:C:H5''  | 1.64                     | 0.62              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:B5:4269:A2M:H5'' | 39:B5:4270:G:H5'   | 1.79                     | 0.62              |
| 46:BE:115:MET:O     | 83:Br:87:ARG:NH1   | 2.32                     | 0.62              |
| 39:B5:1399:G:OP2    | 39:B5:1399:G:N2    | 2.25                     | 0.62              |
| 39:B5:3805:A:N1     | 39:B5:3917:C:N4    | 2.47                     | 0.62              |
| 60:BS:15:ARG:HB3    | 60:BS:27:LEU:HD23  | 1.80                     | 0.62              |
| 88:Bz:383:THR:HA    | 88:Bz:543:THR:HG21 | 1.81                     | 0.62              |
| 39:B5:2250:G:OP2    | 39:B5:2250:G:N2    | 2.33                     | 0.62              |
| 88:Bz:111:THR:H     | 88:Bz:114:ILE:HD12 | 1.64                     | 0.62              |
| 1:A2:985:C:O2'      | 26:An:138:ASP:OD2  | 2.16                     | 0.62              |
| 1:A2:1148:C:OP1     | 6:AE:6:ARG:NH1     | 2.32                     | 0.62              |
| 11:AT:8:U:H4'       | 11:AT:58:C:H4'     | 1.81                     | 0.62              |
| 39:B5:4194:G:H5''   | 39:B5:4195:A:H5''  | 1.80                     | 0.62              |
| 1:A2:1852:MA6:H102  | 1:A2:1853:C:O2'    | 1.99                     | 0.62              |
| 41:B8:71:A:N1       | 41:B8:84:A:O2'     | 2.30                     | 0.62              |
| 1:A2:1864:A:OP2     | 6:AE:4:LYS:NZ      | 2.33                     | 0.62              |
| 11:AT:27:U:OP1      | 87:By:50:LYS:NZ    | 2.25                     | 0.62              |
| 7:AF:244:ASN:ND2    | 7:AF:294:ASP:O     | 2.33                     | 0.62              |
| 20:Ah:67:TRP:NE1    | 20:Ah:191:GLU:OE2  | 2.29                     | 0.62              |
| 8:AG:22:ARG:HH11    | 15:Ac:16:ILE:HG21  | 1.65                     | 0.61              |
| 39:B5:4218:G:O2'    | 80:Bm:100:TYR:O    | 2.18                     | 0.61              |
| 44:BC:327:LYS:NZ    | 47:BF:169:THR:O    | 2.33                     | 0.61              |
| 27:Ao:128:HIS:O     | 27:Ao:130:ARG:NH1  | 2.33                     | 0.61              |
| 79:Bl:30:LYS:HB2    | 79:Bl:33:ASN:HB2   | 1.81                     | 0.61              |
| 39:B5:3449:A:OP2    | 39:B5:3467:G:N2    | 2.27                     | 0.61              |
| 39:B5:4361:C:H5''   | 43:BB:357:ARG:HE   | 1.65                     | 0.61              |
| 1:A2:1014:U:OP1     | 1:A2:1130:G:O2'    | 2.19                     | 0.61              |
| 7:AF:133:ASN:HB3    | 7:AF:139:LYS:HE3   | 1.83                     | 0.61              |
| 39:B5:4666:G:N2     | 39:B5:4666:G:OP2   | 2.33                     | 0.61              |
| 1:A2:99:A2M:HM'2    | 1:A2:100:U:H5'     | 1.83                     | 0.61              |
| 7:AF:11:LEU:HB2     | 7:AF:307:VAL:HB    | 1.83                     | 0.61              |
| 11:AT:11:C:H42      | 11:AT:24:G:H1      | 1.49                     | 0.61              |
| 21:Ai:120:ALA:O     | 21:Ai:125:HIS:ND1  | 2.33                     | 0.61              |
| 21:Ai:138:ARG:NH1   | 21:Ai:153:SER:OG   | 2.33                     | 0.61              |
| 1:A2:165:G:N2       | 1:A2:165:G:OP2     | 2.29                     | 0.61              |
| 11:AT:12:C:OP2      | 95:AT:201:HOH:O    | 2.16                     | 0.61              |
| 52:BK:4370:CYS:HB2  | 52:BK:4377:LYS:HG2 | 1.83                     | 0.61              |
| 86:Bv:94:ASN:O      | 86:Bv:97:LYS:NZ    | 2.30                     | 0.61              |
| 86:Bv:36:ILE:HD11   | 86:Bv:165:LEU:HD12 | 1.83                     | 0.61              |
| 39:B5:3420:U:OP2    | 42:BA:198:ARG:NH2  | 2.34                     | 0.61              |
| 84:Bs:45:MET:SD     | 84:Bs:48:ARG:NH2   | 2.73                     | 0.61              |
| 1:A2:496:U:OP1      | 16:Ad:49:ARG:NH1   | 2.34                     | 0.61              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:A2:1348:PSU:OP1   | 14:Ab:121:ARG:NH1  | 2.34                     | 0.61              |
| 40:B7:105:C:OP2     | 50:BI:203:ARG:NH1  | 2.33                     | 0.61              |
| 1:A2:1486:U:OP1     | 15:Ac:151:LYS:NZ   | 2.33                     | 0.60              |
| 7:AF:120:ILE:HB     | 7:AF:132:TRP:HB2   | 1.83                     | 0.60              |
| 39:B5:1299:G:OP1    | 58:BQ:108:ARG:NH2  | 2.33                     | 0.60              |
| 88:Bz:357:MET:HB3   | 88:Bz:360:PHE:HB3  | 1.83                     | 0.60              |
| 9:AH:3466:U:H4'     | 87:By:58:THR:HG23  | 1.82                     | 0.60              |
| 10:AI:32:N:O2'      | 17:Ae:136:ARG:NH1  | 2.34                     | 0.60              |
| 30:Ar:34:LYS:HB3    | 30:Ar:100:ALA:HA   | 1.82                     | 0.60              |
| 39:B5:2205:U:H2'    | 39:B5:2206:A2M:H8  | 1.82                     | 0.60              |
| 15:Ac:42:THR:OG1    | 15:Ac:45:ARG:O     | 2.15                     | 0.60              |
| 20:Ah:56:ARG:NH1    | 20:Ah:180:GLY:O    | 2.35                     | 0.60              |
| 39:B5:4364:OMG:H5'' | 63:BV:15:ARG:HB2   | 1.81                     | 0.60              |
| 86:Bv:67:VAL:HG12   | 86:Bv:84:HIS:HD2   | 1.67                     | 0.60              |
| 39:B5:1901:A:OP1    | 84:Bs:57:LYS:NZ    | 2.28                     | 0.60              |
| 40:B7:27:G:OP1      | 51:BJ:146:ARG:NH2  | 2.32                     | 0.60              |
| 60:BS:173:ASN:ND2   | 60:BS:175:PHE:O    | 2.32                     | 0.60              |
| 87:By:328:ILE:HB    | 87:By:374:LEU:HD22 | 1.84                     | 0.60              |
| 63:BV:69:LYS:NZ     | 63:BV:71:GLU:OE2   | 2.33                     | 0.60              |
| 12:AZ:77:ILE:HG13   | 12:AZ:99:ILE:HB    | 1.82                     | 0.60              |
| 17:Ae:47:LYS:NZ     | 28:Ap:115:TYR:O    | 2.35                     | 0.60              |
| 39:B5:1394:U:O2'    | 47:BF:33:ARG:NE    | 2.26                     | 0.60              |
| 39:B5:483:G:O2'     | 39:B5:486:C:OP2    | 2.19                     | 0.60              |
| 39:B5:1546:U:OP2    | 39:B5:2699:C:O2'   | 2.19                     | 0.60              |
| 47:BF:104:VAL:HG13  | 47:BF:135:VAL:HG12 | 1.82                     | 0.60              |
| 86:Bv:204:LEU:HD22  | 86:Bv:216:LEU:HD23 | 1.84                     | 0.60              |
| 1:A2:1704:OMC:HM22  | 1:A2:1705:C:H5'    | 1.83                     | 0.60              |
| 39:B5:369:G:N2      | 39:B5:372:A:OP2    | 2.31                     | 0.60              |
| 39:B5:1942:G:N2     | 39:B5:1943:U:O4    | 2.32                     | 0.60              |
| 39:B5:2548:G:O6     | 59:BR:46:LYS:NZ    | 2.26                     | 0.60              |
| 86:Bv:35:GLN:HB2    | 86:Bv:205:TYR:HB2  | 1.84                     | 0.60              |
| 11:AT:13:G:H21      | 11:AT:22:A:H62     | 1.47                     | 0.59              |
| 24:Al:91:LEU:HD22   | 24:Al:106:CYS:HB2  | 1.84                     | 0.59              |
| 39:B5:2422:G:N2     | 39:B5:2425:A:OP2   | 2.28                     | 0.59              |
| 39:B5:4366:OMU:HM22 | 39:B5:4367:C:H5'   | 1.83                     | 0.59              |
| 1:A2:165:G:H2'      | 1:A2:166:A2M:H8    | 1.84                     | 0.59              |
| 1:A2:642:A:OP1      | 21:Ai:40:LYS:NZ    | 2.35                     | 0.59              |
| 1:A2:1311:U:H5''    | 4:AC:130:VAL:HG13  | 1.84                     | 0.59              |
| 30:Ar:36:VAL:HG21   | 30:Ar:71:MET:HE3   | 1.84                     | 0.59              |
| 39:B5:1551:U:O2'    | 57:BP:135:ARG:NH1  | 2.30                     | 0.59              |
| 39:B5:1631:C:OP2    | 95:B5:5407:HOH:O   | 2.16                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:BL:130:LYS:HE2   | 53:BL:132:SER:HB2   | 1.83                     | 0.59              |
| 1:A2:953:G:OP1      | 13:Aa:56:LYS:NZ     | 2.34                     | 0.59              |
| 7:AF:77:PHE:HB3     | 7:AF:89:LEU:HD11    | 1.84                     | 0.59              |
| 18:Af:129:VAL:O     | 64:BW:80:ARG:NH2    | 2.34                     | 0.59              |
| 39:B5:4336:A2M:HM'2 | 39:B5:4337:U:H5'    | 1.83                     | 0.59              |
| 29:Aq:94:GLU:HG2    | 29:Aq:95:ILE:HG13   | 1.84                     | 0.59              |
| 39:B5:4299:A:N7     | 95:B5:5467:HOH:O    | 2.31                     | 0.59              |
| 57:BP:118:GLN:NE2   | 57:BP:147:GLU:OE2   | 2.36                     | 0.59              |
| 88:Bz:169:LYS:HB3   | 88:Bz:230:VAL:HG21  | 1.83                     | 0.59              |
| 33:Au:43:THR:OG1    | 33:Au:45:ARG:NH1    | 2.35                     | 0.59              |
| 39:B5:3619:OMC:HM22 | 39:B5:3620:G:H5'    | 1.84                     | 0.59              |
| 50:BI:87:ILE:HG12   | 50:BI:138:ILE:HG12  | 1.84                     | 0.59              |
| 63:BV:50:ASN:ND2    | 95:BV:301:HOH:O     | 2.35                     | 0.59              |
| 1:A2:905:A:O2'      | 23:Ak:48:LYS:NZ     | 2.33                     | 0.59              |
| 1:A2:1264:U:O2      | 8:AG:16:GLN:NE2     | 2.36                     | 0.59              |
| 1:A2:1529:G:O2'     | 1:A2:1667:C:OP1     | 2.20                     | 0.59              |
| 39:B5:1924:G:H1'    | 39:B5:1942:G:H2'    | 1.84                     | 0.59              |
| 39:B5:2499:U:H5''   | 67:BZ:38:TYR:HB3    | 1.83                     | 0.59              |
| 1:A2:1663:U:O4      | 1:A2:1664:A:N6      | 2.35                     | 0.59              |
| 19:Ag:162:GLN:OE1   | 19:Ag:165:ASN:ND2   | 2.35                     | 0.59              |
| 20:Ah:130:THR:OG1   | 20:Ah:132:GLU:OE1   | 2.21                     | 0.59              |
| 39:B5:3688:G:N2     | 39:B5:3785:C:O2     | 2.36                     | 0.59              |
| 42:BA:36:GLU:OE1    | 42:BA:163:ARG:NH1   | 2.36                     | 0.59              |
| 12:AZ:177:MET:SD    | 12:AZ:180:ARG:NH2   | 2.76                     | 0.59              |
| 17:Ae:71:ARG:NH2    | 17:Ae:148:ASN:OD1   | 2.36                     | 0.59              |
| 18:Af:144:LEU:O     | 64:BW:94:ARG:NH1    | 2.35                     | 0.59              |
| 39:B5:1694:C:O2     | 45:BD:3:PHE:N       | 2.36                     | 0.59              |
| 39:B5:4202:OMC:HM22 | 39:B5:4203:PSU:H5'' | 1.85                     | 0.59              |
| 28:Ap:58:LEU:HB3    | 28:Ap:62:ARG:HD2    | 1.85                     | 0.59              |
| 39:B5:788:G:H2'     | 39:B5:789:G:H8      | 1.66                     | 0.59              |
| 1:A2:1679:A2M:OP2   | 17:Ae:63:LYS:NZ     | 2.35                     | 0.59              |
| 29:Aq:77:GLU:OE2    | 29:Aq:81:ARG:NH2    | 2.35                     | 0.59              |
| 39:B5:3494:PSU:O2'  | 87:By:166:ARG:NH1   | 2.33                     | 0.59              |
| 11:AT:68:A:O2'      | 11:AT:70:C:OP2      | 2.18                     | 0.58              |
| 31:As:104:LEU:HD13  | 31:As:121:ARG:HD3   | 1.84                     | 0.58              |
| 88:Bz:187:ILE:HD11  | 88:Bz:191:LYS:HE3   | 1.85                     | 0.58              |
| 32:At:19:ARG:HB2    | 32:At:117:ALA:HB3   | 1.86                     | 0.58              |
| 33:Au:15:ARG:NH1    | 33:Au:33:GLN:OE1    | 2.36                     | 0.58              |
| 39:B5:734:G:OP2     | 54:BM:71:LYS:NZ     | 2.36                     | 0.58              |
| 62:BU:111:GLU:OE2   | 62:BU:113:ARG:NE    | 2.33                     | 0.58              |
| 2:AA:84:HIS:OXT     | 25:Am:19:ARG:NH1    | 2.36                     | 0.58              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 24:Al:25:ALA:O      | 24:Al:30:GLY:N     | 2.36                     | 0.58              |
| 39:B5:2167:C:O2'    | 72:Be:98:GLU:OE1   | 2.21                     | 0.58              |
| 1:A2:411:G:N7       | 95:A2:2129:HOH:O   | 2.32                     | 0.58              |
| 39:B5:3541:G:OP2    | 39:B5:3541:G:N2    | 2.33                     | 0.58              |
| 39:B5:4610:C:N4     | 60:BS:171:ARG:O    | 2.35                     | 0.58              |
| 62:BU:48:LYS:HG2    | 62:BU:53:ALA:HB2   | 1.86                     | 0.58              |
| 1:A2:71:G:O6        | 18:Af:170:ARG:NH1  | 2.37                     | 0.58              |
| 1:A2:116:OMU:HM22   | 1:A2:117:C:H5'     | 1.86                     | 0.58              |
| 39:B5:1789:A:OP2    | 53:BL:5:ARG:NH2    | 2.35                     | 0.58              |
| 39:B5:1855:G:P      | 95:B5:5401:HOH:O   | 2.58                     | 0.58              |
| 2:AA:23:ARG:HH22    | 2:AA:29:ASN:HD21   | 1.50                     | 0.58              |
| 26:An:92:ALA:HA     | 26:An:125:LYS:HB2  | 1.85                     | 0.58              |
| 39:B5:1297:G:N7     | 58:BQ:104:ARG:NH2  | 2.47                     | 0.58              |
| 40:B7:6:C:H4'       | 45:BD:52:ILE:HD13  | 1.85                     | 0.58              |
| 41:B8:102:G:OP1     | 77:Bj:20:ARG:NH1   | 2.36                     | 0.58              |
| 50:BI:110:ARG:NH1   | 50:BI:113:THR:OG1  | 2.36                     | 0.58              |
| 17:Ae:129:GLY:HA3   | 17:Ae:135:ARG:HH22 | 1.68                     | 0.58              |
| 23:Ak:147:LYS:HD2   | 23:Ak:151:THR:HG21 | 1.84                     | 0.58              |
| 29:Aq:57:LEU:HD13   | 29:Aq:69:ILE:HD11  | 1.86                     | 0.58              |
| 39:B5:74:G:H5''     | 53:BL:59:VAL:HB    | 1.86                     | 0.58              |
| 39:B5:1588:G:O6     | 39:B5:3650:G:O2'   | 2.20                     | 0.58              |
| 39:B5:1631:C:H41    | 39:B5:4124:A:H5''  | 1.69                     | 0.58              |
| 46:BE:181:PRO:HD2   | 46:BE:184:LEU:HD12 | 1.86                     | 0.58              |
| 85:Bt:57:ARG:H      | 85:Bt:57:ARG:HD2   | 1.69                     | 0.58              |
| 86:Bv:21:ASN:HB2    | 86:Bv:26:ARG:HD3   | 1.85                     | 0.58              |
| 9:AH:3466:U:O4'     | 87:By:61:ASN:ND2   | 2.37                     | 0.57              |
| 56:BO:10:ASP:OD2    | 56:BO:37:ARG:NH2   | 2.36                     | 0.57              |
| 88:Bz:356:LYS:HD2   | 88:Bz:361:GLU:HG3  | 1.86                     | 0.57              |
| 21:Ai:134:HIS:ND1   | 21:Ai:163:SER:OG   | 2.37                     | 0.57              |
| 39:B5:3386:G:O2'    | 39:B5:3425:U:OP1   | 2.22                     | 0.57              |
| 39:B5:4416:C:O2'    | 63:BV:15:ARG:NH2   | 2.38                     | 0.57              |
| 39:B5:4744:G:N2     | 39:B5:4780:G:O2'   | 2.36                     | 0.57              |
| 55:BN:53:TYR:HB2    | 55:BN:133:ILE:HD13 | 1.86                     | 0.57              |
| 39:B5:992:C:OP1     | 39:B5:1106:U:O2'   | 2.22                     | 0.57              |
| 39:B5:1937:A:N3     | 39:B5:1958:C:O2'   | 2.36                     | 0.57              |
| 39:B5:2652:G:O2'    | 39:B5:4390:G:OP1   | 2.21                     | 0.57              |
| 39:B5:3557:A2M:HM'2 | 39:B5:3558:C:H5'   | 1.86                     | 0.57              |
| 39:B5:3930:G:H5'    | 42:BA:233:ARG:HB2  | 1.86                     | 0.57              |
| 64:BW:2:LYS:NZ      | 64:BW:4:GLU:OE2    | 2.37                     | 0.57              |
| 67:BZ:25:ILE:HA     | 67:BZ:43:VAL:HG12  | 1.85                     | 0.57              |
| 78:Bk:13:LEU:HD23   | 78:Bk:16:ARG:HH21  | 1.68                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:B5:4335:A:N1    | 39:B5:4367:C:O2'   | 2.37                     | 0.57              |
| 54:BM:29:ASP:OD1   | 54:BM:30:VAL:N     | 2.34                     | 0.57              |
| 1:A2:1594:C:H1'    | 31:As:12:GLN:HE22  | 1.69                     | 0.57              |
| 53:BL:174:LYS:NZ   | 68:Ba:141:GLY:O    | 2.38                     | 0.57              |
| 1:A2:191:A:H62     | 1:A2:208:G:H21     | 1.52                     | 0.57              |
| 1:A2:1569:C:OP1    | 31:As:96:SER:OG    | 2.23                     | 0.57              |
| 21:Ai:170:PRO:O    | 21:Ai:175:ARG:NH1  | 2.36                     | 0.57              |
| 88:Bz:449:LEU:O    | 88:Bz:469:ARG:NH1  | 2.37                     | 0.57              |
| 88:Bz:567:ARG:NH1  | 88:Bz:578:ASN:OD1  | 2.38                     | 0.57              |
| 24:Al:11:VAL:HG13  | 24:Al:13:ASP:H     | 1.70                     | 0.57              |
| 39:B5:1334:G:N2    | 39:B5:1337:G:OP2   | 2.30                     | 0.57              |
| 88:Bz:84:THR:HG21  | 88:Bz:97:LEU:HG    | 1.87                     | 0.57              |
| 2:AA:15:GLU:O      | 2:AA:23:ARG:NE     | 2.33                     | 0.57              |
| 14:Ab:196:ILE:HB   | 14:Ab:223:TYR:HB2  | 1.87                     | 0.57              |
| 57:BP:8:PRO:HG3    | 57:BP:149:ILE:HD13 | 1.85                     | 0.57              |
| 59:BR:44:LEU:HD22  | 59:BR:49:LEU:HD12  | 1.86                     | 0.57              |
| 87:By:299:GLY:HA3  | 87:By:416:ARG:HG3  | 1.86                     | 0.57              |
| 2:AA:11:SER:OG     | 2:AA:14:GLU:OE1    | 2.22                     | 0.57              |
| 12:AZ:63:ARG:HH21  | 33:Au:38:GLU:HA    | 1.70                     | 0.57              |
| 39:B5:1726:A:N3    | 39:B5:3956:U:O2'   | 2.37                     | 0.57              |
| 60:BS:1:MET:HE3    | 60:BS:35:PRO:HD3   | 1.85                     | 0.57              |
| 81:Bo:59:LYS:NZ    | 81:Bo:61:LYS:O     | 2.38                     | 0.57              |
| 1:A2:381:G:N1      | 1:A2:384:G:OP2     | 2.34                     | 0.57              |
| 1:A2:521:A:O2'     | 1:A2:826:A:N3      | 2.37                     | 0.57              |
| 6:AE:44:ILE:O      | 26:An:113:GLN:NE2  | 2.34                     | 0.57              |
| 38:Az:23:ARG:NE    | 39:B5:3539:A:OP1   | 2.32                     | 0.57              |
| 39:B5:2688:A:H61   | 39:B5:3575:C:H42   | 1.51                     | 0.57              |
| 43:BB:261:ARG:HB2  | 56:BO:64:THR:HG21  | 1.87                     | 0.57              |
| 59:BR:39:GLN:OE1   | 59:BR:42:ARG:NH1   | 2.38                     | 0.57              |
| 62:BU:28:PRO:HB2   | 62:BU:34:MET:HG2   | 1.86                     | 0.57              |
| 88:Bz:427:LEU:HD12 | 88:Bz:459:VAL:HG21 | 1.87                     | 0.57              |
| 1:A2:463:OMC:HM22  | 1:A2:464:C:H5'     | 1.86                     | 0.56              |
| 1:A2:1680:A:H2'    | 17:Ae:60:ARG:HD2   | 1.87                     | 0.56              |
| 39:B5:184:U:H3     | 39:B5:253:G:H1     | 1.53                     | 0.56              |
| 39:B5:3991:G:N7    | 95:B5:5477:HOH:O   | 2.33                     | 0.56              |
| 18:Af:58:LYS:HA    | 18:Af:107:SER:HB2  | 1.86                     | 0.56              |
| 23:Ak:119:ASP:O    | 23:Ak:147:LYS:NZ   | 2.30                     | 0.56              |
| 39:B5:2538:A:OP1   | 78:Bk:35:LYS:NZ    | 2.23                     | 0.56              |
| 86:Bv:63:PHE:O     | 86:Bv:152:LYS:NZ   | 2.37                     | 0.56              |
| 1:A2:17:C:O2'      | 1:A2:1195:A:N1     | 2.37                     | 0.56              |
| 15:Ac:177:LEU:HD13 | 15:Ac:182:LEU:HD13 | 1.87                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:B5:1458:A:H4'    | 39:B5:1459:G:H5'   | 1.87                     | 0.56              |
| 39:B5:2338:U:H2'    | 39:B5:2339:G:H8    | 1.70                     | 0.56              |
| 46:BE:120:PRO:O     | 83:Br:112:ARG:NH1  | 2.36                     | 0.56              |
| 53:BL:63:THR:HG21   | 68:Ba:66:ASN:HD22  | 1.69                     | 0.56              |
| 60:BS:74:ARG:O      | 60:BS:76:LYS:NZ    | 2.39                     | 0.56              |
| 7:AF:214:GLY:HA2    | 7:AF:236:ILE:HG13  | 1.87                     | 0.56              |
| 18:Af:5:ILE:HG12    | 18:Af:111:LEU:HB2  | 1.88                     | 0.56              |
| 39:B5:230:G:OP1     | 66:BY:15:ARG:NH1   | 2.35                     | 0.56              |
| 39:B5:632:G:H5''    | 39:B5:633:U:H5'    | 1.86                     | 0.56              |
| 39:B5:4137:G:OP1    | 44:BC:75:ARG:NH1   | 2.35                     | 0.56              |
| 42:BA:180:LEU:HD21  | 82:Bp:22:LEU:HB3   | 1.88                     | 0.56              |
| 39:B5:699:G:OP1     | 72:Be:5:ARG:NH2    | 2.31                     | 0.56              |
| 39:B5:837:U:OP2     | 54:BM:48:GLN:NE2   | 2.39                     | 0.56              |
| 39:B5:3518:U:OP1    | 39:B5:4296:G:O2'   | 2.20                     | 0.56              |
| 39:B5:4304:U:OP2    | 43:BB:246:ARG:NH2  | 2.38                     | 0.56              |
| 1:A2:378:G:H5'      | 20:Ah:98:LYS:HB3   | 1.88                     | 0.56              |
| 1:A2:397:U:OP2      | 23:Ak:79:LYS:NZ    | 2.37                     | 0.56              |
| 1:A2:956:A:N1       | 1:A2:969:U:O2'     | 2.39                     | 0.56              |
| 19:Ag:144:ILE:HB    | 34:Av:52:ILE:HB    | 1.87                     | 0.56              |
| 33:Au:38:GLU:OE2    | 33:Au:51:LYS:NZ    | 2.38                     | 0.56              |
| 48:BG:166:LEU:HD21  | 55:BN:45:PRO:HG2   | 1.86                     | 0.56              |
| 88:Bz:243:PRO:HD2   | 88:Bz:273:GLU:HG2  | 1.86                     | 0.56              |
| 1:A2:1618:G:N1      | 1:A2:1621:A:OP2    | 2.35                     | 0.56              |
| 21:Ai:93:LYS:HB2    | 21:Ai:96:TYR:HD2   | 1.69                     | 0.56              |
| 39:B5:4068:G:N2     | 39:B5:4071:A:OP2   | 2.34                     | 0.56              |
| 39:B5:4381:A:OP1    | 39:B5:4382:PSU:O2' | 2.21                     | 0.56              |
| 88:Bz:244:SER:HA    | 88:Bz:247:LEU:HD12 | 1.88                     | 0.56              |
| 1:A2:1544:U:H5''    | 28:Ap:37:ARG:HH12  | 1.70                     | 0.56              |
| 39:B5:1741:A:O2'    | 39:B5:1776:A:OP1   | 2.22                     | 0.56              |
| 87:By:207:GLU:HG3   | 87:By:211:GLN:HE22 | 1.71                     | 0.56              |
| 12:AZ:33:GLN:HB3    | 12:AZ:154:LEU:HD12 | 1.86                     | 0.56              |
| 17:Ae:49:LEU:HD12   | 28:Ap:50:LYS:HG2   | 1.87                     | 0.56              |
| 39:B5:280:G:OP2     | 55:BN:44:ARG:NH2   | 2.35                     | 0.56              |
| 39:B5:2250:G:N2     | 79:Bl:51:LEU:OXT   | 2.39                     | 0.56              |
| 39:B5:4282:OMC:HM22 | 39:B5:4283:C:H5'   | 1.88                     | 0.56              |
| 39:B5:4366:OMU:OP2  | 39:B5:4416:C:N4    | 2.39                     | 0.56              |
| 50:BI:51:HIS:CD2    | 50:BI:168:SER:HB2  | 2.40                     | 0.56              |
| 87:By:6:SER:OG      | 87:By:7:ALA:N      | 2.38                     | 0.56              |
| 88:Bz:96:ARG:NH1    | 88:Bz:320:GLU:OE2  | 2.38                     | 0.56              |
| 1:A2:98:C:OP2       | 1:A2:427:A:O2'     | 2.24                     | 0.56              |
| 39:B5:835:G:OP1     | 54:BM:23:LYS:NZ    | 2.34                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:B5:1352:C:N4    | 39:B5:1353:G:O6    | 2.39                     | 0.56              |
| 39:B5:4186:G:H4'   | 50:BI:111:LEU:HD13 | 1.88                     | 0.56              |
| 41:B8:81:C:O2'     | 75:Bh:2:ALA:N      | 2.38                     | 0.56              |
| 16:Ad:125:LYS:H    | 16:Ad:142:HIS:HD2  | 1.54                     | 0.55              |
| 30:Ar:16:LEU:HD12  | 30:Ar:33:ILE:HD13  | 1.88                     | 0.55              |
| 39:B5:1125:C:H5    | 46:BE:62:SER:HB2   | 1.70                     | 0.55              |
| 85:Bt:80:LEU:HD23  | 85:Bt:112:ILE:HG23 | 1.88                     | 0.55              |
| 39:B5:2712:U:O2'   | 39:B5:2724:A:N7    | 2.37                     | 0.55              |
| 1:A2:1069:G:N7     | 95:A2:2130:HOH:O   | 2.33                     | 0.55              |
| 17:Ae:58:ALA:HB3   | 17:Ae:62:ARG:HH21  | 1.71                     | 0.55              |
| 39:B5:1214:A:H61   | 39:B5:2054:G:H21   | 1.52                     | 0.55              |
| 39:B5:2146:C:OP1   | 72:Be:107:ASN:ND2  | 2.40                     | 0.55              |
| 41:B8:57:C:OP2     | 77:Bj:68:LYS:NZ    | 2.37                     | 0.55              |
| 45:BD:41:LYS:NZ    | 61:BT:32:ARG:O     | 2.27                     | 0.55              |
| 85:Bt:10:ILE:HG12  | 85:Bt:65:GLN:HG2   | 1.87                     | 0.55              |
| 87:By:166:ARG:HB2  | 87:By:264:PHE:HE2  | 1.71                     | 0.55              |
| 1:A2:1018:U:OP1    | 25:Am:62:GLN:NE2   | 2.34                     | 0.55              |
| 34:Av:45:GLY:O     | 34:Av:68:ARG:NH2   | 2.40                     | 0.55              |
| 39:B5:3997:A:H5''  | 51:BJ:108:GLY:HA3  | 1.88                     | 0.55              |
| 39:B5:4745:U:H4'   | 39:B5:4746:A:H5'   | 1.89                     | 0.55              |
| 20:Ah:162:LEU:HD11 | 20:Ah:191:GLU:HG2  | 1.88                     | 0.55              |
| 39:B5:1341:A:O2'   | 39:B5:1422:C:O2'   | 2.25                     | 0.55              |
| 44:BC:293:LEU:O    | 44:BC:299:GLN:NE2  | 2.40                     | 0.55              |
| 1:A2:1783:G:OP2    | 64:BW:71:ARG:NH2   | 2.39                     | 0.55              |
| 29:Aq:37:GLU:HG3   | 29:Aq:38:ILE:HG23  | 1.89                     | 0.55              |
| 39:B5:2225:A:N1    | 39:B5:2672:U:O2'   | 2.33                     | 0.55              |
| 39:B5:3609:A:OP1   | 95:B5:5408:HOH:O   | 2.18                     | 0.55              |
| 39:B5:3702:G:O2'   | 86:Bv:31:THR:OG1   | 2.24                     | 0.55              |
| 44:BC:201:ARG:NH2  | 95:BC:601:HOH:O    | 2.39                     | 0.55              |
| 16:Ad:31:PRO:HG3   | 16:Ad:43:PRO:HG3   | 1.87                     | 0.55              |
| 43:BB:113:GLU:OE1  | 43:BB:168:MET:N    | 2.39                     | 0.55              |
| 66:BY:30:MET:HB3   | 66:BY:101:PRO:HG2  | 1.89                     | 0.55              |
| 1:A2:421:G:O2'     | 1:A2:661:C:N3      | 2.39                     | 0.55              |
| 1:A2:1222:G:O2'    | 1:A2:1677:U:O2     | 2.25                     | 0.55              |
| 8:AG:20:SER:OG     | 22:Aj:65:ARG:NH1   | 2.40                     | 0.55              |
| 39:B5:198:A:OP2    | 66:BY:126:ARG:NH2  | 2.40                     | 0.55              |
| 39:B5:228:C:O2'    | 66:BY:14:ASN:ND2   | 2.39                     | 0.55              |
| 39:B5:1689:G:H5''  | 50:BI:40:LYS:HG2   | 1.89                     | 0.55              |
| 39:B5:2169:G:OP1   | 72:Be:108:ARG:NH2  | 2.39                     | 0.55              |
| 39:B5:3678:G:H22   | 39:B5:3795:U:H3    | 1.53                     | 0.55              |
| 39:B5:4663:C:O2    | 39:B5:4665:C:N4    | 2.39                     | 0.55              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 67:BZ:36:ARG:NH1    | 67:BZ:38:TYR:OH    | 2.40                     | 0.55              |
| 69:Bb:56:LYS:O      | 69:Bb:60:ASN:ND2   | 2.33                     | 0.55              |
| 84:Bs:82:ILE:HD12   | 84:Bs:86:VAL:HG11  | 1.89                     | 0.55              |
| 86:Bv:89:ALA:HA     | 86:Bv:92:LYS:HD3   | 1.89                     | 0.55              |
| 1:A2:1781:G:OP2     | 64:BW:73:ARG:NH1   | 2.39                     | 0.55              |
| 16:Ad:148:ARG:NH2   | 18:Af:205:GLU:OE1  | 2.37                     | 0.55              |
| 39:B5:303:C:OP2     | 55:BN:68:ARG:NH2   | 2.39                     | 0.55              |
| 56:BO:130:LYS:HB2   | 56:BO:133:ARG:HG2  | 1.89                     | 0.55              |
| 1:A2:328:G:H1'      | 1:A2:329:U:H2'     | 1.88                     | 0.55              |
| 30:Ar:46:ARG:HG2    | 31:As:35:ASP:HB2   | 1.88                     | 0.55              |
| 39:B5:223:G:N3      | 44:BC:223:ASN:ND2  | 2.54                     | 0.55              |
| 39:B5:1805:U:OP1    | 50:BI:4:ARG:NH1    | 2.39                     | 0.55              |
| 39:B5:3457:G:N2     | 39:B5:3460:A:OP2   | 2.33                     | 0.55              |
| 42:BA:3:ARG:HG2     | 42:BA:207:VAL:HG22 | 1.88                     | 0.55              |
| 46:BE:104:ASN:OD1   | 46:BE:108:ARG:NH2  | 2.39                     | 0.55              |
| 48:BG:103:ARG:NH2   | 48:BG:192:ARG:O    | 2.40                     | 0.55              |
| 65:BX:73:HIS:CD2    | 65:BX:115:LYS:HD3  | 2.42                     | 0.55              |
| 72:Be:89:LEU:HD13   | 72:Be:118:LEU:HD22 | 1.89                     | 0.55              |
| 1:A2:228:C:H42      | 1:A2:902:G:H1'     | 1.71                     | 0.54              |
| 12:AZ:76:VAL:HG12   | 12:AZ:123:VAL:HB   | 1.88                     | 0.54              |
| 39:B5:1130:C:H42    | 39:B5:1209:G:H1    | 1.54                     | 0.54              |
| 39:B5:4050:A:OP2    | 39:B5:4051:G:N2    | 2.39                     | 0.54              |
| 43:BB:168:MET:HE1   | 43:BB:173:LEU:HD12 | 1.90                     | 0.54              |
| 1:A2:753:G:O2'      | 1:A2:755:G:O4'     | 2.23                     | 0.54              |
| 13:Aa:179:ASN:HB3   | 13:Aa:183:GLU:HB2  | 1.89                     | 0.54              |
| 14:Ab:171:GLY:O     | 34:Av:98:GLN:NE2   | 2.40                     | 0.54              |
| 39:B5:3812:G:O6     | 42:BA:72:ARG:NH2   | 2.37                     | 0.54              |
| 43:BB:215:GLU:OE2   | 43:BB:349:LYS:NZ   | 2.37                     | 0.54              |
| 1:A2:166:A2M:HM'2   | 1:A2:167:G:H5'     | 1.87                     | 0.54              |
| 29:Aq:29:HIS:HA     | 29:Aq:32:LYS:HE2   | 1.89                     | 0.54              |
| 30:Ar:26:ILE:HG13   | 30:Ar:45:LEU:HD21  | 1.89                     | 0.54              |
| 39:B5:4138:OMG:HM21 | 39:B5:4140:A:H2'   | 1.90                     | 0.54              |
| 1:A2:572:U:O2'      | 36:Ax:60:PHE:O     | 2.22                     | 0.54              |
| 1:A2:1034:G:N1      | 1:A2:1081:A:O2'    | 2.37                     | 0.54              |
| 20:Ah:57:ALA:HB2    | 20:Ah:183:GLY:HA2  | 1.90                     | 0.54              |
| 39:B5:2221:G:N2     | 39:B5:2224:A:OP2   | 2.39                     | 0.54              |
| 49:BH:44:GLU:OE2    | 54:BM:2:VAL:N      | 2.40                     | 0.54              |
| 50:BI:54:SER:HB2    | 50:BI:135:ILE:HD11 | 1.89                     | 0.54              |
| 1:A2:467:G:H8       | 18:Af:59:GLN:HE21  | 1.56                     | 0.54              |
| 1:A2:1085:A:OP1     | 1:A2:1859:G:O2'    | 2.24                     | 0.54              |
| 1:A2:1387:A:OP2     | 15:Ac:160:SER:OG   | 2.18                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AD:102:ARG:HD3   | 5:AD:106:ALA:HB1   | 1.89                     | 0.54              |
| 28:Ap:34:VAL:HG22  | 28:Ap:70:VAL:HB    | 1.89                     | 0.54              |
| 39:B5:1639:A:OP1   | 68:Ba:47:LYS:NZ    | 2.40                     | 0.54              |
| 57:BP:40:HIS:NE2   | 57:BP:110:ASP:O    | 2.33                     | 0.54              |
| 80:Bm:94:MET:HG2   | 80:Bm:105:PRO:HA   | 1.90                     | 0.54              |
| 39:B5:109:G:OP2    | 53:BL:74:ARG:NH2   | 2.41                     | 0.54              |
| 53:BL:81:LEU:HD12  | 53:BL:86:ILE:HB    | 1.88                     | 0.54              |
| 42:BA:101:VAL:HG22 | 42:BA:165:VAL:HG22 | 1.90                     | 0.54              |
| 55:BN:116:LEU:HD22 | 55:BN:135:ILE:HD11 | 1.88                     | 0.54              |
| 75:Bh:13:LYS:NZ    | 75:Bh:16:GLU:OE2   | 2.41                     | 0.54              |
| 84:Bs:19:GLN:NE2   | 84:Bs:23:ASP:OD2   | 2.40                     | 0.54              |
| 1:A2:64:A:OP1      | 18:Af:177:GLN:NE2  | 2.41                     | 0.54              |
| 1:A2:544:C:H2'     | 1:A2:545:G:C8      | 2.43                     | 0.54              |
| 18:Af:2:LYS:HB3    | 18:Af:15:LEU:HD11  | 1.90                     | 0.54              |
| 45:BD:186:GLU:N    | 45:BD:186:GLU:OE1  | 2.40                     | 0.54              |
| 17:Ae:102:LEU:HD21 | 37:Ay:100:VAL:HG21 | 1.89                     | 0.54              |
| 39:B5:1395:U:OP2   | 47:BF:33:ARG:NH2   | 2.41                     | 0.54              |
| 51:BJ:136:ARG:NH2  | 51:BJ:161:GLU:OE1  | 2.41                     | 0.54              |
| 65:BX:82:THR:HG22  | 65:BX:155:ILE:HG23 | 1.90                     | 0.54              |
| 71:Bd:38:PHE:HB3   | 71:Bd:78:ARG:HG2   | 1.88                     | 0.54              |
| 75:Bh:4:ILE:HD12   | 75:Bh:53:SER:HB3   | 1.89                     | 0.54              |
| 1:A2:421:G:OP1     | 34:Av:88:LYS:NZ    | 2.40                     | 0.54              |
| 1:A2:1844:G:N7     | 38:Az:4:LYS:NZ     | 2.46                     | 0.54              |
| 12:AZ:99:ILE:HD11  | 12:AZ:117:ARG:HD2  | 1.89                     | 0.54              |
| 39:B5:2007:C:OP1   | 73:Bf:15:LYS:NZ    | 2.41                     | 0.54              |
| 46:BE:172:SER:OG   | 46:BE:217:ASP:OD2  | 2.25                     | 0.54              |
| 67:BZ:11:VAL:HG12  | 67:BZ:82:PRO:HA    | 1.90                     | 0.54              |
| 73:Bf:41:PHE:HE1   | 73:Bf:110:ILE:HD13 | 1.73                     | 0.54              |
| 86:Bv:140:HIS:HA   | 86:Bv:144:MET:HE1  | 1.90                     | 0.54              |
| 88:Bz:217:LEU:HB3  | 88:Bz:221:GLU:HB2  | 1.89                     | 0.54              |
| 1:A2:1805:OMU:HM22 | 1:A2:1806:G:H5'    | 1.90                     | 0.53              |
| 18:Af:22:ARG:HG2   | 18:Af:25:ARG:HH22  | 1.71                     | 0.53              |
| 51:BJ:40:LEU:HD12  | 51:BJ:70:VAL:HG22  | 1.91                     | 0.53              |
| 84:Bs:69:LEU:HA    | 84:Bs:75:LEU:HD11  | 1.90                     | 0.53              |
| 88:Bz:221:GLU:OE1  | 88:Bz:224:ARG:NH2  | 2.40                     | 0.53              |
| 18:Af:213:LEU:HG   | 18:Af:217:MET:HE2  | 1.89                     | 0.53              |
| 28:Ap:53:GLU:OE1   | 28:Ap:85:ARG:NH2   | 2.41                     | 0.53              |
| 39:B5:394:G:N2     | 39:B5:397:G:OP2    | 2.30                     | 0.53              |
| 39:B5:1811:G:O2'   | 39:B5:3965:A:N3    | 2.41                     | 0.53              |
| 39:B5:2568:A:N6    | 59:BR:88:ARG:O     | 2.42                     | 0.53              |
| 1:A2:1276:G:N2     | 1:A2:1507:A:OP2    | 2.40                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:AE:3:LYS:NZ      | 6:AE:8:ASN:OD1     | 2.42                     | 0.53              |
| 7:AF:256:ILE:HB    | 7:AF:270:LEU:HB2   | 1.90                     | 0.53              |
| 11:AT:5:G:H1       | 11:AT:78:U:H3      | 1.56                     | 0.53              |
| 13:Aa:157:GLN:NE2  | 95:Aa:301:HOH:O    | 2.41                     | 0.53              |
| 30:Ar:7:GLU:HG2    | 30:Ar:8:LYS:HG3    | 1.89                     | 0.53              |
| 35:Aw:71:ARG:NH1   | 35:Aw:82:THR:OG1   | 2.40                     | 0.53              |
| 39:B5:755:G:H1     | 39:B5:800:U:H3     | 1.57                     | 0.53              |
| 42:BA:117:GLU:HG2  | 42:BA:124:GLY:H    | 1.73                     | 0.53              |
| 49:BH:141:LYS:NZ   | 49:BH:142:ASP:OD2  | 2.41                     | 0.53              |
| 39:B5:865:G:N2     | 39:B5:2035:G:O2'   | 2.41                     | 0.53              |
| 41:B8:141:C:H5''   | 55:BN:60:VAL:HG11  | 1.89                     | 0.53              |
| 51:BJ:46:GLN:NE2   | 51:BJ:73:THR:O     | 2.37                     | 0.53              |
| 87:By:119:PRO:HB2  | 87:By:165:THR:HG21 | 1.90                     | 0.53              |
| 7:AF:40:ILE:HB     | 7:AF:59:LEU:HB2    | 1.90                     | 0.53              |
| 31:As:60:THR:HG23  | 31:As:75:MET:HE2   | 1.90                     | 0.53              |
| 39:B5:3432:C:O2'   | 39:B5:3506:A:N3    | 2.32                     | 0.53              |
| 39:B5:4780:G:N1    | 43:BB:389:MET:O    | 2.41                     | 0.53              |
| 50:BI:169:LYS:NZ   | 61:BT:157:GLU:OE2  | 2.29                     | 0.53              |
| 1:A2:355:OMU:HM22  | 1:A2:356:G:H5'     | 1.90                     | 0.53              |
| 23:Ak:18:GLN:HG2   | 23:Ak:33:LEU:HD21  | 1.91                     | 0.53              |
| 25:Am:93:LYS:HA    | 25:Am:150:VAL:HG21 | 1.91                     | 0.53              |
| 39:B5:308:G:O6     | 55:BN:12:ARG:NH1   | 2.42                     | 0.53              |
| 49:BH:120:GLU:OE1  | 49:BH:124:ARG:NH2  | 2.40                     | 0.53              |
| 84:Bs:32:ALA:HB1   | 84:Bs:35:VAL:HG21  | 1.90                     | 0.53              |
| 84:Bs:106:LYS:HE2  | 84:Bs:186:GLY:HA3  | 1.89                     | 0.53              |
| 86:Bv:48:ARG:HH22  | 86:Bv:161:LYS:HD2  | 1.73                     | 0.53              |
| 1:A2:665:A:O2'     | 1:A2:671:A:N1      | 2.35                     | 0.53              |
| 1:A2:1299:G:H4'    | 27:Ao:78:THR:HA    | 1.90                     | 0.53              |
| 1:A2:1494:C:O2'    | 1:A2:1500:U:O4     | 2.24                     | 0.53              |
| 1:A2:1674:U:O2'    | 17:Ae:84:GLY:O     | 2.23                     | 0.53              |
| 1:A2:1842:C:H2'    | 1:A2:1843:4AC:H6   | 1.90                     | 0.53              |
| 7:AF:217:MET:HG2   | 7:AF:229:THR:HG22  | 1.89                     | 0.53              |
| 15:Ac:131:ALA:HA   | 15:Ac:191:PRO:HD3  | 1.91                     | 0.53              |
| 39:B5:869:U:H3'    | 39:B5:2102:G:H22   | 1.74                     | 0.53              |
| 39:B5:1270:A2M:OP2 | 39:B5:4191:U:O2'   | 2.26                     | 0.53              |
| 45:BD:152:ARG:HG3  | 45:BD:154:THR:HG23 | 1.89                     | 0.53              |
| 74:Bg:68:SER:OG    | 74:Bg:71:LYS:NZ    | 2.39                     | 0.53              |
| 1:A2:541:U:H2'     | 1:A2:542:U:H5''    | 1.91                     | 0.53              |
| 1:A2:1315:U:O2'    | 22:Aj:8:ARG:NH2    | 2.41                     | 0.53              |
| 1:A2:1419:C:O2'    | 1:A2:1421:G:OP2    | 2.26                     | 0.53              |
| 1:A2:1500:U:H4'    | 15:Ac:176:LEU:HD13 | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A2:1534:A:OP2    | 17:Ae:164:ARG:NH1  | 2.38                     | 0.53              |
| 39:B5:1809:C:H2'   | 39:B5:1810:A2M:H8  | 1.90                     | 0.53              |
| 8:AG:22:ARG:HH21   | 8:AG:37:ASN:HB2    | 1.73                     | 0.53              |
| 28:Ap:6:PRO:O      | 28:Ap:27:ARG:NH2   | 2.41                     | 0.53              |
| 39:B5:1548:A:H5''  | 39:B5:2682:U:H5''  | 1.91                     | 0.53              |
| 1:A2:191:A:H3'     | 1:A2:192:C:H5''    | 1.89                     | 0.53              |
| 1:A2:382:C:OP2     | 20:Ah:31:ARG:NH2   | 2.42                     | 0.53              |
| 1:A2:745:G:H21     | 19:Ag:109:ARG:HG2  | 1.74                     | 0.53              |
| 1:A2:912:C:H41     | 59:BR:173:ARG:HH22 | 1.57                     | 0.53              |
| 4:AC:116:ARG:NH1   | 4:AC:120:GLU:OE2   | 2.42                     | 0.53              |
| 39:B5:4293:C:O2'   | 39:B5:4295:G:OP1   | 2.27                     | 0.53              |
| 88:Bz:168:ILE:HG12 | 88:Bz:239:MET:HG3  | 1.90                     | 0.53              |
| 17:Ae:45:TYR:OH    | 17:Ae:65:GLN:NE2   | 2.41                     | 0.52              |
| 27:Ao:142:ILE:HD11 | 87:By:112:ILE:HG12 | 1.90                     | 0.52              |
| 39:B5:1772:G:OP1   | 61:BT:120:LYS:NZ   | 2.42                     | 0.52              |
| 39:B5:2364:G:H5'   | 39:B5:2483:G:H1'   | 1.91                     | 0.52              |
| 39:B5:4445:U:H1'   | 39:B5:4446:A:H5''  | 1.89                     | 0.52              |
| 46:BE:277:VAL:HG21 | 73:Bf:1:MET:HA     | 1.91                     | 0.52              |
| 15:Ac:45:ARG:NH2   | 15:Ac:82:GLY:O     | 2.42                     | 0.52              |
| 17:Ae:110:GLN:HE21 | 17:Ae:114:ASN:HD21 | 1.56                     | 0.52              |
| 25:Am:83:ASP:OD1   | 25:Am:83:ASP:N     | 2.42                     | 0.52              |
| 37:Ay:79:ILE:HB    | 37:Ay:83:LEU:HD23  | 1.91                     | 0.52              |
| 39:B5:382:G:N1     | 39:B5:385:A:OP2    | 2.41                     | 0.52              |
| 39:B5:1900:G:OP2   | 84:Bs:59:THR:OG1   | 2.23                     | 0.52              |
| 63:BV:106:VAL:HG12 | 63:BV:112:MET:HA   | 1.91                     | 0.52              |
| 86:Bv:65:VAL:HG22  | 86:Bv:109:ALA:HB3  | 1.92                     | 0.52              |
| 8:AG:52:PHE:HB3    | 32:At:80:PHE:HB3   | 1.92                     | 0.52              |
| 20:Ah:165:GLN:HE22 | 20:Ah:195:LEU:HD11 | 1.73                     | 0.52              |
| 39:B5:1458:A:H62   | 58:BQ:87:THR:HG21  | 1.74                     | 0.52              |
| 39:B5:4311:C:O2    | 43:BB:268:ARG:NH2  | 2.37                     | 0.52              |
| 48:BG:83:PHE:HA    | 48:BG:183:ILE:HD13 | 1.92                     | 0.52              |
| 53:BL:124:LEU:HD11 | 75:Bh:119:TYR:HB2  | 1.90                     | 0.52              |
| 61:BT:18:PRO:HG2   | 61:BT:21:LYS:HB2   | 1.90                     | 0.52              |
| 64:BW:96:GLN:HE21  | 64:BW:100:VAL:HG12 | 1.74                     | 0.52              |
| 85:Bt:64:ILE:HA    | 85:Bt:69:ALA:HA    | 1.91                     | 0.52              |
| 1:A2:1338:4AC:H2'  | 1:A2:1339:G:C8     | 2.44                     | 0.52              |
| 12:AZ:206:ASP:OD1  | 12:AZ:206:ASP:N    | 2.38                     | 0.52              |
| 25:Am:99:ARG:NH2   | 25:Am:119:GLU:OE2  | 2.38                     | 0.52              |
| 28:Ap:117:ARG:HE   | 28:Ap:121:VAL:HG21 | 1.74                     | 0.52              |
| 39:B5:74:G:H1'     | 53:BL:62:PRO:HG3   | 1.92                     | 0.52              |
| 39:B5:2419:G:OP1   | 67:BZ:48:ARG:NH2   | 2.42                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A2:914:A:N6      | 19:Ag:119:SER:O    | 2.42                     | 0.52              |
| 39:B5:856:A:H1'    | 39:B5:2015:G:H5''  | 1.91                     | 0.52              |
| 43:BB:39:LYS:HG2   | 43:BB:40:PRO:HD2   | 1.91                     | 0.52              |
| 47:BF:154:TYR:OH   | 47:BF:187:GLU:OE2  | 2.28                     | 0.52              |
| 51:BJ:35:ARG:NH1   | 51:BJ:123:ILE:O    | 2.35                     | 0.52              |
| 63:BV:85:ARG:NH1   | 63:BV:99:GLU:O     | 2.35                     | 0.52              |
| 72:Be:37:LYS:HD2   | 72:Be:38:PRO:HD2   | 1.91                     | 0.52              |
| 86:Bv:111:LEU:HD21 | 86:Bv:151:VAL:HG21 | 1.92                     | 0.52              |
| 7:AF:236:ILE:HG12  | 7:AF:252:THR:HG22  | 1.92                     | 0.52              |
| 15:Ac:75:LYS:NZ    | 22:Aj:20:VAL:O     | 2.42                     | 0.52              |
| 87:By:360:LYS:N    | 87:By:365:GLU:OE1  | 2.40                     | 0.52              |
| 7:AF:238:ALA:H     | 7:AF:251:ALA:HB3   | 1.75                     | 0.52              |
| 39:B5:4151:G:H21   | 50:BI:103:LEU:HD21 | 1.75                     | 0.52              |
| 39:B5:4717:G:N7    | 95:B5:5488:HOH:O   | 2.34                     | 0.52              |
| 50:BI:55:ASP:OD2   | 50:BI:164:LYS:NZ   | 2.43                     | 0.52              |
| 56:BO:54:TYR:OH    | 56:BO:73:PHE:O     | 2.27                     | 0.52              |
| 84:Bs:29:ILE:HG23  | 84:Bs:86:VAL:HG13  | 1.91                     | 0.52              |
| 27:Ao:123:TYR:OH   | 30:Ar:124:ARG:NH1  | 2.43                     | 0.52              |
| 37:Ay:74:SER:OG    | 37:Ay:79:ILE:O     | 2.18                     | 0.52              |
| 1:A2:115:U:O2'     | 1:A2:382:C:O2      | 2.22                     | 0.52              |
| 24:Al:89:VAL:HG23  | 24:Al:91:LEU:HB2   | 1.91                     | 0.52              |
| 39:B5:1005:G:OP1   | 61:BT:142:ARG:NH1  | 2.41                     | 0.52              |
| 39:B5:1249:C:OP1   | 41:B8:7:U:O2'      | 2.27                     | 0.52              |
| 49:BH:186:THR:O    | 49:BH:189:GLN:NE2  | 2.42                     | 0.52              |
| 60:BS:99:ASP:OD1   | 60:BS:100:LEU:N    | 2.43                     | 0.52              |
| 86:Bv:32:VAL:HA    | 86:Bv:208:SER:HA   | 1.92                     | 0.52              |
| 7:AF:39:THR:HG22   | 7:AF:60:ARG:HG2    | 1.91                     | 0.52              |
| 39:B5:347:A:O2'    | 44:BC:50:GLN:NE2   | 2.40                     | 0.52              |
| 50:BI:66:GLU:OE2   | 50:BI:69:ARG:NH2   | 2.43                     | 0.52              |
| 61:BT:94:GLU:OE1   | 61:BT:94:GLU:N     | 2.40                     | 0.52              |
| 81:Bo:6:LYS:HE3    | 81:Bo:94:GLY:HA3   | 1.92                     | 0.52              |
| 88:Bz:31:VAL:HG12  | 88:Bz:36:LYS:HB2   | 1.92                     | 0.52              |
| 39:B5:2257:G:H2'   | 39:B5:2258:OMU:H6  | 1.91                     | 0.51              |
| 41:B8:65:A:O2'     | 75:Bh:10:ARG:NH2   | 2.43                     | 0.51              |
| 62:BU:47:ILE:HD12  | 62:BU:63:ILE:HD11  | 1.92                     | 0.51              |
| 1:A2:35:C:H5''     | 1:A2:580:C:H5''    | 1.92                     | 0.51              |
| 1:A2:1031:A:H2'    | 1:A2:1032:A2M:H8   | 1.91                     | 0.51              |
| 1:A2:1329:OMG:HM22 | 1:A2:1330:U:H5'    | 1.92                     | 0.51              |
| 14:Ab:102:LEU:HD22 | 14:Ab:130:ILE:HG12 | 1.91                     | 0.51              |
| 39:B5:4735:C:OP1   | 71:Bd:32:ARG:NH1   | 2.43                     | 0.51              |
| 43:BB:224:LYS:HG2  | 43:BB:340:THR:HG22 | 1.90                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BQ:122:THR:OG1  | 58:BQ:124:ASP:OD1  | 2.29                     | 0.51              |
| 74:Bg:64:LEU:HD23  | 74:Bg:67:LEU:HD12  | 1.93                     | 0.51              |
| 1:A2:195:C:H42     | 1:A2:204:G:H1      | 1.59                     | 0.51              |
| 1:A2:523:A:H5''    | 21:Ai:145:PRO:HD2  | 1.91                     | 0.51              |
| 1:A2:832:G:O6      | 36:Ax:11:LYS:NZ    | 2.44                     | 0.51              |
| 19:Ag:117:PRO:HB2  | 19:Ag:120:ARG:HD3  | 1.92                     | 0.51              |
| 39:B5:2146:C:H5''  | 72:Be:104:SER:HB3  | 1.92                     | 0.51              |
| 85:Bt:85:LEU:HD23  | 85:Bt:104:ILE:HD11 | 1.92                     | 0.51              |
| 1:A2:1092:C:O2'    | 34:Av:2:VAL:N      | 2.33                     | 0.51              |
| 7:AF:29:ASP:OD1    | 7:AF:47:ARG:NH1    | 2.30                     | 0.51              |
| 39:B5:151:G:OP2    | 55:BN:4:TYR:OH     | 2.21                     | 0.51              |
| 39:B5:1869:U:OP2   | 56:BO:49:ARG:NH1   | 2.38                     | 0.51              |
| 49:BH:48:LEU:HD11  | 49:BH:56:ARG:HH11  | 1.76                     | 0.51              |
| 88:Bz:169:LYS:HG2  | 88:Bz:240:PHE:HA   | 1.93                     | 0.51              |
| 15:Ac:32:ASP:OD2   | 15:Ac:65:ARG:NH1   | 2.44                     | 0.51              |
| 16:Ad:45:ILE:HA    | 16:Ad:61:VAL:HG11  | 1.92                     | 0.51              |
| 16:Ad:143:ASP:OD1  | 16:Ad:143:ASP:N    | 2.36                     | 0.51              |
| 22:Aj:37:ASP:OD1   | 22:Aj:37:ASP:N     | 2.42                     | 0.51              |
| 28:Ap:97:GLN:HB2   | 28:Ap:105:LYS:HG3  | 1.92                     | 0.51              |
| 40:B7:49:A:H3'     | 45:BD:225:GLN:HE21 | 1.76                     | 0.51              |
| 41:B8:102:G:OP2    | 41:B8:104:A:O2'    | 2.29                     | 0.51              |
| 45:BD:55:VAL:HG13  | 45:BD:60:ILE:HG12  | 1.91                     | 0.51              |
| 87:By:32:THR:H     | 87:By:67:ASN:HD21  | 1.56                     | 0.51              |
| 1:A2:688:C:O3'     | 19:Ag:116:ARG:NH2  | 2.43                     | 0.51              |
| 24:Al:37:GLU:HA    | 24:Al:40:LYS:HD2   | 1.93                     | 0.51              |
| 39:B5:3682:U:H2'   | 39:B5:3683:G:H8    | 1.76                     | 0.51              |
| 1:A2:121:OMU:HM22  | 1:A2:122:G:H5'     | 1.93                     | 0.51              |
| 1:A2:1528:C:OP1    | 28:Ap:142:GLN:NE2  | 2.43                     | 0.51              |
| 30:Ar:14:ARG:NH1   | 30:Ar:19:ASN:OD1   | 2.37                     | 0.51              |
| 31:As:116:ASP:OD1  | 31:As:116:ASP:N    | 2.43                     | 0.51              |
| 39:B5:407:A:O2'    | 39:B5:410:A:OP1    | 2.22                     | 0.51              |
| 39:B5:1105:C:O2    | 69:Bb:91:ARG:NE    | 2.38                     | 0.51              |
| 39:B5:3480:A:O2'   | 42:BA:223:SER:OG   | 2.23                     | 0.51              |
| 51:BJ:81:GLU:OE2   | 51:BJ:85:LYS:NZ    | 2.39                     | 0.51              |
| 75:Bh:80:PRO:HD2   | 75:Bh:83:LEU:HD12  | 1.92                     | 0.51              |
| 12:AZ:145:ILE:HG12 | 12:AZ:159:ILE:HB   | 1.93                     | 0.51              |
| 15:Ac:213:PRO:HG3  | 29:Aq:19:LYS:HB3   | 1.92                     | 0.51              |
| 18:Af:103:ASP:OD2  | 18:Af:105:ASN:ND2  | 2.38                     | 0.51              |
| 39:B5:239:C:OP1    | 66:BY:46:SER:OG    | 2.28                     | 0.51              |
| 46:BE:182:LEU:HD12 | 46:BE:186:ARG:HA   | 1.92                     | 0.51              |
| 46:BE:189:LEU:HD21 | 46:BE:256:VAL:HG21 | 1.93                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A2:1785:G:OP2     | 64:BW:71:ARG:NH2    | 2.43                     | 0.51              |
| 39:B5:238:C:OP2     | 66:BY:45:ARG:NH2    | 2.43                     | 0.51              |
| 39:B5:4011:U:N3     | 45:BD:17:GLN:O      | 2.40                     | 0.51              |
| 43:BB:317:LEU:HD22  | 43:BB:382:VAL:HG13  | 1.92                     | 0.51              |
| 43:BB:350:SER:OG    | 43:BB:354:GLN:NE2   | 2.43                     | 0.51              |
| 39:B5:1741:A:H5''   | 39:B5:1742:G:H5'    | 1.92                     | 0.51              |
| 39:B5:2654:G:N2     | 39:B5:2657:C:OP2    | 2.34                     | 0.51              |
| 1:A2:144:U:OP2      | 18:Af:139:SER:OG    | 2.30                     | 0.50              |
| 1:A2:923:A:OP2      | 34:Av:28:ARG:NH2    | 2.44                     | 0.50              |
| 12:AZ:144:THR:OG1   | 12:AZ:156:TYR:O     | 2.29                     | 0.50              |
| 39:B5:88:A:OP2      | 58:BQ:173:LYS:NZ    | 2.35                     | 0.50              |
| 39:B5:3852:G:N2     | 48:BG:43:GLN:O      | 2.44                     | 0.50              |
| 87:By:78:VAL:HG23   | 87:By:95:VAL:HG11   | 1.93                     | 0.50              |
| 1:A2:454:C:O2'      | 18:Af:92:ARG:O      | 2.21                     | 0.50              |
| 1:A2:1448:OMG:HM22  | 1:A2:1449:A:H5'     | 1.93                     | 0.50              |
| 39:B5:1701:C:H2'    | 39:B5:1702:C:C6     | 2.46                     | 0.50              |
| 39:B5:2223:G:N2     | 39:B5:2267:OMG:H5'' | 2.27                     | 0.50              |
| 39:B5:4649:A:H4'    | 43:BB:95:THR:HG22   | 1.93                     | 0.50              |
| 57:BP:52:THR:HG23   | 57:BP:85:LYS:HG3    | 1.93                     | 0.50              |
| 1:A2:62:G:H1'       | 1:A2:172:OMU:HM23   | 1.92                     | 0.50              |
| 13:Aa:129:THR:OG1   | 13:Aa:131:ASP:OD1   | 2.24                     | 0.50              |
| 39:B5:1859:C:H3'    | 39:B5:1860:C:H5''   | 1.93                     | 0.50              |
| 39:B5:3762:G:H2'    | 39:B5:3763:G:H8     | 1.76                     | 0.50              |
| 57:BP:115:GLU:OE1   | 57:BP:151:THR:OG1   | 2.27                     | 0.50              |
| 72:Be:78:LEU:O      | 83:Br:20:ARG:NH1    | 2.44                     | 0.50              |
| 1:A2:864:PSU:O2     | 1:A2:865:A:N6       | 2.45                     | 0.50              |
| 1:A2:1227:G:N1      | 1:A2:1640:G7M:OP2   | 2.23                     | 0.50              |
| 30:Ar:22:GLY:HA2    | 30:Ar:56:ALA:HB3    | 1.92                     | 0.50              |
| 39:B5:1632:PSU:H4'  | 39:B5:1635:G:C2     | 2.46                     | 0.50              |
| 39:B5:3974:OMG:H5'' | 39:B5:3975:U:O4'    | 2.11                     | 0.50              |
| 12:AZ:198:MET:HG2   | 12:AZ:200:ASP:H     | 1.76                     | 0.50              |
| 15:Ac:132:LYS:HE3   | 15:Ac:191:PRO:HA    | 1.94                     | 0.50              |
| 39:B5:58:G:H4'      | 39:B5:59:A:H4'      | 1.94                     | 0.50              |
| 39:B5:1962:C:OP2    | 84:Bs:83:ARG:NH2    | 2.44                     | 0.50              |
| 39:B5:2601:G:O2'    | 39:B5:2608:A:N3     | 2.35                     | 0.50              |
| 44:BC:39:PHE:O      | 44:BC:43:ASN:ND2    | 2.40                     | 0.50              |
| 59:BR:87:ALA:O      | 95:BR:301:HOH:O     | 2.19                     | 0.50              |
| 1:A2:930:G:OP1      | 70:Bc:5:LYS:NZ      | 2.41                     | 0.50              |
| 1:A2:1334:U:H5'     | 15:Ac:147:ALA:HB2   | 1.94                     | 0.50              |
| 12:AZ:17:LYS:HB3    | 12:AZ:173:LEU:HD11  | 1.94                     | 0.50              |
| 23:Ak:104:LYS:O     | 35:Aw:11:ARG:NH2    | 2.43                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:B5:237:G:N7     | 95:B5:5490:HOH:O   | 2.35                     | 0.50              |
| 39:B5:1109:G:H2'   | 39:B5:1110:G:H8    | 1.76                     | 0.50              |
| 39:B5:4051:G:O5'   | 61:BT:83:LYS:NZ    | 2.45                     | 0.50              |
| 1:A2:1448:OMG:OP1  | 32:At:85:HIS:ND1   | 2.44                     | 0.50              |
| 14:Ab:232:THR:HG22 | 14:Ab:235:ASN:H    | 1.77                     | 0.50              |
| 39:B5:2517:A:N6    | 82:Bp:41:PHE:O     | 2.42                     | 0.50              |
| 39:B5:4224:G:O2'   | 39:B5:4348:A:N1    | 2.41                     | 0.50              |
| 1:A2:49:C:H2'      | 1:A2:473:C:H41     | 1.77                     | 0.50              |
| 1:A2:86:C:O2'      | 1:A2:171:A:N1      | 2.41                     | 0.50              |
| 1:A2:309:G:OP1     | 20:Ah:53:LYS:NZ    | 2.41                     | 0.50              |
| 7:AF:239:LEU:HD22  | 7:AF:248:LEU:HD11  | 1.94                     | 0.50              |
| 16:Ad:151:ASP:HB3  | 16:Ad:154:ILE:HG13 | 1.93                     | 0.50              |
| 18:Af:78:SER:HB3   | 18:Af:92:ARG:HG2   | 1.94                     | 0.50              |
| 39:B5:158:A:H5''   | 39:B5:159:C:H2'    | 1.94                     | 0.50              |
| 39:B5:1070:U:O2    | 45:BD:286:SER:OG   | 2.29                     | 0.50              |
| 47:BF:126:LYS:HB2  | 61:BT:133:ALA:HB3  | 1.94                     | 0.50              |
| 50:BI:48:LEU:HB2   | 50:BI:142:LEU:HD23 | 1.93                     | 0.50              |
| 63:BV:13:LYS:HD2   | 63:BV:128:LEU:HD21 | 1.94                     | 0.50              |
| 71:Bd:46:LEU:HD11  | 71:Bd:73:TRP:HE1   | 1.77                     | 0.50              |
| 84:Bs:54:LEU:O     | 84:Bs:88:PHE:N     | 2.42                     | 0.50              |
| 88:Bz:412:LYS:HB3  | 88:Bz:485:ILE:HA   | 1.93                     | 0.50              |
| 1:A2:469:A2M:HM'2  | 1:A2:470:A:H5'     | 1.94                     | 0.50              |
| 15:Ac:123:LEU:HD22 | 15:Ac:152:PHE:HB3  | 1.94                     | 0.50              |
| 24:Al:39:ALA:HA    | 24:Al:42:LEU:HB2   | 1.94                     | 0.50              |
| 30:Ar:16:LEU:HD21  | 30:Ar:72:GLN:HE21  | 1.77                     | 0.50              |
| 39:B5:150:U:OP2    | 48:BG:200:THR:OG1  | 2.22                     | 0.50              |
| 39:B5:1453:G:OP1   | 58:BQ:150:ARG:NH1  | 2.45                     | 0.50              |
| 39:B5:1829:G:OP2   | 39:B5:1829:G:N2    | 2.32                     | 0.50              |
| 39:B5:1846:A:H4'   | 47:BF:222:LYS:HE3  | 1.92                     | 0.50              |
| 39:B5:2146:C:O2'   | 39:B5:2175:A:N1    | 2.42                     | 0.50              |
| 39:B5:4705:A:H5'   | 43:BB:128:LYS:HG3  | 1.94                     | 0.50              |
| 42:BA:102:LEU:HB2  | 42:BA:107:MET:HE3  | 1.94                     | 0.50              |
| 50:BI:102:MET:HA   | 50:BI:106:ALA:HB3  | 1.92                     | 0.50              |
| 1:A2:1061:A:O2'    | 1:A2:1063:A:N7     | 2.41                     | 0.49              |
| 5:AD:91:LEU:HD23   | 5:AD:91:LEU:H      | 1.76                     | 0.49              |
| 7:AF:150:TRP:NE1   | 29:Aq:37:GLU:OE1   | 2.45                     | 0.49              |
| 10:AI:75:C:O2'     | 81:Bo:54:PRO:O     | 2.25                     | 0.49              |
| 10:AI:76:A:O2'     | 39:B5:4087:C:N3    | 2.43                     | 0.49              |
| 14:Ab:128:VAL:HG11 | 14:Ab:155:ILE:HG12 | 1.94                     | 0.49              |
| 39:B5:1736:G:OP1   | 47:BF:103:LYS:NZ   | 2.45                     | 0.49              |
| 45:BD:122:GLN:NE2  | 45:BD:126:THR:OG1  | 2.45                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 71:Bd:54:MET:HE3    | 71:Bd:60:PRO:HA    | 1.94                     | 0.49              |
| 1:A2:1488:A:H1'     | 14:Ab:118:ALA:HB1  | 1.95                     | 0.49              |
| 12:AZ:89:LYS:NZ     | 29:Aq:83:ASN:OD1   | 2.45                     | 0.49              |
| 15:Ac:48:ILE:HG13   | 15:Ac:86:LEU:HG    | 1.94                     | 0.49              |
| 39:B5:1984:G:O6     | 39:B5:3602:C:O2'   | 2.29                     | 0.49              |
| 39:B5:2338:U:H2'    | 39:B5:2339:G:C8    | 2.46                     | 0.49              |
| 39:B5:4350:G:N2     | 39:B5:4353:A:OP2   | 2.45                     | 0.49              |
| 42:BA:206:PRO:HG3   | 42:BA:213:GLY:HA3  | 1.94                     | 0.49              |
| 43:BB:85:VAL:HG22   | 43:BB:204:GLN:HG2  | 1.94                     | 0.49              |
| 58:BQ:151:HIS:ND1   | 58:BQ:164:LYS:O    | 2.44                     | 0.49              |
| 62:BU:90:TYR:O      | 62:BU:94:ASN:ND2   | 2.44                     | 0.49              |
| 88:Bz:411:TYR:HD1   | 88:Bz:484:LEU:HD13 | 1.77                     | 0.49              |
| 88:Bz:441:PHE:HE2   | 88:Bz:446:MET:HE2  | 1.76                     | 0.49              |
| 5:AD:123:PHE:HB3    | 9:AH:3477:G:N7     | 2.27                     | 0.49              |
| 12:AZ:8:LEU:HD11    | 33:Au:39:VAL:HG11  | 1.95                     | 0.49              |
| 12:AZ:77:ILE:HD11   | 12:AZ:99:ILE:HD12  | 1.93                     | 0.49              |
| 39:B5:724:G:OP2     | 47:BF:75:ARG:NE    | 2.46                     | 0.49              |
| 39:B5:2552:C:OP2    | 59:BR:43:LYS:NZ    | 2.40                     | 0.49              |
| 1:A2:398:G:OP2      | 23:Ak:108:ASN:ND2  | 2.46                     | 0.49              |
| 3:AB:27:CYS:SG      | 17:Ae:126:THR:HG21 | 2.51                     | 0.49              |
| 18:Af:138:ALA:HA    | 18:Af:176:ILE:HD11 | 1.95                     | 0.49              |
| 19:Ag:57:ARG:NH2    | 19:Ag:89:GLY:O     | 2.46                     | 0.49              |
| 39:B5:2249:G:N7     | 79:Bl:2:SER:N      | 2.60                     | 0.49              |
| 39:B5:2651:G:O3'    | 59:BR:60:ARG:NH1   | 2.45                     | 0.49              |
| 51:BJ:160:GLU:OE1   | 51:BJ:160:GLU:N    | 2.45                     | 0.49              |
| 57:BP:64:ASN:ND2    | 57:BP:80:GLN:OE1   | 2.41                     | 0.49              |
| 65:BX:82:THR:HG21   | 75:Bh:37:THR:HG22  | 1.93                     | 0.49              |
| 1:A2:46:A:OP2       | 95:A2:2104:HOH:O   | 2.18                     | 0.49              |
| 1:A2:1755:G:H1      | 1:A2:1779:C:H42    | 1.59                     | 0.49              |
| 7:AF:119:GLN:HB3    | 7:AF:131:LEU:HD11  | 1.93                     | 0.49              |
| 39:B5:158:A:N1      | 39:B5:276:C:O2'    | 2.42                     | 0.49              |
| 39:B5:172:C:N3      | 39:B5:266:C:N4     | 2.60                     | 0.49              |
| 39:B5:1601:A:O2'    | 77:Bj:49:TRP:O     | 2.26                     | 0.49              |
| 39:B5:2258:OMU:HM22 | 39:B5:2259:G:H5'   | 1.95                     | 0.49              |
| 46:BE:45:HIS:ND1    | 46:BE:46:CYS:O     | 2.44                     | 0.49              |
| 1:A2:434:A:H5''     | 20:Ah:22:HIS:HB3   | 1.94                     | 0.49              |
| 1:A2:589:G:OP2      | 1:A2:589:G:N2      | 2.36                     | 0.49              |
| 27:Ao:56:LEU:HD23   | 27:Ao:83:MET:HG2   | 1.95                     | 0.49              |
| 28:Ap:16:LYS:HG3    | 28:Ap:17:LYS:H     | 1.77                     | 0.49              |
| 39:B5:1866:U:OP1    | 39:B5:1888:U:O2'   | 2.26                     | 0.49              |
| 39:B5:2400:G:H1     | 39:B5:2413:U:H3    | 1.61                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:B5:2602:G:O2'    | 39:B5:2605:G:N2    | 2.45                     | 0.49              |
| 39:B5:2658:A2M:HM'2 | 39:B5:2659:G:H5'   | 1.95                     | 0.49              |
| 41:B8:149:G:H21     | 48:BG:64:GLN:HE22  | 1.61                     | 0.49              |
| 85:Bt:133:LEU:HD11  | 85:Bt:151:ILE:HG23 | 1.93                     | 0.49              |
| 16:Ad:44:LEU:HD21   | 16:Ad:72:ILE:HD11  | 1.95                     | 0.49              |
| 39:B5:4632:A:OP1    | 56:BO:188:LYS:NZ   | 2.45                     | 0.49              |
| 7:AF:203:ASP:OD1    | 7:AF:205:SER:OG    | 2.29                     | 0.49              |
| 12:AZ:41:ARG:HE     | 12:AZ:45:GLY:HA2   | 1.78                     | 0.49              |
| 13:Aa:30:TRP:CE2    | 26:An:19:PRO:HD3   | 2.47                     | 0.49              |
| 16:Ad:112:HIS:NE2   | 16:Ad:237:SER:O    | 2.45                     | 0.49              |
| 25:Am:101:HIS:HA    | 25:Am:104:ARG:HH21 | 1.78                     | 0.49              |
| 42:BA:204:MET:HB3   | 42:BA:208:GLU:HG3  | 1.95                     | 0.49              |
| 51:BJ:90:ARG:NH2    | 51:BJ:108:GLY:O    | 2.46                     | 0.49              |
| 84:Bs:58:ASN:ND2    | 84:Bs:84:GLY:O     | 2.37                     | 0.49              |
| 1:A2:686:A:H5''     | 34:Av:31:SER:HB3   | 1.95                     | 0.49              |
| 1:A2:1059:A:OP1     | 11:AT:38:A:O2'     | 2.30                     | 0.49              |
| 1:A2:1162:U:O4      | 35:Aw:2:GLY:N      | 2.46                     | 0.49              |
| 1:A2:1446:PSU:O2    | 1:A2:1447:A:N6     | 2.45                     | 0.49              |
| 28:Ap:19:ALA:HB2    | 28:Ap:75:GLY:HA3   | 1.95                     | 0.49              |
| 28:Ap:89:SER:HB3    | 28:Ap:112:LEU:HD13 | 1.94                     | 0.49              |
| 66:BY:31:SER:HA     | 66:BY:48:PRO:HA    | 1.95                     | 0.49              |
| 67:BZ:50:PRO:HD3    | 67:BZ:68:ILE:HG12  | 1.95                     | 0.49              |
| 68:Ba:89:ASN:OD1    | 68:Ba:92:LYS:NZ    | 2.45                     | 0.49              |
| 74:Bg:60:ARG:HB2    | 74:Bg:63:VAL:HG23  | 1.95                     | 0.49              |
| 85:Bt:14:TYR:O      | 85:Bt:31:LYS:NZ    | 2.39                     | 0.49              |
| 88:Bz:332:LYS:H     | 88:Bz:332:LYS:HD2  | 1.78                     | 0.49              |
| 88:Bz:379:GLY:HA3   | 88:Bz:535:PHE:HB2  | 1.93                     | 0.49              |
| 1:A2:35:C:H2'       | 1:A2:36:PSU:H6     | 1.78                     | 0.49              |
| 1:A2:1098:G:H4'     | 12:AZ:32:PHE:CD1   | 2.48                     | 0.49              |
| 1:A2:1249:B8N:O2'   | 28:Ap:145:TYR:O    | 2.30                     | 0.49              |
| 1:A2:1544:U:OP2     | 31:As:62:ARG:NH2   | 2.31                     | 0.49              |
| 7:AF:42:MET:O       | 7:AF:56:GLN:N      | 2.44                     | 0.49              |
| 8:AG:17:GLY:O       | 8:AG:27:ARG:NH1    | 2.46                     | 0.49              |
| 12:AZ:85:ARG:NH2    | 29:Aq:82:ASP:O     | 2.44                     | 0.49              |
| 16:Ad:43:PRO:HD2    | 16:Ad:46:ILE:HD12  | 1.95                     | 0.49              |
| 30:Ar:35:GLY:O      | 30:Ar:97:GLN:NE2   | 2.46                     | 0.49              |
| 39:B5:1105:C:C5     | 69:Bb:92:LYS:HD2   | 2.47                     | 0.49              |
| 39:B5:2178:C:H2'    | 39:B5:2179:G:H8    | 1.78                     | 0.49              |
| 67:BZ:87:VAL:HG12   | 67:BZ:89:ILE:HG13  | 1.95                     | 0.49              |
| 1:A2:465:A:OP1      | 88:Bz:576:ARG:NH1  | 2.45                     | 0.48              |
| 39:B5:2745:G:OP2    | 39:B5:3328:A:N6    | 2.38                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:B5:4254:C:H5''  | 63:BV:43:LYS:HD3   | 1.96                     | 0.48              |
| 44:BC:133:LEU:HD13 | 83:Br:6:GLN:HE21   | 1.77                     | 0.48              |
| 86:Bv:204:LEU:N    | 86:Bv:216:LEU:O    | 2.41                     | 0.48              |
| 87:By:283:GLU:HG3  | 87:By:392:VAL:HG12 | 1.94                     | 0.48              |
| 1:A2:1532:A:H4'    | 1:A2:1606:G:H4'    | 1.94                     | 0.48              |
| 2:AA:28:PRO:HG3    | 25:Am:17:PRO:HG3   | 1.94                     | 0.48              |
| 16:Ad:11:ARG:HA    | 16:Ad:28:ALA:HB2   | 1.94                     | 0.48              |
| 16:Ad:124:CYS:HB3  | 16:Ad:141:THR:HB   | 1.95                     | 0.48              |
| 19:Ag:112:ASN:OD1  | 19:Ag:113:LYS:N    | 2.43                     | 0.48              |
| 20:Ah:22:HIS:ND1   | 20:Ah:23:LYS:O     | 2.38                     | 0.48              |
| 39:B5:1624:A:N3    | 39:B5:1791:U:O2'   | 2.41                     | 0.48              |
| 39:B5:4213:A:O2'   | 39:B5:4256:A:N3    | 2.43                     | 0.48              |
| 51:BJ:15:LEU:HD12  | 51:BJ:165:TRP:HB2  | 1.93                     | 0.48              |
| 64:BW:71:ARG:NH1   | 64:BW:71:ARG:HA    | 2.28                     | 0.48              |
| 84:Bs:26:LYS:NZ    | 84:Bs:193:PHE:O    | 2.43                     | 0.48              |
| 1:A2:75:G:O2'      | 1:A2:77:A:OP1      | 2.31                     | 0.48              |
| 1:A2:953:G:H21     | 26:An:52:THR:HG21  | 1.77                     | 0.48              |
| 10:AI:8:N:H4'      | 10:AI:48:N:H4'     | 1.95                     | 0.48              |
| 19:Ag:160:LYS:HA   | 19:Ag:163:GLN:HB2  | 1.96                     | 0.48              |
| 26:An:151:LEU:H    | 26:An:151:LEU:HD23 | 1.77                     | 0.48              |
| 35:Aw:6:GLY:O      | 35:Aw:9:THR:OG1    | 2.31                     | 0.48              |
| 39:B5:62:A:N3      | 39:B5:77:U:O2'     | 2.40                     | 0.48              |
| 39:B5:307:A:OP1    | 76:Bi:86:LYS:NZ    | 2.47                     | 0.48              |
| 39:B5:684:C:OP2    | 46:BE:114:LYS:NZ   | 2.44                     | 0.48              |
| 39:B5:2318:G:N2    | 65:BX:51:THR:O     | 2.42                     | 0.48              |
| 66:BY:28:LYS:O     | 66:BY:31:SER:OG    | 2.27                     | 0.48              |
| 67:BZ:95:VAL:HG13  | 67:BZ:96:VAL:HG23  | 1.96                     | 0.48              |
| 1:A2:1100:G:H22    | 1:A2:1134:A:H2     | 1.60                     | 0.48              |
| 1:A2:1118:C:O2'    | 1:A2:1119:C:O4'    | 2.30                     | 0.48              |
| 32:At:50:VAL:HG12  | 32:At:91:LEU:HD22  | 1.95                     | 0.48              |
| 36:Ax:18:LEU:O     | 36:Ax:85:ASN:ND2   | 2.47                     | 0.48              |
| 39:B5:458:C:OP2    | 46:BE:117:ARG:NH1  | 2.47                     | 0.48              |
| 39:B5:2204:G:O2'   | 39:B5:3591:G:O6    | 2.27                     | 0.48              |
| 39:B5:4437:A:O2'   | 49:BH:68:ALA:O     | 2.28                     | 0.48              |
| 88:Bz:346:CYS:SG   | 88:Bz:348:TYR:OH   | 2.72                     | 0.48              |
| 1:A2:875:G:H2'     | 1:A2:876:A:H8      | 1.79                     | 0.48              |
| 39:B5:2169:G:H5''  | 72:Be:127:ALA:HB2  | 1.94                     | 0.48              |
| 42:BA:137:ILE:HD11 | 42:BA:149:LYS:HB2  | 1.95                     | 0.48              |
| 85:Bt:130:LYS:HD2  | 85:Bt:155:ILE:HG21 | 1.95                     | 0.48              |
| 1:A2:74:G:H1       | 18:Af:171:THR:N    | 2.11                     | 0.48              |
| 17:Ae:164:ARG:HB3  | 37:Ay:41:ARG:HH12  | 1.78                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:Am:20:ARG:HH21   | 34:Av:56:HIS:HB3   | 1.77                     | 0.48              |
| 26:An:95:ILE:HB     | 26:An:129:ILE:HG12 | 1.95                     | 0.48              |
| 39:B5:3978:U:O4     | 81:Bo:8:ARG:NH2    | 2.46                     | 0.48              |
| 46:BE:97:LYS:HD2    | 46:BE:110:VAL:HG21 | 1.96                     | 0.48              |
| 53:BL:12:PRO:HB2    | 53:BL:14:PHE:HD2   | 1.78                     | 0.48              |
| 73:Bf:36:ARG:HB2    | 73:Bf:80:ASN:HA    | 1.95                     | 0.48              |
| 1:A2:497:C:OP1      | 16:Ad:49:ARG:NH2   | 2.37                     | 0.48              |
| 1:A2:862:A:N6       | 19:Ag:106:ARG:HG2  | 2.29                     | 0.48              |
| 1:A2:1275:G:N7      | 8:AG:7:TYR:OH      | 2.44                     | 0.48              |
| 1:A2:1550:U:OP1     | 8:AG:34:TYR:OH     | 2.21                     | 0.48              |
| 1:A2:1567:G:N7      | 31:As:101:ARG:NH2  | 2.62                     | 0.48              |
| 13:Aa:32:ASP:OD1    | 13:Aa:46:LYS:NZ    | 2.45                     | 0.48              |
| 39:B5:48:G:OP1      | 55:BN:192:TRP:NE1  | 2.38                     | 0.48              |
| 39:B5:3450:A2M:HM'2 | 39:B5:3451:A:H5'   | 1.95                     | 0.48              |
| 56:BO:125:LYS:HG2   | 56:BO:129:LEU:HD12 | 1.96                     | 0.48              |
| 70:Bc:4:ALA:O       | 70:Bc:7:THR:OG1    | 2.29                     | 0.48              |
| 87:By:312:LEU:HD12  | 87:By:317:VAL:HG11 | 1.95                     | 0.48              |
| 87:By:335:CYS:HB2   | 87:By:366:HIS:HA   | 1.95                     | 0.48              |
| 1:A2:549:C:H4'      | 1:A2:550:C:O5'     | 2.14                     | 0.48              |
| 1:A2:1266:A:OP1     | 95:A2:2105:HOH:O   | 2.19                     | 0.48              |
| 1:A2:1338:4AC:H2'   | 1:A2:1339:G:H8     | 1.79                     | 0.48              |
| 1:A2:1809:U:H2'     | 1:A2:1810:A:C8     | 2.48                     | 0.48              |
| 11:AT:9:G:H21       | 11:AT:45:G:H2'     | 1.78                     | 0.48              |
| 16:Ad:80:ILE:HG13   | 16:Ad:81:THR:HG23  | 1.94                     | 0.48              |
| 39:B5:1844:U:OP2    | 73:Bf:76:ARG:NH1   | 2.40                     | 0.48              |
| 39:B5:2385:G:H4'    | 41:B8:128:C:H4'    | 1.96                     | 0.48              |
| 49:BH:41:ILE:HG22   | 49:BH:43:VAL:HG13  | 1.96                     | 0.48              |
| 53:BL:90:VAL:O      | 53:BL:93:THR:OG1   | 2.26                     | 0.48              |
| 68:Ba:100:ILE:HG13  | 68:Ba:123:ILE:HB   | 1.95                     | 0.48              |
| 1:A2:602:OMG:HM22   | 1:A2:603:G:H5'     | 1.95                     | 0.48              |
| 1:A2:824:U:N3       | 21:Ai:143:ASN:OD1  | 2.43                     | 0.48              |
| 39:B5:4316:G:H2'    | 39:B5:4317:A2M:H8  | 1.96                     | 0.48              |
| 50:BI:187:GLU:HG3   | 50:BI:189:ARG:HG3  | 1.94                     | 0.48              |
| 1:A2:465:A:H5'      | 1:A2:466:A:C8      | 2.49                     | 0.48              |
| 1:A2:535:G:H2'      | 1:A2:536:G:C8      | 2.49                     | 0.48              |
| 3:AB:32:VAL:HG11    | 3:AB:56:LEU:HD12   | 1.95                     | 0.48              |
| 39:B5:642:G:H2'     | 39:B5:643:A:H8     | 1.79                     | 0.48              |
| 39:B5:788:G:H2'     | 39:B5:789:G:C8     | 2.48                     | 0.48              |
| 77:Bj:27:TYR:HA     | 77:Bj:34:CYS:HA    | 1.96                     | 0.48              |
| 1:A2:1758:G:H1      | 1:A2:1776:U:H3     | 1.62                     | 0.47              |
| 1:A2:1865:U:H5'     | 6:AE:79:ILE:HD11   | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AZ:9:GLN:O      | 12:AZ:11:LYS:NZ    | 2.43                     | 0.47              |
| 13:Aa:44:ILE:HD12  | 13:Aa:69:VAL:HG21  | 1.96                     | 0.47              |
| 28:Ap:131:LYS:HB2  | 28:Ap:140:ARG:HH12 | 1.79                     | 0.47              |
| 39:B5:66:A:O2'     | 39:B5:326:C:O2     | 2.28                     | 0.47              |
| 39:B5:2028:G:OP2   | 44:BC:294:LYS:NZ   | 2.44                     | 0.47              |
| 51:BJ:13:ARG:O     | 51:BJ:136:ARG:NH1  | 2.47                     | 0.47              |
| 81:Bo:74:GLU:HB3   | 81:Bo:77:CYS:HB3   | 1.96                     | 0.47              |
| 87:By:323:TYR:HB2  | 87:By:408:GLY:HA3  | 1.95                     | 0.47              |
| 1:A2:868:OMG:H5''  | 23:Ak:149:ALA:HB2  | 1.96                     | 0.47              |
| 1:A2:1320:U:H2'    | 1:A2:1321:G:C8     | 2.48                     | 0.47              |
| 1:A2:1446:PSU:H1'  | 1:A2:1581:A:N6     | 2.29                     | 0.47              |
| 11:AT:9:G:N1       | 11:AT:21:A:H2'     | 2.30                     | 0.47              |
| 17:Ae:40:ALA:HB1   | 17:Ae:45:TYR:CG    | 2.49                     | 0.47              |
| 23:Ak:126:VAL:HG12 | 23:Ak:145:VAL:HG22 | 1.95                     | 0.47              |
| 26:An:101:GLY:HA3  | 26:An:134:PRO:HG2  | 1.96                     | 0.47              |
| 39:B5:4627:C:H2'   | 39:B5:4628:G:H8    | 1.79                     | 0.47              |
| 44:BC:218:VAL:HA   | 44:BC:229:LEU:HG   | 1.95                     | 0.47              |
| 45:BD:65:ALA:HB2   | 45:BD:74:ILE:HD13  | 1.95                     | 0.47              |
| 56:BO:74:ARG:NH1   | 56:BO:145:VAL:O    | 2.46                     | 0.47              |
| 85:Bt:133:LEU:HD22 | 85:Bt:152:ILE:HD12 | 1.97                     | 0.47              |
| 7:AF:25:PRO:HA     | 7:AF:293:ALA:HB2   | 1.97                     | 0.47              |
| 14:Ab:81:ILE:HG23  | 14:Ab:86:LEU:HB2   | 1.95                     | 0.47              |
| 19:Ag:8:ILE:HD13   | 19:Ag:16:PRO:HB3   | 1.95                     | 0.47              |
| 20:Ah:11:ARG:NH1   | 20:Ah:15:GLY:O     | 2.44                     | 0.47              |
| 39:B5:3954:U:OP2   | 61:BT:4:THR:OG1    | 2.31                     | 0.47              |
| 39:B5:4060:C:O2'   | 69:Bb:36:ASP:OD1   | 2.28                     | 0.47              |
| 88:Bz:354:LYS:HG2  | 88:Bz:363:ALA:HA   | 1.95                     | 0.47              |
| 1:A2:1566:C:OP2    | 31:As:101:ARG:NH1  | 2.47                     | 0.47              |
| 1:A2:1861:A:N7     | 6:AE:34:LYS:NZ     | 2.63                     | 0.47              |
| 6:AE:24:THR:HG21   | 6:AE:71:LEU:HD22   | 1.95                     | 0.47              |
| 13:Aa:30:TRP:CE2   | 13:Aa:48:LEU:HD13  | 2.49                     | 0.47              |
| 35:Aw:60:LYS:HG3   | 35:Aw:116:PRO:HG3  | 1.96                     | 0.47              |
| 39:B5:1737:G:O2'   | 61:BT:60:LYS:NZ    | 2.47                     | 0.47              |
| 39:B5:4508:G:OP2   | 56:BO:37:ARG:NH1   | 2.41                     | 0.47              |
| 45:BD:37:VAL:HG12  | 45:BD:50:ARG:HD3   | 1.95                     | 0.47              |
| 46:BE:136:PHE:O    | 46:BE:141:ARG:NH2  | 2.47                     | 0.47              |
| 48:BG:229:ARG:NE   | 48:BG:232:GLU:OE2  | 2.48                     | 0.47              |
| 1:A2:168:C:OP1     | 18:Af:131:ARG:NH2  | 2.47                     | 0.47              |
| 1:A2:1651:A:H5''   | 28:Ap:139:ALA:HB2  | 1.95                     | 0.47              |
| 21:Ai:110:LEU:HB2  | 21:Ai:147:PHE:HB3  | 1.95                     | 0.47              |
| 39:B5:85:G:O2'     | 39:B5:97:G:O6      | 2.26                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:B5:2366:G:OP1    | 59:BR:16:ARG:NH2   | 2.40                     | 0.47              |
| 45:BD:125:VAL:HG11  | 45:BD:199:ILE:HG21 | 1.95                     | 0.47              |
| 55:BN:8:GLN:OE1     | 55:BN:50:ARG:NH2   | 2.47                     | 0.47              |
| 66:BY:112:ASP:OD1   | 66:BY:112:ASP:N    | 2.47                     | 0.47              |
| 86:Bv:128:LEU:HD13  | 86:Bv:135:PRO:HD3  | 1.96                     | 0.47              |
| 1:A2:583:U:H1'      | 36:Ax:33:ALA:HB2   | 1.96                     | 0.47              |
| 1:A2:630:A:O2'      | 1:A2:632:U:OP1     | 2.32                     | 0.47              |
| 2:AA:16:LYS:HA      | 2:AA:23:ARG:HH21   | 1.79                     | 0.47              |
| 7:AF:78:ALA:HB3     | 7:AF:90:TRP:HB2    | 1.95                     | 0.47              |
| 36:Ax:87:PRO:HD2    | 36:Ax:90:ARG:HD2   | 1.97                     | 0.47              |
| 39:B5:3835:G:H2'    | 39:B5:3836:G:H8    | 1.79                     | 0.47              |
| 39:B5:4381:A:H3'    | 39:B5:4382:PSU:H4' | 1.97                     | 0.47              |
| 42:BA:140:ASN:ND2   | 42:BA:143:THR:OG1  | 2.47                     | 0.47              |
| 49:BH:59:LYS:HE2    | 49:BH:66:GLU:HB3   | 1.96                     | 0.47              |
| 6:AE:23:CYS:O       | 26:An:142:ARG:NH1  | 2.48                     | 0.47              |
| 11:AT:56:C:H2'      | 11:AT:57:G:C8      | 2.50                     | 0.47              |
| 20:Ah:113:TYR:OH    | 20:Ah:156:ALA:O    | 2.31                     | 0.47              |
| 22:Aj:63:ALA:HB3    | 22:Aj:68:TYR:HE2   | 1.79                     | 0.47              |
| 36:Ax:117:VAL:HG11  | 36:Ax:125:VAL:HG21 | 1.96                     | 0.47              |
| 39:B5:2245:G:O2'    | 74:Bg:10:ARG:O     | 2.32                     | 0.47              |
| 39:B5:4073:C:OP1    | 61:BT:70:HIS:NE2   | 2.47                     | 0.47              |
| 39:B5:4741:U:OP2    | 43:BB:385:LYS:NZ   | 2.34                     | 0.47              |
| 40:B7:117:G:H5''    | 45:BD:256:LYS:HD2  | 1.97                     | 0.47              |
| 45:BD:223:PHE:HB3   | 45:BD:226:TYR:HB2  | 1.95                     | 0.47              |
| 87:By:358:THR:HA    | 87:By:365:GLU:HB3  | 1.96                     | 0.47              |
| 88:Bz:188:LEU:HD22  | 88:Bz:232:ILE:HD12 | 1.95                     | 0.47              |
| 12:AZ:13:GLU:HG2    | 12:AZ:17:LYS:HE2   | 1.96                     | 0.47              |
| 13:Aa:175:GLU:O     | 13:Aa:187:LYS:NZ   | 2.47                     | 0.47              |
| 39:B5:19:G:P        | 75:Bh:93:ARG:HE    | 2.38                     | 0.47              |
| 39:B5:404:U:O3'     | 66:BY:87:ARG:NH2   | 2.46                     | 0.47              |
| 39:B5:420:A:HO2'    | 39:B5:1275:C:HO2'  | 1.59                     | 0.47              |
| 39:B5:2329:G:OP2    | 39:B5:2332:C:N4    | 2.45                     | 0.47              |
| 39:B5:3599:A2M:HM'3 | 39:B5:3612:G:H21   | 1.80                     | 0.47              |
| 39:B5:4283:C:H2'    | 39:B5:4284:G:C8    | 2.50                     | 0.47              |
| 48:BG:51:LEU:O      | 48:BG:55:VAL:HG23  | 2.15                     | 0.47              |
| 84:Bs:161:ILE:HG21  | 84:Bs:167:VAL:HG22 | 1.96                     | 0.47              |
| 1:A2:485:A2M:O5'    | 1:A2:485:A2M:H8    | 2.15                     | 0.47              |
| 1:A2:571:C:O2'      | 36:Ax:34:THR:O     | 2.28                     | 0.47              |
| 11:AT:65:PSU:N3     | 11:AT:68:A:OP2     | 2.42                     | 0.47              |
| 12:AZ:79:SER:HA     | 12:AZ:101:GLY:HA2  | 1.97                     | 0.47              |
| 37:Ay:58:LEU:HD12   | 37:Ay:62:VAL:HG21  | 1.97                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:B5:1283:U:OP1    | 68:Ba:8:THR:OG1    | 2.30                     | 0.47              |
| 39:B5:1532:G:O2'    | 39:B5:1567:G:H4'   | 2.14                     | 0.47              |
| 39:B5:3380:A:H1'    | 39:B5:3517:A2M:N6  | 2.30                     | 0.47              |
| 47:BF:189:LEU:HD21  | 47:BF:207:LEU:HD21 | 1.96                     | 0.47              |
| 55:BN:42:PRO:HG3    | 55:BN:61:ILE:HG13  | 1.95                     | 0.47              |
| 64:BW:60:LYS:HB3    | 64:BW:63:GLN:HB2   | 1.97                     | 0.47              |
| 88:Bz:423:SER:HA    | 88:Bz:458:GLU:HA   | 1.97                     | 0.47              |
| 1:A2:751:C:H2'      | 1:A2:752:G:C8      | 2.49                     | 0.47              |
| 1:A2:1240:U:H5''    | 27:Ao:124:LYS:HD3  | 1.97                     | 0.47              |
| 39:B5:1449:U:H2'    | 39:B5:1450:G:H8    | 1.80                     | 0.47              |
| 39:B5:3599:A2M:HM'3 | 39:B5:3612:G:N2    | 2.30                     | 0.47              |
| 39:B5:4486:G:H2'    | 39:B5:4489:G:H5'   | 1.97                     | 0.47              |
| 43:BB:220:ILE:HG12  | 43:BB:278:THR:HG23 | 1.97                     | 0.47              |
| 86:Bv:26:ARG:HG3    | 86:Bv:30:GLU:HG3   | 1.97                     | 0.47              |
| 1:A2:4:C:H4'        | 14:Ab:207:ALA:HB2  | 1.97                     | 0.46              |
| 1:A2:1804:U:H2'     | 1:A2:1805:OMU:H6   | 1.97                     | 0.46              |
| 7:AF:152:SER:HB2    | 7:AF:168:CYS:SG    | 2.55                     | 0.46              |
| 39:B5:1341:A:N1     | 39:B5:1453:G:O2'   | 2.42                     | 0.46              |
| 39:B5:1827:A:N6     | 39:B5:3605:G:O2'   | 2.48                     | 0.46              |
| 39:B5:4794:G:N2     | 71:Bd:118:GLN:OE1  | 2.42                     | 0.46              |
| 43:BB:95:THR:OG1    | 43:BB:98:GLY:O     | 2.26                     | 0.46              |
| 44:BC:159:GLU:HA    | 44:BC:217:ILE:HB   | 1.97                     | 0.46              |
| 44:BC:221:PHE:HB3   | 44:BC:227:ILE:HG21 | 1.97                     | 0.46              |
| 51:BJ:159:LYS:HG2   | 51:BJ:163:MET:HE2  | 1.96                     | 0.46              |
| 53:BL:7:GLY:O       | 68:Ba:49:HIS:NE2   | 2.41                     | 0.46              |
| 62:BU:36:ALA:HB3    | 62:BU:65:ARG:HH21  | 1.80                     | 0.46              |
| 1:A2:156:G:OP1      | 18:Af:2:LYS:NZ     | 2.43                     | 0.46              |
| 1:A2:518:OMC:HM22   | 1:A2:519:G:H5'     | 1.97                     | 0.46              |
| 1:A2:526:A:H2'      | 1:A2:527:A:H8      | 1.80                     | 0.46              |
| 1:A2:563:U:H2'      | 1:A2:564:G:C8      | 2.49                     | 0.46              |
| 1:A2:1230:G:OP1     | 37:Ay:32:LYS:NZ    | 2.48                     | 0.46              |
| 21:Ai:160:SER:HB3   | 21:Ai:163:SER:HB2  | 1.97                     | 0.46              |
| 42:BA:118:GLU:HG3   | 42:BA:156:LYS:HZ3  | 1.81                     | 0.46              |
| 46:BE:246:THR:HG22  | 46:BE:248:GLN:H    | 1.78                     | 0.46              |
| 56:BO:128:ARG:NH1   | 60:BS:162:GLN:OE1  | 2.44                     | 0.46              |
| 85:Bt:18:THR:OG1    | 85:Bt:21:GLU:O     | 2.27                     | 0.46              |
| 85:Bt:52:ASP:OD1    | 85:Bt:52:ASP:N     | 2.45                     | 0.46              |
| 87:By:251:LEU:HD13  | 87:By:278:VAL:HG21 | 1.97                     | 0.46              |
| 1:A2:1678:U:H2'     | 1:A2:1679:A2M:H8   | 1.96                     | 0.46              |
| 1:A2:1732:A:H2'     | 1:A2:1733:G:C8     | 2.50                     | 0.46              |
| 4:AC:102:VAL:HG21   | 24:Al:35:ILE:HG21  | 1.98                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:Ag:37:LYS:HE3    | 19:Ag:41:ARG:HE    | 1.79                     | 0.46              |
| 39:B5:519:C:H2'     | 39:B5:520:G:H8     | 1.80                     | 0.46              |
| 39:B5:1225:G:H5'    | 44:BC:323:ARG:HB2  | 1.96                     | 0.46              |
| 39:B5:2205:U:OP1    | 57:BP:82:ARG:NH2   | 2.49                     | 0.46              |
| 39:B5:3476:OMG:HM22 | 39:B5:3477:U:H5'   | 1.97                     | 0.46              |
| 40:B7:6:C:O2'       | 45:BD:50:ARG:NH2   | 2.48                     | 0.46              |
| 88:Bz:121:LYS:HE2   | 88:Bz:127:GLN:HB2  | 1.98                     | 0.46              |
| 1:A2:381:G:OP1      | 20:Ah:56:ARG:NH2   | 2.48                     | 0.46              |
| 1:A2:660:G:H21      | 35:Aw:17:ARG:NH2   | 2.13                     | 0.46              |
| 1:A2:985:C:HO2'     | 26:An:138:ASP:CG   | 2.24                     | 0.46              |
| 12:AZ:66:VAL:HG21   | 12:AZ:185:MET:HB2  | 1.97                     | 0.46              |
| 39:B5:4323:U:H2'    | 39:B5:4324:G:C8    | 2.50                     | 0.46              |
| 39:B5:4367:C:OP1    | 63:BV:48:ARG:HD2   | 2.15                     | 0.46              |
| 39:B5:4668:C:H5''   | 54:BM:114:LYS:HD2  | 1.98                     | 0.46              |
| 43:BB:41:VAL:HA     | 43:BB:187:GLY:HA3  | 1.97                     | 0.46              |
| 44:BC:317:ASN:HD22  | 44:BC:320:LYS:HD3  | 1.80                     | 0.46              |
| 46:BE:193:HIS:HB3   | 46:BE:196:PHE:HD2  | 1.79                     | 0.46              |
| 48:BG:150:LYS:HE3   | 48:BG:177:MET:HE3  | 1.97                     | 0.46              |
| 49:BH:95:VAL:HG22   | 80:Bm:82:LEU:HB3   | 1.98                     | 0.46              |
| 72:Be:35:TRP:CZ2    | 72:Be:56:PRO:HD2   | 2.51                     | 0.46              |
| 85:Bt:90:ARG:HD3    | 85:Bt:90:ARG:H     | 1.79                     | 0.46              |
| 1:A2:753:G:H1       | 1:A2:792:C:H42     | 1.64                     | 0.46              |
| 1:A2:963:A:N1       | 1:A2:1056:A:O2'    | 2.48                     | 0.46              |
| 18:Af:162:LEU:HD12  | 18:Af:170:ARG:HD2  | 1.96                     | 0.46              |
| 22:Aj:24:LYS:HB2    | 22:Aj:66:HIS:CE1   | 2.50                     | 0.46              |
| 31:As:116:ASP:HB3   | 31:As:122:LYS:HD3  | 1.97                     | 0.46              |
| 39:B5:2301:C:H5''   | 55:BN:67:ARG:HD2   | 1.97                     | 0.46              |
| 40:B7:120:U:H3'     | 45:BD:262:LYS:HE2  | 1.98                     | 0.46              |
| 43:BB:231:VAL:HG21  | 43:BB:251:VAL:HG23 | 1.98                     | 0.46              |
| 51:BJ:144:LYS:HE3   | 51:BJ:147:ARG:O    | 2.15                     | 0.46              |
| 60:BS:154:LEU:HB3   | 60:BS:157:ARG:HD3  | 1.98                     | 0.46              |
| 1:A2:1522:C:H5'     | 27:Ao:126:VAL:HB   | 1.98                     | 0.46              |
| 1:A2:1564:G:OP1     | 31:As:121:ARG:NH1  | 2.47                     | 0.46              |
| 1:A2:1783:G:H3'     | 1:A2:1784:C:H4'    | 1.98                     | 0.46              |
| 18:Af:164:LYS:HG2   | 18:Af:165:GLU:H    | 1.81                     | 0.46              |
| 19:Ag:100:ILE:HG12  | 19:Ag:125:VAL:HG21 | 1.98                     | 0.46              |
| 21:Ai:107:GLU:HA    | 21:Ai:112:THR:HG21 | 1.97                     | 0.46              |
| 40:B7:48:G:OP1      | 45:BD:226:TYR:OH   | 2.32                     | 0.46              |
| 45:BD:108:ARG:CZ    | 45:BD:253:TYR:HB2  | 2.46                     | 0.46              |
| 50:BI:107:GLY:HA2   | 50:BI:111:LEU:HD21 | 1.97                     | 0.46              |
| 50:BI:145:LYS:HE2   | 50:BI:167:ILE:HG13 | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:BZ:92:ASP:HB3   | 67:BZ:95:VAL:HG12  | 1.98                     | 0.46              |
| 88:Bz:264:ASN:HB2  | 88:Bz:267:ARG:HG3  | 1.98                     | 0.46              |
| 1:A2:1172:G:O2'    | 1:A2:1188:G:O6     | 2.33                     | 0.46              |
| 1:A2:1830:G:H1'    | 1:A2:1851:MA6:H2   | 1.98                     | 0.46              |
| 9:AH:3458:C:H42    | 17:Ae:135:ARG:HH12 | 1.64                     | 0.46              |
| 18:Af:148:SER:N    | 18:Af:151:ASP:OD2  | 2.48                     | 0.46              |
| 24:Al:75:ASN:OD1   | 24:Al:75:ASN:N     | 2.48                     | 0.46              |
| 32:At:20:ILE:HG12  | 32:At:98:VAL:HG21  | 1.98                     | 0.46              |
| 39:B5:178:C:H2'    | 39:B5:179:G:C8     | 2.50                     | 0.46              |
| 39:B5:1891:G:OP1   | 60:BS:139:ARG:NE   | 2.46                     | 0.46              |
| 39:B5:3413:G:OP2   | 42:BA:128:ARG:NH2  | 2.48                     | 0.46              |
| 39:B5:3909:U:OP2   | 48:BG:53:ARG:NH1   | 2.43                     | 0.46              |
| 39:B5:4261:G:H5''  | 43:BB:3:HIS:CE1    | 2.51                     | 0.46              |
| 1:A2:658:U:O2      | 95:A2:2106:HOH:O   | 2.20                     | 0.46              |
| 1:A2:1525:G:O2'    | 11:AT:30:G:OP1     | 2.33                     | 0.46              |
| 12:AZ:77:ILE:HG21  | 12:AZ:133:PRO:HG3  | 1.98                     | 0.46              |
| 22:Aj:61:GLN:O     | 22:Aj:68:TYR:N     | 2.49                     | 0.46              |
| 39:B5:1473:A:N6    | 53:BL:19:GLN:OE1   | 2.47                     | 0.46              |
| 39:B5:2318:G:H4'   | 39:B5:2319:G:H8    | 1.80                     | 0.46              |
| 39:B5:3894:C:OP1   | 67:BZ:59:LYS:NZ    | 2.31                     | 0.46              |
| 39:B5:4620:U:C4    | 54:BM:113:MET:HG3  | 2.50                     | 0.46              |
| 42:BA:20:VAL:HG12  | 42:BA:23:ARG:HD2   | 1.96                     | 0.46              |
| 1:A2:613:U:H4'     | 5:AD:89:GLN:NE2    | 2.31                     | 0.46              |
| 1:A2:1233:PSU:H2'  | 1:A2:1234:G:H8     | 1.81                     | 0.46              |
| 1:A2:1521:G:H21    | 27:Ao:126:VAL:HG11 | 1.80                     | 0.46              |
| 11:AT:20:U:H2'     | 11:AT:21:A:O4'     | 2.15                     | 0.46              |
| 33:AU:33:GLN:HE21  | 33:AU:52:THR:HG21  | 1.81                     | 0.46              |
| 39:B5:878:G:O2'    | 44:BC:333:LYS:NZ   | 2.39                     | 0.46              |
| 39:B5:1757:G:OP2   | 39:B5:1757:G:N2    | 2.32                     | 0.46              |
| 39:B5:1820:OMC:OP2 | 95:B5:5413:HOH:O   | 2.20                     | 0.46              |
| 44:BC:108:TRP:O    | 55:BN:204:ARG:NH2  | 2.49                     | 0.46              |
| 88:Bz:395:ARG:NH1  | 88:Bz:407:LEU:O    | 2.49                     | 0.46              |
| 7:AF:91:ASP:OD2    | 7:AF:93:THR:OG1    | 2.27                     | 0.46              |
| 14:Ab:110:MET:HG3  | 14:Ab:125:LYS:HB3  | 1.97                     | 0.46              |
| 17:Ae:80:GLY:HA2   | 17:Ae:83:ASN:ND2   | 2.30                     | 0.46              |
| 39:B5:99:A:H5''    | 55:BN:184:ILE:HD12 | 1.98                     | 0.46              |
| 39:B5:1784:U:H2'   | 39:B5:1785:G:H8    | 1.81                     | 0.46              |
| 39:B5:2597:G:N7    | 95:B5:5497:HOH:O   | 2.36                     | 0.46              |
| 39:B5:3486:G:H1    | 39:B5:3502:PSU:HN3 | 1.64                     | 0.46              |
| 41:B8:58:G:N7      | 77:Bj:63:ARG:NH1   | 2.56                     | 0.46              |
| 86:Bv:207:LYS:HB3  | 86:Bv:213:PRO:HA   | 1.98                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:AF:278:SER:HB2    | 7:AF:281:ALA:HB3   | 1.98                     | 0.45              |
| 15:Ac:39:VAL:HG22   | 15:Ac:48:ILE:HG22  | 1.97                     | 0.45              |
| 29:Aq:44:LYS:HG3    | 29:Aq:47:ARG:HH21  | 1.81                     | 0.45              |
| 39:B5:793:C:N3      | 39:B5:794:G:N1     | 2.64                     | 0.45              |
| 39:B5:1270:A2M:HM'2 | 39:B5:1271:C:O4'   | 2.15                     | 0.45              |
| 39:B5:2544:U:H2'    | 39:B5:2545:C:C6    | 2.52                     | 0.45              |
| 39:B5:3502:PSU:H2'  | 39:B5:3503:C:C6    | 2.51                     | 0.45              |
| 41:B8:90:C:H2'      | 41:B8:91:A:C8      | 2.51                     | 0.45              |
| 44:BC:66:SER:HA     | 44:BC:77:PRO:HA    | 1.96                     | 0.45              |
| 87:By:113:ASP:N     | 87:By:113:ASP:OD1  | 2.49                     | 0.45              |
| 1:A2:661:C:OP1      | 35:Aw:17:ARG:NH2   | 2.46                     | 0.45              |
| 1:A2:1666:G:OP1     | 31:As:91:HIS:NE2   | 2.34                     | 0.45              |
| 18:Af:121:ILE:O     | 18:Af:125:THR:OG1  | 2.33                     | 0.45              |
| 20:Ah:3:ILE:O       | 20:Ah:30:GLY:N     | 2.45                     | 0.45              |
| 1:A2:26:U:H2'       | 1:A2:27:A2M:H8     | 1.97                     | 0.45              |
| 1:A2:65:C:C6        | 18:Af:174:PRO:HB3  | 2.51                     | 0.45              |
| 14:Ab:252:THR:OG1   | 14:Ab:254:ASP:OD1  | 2.26                     | 0.45              |
| 16:Ad:100:ARG:HB2   | 16:Ad:114:ILE:HD13 | 1.97                     | 0.45              |
| 17:Ae:126:THR:HG23  | 17:Ae:128:ILE:HG13 | 1.99                     | 0.45              |
| 26:An:98:ARG:HB3    | 26:An:132:VAL:HG23 | 1.98                     | 0.45              |
| 39:B5:2742:C:OP1    | 59:BR:108:ARG:NH2  | 2.36                     | 0.45              |
| 39:B5:3588:A:H5''   | 57:BP:83:TRP:O     | 2.16                     | 0.45              |
| 42:BA:2:GLY:HA2     | 42:BA:207:VAL:HG23 | 1.97                     | 0.45              |
| 43:BB:77:THR:HG21   | 43:BB:337:VAL:HG22 | 1.98                     | 0.45              |
| 46:BE:167:PHE:HA    | 46:BE:178:VAL:HG12 | 1.97                     | 0.45              |
| 84:Bs:53:VAL:HG22   | 84:Bs:89:VAL:HG13  | 1.99                     | 0.45              |
| 84:Bs:65:ILE:HG23   | 84:Bs:75:LEU:HD13  | 1.99                     | 0.45              |
| 87:By:152:ASP:OD1   | 87:By:153:GLY:N    | 2.48                     | 0.45              |
| 1:A2:1787:U:H2'     | 1:A2:1788:G:H8     | 1.81                     | 0.45              |
| 7:AF:32:LEU:HD21    | 7:AF:92:LEU:HD11   | 1.99                     | 0.45              |
| 8:AG:33:LYS:HE2     | 8:AG:34:TYR:CZ     | 2.51                     | 0.45              |
| 11:AT:52:U:H2'      | 11:AT:53:G:C8      | 2.52                     | 0.45              |
| 35:Aw:28:LYS:HE2    | 35:Aw:32:LEU:HD22  | 1.99                     | 0.45              |
| 39:B5:2515:C:OP1    | 82:Bp:44:LYS:NZ    | 2.42                     | 0.45              |
| 39:B5:4012:G:N3     | 39:B5:4012:G:H2'   | 2.32                     | 0.45              |
| 41:B8:47:C:H1'      | 41:B8:61:A:H2'     | 1.97                     | 0.45              |
| 57:BP:131:ARG:HG3   | 57:BP:137:ASN:ND2  | 2.31                     | 0.45              |
| 87:By:87:LYS:HD3    | 87:By:88:VAL:H     | 1.81                     | 0.45              |
| 2:AA:67:THR:OG1     | 2:AA:70:LYS:O      | 2.34                     | 0.45              |
| 7:AF:154:VAL:O      | 7:AF:155:ARG:NH1   | 2.45                     | 0.45              |
| 13:Aa:99:ASN:OD1    | 13:Aa:100:PHE:N    | 2.49                     | 0.45              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 15:Ac:163:PRO:O     | 15:Ac:167:TYR:HB2 | 2.17                     | 0.45              |
| 39:B5:639:G:H2'     | 39:B5:640:G:H8    | 1.81                     | 0.45              |
| 39:B5:827:C:H2'     | 39:B5:828:A:C8    | 2.52                     | 0.45              |
| 39:B5:1284:OMC:HM22 | 39:B5:1285:U:H5'  | 1.98                     | 0.45              |
| 39:B5:1743:A:H5'    | 39:B5:1745:G:O4'  | 2.16                     | 0.45              |
| 39:B5:1980:A:N7     | 39:B5:4180:C:O2'  | 2.47                     | 0.45              |
| 39:B5:4621:U:OP1    | 54:BM:117:LYS:NZ  | 2.35                     | 0.45              |
| 41:B8:30:U:OP1      | 53:BL:34:ARG:NH2  | 2.44                     | 0.45              |
| 46:BE:155:ILE:O     | 46:BE:162:GLY:N   | 2.37                     | 0.45              |
| 59:BR:12:SER:OG     | 59:BR:17:CYS:O    | 2.24                     | 0.45              |
| 71:Bd:37:GLY:O      | 71:Bd:41:ARG:HG3  | 2.16                     | 0.45              |
| 84:Bs:47:LEU:HB3    | 84:Bs:51:ALA:HB3  | 1.98                     | 0.45              |
| 86:Bv:205:TYR:HD2   | 86:Bv:213:PRO:HB2 | 1.81                     | 0.45              |
| 88:Bz:85:HIS:HD2    | 88:Bz:129:PRO:HA  | 1.82                     | 0.45              |
| 1:A2:1330:U:O2'     | 1:A2:1333:A:OP2   | 2.23                     | 0.45              |
| 39:B5:529:U:O2      | 39:B5:627:G:N2    | 2.50                     | 0.45              |
| 39:B5:779:G:H2'     | 39:B5:780:G:H8    | 1.82                     | 0.45              |
| 39:B5:1572:G:H1'    | 39:B5:2356:A:N6   | 2.32                     | 0.45              |
| 39:B5:1672:G:N3     | 39:B5:3960:A:H2'  | 2.32                     | 0.45              |
| 39:B5:2243:G:H21    | 74:Bg:6:THR:HG22  | 1.80                     | 0.45              |
| 39:B5:2328:U:H2'    | 39:B5:2329:G:C8   | 2.51                     | 0.45              |
| 39:B5:2691:G:O2'    | 39:B5:3570:U:O4   | 2.26                     | 0.45              |
| 47:BF:121:PHE:O     | 47:BF:204:ASN:ND2 | 2.47                     | 0.45              |
| 52:BK:4374:GLY:HA3  | 57:BP:126:ARG:O   | 2.17                     | 0.45              |
| 58:BQ:172:ARG:HA    | 58:BQ:176:ARG:HD2 | 1.98                     | 0.45              |
| 1:A2:1229:A:H2'     | 1:A2:1230:G:C8    | 2.52                     | 0.45              |
| 7:AF:11:LEU:HB3     | 7:AF:43:TRP:CZ3   | 2.51                     | 0.45              |
| 16:Ad:86:PHE:CD2    | 16:Ad:87:MET:HG2  | 2.51                     | 0.45              |
| 20:Ah:80:ASP:OD1    | 20:Ah:81:VAL:N    | 2.47                     | 0.45              |
| 36:Ax:79:LEU:HG     | 36:Ax:83:LYS:HE3  | 1.97                     | 0.45              |
| 39:B5:1381:G:N1     | 39:B5:1413:C:OP2  | 2.44                     | 0.45              |
| 39:B5:2329:G:H2'    | 39:B5:2330:G:C8   | 2.51                     | 0.45              |
| 39:B5:2647:OMC:HM22 | 39:B5:2648:C:H5'  | 1.98                     | 0.45              |
| 39:B5:3562:A2M:HM'2 | 39:B5:3563:U:H5'  | 1.98                     | 0.45              |
| 39:B5:4270:G:C2     | 43:BB:252:ALA:HB1 | 2.52                     | 0.45              |
| 39:B5:4641:C:H2'    | 39:B5:4642:G:C8   | 2.52                     | 0.45              |
| 72:Be:23:HIS:HD2    | 72:Be:43:ASN:HD21 | 1.65                     | 0.45              |
| 73:Bf:7:CYS:HB2     | 73:Bf:103:VAL:HB  | 1.99                     | 0.45              |
| 87:By:145:LYS:O     | 87:By:222:ALA:N   | 2.47                     | 0.45              |
| 88:Bz:417:SER:OG    | 88:Bz:419:LYS:NZ  | 2.44                     | 0.45              |
| 1:A2:858:U:H2'      | 1:A2:859:A:C8     | 2.52                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 15:Ac:50:ILE:HD11   | 15:Ac:86:LEU:HD23  | 1.98                     | 0.45              |
| 16:Ad:100:ARG:NH2   | 16:Ad:118:GLU:O    | 2.50                     | 0.45              |
| 21:Ai:93:LYS:HB2    | 21:Ai:96:TYR:CD2   | 2.52                     | 0.45              |
| 39:B5:2473:U:OP1    | 62:BU:48:LYS:NZ    | 2.30                     | 0.45              |
| 39:B5:3524:OMG:HM22 | 39:B5:3525:U:H5'   | 1.97                     | 0.45              |
| 40:B7:47:G:H21      | 45:BD:222:GLN:HE22 | 1.63                     | 0.45              |
| 49:BH:173:ARG:NH1   | 80:Bm:125:LYS:O    | 2.43                     | 0.45              |
| 53:BL:40:GLN:O      | 53:BL:44:ARG:HG3   | 2.17                     | 0.45              |
| 88:Bz:255:ALA:O     | 88:Bz:258:THR:OG1  | 2.35                     | 0.45              |
| 1:A2:1316:U:H4'     | 22:Aj:2:LEU:HG     | 1.99                     | 0.45              |
| 25:Am:40:LEU:HB3    | 25:Am:45:LEU:HD12  | 1.98                     | 0.45              |
| 25:Am:48:SER:OG     | 25:Am:86:GLU:OE2   | 2.32                     | 0.45              |
| 31:As:76:THR:HG21   | 31:As:97:LYS:HG2   | 1.99                     | 0.45              |
| 36:Ax:7:ILE:HG22    | 36:Ax:27:VAL:HG22  | 1.99                     | 0.45              |
| 39:B5:2388:U:OP2    | 41:B8:125:C:N4     | 2.50                     | 0.45              |
| 39:B5:2539:A:H62    | 78:Bk:35:LYS:NZ    | 2.15                     | 0.45              |
| 47:BF:181:TYR:CZ    | 47:BF:202:GLU:HG2  | 2.52                     | 0.45              |
| 49:BH:63:ASN:O      | 49:BH:67:LEU:HG    | 2.17                     | 0.45              |
| 83:Br:63:VAL:HG22   | 83:Br:79:ARG:HG2   | 1.98                     | 0.45              |
| 87:By:32:THR:O      | 87:By:32:THR:OG1   | 2.28                     | 0.45              |
| 1:A2:51:U:H2'       | 1:A2:52:G:C8       | 2.52                     | 0.45              |
| 1:A2:1411:C:H2'     | 1:A2:1412:G:C8     | 2.52                     | 0.45              |
| 1:A2:1601:G:H4'     | 37:Ay:43:LYS:HE3   | 1.99                     | 0.45              |
| 5:AD:112:TYR:CG     | 21:Ai:33:GLY:HA3   | 2.52                     | 0.45              |
| 7:AF:5:MET:HG2      | 7:AF:312:VAL:HG22  | 1.99                     | 0.45              |
| 17:Ae:124:ASP:OD1   | 17:Ae:125:SER:N    | 2.44                     | 0.45              |
| 30:Ar:46:ARG:HH22   | 30:Ar:52:LEU:HD11  | 1.81                     | 0.45              |
| 35:Aw:131:LEU:HD11  | 35:Aw:135:LYS:HE3  | 1.98                     | 0.45              |
| 39:B5:267:G:OP1     | 75:Bh:109:ARG:NH2  | 2.45                     | 0.45              |
| 39:B5:3942:OMG:HM22 | 39:B5:3943:G:H5'   | 1.99                     | 0.45              |
| 41:B8:92:U:H2'      | 41:B8:93:C:O4'     | 2.17                     | 0.45              |
| 44:BC:60:HIS:NE2    | 44:BC:100:ARG:HD3  | 2.32                     | 0.45              |
| 45:BD:202:GLN:HE22  | 45:BD:237:GLU:HB2  | 1.81                     | 0.45              |
| 51:BJ:152:GLY:O     | 51:BJ:156:ARG:HG3  | 2.17                     | 0.45              |
| 63:BV:87:SER:HB3    | 64:BW:19:ARG:HH21  | 1.82                     | 0.45              |
| 87:By:89:PRO:HG2    | 87:By:93:LEU:HG    | 1.98                     | 0.45              |
| 14:Ab:169:TYR:OH    | 14:Ab:175:GLY:O    | 2.25                     | 0.44              |
| 21:Ai:83:ARG:HH21   | 21:Ai:150:ARG:NH1  | 2.15                     | 0.44              |
| 28:Ap:86:GLN:HE22   | 28:Ap:122:ALA:HB2  | 1.82                     | 0.44              |
| 34:Av:101:PHE:HA    | 34:Av:113:HIS:CE1  | 2.52                     | 0.44              |
| 39:B5:1217:G:H5''   | 69:Bb:117:ARG:HG2  | 1.99                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 43:BB:317:LEU:HB2   | 43:BB:372:SER:HB2  | 1.99                     | 0.44              |
| 58:BQ:53:MET:SD     | 58:BQ:143:ARG:NH2  | 2.90                     | 0.44              |
| 66:BY:2:LYS:HE3     | 66:BY:2:LYS:HB3    | 1.71                     | 0.44              |
| 78:Bk:33:LYS:HG2    | 78:Bk:46:VAL:HG22  | 1.98                     | 0.44              |
| 81:Bo:26:TYR:HB3    | 81:Bo:67:VAL:HB    | 1.99                     | 0.44              |
| 1:A2:656:A:H4'      | 1:A2:657:G:H3'     | 1.98                     | 0.44              |
| 1:A2:1631:A:H5''    | 30:Ar:37:GLY:H     | 1.81                     | 0.44              |
| 39:B5:769:C:H2'     | 39:B5:770:G:C8     | 2.53                     | 0.44              |
| 39:B5:1704:A:C6     | 39:B5:1705:A:H1'   | 2.52                     | 0.44              |
| 39:B5:1993:U:OP2    | 56:BO:44:SER:OG    | 2.33                     | 0.44              |
| 39:B5:2386:A:H2'    | 39:B5:2387:G:C8    | 2.53                     | 0.44              |
| 39:B5:4436:G:N1     | 39:B5:4445:U:OP1   | 2.41                     | 0.44              |
| 41:B8:8:U:H2'       | 41:B8:9:A:C8       | 2.52                     | 0.44              |
| 1:A2:1018:U:H5'     | 25:Am:55:ARG:HE    | 1.82                     | 0.44              |
| 1:A2:1599:G:OP1     | 37:Ay:80:ARG:NH1   | 2.50                     | 0.44              |
| 15:Ac:106:ARG:HG3   | 15:Ac:175:VAL:HB   | 2.00                     | 0.44              |
| 29:Aq:109:LEU:HG    | 29:Aq:111:PHE:CD1  | 2.52                     | 0.44              |
| 39:B5:231:U:O2      | 66:BY:103:LYS:NZ   | 2.41                     | 0.44              |
| 39:B5:2208:OMC:HM21 | 39:B5:2671:U:H2'   | 1.99                     | 0.44              |
| 39:B5:2632:A:H1'    | 79:Bl:45:ARG:HH22  | 1.81                     | 0.44              |
| 39:B5:3468:A:H2'    | 39:B5:3469:A:C8    | 2.52                     | 0.44              |
| 39:B5:3699:G:N2     | 86:Bv:164:CYS:SG   | 2.90                     | 0.44              |
| 88:Bz:21:CYS:HB3    | 88:Bz:67:PHE:HE2   | 1.82                     | 0.44              |
| 88:Bz:240:PHE:HB2   | 88:Bz:271:VAL:HG23 | 2.00                     | 0.44              |
| 1:A2:519:G:H2'      | 1:A2:520:A:H8      | 1.82                     | 0.44              |
| 1:A2:869:G:C2       | 19:Ag:115:LYS:HE2  | 2.53                     | 0.44              |
| 1:A2:944:U:O2'      | 26:An:135:ILE:O    | 2.35                     | 0.44              |
| 1:A2:1272:C:OP1     | 4:AC:90:LYS:NZ     | 2.43                     | 0.44              |
| 1:A2:1643:U:H2'     | 1:A2:1644:PSU:H6   | 1.82                     | 0.44              |
| 14:Ab:187:ARG:HD2   | 14:Ab:192:LEU:HD12 | 1.99                     | 0.44              |
| 33:Au:1:AME:HT23    | 33:Au:1:AME:HA     | 1.61                     | 0.44              |
| 39:B5:181:C:H2'     | 39:B5:182:G:C8     | 2.52                     | 0.44              |
| 39:B5:795:A:H3'     | 39:B5:796:C:C6     | 2.53                     | 0.44              |
| 39:B5:1303:G:H4'    | 55:BN:203:TYR:HB2  | 2.00                     | 0.44              |
| 39:B5:1701:C:H2'    | 39:B5:1702:C:H6    | 1.83                     | 0.44              |
| 39:B5:4043:G:H22    | 39:B5:4059:A:H2    | 1.66                     | 0.44              |
| 39:B5:4383:OMG:HM22 | 39:B5:4384:U:H5'   | 1.99                     | 0.44              |
| 47:BF:135:VAL:HG23  | 47:BF:139:ILE:HD13 | 1.99                     | 0.44              |
| 55:BN:181:HIS:O     | 55:BN:195:ARG:NH2  | 2.40                     | 0.44              |
| 84:Bs:27:CYS:HB3    | 84:Bs:90:PHE:CD2   | 2.52                     | 0.44              |
| 84:Bs:122:THR:HG22  | 84:Bs:159:GLN:HG2  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:Bt:111:ASN:OD1  | 85:Bt:112:ILE:N    | 2.50                     | 0.44              |
| 88:Bz:108:LEU:HB2  | 88:Bz:272:VAL:HG22 | 1.98                     | 0.44              |
| 88:Bz:325:ARG:NH2  | 88:Bz:495:GLU:OE2  | 2.43                     | 0.44              |
| 1:A2:380:C:O2      | 20:Ah:5:ARG:NE     | 2.49                     | 0.44              |
| 1:A2:1598:C:H4'    | 1:A2:1604:G:C6     | 2.53                     | 0.44              |
| 17:Ae:131:ALA:HB2  | 17:Ae:135:ARG:HE   | 1.83                     | 0.44              |
| 18:Af:162:LEU:HD11 | 18:Af:172:LYS:HB2  | 2.00                     | 0.44              |
| 19:Ag:135:PHE:CG   | 19:Ag:136:PRO:HA   | 2.52                     | 0.44              |
| 32:At:20:ILE:HG13  | 32:At:116:ILE:HG13 | 2.00                     | 0.44              |
| 39:B5:26:C:O2'     | 39:B5:338:A:N3     | 2.46                     | 0.44              |
| 39:B5:741:A:N6     | 39:B5:810:U:O2     | 2.51                     | 0.44              |
| 39:B5:2118:G:H2'   | 39:B5:2119:A:C8    | 2.52                     | 0.44              |
| 39:B5:2335:C:H2'   | 39:B5:2336:G:C8    | 2.52                     | 0.44              |
| 39:B5:4061:A:OP1   | 61:BT:69:GLN:NE2   | 2.50                     | 0.44              |
| 44:BC:14:LYS:HA    | 44:BC:173:LYS:HD3  | 1.99                     | 0.44              |
| 51:BJ:32:ARG:HD2   | 51:BJ:35:ARG:HH22  | 1.82                     | 0.44              |
| 67:BZ:76:ASN:OD1   | 67:BZ:77:TYR:N     | 2.50                     | 0.44              |
| 81:Bo:33:LEU:HA    | 81:Bo:38:LYS:HG2   | 1.99                     | 0.44              |
| 1:A2:77:A:N3       | 18:Af:176:ILE:HG22 | 2.32                     | 0.44              |
| 1:A2:1338:4AC:O5'  | 1:A2:1338:4AC:H6   | 2.18                     | 0.44              |
| 3:AB:47:LYS:NZ     | 17:Ae:125:SER:O    | 2.46                     | 0.44              |
| 13:Aa:225:LEU:HD23 | 48:BG:264:LYS:HG3  | 2.00                     | 0.44              |
| 39:B5:1638:PSU:OP1 | 68:Ba:44:ASN:ND2   | 2.47                     | 0.44              |
| 75:Bh:70:ARG:HG2   | 75:Bh:83:LEU:HD22  | 2.00                     | 0.44              |
| 1:A2:1241:A:N3     | 1:A2:1268:C:O2'    | 2.50                     | 0.44              |
| 1:A2:1776:U:H2'    | 1:A2:1777:G:C8     | 2.52                     | 0.44              |
| 8:AG:30:LEU:HA     | 8:AG:39:CYS:HA     | 2.00                     | 0.44              |
| 15:Ac:154:ASP:OD1  | 15:Ac:154:ASP:N    | 2.50                     | 0.44              |
| 17:Ae:14:THR:HB    | 17:Ae:15:PRO:HD3   | 1.98                     | 0.44              |
| 39:B5:442:G:N7     | 95:B5:5498:HOH:O   | 2.36                     | 0.44              |
| 39:B5:1510:G:N7    | 82:Bp:4:ARG:NH2    | 2.61                     | 0.44              |
| 39:B5:1818:C:O2'   | 39:B5:1830:A:N3    | 2.44                     | 0.44              |
| 39:B5:2362:U:O2'   | 39:B5:2373:U:O2    | 2.32                     | 0.44              |
| 39:B5:3353:A:HO2'  | 39:B5:4404:G:HO2'  | 1.65                     | 0.44              |
| 59:BR:15:LEU:HD13  | 59:BR:52:ARG:HB2   | 1.98                     | 0.44              |
| 70:Bc:47:ILE:HD12  | 70:Bc:94:LEU:HD11  | 2.00                     | 0.44              |
| 86:Bv:52:THR:HG22  | 86:Bv:156:LYS:HG2  | 2.00                     | 0.44              |
| 1:A2:533:C:H2'     | 1:A2:534:A:C8      | 2.53                     | 0.44              |
| 1:A2:549:C:H4'     | 1:A2:550:C:C5'     | 2.48                     | 0.44              |
| 1:A2:599:G:O2'     | 1:A2:606:A:N1      | 2.50                     | 0.44              |
| 1:A2:1032:A2M:HM'2 | 1:A2:1033:C:H5'    | 2.00                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:A2:1080:C:O2'     | 1:A2:1183:A:N1     | 2.47                     | 0.44              |
| 16:Ad:54:TYR:OH     | 16:Ad:97:GLU:OE1   | 2.32                     | 0.44              |
| 30:Ar:116:LYS:HG3   | 39:B5:1704:A:C6    | 2.52                     | 0.44              |
| 39:B5:300:A:H2'     | 39:B5:301:G:C8     | 2.53                     | 0.44              |
| 39:B5:1673:G:N2     | 39:B5:1674:U:O4    | 2.38                     | 0.44              |
| 39:B5:1712:U:H2'    | 39:B5:1713:C:C6    | 2.53                     | 0.44              |
| 39:B5:1943:U:H2'    | 39:B5:1944:G:C8    | 2.52                     | 0.44              |
| 39:B5:2667:OMC:HM22 | 39:B5:2668:A:H5'   | 2.00                     | 0.44              |
| 39:B5:3421:G:O2'    | 39:B5:3550:UY1:OP2 | 2.32                     | 0.44              |
| 39:B5:4193:5MC:O2'  | 95:B5:5411:HOH:O   | 2.20                     | 0.44              |
| 40:B7:74:A:N1       | 40:B7:100:A:H5''   | 2.32                     | 0.44              |
| 42:BA:173:GLY:O     | 82:Bp:69:TRP:NE1   | 2.50                     | 0.44              |
| 70:Bc:99:PRO:HG3    | 70:Bc:105:ILE:HG13 | 2.00                     | 0.44              |
| 85:Bt:114:ARG:HH21  | 85:Bt:164:ALA:HB2  | 1.82                     | 0.44              |
| 1:A2:282:C:N4       | 1:A2:892:G:O4'     | 2.50                     | 0.44              |
| 1:A2:1167:G:O6      | 35:Aw:25:LYS:NZ    | 2.51                     | 0.44              |
| 20:Ah:89:GLU:OE1    | 20:Ah:92:ARG:NH2   | 2.51                     | 0.44              |
| 21:Ai:53:ILE:HD13   | 21:Ai:81:LEU:HD21  | 2.00                     | 0.44              |
| 21:Ai:107:GLU:O     | 21:Ai:113:GLN:NE2  | 2.50                     | 0.44              |
| 24:Al:49:LEU:HB3    | 24:Al:111:VAL:HB   | 1.99                     | 0.44              |
| 30:Ar:48:ALA:HB2    | 30:Ar:70:ILE:HD12  | 1.99                     | 0.44              |
| 39:B5:3374:A:C4     | 77:Bj:3:LYS:HB3    | 2.52                     | 0.44              |
| 39:B5:3701:G:H2'    | 39:B5:3702:G:C8    | 2.53                     | 0.44              |
| 39:B5:3783:U:H2'    | 39:B5:3784:A:C8    | 2.53                     | 0.44              |
| 43:BB:43:LEU:HD12   | 43:BB:205:VAL:HG11 | 2.00                     | 0.44              |
| 45:BD:51:MET:HE3    | 45:BD:105:LEU:HD23 | 1.98                     | 0.44              |
| 51:BJ:52:LYS:HB3    | 51:BJ:65:ASN:HA    | 2.00                     | 0.44              |
| 84:Bs:5:ASP:OD1     | 84:Bs:6:ARG:N      | 2.51                     | 0.44              |
| 88:Bz:106:LEU:HD13  | 88:Bz:285:PHE:CE2  | 2.52                     | 0.44              |
| 1:A2:1649:G:O2'     | 1:A2:1675:G:O6     | 2.33                     | 0.43              |
| 13:Aa:86:LEU:HB3    | 13:Aa:98:THR:HB    | 1.98                     | 0.43              |
| 13:Aa:168:MET:HG2   | 13:Aa:197:ILE:HG21 | 2.00                     | 0.43              |
| 26:An:86:LYS:NZ     | 26:An:122:SER:O    | 2.41                     | 0.43              |
| 39:B5:2141:U:OP1    | 44:BC:204:ARG:NH2  | 2.50                     | 0.43              |
| 43:BB:86:VAL:HG13   | 43:BB:162:VAL:HG13 | 2.00                     | 0.43              |
| 45:BD:70:GLU:H      | 45:BD:70:GLU:CD    | 2.26                     | 0.43              |
| 65:BX:64:SER:HB2    | 75:Bh:69:LEU:HD13  | 2.00                     | 0.43              |
| 78:Bk:30:ASP:OD1    | 78:Bk:30:ASP:N     | 2.50                     | 0.43              |
| 1:A2:1233:PSU:H2'   | 1:A2:1234:G:C8     | 2.52                     | 0.43              |
| 1:A2:1321:G:H2'     | 1:A2:1322:G:O4'    | 2.18                     | 0.43              |
| 7:AF:226:HIS:NE2    | 7:AF:229:THR:HG23  | 2.32                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AZ:189:ILE:HG22 | 12:AZ:191:ARG:H    | 1.83                     | 0.43              |
| 15:Ac:115:VAL:HG21 | 15:Ac:142:LEU:HD22 | 2.00                     | 0.43              |
| 39:B5:1991:G:O2'   | 39:B5:1996:A:N1    | 2.48                     | 0.43              |
| 39:B5:3976:C:O2'   | 39:B5:3980:A:N1    | 2.45                     | 0.43              |
| 42:BA:48:ILE:HD13  | 82:Bp:65:ALA:HB2   | 2.00                     | 0.43              |
| 43:BB:395:ASP:O    | 43:BB:399:LYS:HG3  | 2.18                     | 0.43              |
| 50:BI:53:VAL:HG11  | 61:BT:158:PHE:CZ   | 2.47                     | 0.43              |
| 84:Bs:30:VAL:HG12  | 84:Bs:189:ILE:HG12 | 1.99                     | 0.43              |
| 85:Bt:97:ASN:ND2   | 85:Bt:97:ASN:O     | 2.51                     | 0.43              |
| 88:Bz:8:ILE:HG22   | 88:Bz:75:LEU:HD21  | 2.01                     | 0.43              |
| 39:B5:1315:A:N1    | 41:B8:28:C:O2'     | 2.50                     | 0.43              |
| 39:B5:3835:G:H2'   | 39:B5:3836:G:C8    | 2.53                     | 0.43              |
| 66:BY:134:LYS:HE3  | 66:BY:134:LYS:HB3  | 1.87                     | 0.43              |
| 72:Be:104:SER:O    | 72:Be:108:ARG:HG3  | 2.17                     | 0.43              |
| 73:Bf:76:ARG:NH2   | 95:Bf:301:HOH:O    | 2.51                     | 0.43              |
| 80:Bm:113:LYS:HG2  | 80:Bm:117:HIS:HE1  | 1.83                     | 0.43              |
| 88:Bz:114:ILE:HG21 | 88:Bz:289:LEU:HB3  | 1.99                     | 0.43              |
| 1:A2:67:C:H41      | 18:Af:163:ASN:HA   | 1.83                     | 0.43              |
| 1:A2:220:U:H2'     | 1:A2:221:A:C8      | 2.53                     | 0.43              |
| 1:A2:1627:C:OP2    | 89:A2:1901:SPD:N10 | 2.52                     | 0.43              |
| 39:B5:86:U:HO2'    | 68:Ba:65:ARG:HH21  | 1.59                     | 0.43              |
| 39:B5:1394:U:HO2'  | 47:BF:33:ARG:NE    | 2.10                     | 0.43              |
| 39:B5:1568:A:H5'   | 42:BA:183:GLY:HA2  | 2.00                     | 0.43              |
| 39:B5:3660:A:OP1   | 55:BN:90:ASN:ND2   | 2.51                     | 0.43              |
| 41:B8:60:G:O6      | 75:Bh:62:ASN:ND2   | 2.30                     | 0.43              |
| 47:BF:240:ASN:O    | 47:BF:244:ARG:HG2  | 2.19                     | 0.43              |
| 49:BH:94:SER:HB3   | 49:BH:142:ASP:HB3  | 2.00                     | 0.43              |
| 86:Bv:60:ARG:O     | 86:Bv:171:HIS:ND1  | 2.52                     | 0.43              |
| 87:By:323:TYR:CE2  | 87:By:325:ASN:HB2  | 2.53                     | 0.43              |
| 87:By:333:LEU:HB3  | 87:By:366:HIS:HB3  | 2.00                     | 0.43              |
| 1:A2:585:A:OP1     | 21:Ai:169:ARG:NH2  | 2.50                     | 0.43              |
| 1:A2:590:G:N2      | 5:AD:97:GLU:OE2    | 2.52                     | 0.43              |
| 1:A2:657:G:H5'     | 1:A2:663:G:N2      | 2.34                     | 0.43              |
| 1:A2:894:U:H2'     | 1:A2:895:G:H8      | 1.83                     | 0.43              |
| 1:A2:1260:A:H1'    | 1:A2:1265:C:N4     | 2.33                     | 0.43              |
| 1:A2:1744:G:H21    | 1:A2:1792:A:H62    | 1.67                     | 0.43              |
| 7:AF:107:ASP:OD1   | 7:AF:107:ASP:N     | 2.51                     | 0.43              |
| 16:Ad:55:ALA:HB1   | 16:Ad:60:GLU:HB2   | 2.00                     | 0.43              |
| 24:Al:72:HIS:CD2   | 24:Al:74:ILE:HD11  | 2.53                     | 0.43              |
| 39:B5:1733:A:H5''  | 39:B5:3960:A:H61   | 1.83                     | 0.43              |
| 39:B5:1793:G:N2    | 39:B5:4140:A:O4'   | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:B5:2036:A:H3'   | 39:B5:2037:G:H5'   | 2.00                     | 0.43              |
| 41:B8:140:C:H2'    | 41:B8:141:C:C6     | 2.54                     | 0.43              |
| 1:A2:542:U:H2'     | 1:A2:543:U:C6      | 2.53                     | 0.43              |
| 1:A2:940:U:OP1     | 82:Bp:85:ARG:NH2   | 2.52                     | 0.43              |
| 1:A2:1809:U:H2'    | 1:A2:1810:A:H8     | 1.83                     | 0.43              |
| 7:AF:64:HIS:HB3    | 7:AF:83:TRP:HB2    | 2.00                     | 0.43              |
| 15:Ac:68:GLU:HG3   | 22:Aj:93:THR:HG21  | 2.00                     | 0.43              |
| 39:B5:1478:A:N3    | 39:B5:4135:C:O2'   | 2.49                     | 0.43              |
| 39:B5:2372:A:OP1   | 95:B5:5414:HOH:O   | 2.21                     | 0.43              |
| 39:B5:3430:G:OP2   | 42:BA:245:ARG:NH2  | 2.40                     | 0.43              |
| 44:BC:92:PHE:O     | 44:BC:100:ARG:NH1  | 2.51                     | 0.43              |
| 44:BC:328:LEU:HB3  | 47:BF:186:MET:HG3  | 2.00                     | 0.43              |
| 50:BI:99:ILE:HG22  | 50:BI:123:GLN:HB2  | 2.00                     | 0.43              |
| 51:BJ:101:ASP:OD1  | 51:BJ:101:ASP:N    | 2.42                     | 0.43              |
| 54:BM:108:ASP:HB3  | 56:BO:199:HIS:CD2  | 2.53                     | 0.43              |
| 88:Bz:123:LEU:HD13 | 88:Bz:270:ILE:HD13 | 2.00                     | 0.43              |
| 1:A2:887:A:H62     | 1:A2:901:C:H42     | 1.66                     | 0.43              |
| 1:A2:1611:G:OP1    | 30:Ar:125:HIS:NE2  | 2.39                     | 0.43              |
| 16:Ad:125:LYS:H    | 16:Ad:142:HIS:CD2  | 2.36                     | 0.43              |
| 25:Am:87:ASP:N     | 25:Am:87:ASP:OD1   | 2.49                     | 0.43              |
| 39:B5:417:G:H1'    | 41:B8:16:G:N2      | 2.33                     | 0.43              |
| 39:B5:521:C:H2'    | 39:B5:522:U:C6     | 2.53                     | 0.43              |
| 39:B5:866:A:H8     | 47:BF:22:ARG:HD3   | 1.83                     | 0.43              |
| 39:B5:1065:G:H2'   | 39:B5:1066:A:C8    | 2.54                     | 0.43              |
| 39:B5:1095:C:H2'   | 39:B5:1096:G:C8    | 2.54                     | 0.43              |
| 39:B5:1779:G:OP2   | 47:BF:201:LYS:NZ   | 2.50                     | 0.43              |
| 47:BF:219:MET:HB3  | 47:BF:231:ASP:OD2  | 2.19                     | 0.43              |
| 51:BJ:14:GLU:OE2   | 51:BJ:16:ARG:NH2   | 2.46                     | 0.43              |
| 75:Bh:6:ALA:O      | 75:Bh:10:ARG:HG3   | 2.18                     | 0.43              |
| 82:Bp:7:LYS:O      | 82:Bp:27:LYS:NZ    | 2.44                     | 0.43              |
| 86:Bv:90:LEU:HB3   | 86:Bv:123:ILE:HD12 | 2.01                     | 0.43              |
| 87:By:359:ASP:N    | 87:By:365:GLU:OE1  | 2.52                     | 0.43              |
| 1:A2:442:C:O2'     | 18:Af:92:ARG:NH2   | 2.51                     | 0.43              |
| 11:AT:61:G:H2'     | 11:AT:62:G:C8      | 2.53                     | 0.43              |
| 39:B5:398:A2M:H8   | 39:B5:398:A2M:O5'  | 2.19                     | 0.43              |
| 39:B5:2282:G:H5'   | 39:B5:2621:G:OP2   | 2.18                     | 0.43              |
| 42:BA:6:ARG:HH12   | 42:BA:199:VAL:H    | 1.65                     | 0.43              |
| 64:BW:63:GLN:OE1   | 64:BW:63:GLN:N     | 2.44                     | 0.43              |
| 68:Ba:85:GLN:HA    | 68:Ba:88:VAL:HG22  | 2.00                     | 0.43              |
| 71:Bd:92:ARG:HA    | 71:Bd:102:LEU:HD23 | 2.00                     | 0.43              |
| 1:A2:869:G:C5      | 19:Ag:115:LYS:HG2  | 2.54                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A2:1038:G:H4'     | 1:A2:1846:A:H4'     | 2.00                     | 0.43              |
| 16:Ad:18:TRP:C      | 16:Ad:51:ARG:HH22   | 2.26                     | 0.43              |
| 16:Ad:175:PHE:HE1   | 16:Ad:225:ILE:HG21  | 1.84                     | 0.43              |
| 21:Ai:54:ARG:NH1    | 21:Ai:98:LEU:O      | 2.52                     | 0.43              |
| 24:Al:79:VAL:HG11   | 24:Al:85:LEU:HB2    | 2.01                     | 0.43              |
| 39:B5:512:U:O5'     | 53:BL:163:LYS:NZ    | 2.51                     | 0.43              |
| 39:B5:526:C:H2'     | 39:B5:527:G:C8      | 2.53                     | 0.43              |
| 39:B5:1471:G:O2'    | 53:BL:18:TRP:NE1    | 2.46                     | 0.43              |
| 39:B5:2207:OMG:HM22 | 39:B5:2208:OMC:H5'' | 2.00                     | 0.43              |
| 39:B5:4006:U:H2'    | 39:B5:4007:C:C6     | 2.54                     | 0.43              |
| 49:BH:115:ARG:HG2   | 49:BH:123:ILE:HG12  | 2.01                     | 0.43              |
| 72:Be:58:ILE:HD12   | 72:Be:58:ILE:HA     | 1.91                     | 0.43              |
| 77:Bj:39:TYR:CG     | 77:Bj:40:PRO:HA     | 2.53                     | 0.43              |
| 1:A2:1828:U:O2'     | 39:B5:3498:A:N1     | 2.44                     | 0.43              |
| 17:Ae:73:THR:O      | 17:Ae:89:THR:HG21   | 2.19                     | 0.43              |
| 26:An:68:GLU:OE2    | 95:An:201:HOH:O     | 2.20                     | 0.43              |
| 39:B5:156:G:OP2     | 75:Bh:106:LYS:NZ    | 2.52                     | 0.43              |
| 39:B5:440:U:O2'     | 73:Bf:91:ASN:O      | 2.33                     | 0.43              |
| 39:B5:519:C:H2'     | 39:B5:520:G:C8      | 2.53                     | 0.43              |
| 39:B5:766:C:H2'     | 39:B5:767:G:C8      | 2.54                     | 0.43              |
| 39:B5:1386:C:H2'    | 39:B5:1387:G:O4'    | 2.19                     | 0.43              |
| 39:B5:2142:G:OP1    | 44:BC:182:LYS:NZ    | 2.33                     | 0.43              |
| 39:B5:2687:A:O2'    | 39:B5:4377:G:H4'    | 2.18                     | 0.43              |
| 39:B5:3439:U:H2'    | 39:B5:3440:C:C6     | 2.54                     | 0.43              |
| 39:B5:4324:G:H2'    | 39:B5:4325:PSU:H6   | 1.84                     | 0.43              |
| 39:B5:4452:G:N7     | 95:B5:5501:HOH:O    | 2.37                     | 0.43              |
| 49:BH:14:GLU:H      | 49:BH:14:GLU:CD     | 2.27                     | 0.43              |
| 53:BL:5:ARG:HB3     | 53:BL:6:ASN:H       | 1.62                     | 0.43              |
| 73:Bf:36:ARG:NH1    | 73:Bf:79:GLY:O      | 2.44                     | 0.43              |
| 81:Bo:30:LYS:HE3    | 81:Bo:30:LYS:HB2    | 1.87                     | 0.43              |
| 1:A2:106:C:OP1      | 1:A2:432:G:O2'      | 2.35                     | 0.42              |
| 1:A2:109:PSU:O4     | 23:Ak:71:ARG:NH2    | 2.52                     | 0.42              |
| 1:A2:445:G:O6       | 20:Ah:26:LYS:HE3    | 2.19                     | 0.42              |
| 1:A2:1783:G:O6      | 64:BW:74:ARG:NH2    | 2.48                     | 0.42              |
| 8:AG:3:HIS:HB3      | 8:AG:6:LEU:HB2      | 2.01                     | 0.42              |
| 12:AZ:176:TRP:HE1   | 12:AZ:197:VAL:HG23  | 1.83                     | 0.42              |
| 39:B5:135:G:N7      | 75:Bh:97:LYS:HE3    | 2.34                     | 0.42              |
| 39:B5:1072:C:H1'    | 39:B5:1074:C:C2     | 2.54                     | 0.42              |
| 39:B5:1423:C:OP1    | 68:Ba:132:ARG:NH2   | 2.39                     | 0.42              |
| 39:B5:1877:C:O2     | 95:B5:5416:HOH:O    | 2.22                     | 0.42              |
| 39:B5:2359:G:OP1    | 74:Bg:60:ARG:NH2    | 2.45                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:B5:3465:A:H2'    | 39:B5:3466:PSU:O4' | 2.19                     | 0.42              |
| 44:BC:76:ILE:HD12   | 44:BC:77:PRO:HD2   | 2.01                     | 0.42              |
| 45:BD:152:ARG:O     | 45:BD:157:ASN:ND2  | 2.52                     | 0.42              |
| 70:Bc:45:LEU:HD21   | 70:Bc:108:MET:HE3  | 2.01                     | 0.42              |
| 85:Bt:108:GLU:HA    | 85:Bt:111:ASN:HD21 | 1.83                     | 0.42              |
| 1:A2:77:A:C4        | 18:Af:176:ILE:HG22 | 2.54                     | 0.42              |
| 1:A2:172:OMU:H6     | 1:A2:315:U:H1'     | 2.00                     | 0.42              |
| 1:A2:908:G:H2'      | 1:A2:909:A:C8      | 2.54                     | 0.42              |
| 39:B5:375:G:OP1     | 44:BC:62:THR:OG1   | 2.32                     | 0.42              |
| 39:B5:3404:G:OP2    | 39:B5:3404:G:N2    | 2.51                     | 0.42              |
| 39:B5:3631:OMG:HM22 | 39:B5:3632:G:H5'   | 2.01                     | 0.42              |
| 39:B5:4675:G:C5     | 46:BE:186:ARG:HD3  | 2.54                     | 0.42              |
| 48:BG:187:LYS:HB2   | 48:BG:198:THR:HG23 | 2.02                     | 0.42              |
| 53:BL:107:THR:HG22  | 76:Bi:20:ASN:HB3   | 2.00                     | 0.42              |
| 63:BV:21:PRO:HA     | 63:BV:54:ALA:HA    | 2.00                     | 0.42              |
| 87:By:220:ASN:OD1   | 87:By:221:VAL:N    | 2.52                     | 0.42              |
| 88:Bz:192:ASP:HA    | 88:Bz:232:ILE:HG23 | 2.00                     | 0.42              |
| 88:Bz:333:VAL:HG21  | 88:Bz:597:LEU:HD11 | 2.00                     | 0.42              |
| 1:A2:1102:U:H2'     | 1:A2:1103:G:C8     | 2.55                     | 0.42              |
| 1:A2:1399:G:HO2'    | 7:AF:88:ARG:HH21   | 1.65                     | 0.42              |
| 1:A2:1598:C:N4      | 1:A2:1599:G:O6     | 2.52                     | 0.42              |
| 1:A2:1734:U:H2'     | 1:A2:1735:G:O4'    | 2.19                     | 0.42              |
| 12:AZ:58:LEU:HD11   | 12:AZ:178:LEU:HB2  | 2.00                     | 0.42              |
| 14:Ab:254:ASP:HB2   | 33:Au:1:AME:HT22   | 2.01                     | 0.42              |
| 16:Ad:153:LEU:HD13  | 18:Af:216:ARG:HD2  | 2.02                     | 0.42              |
| 29:Aq:56:HIS:HA     | 29:Aq:59:LYS:HE2   | 2.01                     | 0.42              |
| 31:As:35:ASP:OD1    | 31:As:35:ASP:N     | 2.50                     | 0.42              |
| 36:Ax:23:MET:N      | 36:Ax:23:MET:SD    | 2.92                     | 0.42              |
| 39:B5:260:C:H2'     | 39:B5:261:G:H8     | 1.83                     | 0.42              |
| 39:B5:819:C:H2'     | 39:B5:820:G:H8     | 1.85                     | 0.42              |
| 43:BB:161:ARG:HG2   | 43:BB:184:GLN:HA   | 2.01                     | 0.42              |
| 46:BE:59:TYR:HB3    | 46:BE:63:ALA:HB3   | 2.00                     | 0.42              |
| 55:BN:143:ARG:NH1   | 75:Bh:95:LEU:HD23  | 2.34                     | 0.42              |
| 88:Bz:371:ASP:HB2   | 88:Bz:512:LYS:O    | 2.19                     | 0.42              |
| 1:A2:496:U:H4'      | 16:Ad:24:THR:HG22  | 2.01                     | 0.42              |
| 1:A2:526:A:H2'      | 1:A2:527:A:C8      | 2.54                     | 0.42              |
| 1:A2:1473:C:O2'     | 7:AF:15:ASN:ND2    | 2.50                     | 0.42              |
| 1:A2:1607:G:N2      | 1:A2:1633:G:H1'    | 2.33                     | 0.42              |
| 3:AB:36:ASP:OD1     | 3:AB:36:ASP:N      | 2.51                     | 0.42              |
| 13:Aa:48:LEU:O      | 26:An:51:GLU:HG3   | 2.19                     | 0.42              |
| 20:Ah:81:VAL:HG22   | 20:Ah:102:VAL:HG12 | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:Ax:117:VAL:HG23 | 36:Ax:122:LYS:HG2  | 1.99                     | 0.42              |
| 39:B5:3450:A2M:H8  | 39:B5:3450:A2M:O5' | 2.19                     | 0.42              |
| 40:B7:27:G:H21     | 40:B7:55:A:N6      | 2.16                     | 0.42              |
| 45:BD:62:CYS:HB3   | 45:BD:105:LEU:HD22 | 2.02                     | 0.42              |
| 46:BE:78:PRO:O     | 46:BE:84:ARG:NE    | 2.52                     | 0.42              |
| 56:BO:8:VAL:HG12   | 56:BO:117:ARG:HG3  | 2.01                     | 0.42              |
| 57:BP:60:PHE:CE1   | 57:BP:82:ARG:HB2   | 2.55                     | 0.42              |
| 82:Bp:26:VAL:HG22  | 82:Bp:30:GLU:HG2   | 2.02                     | 0.42              |
| 84:Bs:41:GLN:HE21  | 84:Bs:45:MET:HE1   | 1.84                     | 0.42              |
| 88:Bz:442:VAL:HA   | 88:Bz:446:MET:HB2  | 2.01                     | 0.42              |
| 1:A2:830:C:OP1     | 16:Ad:21:ASP:HB2   | 2.19                     | 0.42              |
| 1:A2:1704:OMC:N3   | 1:A2:1833:6MZ:H9   | 2.35                     | 0.42              |
| 7:AF:87:LEU:HD21   | 7:AF:108:VAL:HG11  | 2.02                     | 0.42              |
| 11:AT:72:C:H2'     | 11:AT:73:C:C6      | 2.54                     | 0.42              |
| 13:Aa:27:LYS:HA    | 13:Aa:51:ARG:NH1   | 2.34                     | 0.42              |
| 15:Ac:135:GLU:HG3  | 15:Ac:153:VAL:HG12 | 2.01                     | 0.42              |
| 16:Ad:160:ILE:HG22 | 16:Ad:172:PHE:HB3  | 2.02                     | 0.42              |
| 28:Ap:24:HIS:HE1   | 28:Ap:26:LYS:HD3   | 1.85                     | 0.42              |
| 29:Aq:99:ASP:OD1   | 29:Aq:102:THR:N    | 2.45                     | 0.42              |
| 30:Ar:80:PRO:HG2   | 30:Ar:83:PHE:HB2   | 2.02                     | 0.42              |
| 39:B5:642:G:H2'    | 39:B5:643:A:C8     | 2.55                     | 0.42              |
| 39:B5:1223:A:O2'   | 39:B5:1225:G:N7    | 2.47                     | 0.42              |
| 39:B5:2302:G:H2'   | 39:B5:2304:G:OP2   | 2.20                     | 0.42              |
| 39:B5:3682:U:H3    | 39:B5:3790:A:H61   | 1.65                     | 0.42              |
| 39:B5:4220:A:H5''  | 80:Bm:125:LYS:HD2  | 2.01                     | 0.42              |
| 43:BB:93:VAL:HG23  | 43:BB:102:PHE:HB2  | 2.01                     | 0.42              |
| 56:BO:125:LYS:HE3  | 56:BO:125:LYS:HB3  | 1.90                     | 0.42              |
| 60:BS:112:ASP:OD1  | 60:BS:116:ARG:NH1  | 2.38                     | 0.42              |
| 84:Bs:93:GLU:HG2   | 84:Bs:94:ASP:H     | 1.84                     | 0.42              |
| 87:By:321:ILE:HG12 | 87:By:410:GLY:O    | 2.19                     | 0.42              |
| 1:A2:533:C:H2'     | 1:A2:534:A:H8      | 1.84                     | 0.42              |
| 1:A2:840:C:H42     | 36:Ax:48:TYR:HA    | 1.85                     | 0.42              |
| 1:A2:1011:G:H2'    | 1:A2:1012:A:C8     | 2.54                     | 0.42              |
| 1:A2:1366:G:H2'    | 1:A2:1367:G:C8     | 2.55                     | 0.42              |
| 6:AE:22:ARG:NH2    | 26:An:145:GLY:O    | 2.53                     | 0.42              |
| 18:Af:102:VAL:HG13 | 18:Af:106:LEU:HD12 | 2.01                     | 0.42              |
| 22:Aj:51:SER:OG    | 22:Aj:55:ARG:NH1   | 2.53                     | 0.42              |
| 39:B5:681:U:OP1    | 46:BE:100:GLY:N    | 2.45                     | 0.42              |
| 39:B5:1343:G:H2'   | 39:B5:1344:G:C8    | 2.55                     | 0.42              |
| 39:B5:2335:C:H2'   | 39:B5:2336:G:H8    | 1.85                     | 0.42              |
| 39:B5:4268:G:O2'   | 39:B5:4271:C:OP2   | 2.29                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 40:B7:46:C:OP1      | 45:BD:158:LYS:N    | 2.47                     | 0.42              |
| 43:BB:396:ARG:HA    | 43:BB:399:LYS:HD2  | 2.02                     | 0.42              |
| 47:BF:86:PRO:HG3    | 47:BF:143:TYR:CG   | 2.55                     | 0.42              |
| 54:BM:24:LEU:HD11   | 54:BM:86:TRP:CG    | 2.55                     | 0.42              |
| 60:BS:147:ASP:HB3   | 60:BS:150:ILE:HB   | 2.00                     | 0.42              |
| 88:Bz:137:PRO:HA    | 88:Bz:138:PRO:HD3  | 1.93                     | 0.42              |
| 88:Bz:159:ILE:HA    | 88:Bz:164:LEU:HB2  | 2.00                     | 0.42              |
| 13:Aa:65:ARG:HE     | 26:An:50:LYS:HD3   | 1.84                     | 0.42              |
| 18:Af:67:VAL:HG12   | 18:Af:69:THR:HG22  | 2.00                     | 0.42              |
| 39:B5:1216:C:H42    | 46:BE:81:ARG:HG2   | 1.85                     | 0.42              |
| 39:B5:1298:A:H5'    | 58:BQ:108:ARG:HH21 | 1.85                     | 0.42              |
| 39:B5:1580:OMG:HM23 | 55:BN:81:TYR:HE1   | 1.85                     | 0.42              |
| 39:B5:4270:G:N3     | 43:BB:252:ALA:HB1  | 2.34                     | 0.42              |
| 48:BG:165:GLU:OE2   | 55:BN:26:ARG:NH1   | 2.52                     | 0.42              |
| 60:BS:93:MET:HE1    | 60:BS:117:HIS:CE1  | 2.54                     | 0.42              |
| 69:Bb:36:ASP:HB3    | 69:Bb:39:PHE:HB3   | 2.01                     | 0.42              |
| 70:Bc:47:ILE:HB     | 70:Bc:94:LEU:HG    | 2.02                     | 0.42              |
| 85:Bt:124:GLU:OE1   | 85:Bt:124:GLU:N    | 2.53                     | 0.42              |
| 88:Bz:193:GLU:HB3   | 88:Bz:234:LYS:NZ   | 2.34                     | 0.42              |
| 88:Bz:519:GLU:HG3   | 88:Bz:521:ASP:H    | 1.84                     | 0.42              |
| 1:A2:582:U:OP1      | 21:Ai:133:ARG:NH1  | 2.52                     | 0.42              |
| 1:A2:914:A:N3       | 19:Ag:66:VAL:HG11  | 2.35                     | 0.42              |
| 1:A2:1289:OMU:HM22  | 1:A2:1290:U:H5'    | 2.00                     | 0.42              |
| 1:A2:1751:C:N4      | 64:BW:74:ARG:HH21  | 2.17                     | 0.42              |
| 30:Ar:98:VAL:HG11   | 30:Ar:106:LYS:HG3  | 2.02                     | 0.42              |
| 39:B5:624:G:H2'     | 39:B5:625:G:C8     | 2.54                     | 0.42              |
| 39:B5:769:C:H2'     | 39:B5:770:G:H8     | 1.84                     | 0.42              |
| 39:B5:2499:U:OP1    | 67:BZ:78:ASN:ND2   | 2.53                     | 0.42              |
| 39:B5:4222:C:O2'    | 39:B5:4224:G:OP2   | 2.31                     | 0.42              |
| 44:BC:137:VAL:HG21  | 44:BC:150:LEU:HD21 | 2.02                     | 0.42              |
| 88:Bz:86:ARG:HD2    | 88:Bz:93:LYS:HG3   | 2.01                     | 0.42              |
| 1:A2:751:C:H2'      | 1:A2:752:G:H8      | 1.85                     | 0.42              |
| 1:A2:1770:C:H2'     | 1:A2:1771:G:C8     | 2.55                     | 0.42              |
| 11:AT:13:G:H2'      | 11:AT:14:A:C8      | 2.55                     | 0.42              |
| 15:Ac:70:THR:HA     | 15:Ac:86:LEU:HD13  | 2.01                     | 0.42              |
| 21:Ai:21:GLU:HB2    | 21:Ai:24:ARG:HB3   | 2.02                     | 0.42              |
| 39:B5:1093:C:H2'    | 39:B5:1094:A:C8    | 2.55                     | 0.42              |
| 39:B5:2141:U:O4     | 44:BC:188:ARG:NH2  | 2.52                     | 0.42              |
| 39:B5:2742:C:P      | 59:BR:108:ARG:HH22 | 2.42                     | 0.42              |
| 40:B7:36:C:H2'      | 40:B7:37:G:C8      | 2.55                     | 0.42              |
| 46:BE:164:ARG:O     | 46:BE:185:ASN:ND2  | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BO:185:VAL:O    | 56:BO:189:ILE:HG12 | 2.20                     | 0.42              |
| 63:BV:89:ARG:HB2   | 63:BV:95:PHE:CE2   | 2.54                     | 0.42              |
| 64:BW:102:LYS:HG2  | 64:BW:105:ARG:NH2  | 2.34                     | 0.42              |
| 67:BZ:48:ARG:HB3   | 67:BZ:69:LYS:HB3   | 2.02                     | 0.42              |
| 72:Be:105:SER:HB3  | 72:Be:128:ARG:HB3  | 2.01                     | 0.42              |
| 88:Bz:13:HIS:HA    | 88:Bz:47:ILE:HD11  | 2.02                     | 0.42              |
| 1:A2:1125:C:H5''   | 13:Aa:150:ILE:HG12 | 2.02                     | 0.42              |
| 16:Ad:87:MET:HE1   | 16:Ad:236:ILE:HG21 | 2.02                     | 0.42              |
| 30:Ar:55:ARG:HB2   | 30:Ar:58:GLU:HG3   | 2.02                     | 0.42              |
| 39:B5:229:G:H5''   | 66:BY:11:ARG:HG3   | 2.02                     | 0.42              |
| 39:B5:1093:C:H2'   | 39:B5:1094:A:H8    | 1.85                     | 0.42              |
| 39:B5:1095:C:H2'   | 39:B5:1096:G:H8    | 1.85                     | 0.42              |
| 39:B5:1290:C:H2'   | 39:B5:1291:G:H8    | 1.85                     | 0.42              |
| 39:B5:1520:A:C5    | 39:B5:1521:C:H1'   | 2.55                     | 0.42              |
| 39:B5:3422:U:O2'   | 39:B5:3549:A:N3    | 2.44                     | 0.42              |
| 41:B8:29:G:H5''    | 53:BL:27:ASN:HB3   | 2.02                     | 0.42              |
| 75:Bh:87:LYS:HE3   | 75:Bh:91:MET:HE2   | 2.01                     | 0.42              |
| 85:Bt:148:PRO:HA   | 85:Bt:151:ILE:HG22 | 2.02                     | 0.42              |
| 86:Bv:35:GLN:HG3   | 86:Bv:166:ALA:HB2  | 2.02                     | 0.42              |
| 86:Bv:205:TYR:HA   | 86:Bv:214:GLN:O    | 2.19                     | 0.42              |
| 88:Bz:82:GLU:CD    | 88:Bz:96:ARG:HE    | 2.28                     | 0.42              |
| 1:A2:240:G:H2'     | 1:A2:241:G:C8      | 2.55                     | 0.41              |
| 1:A2:617:A:H1'     | 5:AD:86:VAL:HG23   | 2.02                     | 0.41              |
| 1:A2:691:G:H1      | 1:A2:737:C:H42     | 1.68                     | 0.41              |
| 1:A2:1411:C:H2'    | 1:A2:1412:G:H8     | 1.84                     | 0.41              |
| 12:AZ:52:LYS:HB2   | 29:Aq:109:LEU:HD13 | 2.02                     | 0.41              |
| 24:Al:11:VAL:HG21  | 24:Al:16:THR:HG21  | 2.02                     | 0.41              |
| 36:Ax:51:THR:OG1   | 36:Ax:53:ASP:OD1   | 2.36                     | 0.41              |
| 39:B5:90:G:OP2     | 39:B5:92:C:N4      | 2.49                     | 0.41              |
| 39:B5:1215:G:H5''  | 69:Bb:110:ALA:HB1  | 2.02                     | 0.41              |
| 39:B5:1571:U:H2'   | 39:B5:1572:G:H8    | 1.85                     | 0.41              |
| 39:B5:1933:C:H2'   | 39:B5:1934:G:C8    | 2.55                     | 0.41              |
| 39:B5:2122:A:O2'   | 72:Be:48:ARG:NH2   | 2.52                     | 0.41              |
| 39:B5:2719:OMG:C8  | 82:Bp:16:THR:HG22  | 2.55                     | 0.41              |
| 39:B5:4089:U:O2'   | 81:Bo:31:ASP:OD1   | 2.37                     | 0.41              |
| 46:BE:156:LEU:HD11 | 46:BE:198:ILE:HG13 | 2.01                     | 0.41              |
| 55:BN:43:THR:OG1   | 55:BN:131:GLU:OE2  | 2.27                     | 0.41              |
| 55:BN:90:ASN:O     | 81:Bo:48:TYR:OH    | 2.25                     | 0.41              |
| 61:BT:93:ILE:H     | 61:BT:93:ILE:HG13  | 1.64                     | 0.41              |
| 85:Bt:114:ARG:HA   | 85:Bt:117:ARG:HB2  | 2.02                     | 0.41              |
| 87:By:24:LEU:HD21  | 87:By:112:ILE:HD13 | 2.01                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 87:By:280:PHE:HE1  | 87:By:396:SER:HA    | 1.84                     | 0.41              |
| 1:A2:390:A:OP2     | 95:A2:2107:HOH:O    | 2.21                     | 0.41              |
| 7:AF:99:ARG:NH2    | 7:AF:135:LEU:O      | 2.51                     | 0.41              |
| 14:Ab:168:GLY:N    | 14:Ab:179:THR:O     | 2.33                     | 0.41              |
| 17:Ae:42:LYS:HD3   | 17:Ae:42:LYS:HA     | 1.89                     | 0.41              |
| 20:Ah:141:ARG:HB2  | 20:Ah:146:GLN:HE21  | 1.84                     | 0.41              |
| 28:Ap:16:LYS:HA    | 28:Ap:16:LYS:HD2    | 1.79                     | 0.41              |
| 39:B5:197:A:N3     | 39:B5:222:C:O2'     | 2.52                     | 0.41              |
| 39:B5:1645:C:C5    | 58:BQ:13:VAL:HG11   | 2.55                     | 0.41              |
| 39:B5:3818:G:OP1   | 48:BG:252:LYS:NZ    | 2.49                     | 0.41              |
| 39:B5:3954:U:OP1   | 39:B5:4080:U:O2'    | 2.38                     | 0.41              |
| 39:B5:4138:OMG:N3  | 39:B5:4193:5MC:HM52 | 2.35                     | 0.41              |
| 39:B5:4140:A:N6    | 95:B5:5538:HOH:O    | 2.41                     | 0.41              |
| 39:B5:4474:U:H4'   | 39:B5:4705:A:H1'    | 2.02                     | 0.41              |
| 39:B5:4623:G:N7    | 46:BE:275:ARG:NH2   | 2.68                     | 0.41              |
| 39:B5:4641:C:H2'   | 39:B5:4642:G:H8     | 1.84                     | 0.41              |
| 39:B5:4792:U:H3'   | 39:B5:4793:C:C6     | 2.55                     | 0.41              |
| 45:BD:208:MET:HB2  | 45:BD:233:PRO:HG3   | 2.02                     | 0.41              |
| 53:BL:205:GLN:O    | 53:BL:208:GLU:HG2   | 2.19                     | 0.41              |
| 85:Bt:17:CYS:SG    | 85:Bt:18:THR:N      | 2.93                     | 0.41              |
| 87:By:185:GLN:HE21 | 87:By:185:GLN:HB2   | 1.67                     | 0.41              |
| 87:By:323:TYR:N    | 87:By:408:GLY:O     | 2.53                     | 0.41              |
| 87:By:329:MET:HA   | 87:By:373:PRO:HA    | 2.02                     | 0.41              |
| 1:A2:192:C:H4'     | 1:A2:192:C:OP1      | 2.19                     | 0.41              |
| 1:A2:1218:A:P      | 95:Ap:201:HOH:O     | 2.79                     | 0.41              |
| 4:AC:126:CYS:HB2   | 4:AC:130:VAL:HB     | 2.01                     | 0.41              |
| 20:Ah:114:GLU:OE2  | 20:Ah:123:ARG:NH2   | 2.54                     | 0.41              |
| 39:B5:315:G:OP2    | 39:B5:4100:U:O2'    | 2.35                     | 0.41              |
| 39:B5:1784:U:H2'   | 39:B5:1785:G:C8     | 2.55                     | 0.41              |
| 39:B5:1823:C:H4'   | 39:B5:2009:U:C4     | 2.55                     | 0.41              |
| 39:B5:2583:U:O4'   | 42:BA:187:HIS:HB3   | 2.20                     | 0.41              |
| 39:B5:3468:A:O2'   | 39:B5:3664:U:O2'    | 2.34                     | 0.41              |
| 39:B5:3797:U:H2'   | 39:B5:3798:U:C6     | 2.55                     | 0.41              |
| 43:BB:248:LEU:HD12 | 43:BB:249:ARG:HG3   | 2.03                     | 0.41              |
| 57:BP:94:MET:HE1   | 57:BP:146:ILE:HB    | 2.02                     | 0.41              |
| 69:Bb:48:LYS:O     | 69:Bb:51:LYS:NZ     | 2.54                     | 0.41              |
| 84:Bs:20:LEU:HD11  | 84:Bs:54:LEU:HG     | 2.02                     | 0.41              |
| 85:Bt:28:LEU:HD13  | 85:Bt:42:VAL:HG23   | 2.02                     | 0.41              |
| 86:Bv:117:ILE:HD13 | 86:Bv:137:LEU:HD21  | 2.02                     | 0.41              |
| 87:By:32:THR:H     | 87:By:67:ASN:ND2    | 2.17                     | 0.41              |
| 88:Bz:567:ARG:O    | 88:Bz:576:ARG:N     | 2.51                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A2:65:C:C2      | 18:Af:133:LEU:HD22 | 2.55                     | 0.41              |
| 1:A2:77:A:O2'     | 18:Af:174:PRO:O    | 2.36                     | 0.41              |
| 1:A2:507:G:OP1    | 36:Ax:108:LYS:NZ   | 2.38                     | 0.41              |
| 1:A2:572:U:H5''   | 36:Ax:37:LYS:HG3   | 2.02                     | 0.41              |
| 1:A2:1684:C:C2    | 3:AB:24:GLN:HG3    | 2.55                     | 0.41              |
| 1:A2:1754:C:H2'   | 1:A2:1755:G:C8     | 2.55                     | 0.41              |
| 1:A2:1837:G:OP1   | 1:A2:1840:U:H4'    | 2.20                     | 0.41              |
| 11:AT:61:G:H1     | 11:AT:73:C:H42     | 1.68                     | 0.41              |
| 15:Ac:8:LYS:HE3   | 32:At:59:LYS:HD2   | 2.02                     | 0.41              |
| 39:B5:443:G:H5''  | 73:Bf:54:LYS:HB3   | 2.01                     | 0.41              |
| 39:B5:1015:U:H3   | 39:B5:1086:G:H1    | 1.68                     | 0.41              |
| 39:B5:2110:U:OP1  | 83:Br:37:SER:OG    | 2.25                     | 0.41              |
| 43:BB:19:ARG:HB2  | 43:BB:234:ARG:NH2  | 2.35                     | 0.41              |
| 58:BQ:63:LEU:N    | 58:BQ:87:THR:O     | 2.53                     | 0.41              |
| 72:Be:124:ASN:N   | 72:Be:124:ASN:OD1  | 2.53                     | 0.41              |
| 83:Br:28:GLU:OE2  | 83:Br:31:ASN:ND2   | 2.53                     | 0.41              |
| 87:By:181:GLY:HA3 | 87:By:190:PHE:CE2  | 2.55                     | 0.41              |
| 88:Bz:425:ARG:HB2 | 88:Bz:455:ILE:HG12 | 2.03                     | 0.41              |
| 1:A2:229:A:H2'    | 1:A2:230:A:C8      | 2.56                     | 0.41              |
| 1:A2:1489:C:H3'   | 1:A2:1490:A:H4'    | 2.02                     | 0.41              |
| 12:AZ:5:LEU:O     | 12:AZ:9:GLN:HG2    | 2.20                     | 0.41              |
| 16:Ad:44:LEU:HD11 | 16:Ad:72:ILE:HD11  | 2.01                     | 0.41              |
| 18:Af:137:ARG:HD3 | 18:Af:178:ARG:NH2  | 2.35                     | 0.41              |
| 19:Ag:65:PRO:HD2  | 19:Ag:68:GLN:HE21  | 1.86                     | 0.41              |
| 26:An:16:SER:OG   | 26:An:17:LEU:N     | 2.47                     | 0.41              |
| 29:Aq:87:GLU:N    | 29:Aq:87:GLU:OE1   | 2.54                     | 0.41              |
| 39:B5:78:U:H5''   | 55:BN:185:GLY:HA2  | 2.03                     | 0.41              |
| 39:B5:175:C:H2'   | 39:B5:176:G:H8     | 1.86                     | 0.41              |
| 39:B5:819:C:H2'   | 39:B5:820:G:C8     | 2.54                     | 0.41              |
| 39:B5:1016:C:O2'  | 39:B5:1059:G:O4'   | 2.37                     | 0.41              |
| 39:B5:3693:G:O2'  | 39:B5:3771:G:N2    | 2.53                     | 0.41              |
| 39:B5:4088:C:O3'  | 81:Bo:37:GLY:HA3   | 2.20                     | 0.41              |
| 45:BD:119:TYR:OH  | 45:BD:139:PRO:O    | 2.36                     | 0.41              |
| 70:Bc:38:ILE:HG21 | 70:Bc:63:TYR:HB3   | 2.02                     | 0.41              |
| 80:Bm:112:LYS:HB3 | 80:Bm:114:LYS:HG2  | 2.03                     | 0.41              |
| 85:Bt:117:ARG:NH2 | 85:Bt:122:ALA:O    | 2.53                     | 0.41              |
| 1:A2:605:A:N3     | 1:A2:640:C:O2'     | 2.52                     | 0.41              |
| 1:A2:869:G:N3     | 19:Ag:115:LYS:HE2  | 2.36                     | 0.41              |
| 1:A2:915:U:OP1    | 19:Ag:67:PRO:HG3   | 2.21                     | 0.41              |
| 12:AZ:63:ARG:NH1  | 33:Au:78:ILE:HG23  | 2.36                     | 0.41              |
| 14:Ab:192:LEU:HB3 | 14:Ab:227:ARG:HG2  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:Ad:62:LYS:HE3  | 16:Ad:62:LYS:HB3   | 1.92                     | 0.41              |
| 27:Ao:60:LEU:HD22 | 27:Ao:92:SER:HB3   | 2.02                     | 0.41              |
| 37:Ay:42:ASP:OD1  | 37:Ay:42:ASP:N     | 2.50                     | 0.41              |
| 39:B5:49:U:OP2    | 55:BN:189:ARG:NH1  | 2.53                     | 0.41              |
| 39:B5:1654:A:O2'  | 39:B5:2042:A:O2'   | 2.29                     | 0.41              |
| 39:B5:1705:A:H2'  | 39:B5:1706:A:O4'   | 2.21                     | 0.41              |
| 39:B5:1928:G:H2'  | 39:B5:1929:A:C8    | 2.56                     | 0.41              |
| 39:B5:1941:A:C6   | 85:Bt:138:SER:HB3  | 2.56                     | 0.41              |
| 39:B5:3886:G:H2'  | 39:B5:3887:G:H8    | 1.85                     | 0.41              |
| 39:B5:4118:U:OP2  | 81:Bo:61:LYS:HG2   | 2.20                     | 0.41              |
| 39:B5:4277:U:H5   | 87:By:183:ALA:HA   | 1.85                     | 0.41              |
| 39:B5:4508:G:H5'' | 56:BO:12:ARG:CZ    | 2.51                     | 0.41              |
| 50:BI:205:PRO:HD2 | 50:BI:208:LYS:NZ   | 2.36                     | 0.41              |
| 67:BZ:22:LYS:NZ   | 67:BZ:132:GLN:O    | 2.45                     | 0.41              |
| 71:Bd:114:PHE:HA  | 71:Bd:117:LEU:HD12 | 2.01                     | 0.41              |
| 83:Br:56:ASP:OD1  | 83:Br:56:ASP:N     | 2.54                     | 0.41              |
| 1:A2:222:U:H5''   | 23:Ak:17:PHE:CG    | 2.56                     | 0.41              |
| 1:A2:399:A:OP1    | 1:A2:400:C:O2'     | 2.31                     | 0.41              |
| 1:A2:1375:C:H2'   | 1:A2:1376:G:O4'    | 2.21                     | 0.41              |
| 4:AC:117:LEU:H    | 4:AC:117:LEU:HD12  | 1.85                     | 0.41              |
| 39:B5:74:G:O6     | 53:BL:103:ARG:NH2  | 2.54                     | 0.41              |
| 39:B5:673:C:H2'   | 39:B5:674:G:C8     | 2.55                     | 0.41              |
| 39:B5:1704:A:N6   | 39:B5:1705:A:N3    | 2.68                     | 0.41              |
| 39:B5:2277:G:O2'  | 39:B5:2370:A:N1    | 2.54                     | 0.41              |
| 39:B5:2599:G:O6   | 67:BZ:51:ARG:NH2   | 2.41                     | 0.41              |
| 39:B5:3701:G:H1'  | 86:Bv:166:ALA:HB3  | 2.02                     | 0.41              |
| 39:B5:3791:U:H2'  | 39:B5:3792:C:C6    | 2.56                     | 0.41              |
| 55:BN:94:PHE:CE2  | 55:BN:96:ARG:HB2   | 2.55                     | 0.41              |
| 55:BN:146:PRO:HB2 | 75:Bh:104:THR:HG23 | 2.03                     | 0.41              |
| 60:BS:30:MET:HE2  | 60:BS:30:MET:HB3   | 1.94                     | 0.41              |
| 78:Bk:57:LYS:NZ   | 78:Bk:68:GLU:OE2   | 2.37                     | 0.41              |
| 1:A2:360:U:OP1    | 35:Aw:22:TRP:NE1   | 2.50                     | 0.41              |
| 1:A2:1051:A:H62   | 1:A2:1069:G:H21    | 1.69                     | 0.41              |
| 1:A2:1521:G:N2    | 27:Ao:126:VAL:HG11 | 2.35                     | 0.41              |
| 1:A2:1561:U:H2'   | 1:A2:1562:A:H8     | 1.84                     | 0.41              |
| 11:AT:86:A:H5''   | 52:BK:4400:LEU:O   | 2.21                     | 0.41              |
| 13:Aa:117:TRP:HB3 | 13:Aa:153:THR:HG22 | 2.02                     | 0.41              |
| 18:Af:162:LEU:HB2 | 18:Af:170:ARG:HB3  | 2.02                     | 0.41              |
| 39:B5:1508:A:O2'  | 82:Bp:9:GLY:O      | 2.33                     | 0.41              |
| 39:B5:1692:G:H21  | 45:BD:3:PHE:HD2    | 1.69                     | 0.41              |
| 39:B5:1907:G:H2'  | 39:B5:1908:G:C8    | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:B5:2127:G:OP1   | 68:Ba:7:LYS:NZ     | 2.52                     | 0.41              |
| 39:B5:2418:U:H5''  | 39:B5:2419:G:H5'   | 2.03                     | 0.41              |
| 39:B5:3548:A:OP1   | 39:B5:3550:UY1:N1  | 2.54                     | 0.41              |
| 39:B5:3687:G:O2'   | 39:B5:3688:G:O4'   | 2.39                     | 0.41              |
| 39:B5:4431:U:H2'   | 39:B5:4432:G:C8    | 2.56                     | 0.41              |
| 41:B8:36:G:C5      | 75:Bh:89:ARG:HD3   | 2.56                     | 0.41              |
| 48:BG:165:GLU:OE1  | 55:BN:26:ARG:NH2   | 2.41                     | 0.41              |
| 57:BP:94:MET:HE3   | 57:BP:94:MET:HB2   | 1.98                     | 0.41              |
| 73:Bf:40:GLU:O     | 73:Bf:109:ARG:NH2  | 2.53                     | 0.41              |
| 1:A2:541:U:H3      | 1:A2:544:C:H42     | 1.67                     | 0.41              |
| 1:A2:894:U:H2'     | 1:A2:895:G:C8      | 2.55                     | 0.41              |
| 1:A2:992:G:C6      | 1:A2:1135:G:H4'    | 2.56                     | 0.41              |
| 1:A2:1806:G:H2'    | 1:A2:1807:A:C8     | 2.56                     | 0.41              |
| 10:AI:71:N:H5''    | 39:B5:3471:C:O2'   | 2.20                     | 0.41              |
| 11:AT:46:G:H2'     | 11:AT:47:G:C8      | 2.56                     | 0.41              |
| 16:Ad:107:GLY:HA2  | 16:Ad:189:LEU:HG   | 2.02                     | 0.41              |
| 24:Al:52:LEU:HD21  | 24:Al:62:VAL:HG13  | 2.03                     | 0.41              |
| 30:Ar:7:GLU:H      | 30:Ar:7:GLU:CD     | 2.28                     | 0.41              |
| 35:Aw:17:ARG:HH11  | 35:Aw:17:ARG:HA    | 1.85                     | 0.41              |
| 36:Ax:21:LYS:HB2   | 36:Ax:75:ILE:HB    | 2.03                     | 0.41              |
| 39:B5:48:G:H5'     | 55:BN:192:TRP:CD1  | 2.56                     | 0.41              |
| 39:B5:120:A:N1     | 39:B5:148:A:O2'    | 2.49                     | 0.41              |
| 39:B5:419:A:N3     | 39:B5:1276:C:O2'   | 2.50                     | 0.41              |
| 39:B5:480:C:OP1    | 83:Br:67:ARG:NH1   | 2.47                     | 0.41              |
| 39:B5:624:G:H2'    | 39:B5:625:G:H8     | 1.85                     | 0.41              |
| 39:B5:778:C:H2'    | 39:B5:779:G:C8     | 2.56                     | 0.41              |
| 39:B5:790:G:O2'    | 39:B5:792:G:O4'    | 2.38                     | 0.41              |
| 39:B5:1271:C:H2'   | 39:B5:1272:G:C8    | 2.55                     | 0.41              |
| 39:B5:2317:G:H22   | 39:B5:2346:G:H5''  | 1.86                     | 0.41              |
| 39:B5:2625:U:OP2   | 79:Bl:10:LYS:NZ    | 2.45                     | 0.41              |
| 39:B5:3685:G:H2'   | 39:B5:3686:A:C8    | 2.56                     | 0.41              |
| 39:B5:4450:C:H2'   | 39:B5:4451:A:C8    | 2.56                     | 0.41              |
| 43:BB:353:VAL:HG12 | 43:BB:355:THR:HG23 | 2.02                     | 0.41              |
| 79:Bl:42:ARG:HG3   | 79:Bl:47:THR:HG23  | 2.03                     | 0.41              |
| 80:Bm:113:LYS:HG2  | 80:Bm:117:HIS:CE1  | 2.56                     | 0.41              |
| 87:By:33:SER:HA    | 87:By:71:VAL:HG22  | 2.03                     | 0.41              |
| 87:By:280:PHE:CZ   | 87:By:284:LYS:HD2  | 2.55                     | 0.41              |
| 88:Bz:73:VAL:HG21  | 88:Bz:295:ALA:HB1  | 2.03                     | 0.41              |
| 1:A2:74:G:H1       | 18:Af:171:THR:H    | 1.69                     | 0.41              |
| 11:AT:79:C:H2'     | 11:AT:80:G:C8      | 2.56                     | 0.41              |
| 12:AZ:118:GLU:OE2  | 14:Ab:65:LYS:N     | 2.46                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AZ:137:ALA:HB1  | 12:AZ:142:LEU:HB3  | 2.03                     | 0.41              |
| 20:Ah:142:SER:HB3  | 20:Ah:145:ILE:HG12 | 2.03                     | 0.41              |
| 21:Ai:158:ASP:OD1  | 21:Ai:158:ASP:N    | 2.52                     | 0.41              |
| 39:B5:63:G:OP1     | 55:BN:169:ARG:NH2  | 2.55                     | 0.41              |
| 39:B5:1549:C:O2'   | 39:B5:1552:G:H1'   | 2.21                     | 0.41              |
| 39:B5:1984:G:O2'   | 39:B5:1985:G:H5''  | 2.21                     | 0.41              |
| 39:B5:2102:G:O2'   | 46:BE:111:LYS:NZ   | 2.34                     | 0.41              |
| 39:B5:3602:C:H2'   | 39:B5:3603:A:C8    | 2.56                     | 0.41              |
| 44:BC:71:ARG:CZ    | 52:BK:4389:PRO:HD3 | 2.51                     | 0.41              |
| 1:A2:683:U:H2'     | 1:A2:684:OMG:O4'   | 2.21                     | 0.40              |
| 1:A2:849:U:H2'     | 1:A2:850:A:H8      | 1.85                     | 0.40              |
| 1:A2:1671:C:H2'    | 1:A2:1672:G:C8     | 2.56                     | 0.40              |
| 7:AF:159:ASN:HD22  | 7:AF:159:ASN:H     | 1.69                     | 0.40              |
| 13:Aa:108:ASP:OD1  | 13:Aa:108:ASP:N    | 2.43                     | 0.40              |
| 21:Ai:3:VAL:HG21   | 21:Ai:5:ARG:HD2    | 2.03                     | 0.40              |
| 39:B5:62:A:OP2     | 95:B5:5417:HOH:O   | 2.22                     | 0.40              |
| 39:B5:300:A:H2'    | 39:B5:301:G:H8     | 1.86                     | 0.40              |
| 39:B5:3686:A:H2'   | 39:B5:3687:G:C8    | 2.56                     | 0.40              |
| 39:B5:4368:A:H4'   | 43:BB:13:SER:HB2   | 2.04                     | 0.40              |
| 39:B5:4599:G:H2'   | 39:B5:4600:G:H8    | 1.86                     | 0.40              |
| 39:B5:4627:C:H2'   | 39:B5:4628:G:C8    | 2.56                     | 0.40              |
| 40:B7:55:A:O2'     | 51:BJ:151:ILE:O    | 2.23                     | 0.40              |
| 45:BD:208:MET:HE3  | 45:BD:233:PRO:HG3  | 2.03                     | 0.40              |
| 62:BU:27:HIS:HB3   | 62:BU:114:TYR:HE1  | 1.86                     | 0.40              |
| 1:A2:1241:A:H5''   | 27:Ao:140:ARG:NH2  | 2.36                     | 0.40              |
| 7:AF:194:TYR:HE1   | 7:AF:196:ASN:HD21  | 1.68                     | 0.40              |
| 11:AT:35:A:H2'     | 11:AT:36:A:C8      | 2.56                     | 0.40              |
| 13:Aa:123:ALA:HB2  | 13:Aa:165:ARG:HG3  | 2.02                     | 0.40              |
| 14:Ab:172:ASN:HD22 | 21:Ai:95:ASP:CG    | 2.29                     | 0.40              |
| 31:As:65:TYR:HE1   | 31:As:128:GLN:HG3  | 1.87                     | 0.40              |
| 39:B5:681:U:C4     | 46:BE:98:PRO:HG2   | 2.56                     | 0.40              |
| 39:B5:1430:G:H2'   | 39:B5:1431:C:C6    | 2.56                     | 0.40              |
| 39:B5:4052:OMU:OP2 | 58:BQ:159:PRO:HD2  | 2.21                     | 0.40              |
| 39:B5:4667:C:O2    | 54:BM:118:MET:HE1  | 2.22                     | 0.40              |
| 41:B8:30:U:H2'     | 41:B8:31:G:C8      | 2.56                     | 0.40              |
| 45:BD:116:ASP:OD1  | 45:BD:116:ASP:N    | 2.53                     | 0.40              |
| 45:BD:202:GLN:NE2  | 45:BD:237:GLU:HB2  | 2.37                     | 0.40              |
| 72:Be:82:VAL:HG13  | 72:Be:114:ARG:HG2  | 2.03                     | 0.40              |
| 88:Bz:436:TYR:CZ   | 88:Bz:437:THR:HG23 | 2.56                     | 0.40              |
| 1:A2:53:C:O2'      | 1:A2:508:G:N7      | 2.49                     | 0.40              |
| 1:A2:64:A:H2       | 1:A2:83:A:H62      | 1.69                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A2:317:G:H3'     | 18:Af:183:ARG:HH12 | 1.87                     | 0.40              |
| 1:A2:695:G:H1      | 1:A2:733:U:H3      | 1.70                     | 0.40              |
| 1:A2:982:A:H2'     | 1:A2:983:G:C8      | 2.56                     | 0.40              |
| 18:Af:44:GLU:H     | 18:Af:44:GLU:CD    | 2.29                     | 0.40              |
| 30:Ar:132:ARG:HB2  | 30:Ar:134:GLN:HE22 | 1.84                     | 0.40              |
| 31:As:39:LEU:HD21  | 31:As:52:TRP:CZ3   | 2.56                     | 0.40              |
| 39:B5:252:C:H2'    | 39:B5:253:G:C8     | 2.57                     | 0.40              |
| 39:B5:1068:U:H2'   | 39:B5:1069:G:C8    | 2.56                     | 0.40              |
| 39:B5:1265:G:H2'   | 39:B5:3608:A:N7    | 2.36                     | 0.40              |
| 39:B5:1508:A:OP2   | 82:Bp:4:ARG:HD2    | 2.21                     | 0.40              |
| 39:B5:2573:U:H2'   | 39:B5:2574:C:C6    | 2.56                     | 0.40              |
| 39:B5:2592:C:H2'   | 39:B5:2593:G:C8    | 2.56                     | 0.40              |
| 39:B5:4447:A:HO2'  | 49:BH:40:HIS:CE1   | 2.35                     | 0.40              |
| 42:BA:177:LYS:HG3  | 82:Bp:26:VAL:HG23  | 2.03                     | 0.40              |
| 81:Bo:28:LYS:NZ    | 81:Bo:31:ASP:OD1   | 2.53                     | 0.40              |
| 87:By:256:ILE:HD12 | 87:By:263:GLY:HA3  | 2.04                     | 0.40              |
| 1:A2:503:C:O4'     | 16:Ad:66:MET:HG3   | 2.21                     | 0.40              |
| 1:A2:1044:G:H2'    | 1:A2:1045:G:O4'    | 2.22                     | 0.40              |
| 1:A2:1084:A:N7     | 1:A2:1842:C:O2'    | 2.45                     | 0.40              |
| 1:A2:1657:G:H1     | 1:A2:1669:U:H3     | 1.69                     | 0.40              |
| 2:AA:23:ARG:O      | 34:Av:60:LYS:NZ    | 2.54                     | 0.40              |
| 2:AA:54:VAL:HG12   | 2:AA:63:LEU:HD12   | 2.04                     | 0.40              |
| 25:Am:100:LYS:O    | 25:Am:103:GLU:HG2  | 2.21                     | 0.40              |
| 25:Am:140:LYS:HD2  | 25:Am:140:LYS:HA   | 1.90                     | 0.40              |
| 39:B5:91:G:H4'     | 81:Bo:53:MLZ:HE2   | 2.02                     | 0.40              |
| 39:B5:106:A:H1'    | 39:B5:336:A:N3     | 2.36                     | 0.40              |
| 39:B5:478:G:H2'    | 39:B5:479:G:C8     | 2.57                     | 0.40              |
| 39:B5:1250:C:H2'   | 39:B5:1251:A:C8    | 2.56                     | 0.40              |
| 39:B5:1680:G:O6    | 40:B7:103:A:O2'    | 2.26                     | 0.40              |
| 39:B5:2254:C:H2'   | 39:B5:2255:A:C8    | 2.56                     | 0.40              |
| 39:B5:4516:G:H5''  | 56:BO:176:ARG:HD3  | 2.02                     | 0.40              |
| 43:BB:17:LEU:HD21  | 43:BB:235:TRP:HH2  | 1.85                     | 0.40              |
| 46:BE:165:VAL:HG11 | 46:BE:187:VAL:HG11 | 2.02                     | 0.40              |
| 59:BR:70:ARG:HD3   | 59:BR:76:MET:HE2   | 2.03                     | 0.40              |
| 60:BS:83:ARG:HH21  | 60:BS:90:THR:HG21  | 1.87                     | 0.40              |
| 64:BW:34:ALA:HA    | 64:BW:37:GLU:HB3   | 2.04                     | 0.40              |
| 76:Bi:73:ILE:O     | 76:Bi:77:VAL:HG22  | 2.21                     | 0.40              |
| 1:A2:43:U:OP2      | 1:A2:486:A:N6      | 2.42                     | 0.40              |
| 1:A2:381:G:OP1     | 20:Ah:31:ARG:NE    | 2.40                     | 0.40              |
| 1:A2:997:A:P       | 25:Am:114:ARG:HH22 | 2.44                     | 0.40              |
| 1:A2:1347:U:H2'    | 1:A2:1348:PSU:H6   | 1.86                     | 0.40              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:A2:1446:PSU:H1'   | 1:A2:1581:A:H61   | 1.86                     | 0.40              |
| 1:A2:1737:G:H2'     | 1:A2:1738:G:C8    | 2.57                     | 0.40              |
| 1:A2:1837:G:OP1     | 95:A2:2108:HOH:O  | 2.22                     | 0.40              |
| 20:Ah:106:SER:HB3   | 20:Ah:171:LEU:HG  | 2.02                     | 0.40              |
| 22:Aj:32:HIS:CD2    | 22:Aj:34:GLU:H    | 2.40                     | 0.40              |
| 35:Aw:115:ILE:HA    | 35:Aw:116:PRO:HD3 | 1.95                     | 0.40              |
| 39:B5:484:G:H3'     | 39:B5:485:U:H2'   | 2.03                     | 0.40              |
| 39:B5:716:G:OP1     | 39:B5:835:G:N1    | 2.42                     | 0.40              |
| 39:B5:842:G:OP1     | 47:BF:244:ARG:NH2 | 2.54                     | 0.40              |
| 39:B5:1276:C:H2'    | 39:B5:1277:A:C8   | 2.57                     | 0.40              |
| 39:B5:2399:G:H2'    | 39:B5:2400:G:C8   | 2.56                     | 0.40              |
| 42:BA:80:GLU:HB2    | 42:BA:170:ALA:HA  | 2.03                     | 0.40              |
| 52:BK:4387:ARG:HH11 | 52:BK:4388:GLU:H  | 1.69                     | 0.40              |
| 55:BN:149:GLN:O     | 55:BN:152:THR:OG1 | 2.37                     | 0.40              |
| 86:Bv:60:ARG:HD3    | 86:Bv:173:LYS:HB2 | 2.03                     | 0.40              |
| 88:Bz:353:MET:HB2   | 88:Bz:398:PRO:HB3 | 2.04                     | 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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | AA    | 81/84 (96%)   | 79 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 3   | AB    | 61/69 (88%)   | 61 (100%) | 0       | 0        | 100         | 100 |
| 4   | AC    | 71/156 (46%)  | 69 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 5   | AD    | 55/133 (41%)  | 55 (100%) | 0       | 0        | 100         | 100 |
| 6   | AE    | 99/115 (86%)  | 99 (100%) | 0       | 0        | 100         | 100 |
| 7   | AF    | 311/317 (98%) | 300 (96%) | 11 (4%) | 0        | 100         | 100 |
| 8   | AG    | 53/56 (95%)   | 53 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 12  | AZ    | 219/295 (74%) | 215 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 13  | Aa    | 220/264 (83%) | 218 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 14  | Ab    | 218/293 (74%) | 218 (100%) | 0       | 0        | 100         | 100 |
| 15  | Ac    | 223/281 (79%) | 222 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 16  | Ad    | 260/263 (99%) | 256 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 17  | Ae    | 189/204 (93%) | 184 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 18  | Af    | 235/249 (94%) | 235 (100%) | 0       | 0        | 100         | 100 |
| 19  | Ag    | 188/194 (97%) | 184 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 20  | Ah    | 204/208 (98%) | 203 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 21  | Ai    | 183/194 (94%) | 181 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 22  | Aj    | 94/165 (57%)  | 93 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 23  | Ak    | 152/158 (96%) | 149 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 24  | Al    | 122/132 (92%) | 119 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 25  | Am    | 148/151 (98%) | 147 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 26  | An    | 134/151 (89%) | 133 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 27  | Ao    | 131/145 (90%) | 130 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 28  | Ap    | 139/146 (95%) | 133 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 29  | Aq    | 132/135 (98%) | 132 (100%) | 0       | 0        | 100         | 100 |
| 30  | Ar    | 143/152 (94%) | 141 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 31  | As    | 140/145 (97%) | 139 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 32  | At    | 102/119 (86%) | 101 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 33  | Au    | 81/83 (98%)   | 81 (100%)  | 0       | 0        | 100         | 100 |
| 34  | Av    | 127/130 (98%) | 126 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 35  | Aw    | 138/143 (96%) | 137 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 36  | Ax    | 123/130 (95%) | 121 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 37  | Ay    | 83/124 (67%)  | 83 (100%)  | 0       | 0        | 100         | 100 |
| 38  | Az    | 23/25 (92%)   | 23 (100%)  | 0       | 0        | 100         | 100 |
| 42  | BA    | 250/257 (97%) | 244 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 43  | BB    | 395/403 (98%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 44  | BC    | 360/413 (87%) | 357 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 45  | BD    | 291/297 (98%) | 289 (99%)  | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 46  | BE    | 239/291 (82%) | 235 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 47  | BF    | 224/247 (91%) | 219 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 48  | BG    | 229/266 (86%) | 228 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 49  | BH    | 188/192 (98%) | 188 (100%) | 0       | 0        | 100         | 100 |
| 50  | BI    | 211/214 (99%) | 208 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 51  | BJ    | 168/178 (94%) | 167 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 52  | BK    | 34/1071 (3%)  | 34 (100%)  | 0       | 0        | 100         | 100 |
| 53  | BL    | 208/211 (99%) | 204 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 54  | BM    | 136/218 (62%) | 133 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 55  | BN    | 201/204 (98%) | 196 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 56  | BO    | 197/203 (97%) | 197 (100%) | 0       | 0        | 100         | 100 |
| 57  | BP    | 157/184 (85%) | 156 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 58  | BQ    | 185/188 (98%) | 182 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 59  | BR    | 178/196 (91%) | 178 (100%) | 0       | 0        | 100         | 100 |
| 60  | BS    | 174/176 (99%) | 174 (100%) | 0       | 0        | 100         | 100 |
| 61  | BT    | 157/160 (98%) | 154 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 62  | BU    | 97/128 (76%)  | 95 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 63  | BV    | 137/140 (98%) | 137 (100%) | 0       | 0        | 100         | 100 |
| 64  | BW    | 119/157 (76%) | 119 (100%) | 0       | 0        | 100         | 100 |
| 65  | BX    | 116/156 (74%) | 114 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 66  | BY    | 132/145 (91%) | 131 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 67  | BZ    | 133/136 (98%) | 133 (100%) | 0       | 0        | 100         | 100 |
| 68  | Ba    | 144/148 (97%) | 139 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 69  | Bb    | 103/245 (42%) | 97 (94%)   | 6 (6%)  | 0        | 100         | 100 |
| 70  | Bc    | 106/115 (92%) | 106 (100%) | 0       | 0        | 100         | 100 |
| 71  | Bd    | 105/125 (84%) | 105 (100%) | 0       | 0        | 100         | 100 |
| 72  | Be    | 128/135 (95%) | 128 (100%) | 0       | 0        | 100         | 100 |
| 73  | Bf    | 108/110 (98%) | 108 (100%) | 0       | 0        | 100         | 100 |
| 74  | Bg    | 112/117 (96%) | 111 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 75  | Bh    | 120/123 (98%) | 120 (100%) | 0       | 0        | 100         | 100 |
| 76  | Bi    | 100/105 (95%) | 99 (99%)   | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 77  | Bj    | 84/97 (87%)       | 84 (100%)   | 0        | 0        | 100         | 100 |
| 78  | Bk    | 67/70 (96%)       | 67 (100%)   | 0        | 0        | 100         | 100 |
| 79  | Bl    | 48/51 (94%)       | 48 (100%)   | 0        | 0        | 100         | 100 |
| 80  | Bm    | 49/128 (38%)      | 49 (100%)   | 0        | 0        | 100         | 100 |
| 81  | Bo    | 102/106 (96%)     | 100 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 82  | Bp    | 89/92 (97%)       | 88 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 83  | Br    | 124/137 (90%)     | 122 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 84  | Bs    | 194/318 (61%)     | 190 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 85  | Bt    | 154/165 (93%)     | 153 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 86  | Bv    | 210/217 (97%)     | 203 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 87  | By    | 414/437 (95%)     | 406 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 88  | Bz    | 593/599 (99%)     | 582 (98%)   | 11 (2%)  | 0        | 100         | 100 |
| All | All   | 12952/15680 (83%) | 12789 (99%) | 163 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 2   | AA    | 75/76 (99%)   | 74 (99%)  | 1 (1%)   | 61          | 86  |
| 3   | AB    | 56/62 (90%)   | 55 (98%)  | 1 (2%)   | 51          | 80  |
| 4   | AC    | 66/140 (47%)  | 66 (100%) | 0        | 100         | 100 |
| 5   | AD    | 47/106 (44%)  | 46 (98%)  | 1 (2%)   | 47          | 77  |
| 6   | AE    | 88/98 (90%)   | 85 (97%)  | 3 (3%)   | 32          | 66  |
| 7   | AF    | 272/275 (99%) | 267 (98%) | 5 (2%)   | 51          | 80  |
| 8   | AG    | 48/49 (98%)   | 48 (100%) | 0        | 100         | 100 |
| 12  | AZ    | 182/243 (75%) | 179 (98%) | 3 (2%)   | 55          | 83  |
| 13  | Aa    | 203/231 (88%) | 201 (99%) | 2 (1%)   | 68          | 89  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 14  | Ab    | 185/223 (83%)  | 184 (100%) | 1 (0%)   | 81          | 93  |
| 15  | Ac    | 189/232 (82%)  | 185 (98%)  | 4 (2%)   | 47          | 77  |
| 16  | Ad    | 224/225 (100%) | 224 (100%) | 0        | 100         | 100 |
| 17  | Ae    | 161/170 (95%)  | 161 (100%) | 0        | 100         | 100 |
| 18  | Af    | 207/218 (95%)  | 206 (100%) | 1 (0%)   | 81          | 93  |
| 19  | Ag    | 170/174 (98%)  | 166 (98%)  | 4 (2%)   | 43          | 75  |
| 20  | Ah    | 178/180 (99%)  | 177 (99%)  | 1 (1%)   | 78          | 93  |
| 21  | Ai    | 161/168 (96%)  | 160 (99%)  | 1 (1%)   | 78          | 93  |
| 22  | Aj    | 87/136 (64%)   | 86 (99%)   | 1 (1%)   | 65          | 88  |
| 23  | Ak    | 139/142 (98%)  | 138 (99%)  | 1 (1%)   | 76          | 92  |
| 24  | Al    | 104/108 (96%)  | 100 (96%)  | 4 (4%)   | 29          | 64  |
| 25  | Am    | 130/131 (99%)  | 130 (100%) | 0        | 100         | 100 |
| 26  | An    | 106/119 (89%)  | 104 (98%)  | 2 (2%)   | 50          | 79  |
| 27  | Ao    | 119/130 (92%)  | 119 (100%) | 0        | 100         | 100 |
| 28  | Ap    | 117/121 (97%)  | 117 (100%) | 0        | 100         | 100 |
| 29  | Aq    | 120/121 (99%)  | 120 (100%) | 0        | 100         | 100 |
| 30  | Ar    | 125/131 (95%)  | 122 (98%)  | 3 (2%)   | 43          | 75  |
| 31  | As    | 112/114 (98%)  | 112 (100%) | 0        | 100         | 100 |
| 32  | At    | 94/107 (88%)   | 92 (98%)   | 2 (2%)   | 47          | 77  |
| 33  | Au    | 67/67 (100%)   | 65 (97%)   | 2 (3%)   | 36          | 70  |
| 34  | Av    | 112/113 (99%)  | 112 (100%) | 0        | 100         | 100 |
| 35  | Aw    | 112/114 (98%)  | 109 (97%)  | 3 (3%)   | 39          | 73  |
| 36  | Ax    | 107/112 (96%)  | 106 (99%)  | 1 (1%)   | 70          | 90  |
| 37  | Ay    | 75/102 (74%)   | 74 (99%)   | 1 (1%)   | 61          | 86  |
| 38  | Az    | 24/24 (100%)   | 24 (100%)  | 0        | 100         | 100 |
| 42  | BA    | 194/198 (98%)  | 193 (100%) | 1 (0%)   | 81          | 93  |
| 43  | BB    | 344/347 (99%)  | 342 (99%)  | 2 (1%)   | 78          | 93  |
| 44  | BC    | 302/337 (90%)  | 302 (100%) | 0        | 100         | 100 |
| 45  | BD    | 247/250 (99%)  | 247 (100%) | 0        | 100         | 100 |
| 46  | BE    | 216/251 (86%)  | 214 (99%)  | 2 (1%)   | 70          | 90  |
| 47  | BF    | 197/215 (92%)  | 196 (100%) | 1 (0%)   | 81          | 93  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 48  | BG    | 199/223 (89%)  | 197 (99%)  | 2 (1%)   | 68          | 89  |
| 49  | BH    | 169/171 (99%)  | 169 (100%) | 0        | 100         | 100 |
| 50  | BI    | 180/181 (99%)  | 179 (99%)  | 1 (1%)   | 78          | 93  |
| 51  | BJ    | 143/149 (96%)  | 143 (100%) | 0        | 100         | 100 |
| 52  | BK    | 31/936 (3%)    | 30 (97%)   | 1 (3%)   | 34          | 68  |
| 53  | BL    | 175/176 (99%)  | 171 (98%)  | 4 (2%)   | 44          | 76  |
| 54  | BM    | 117/161 (73%)  | 116 (99%)  | 1 (1%)   | 70          | 90  |
| 55  | BN    | 171/172 (99%)  | 171 (100%) | 0        | 100         | 100 |
| 56  | BO    | 171/173 (99%)  | 171 (100%) | 0        | 100         | 100 |
| 57  | BP    | 140/163 (86%)  | 140 (100%) | 0        | 100         | 100 |
| 58  | BQ    | 164/165 (99%)  | 160 (98%)  | 4 (2%)   | 43          | 75  |
| 59  | BR    | 159/175 (91%)  | 159 (100%) | 0        | 100         | 100 |
| 60  | BS    | 154/154 (100%) | 153 (99%)  | 1 (1%)   | 78          | 93  |
| 61  | BT    | 139/140 (99%)  | 139 (100%) | 0        | 100         | 100 |
| 62  | BU    | 88/113 (78%)   | 88 (100%)  | 0        | 100         | 100 |
| 63  | BV    | 106/107 (99%)  | 105 (99%)  | 1 (1%)   | 70          | 90  |
| 64  | BW    | 100/126 (79%)  | 99 (99%)   | 1 (1%)   | 68          | 89  |
| 65  | BX    | 106/134 (79%)  | 106 (100%) | 0        | 100         | 100 |
| 66  | BY    | 124/135 (92%)  | 123 (99%)  | 1 (1%)   | 73          | 90  |
| 67  | BZ    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 68  | Ba    | 118/119 (99%)  | 118 (100%) | 0        | 100         | 100 |
| 69  | Bb    | 87/183 (48%)   | 87 (100%)  | 0        | 100         | 100 |
| 70  | Bc    | 92/98 (94%)    | 92 (100%)  | 0        | 100         | 100 |
| 71  | Bd    | 98/110 (89%)   | 97 (99%)   | 1 (1%)   | 68          | 89  |
| 72  | Be    | 116/121 (96%)  | 116 (100%) | 0        | 100         | 100 |
| 73  | Bf    | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 74  | Bg    | 98/100 (98%)   | 98 (100%)  | 0        | 100         | 100 |
| 75  | Bh    | 109/110 (99%)  | 109 (100%) | 0        | 100         | 100 |
| 76  | Bi    | 86/89 (97%)    | 85 (99%)   | 1 (1%)   | 63          | 86  |
| 77  | Bj    | 73/80 (91%)    | 72 (99%)   | 1 (1%)   | 59          | 85  |
| 78  | Bk    | 64/65 (98%)    | 62 (97%)   | 2 (3%)   | 35          | 69  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 79  | Bl    | 47/48 (98%)       | 46 (98%)    | 1 (2%)   | 47          | 77  |
| 80  | Bm    | 47/115 (41%)      | 47 (100%)   | 0        | 100         | 100 |
| 81  | Bo    | 92/93 (99%)       | 92 (100%)   | 0        | 100         | 100 |
| 82  | Bp    | 74/75 (99%)       | 73 (99%)    | 1 (1%)   | 59          | 85  |
| 83  | Br    | 109/120 (91%)     | 109 (100%)  | 0        | 100         | 100 |
| 84  | Bs    | 164/258 (64%)     | 163 (99%)   | 1 (1%)   | 78          | 93  |
| 85  | Bt    | 128/137 (93%)     | 125 (98%)   | 3 (2%)   | 44          | 76  |
| 86  | Bv    | 191/195 (98%)     | 185 (97%)   | 6 (3%)   | 35          | 69  |
| 87  | By    | 358/376 (95%)     | 337 (94%)   | 21 (6%)  | 18          | 48  |
| 88  | Bz    | 516/526 (98%)     | 502 (97%)   | 14 (3%)  | 39          | 73  |
| All | All   | 11271/13339 (84%) | 11148 (99%) | 123 (1%) | 63          | 88  |

All (123) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AA    | 74  | THR  |
| 3   | AB    | 14  | VAL  |
| 5   | AD    | 122 | THR  |
| 6   | AE    | 21  | ILE  |
| 6   | AE    | 40  | VAL  |
| 6   | AE    | 75  | VAL  |
| 7   | AF    | 107 | ASP  |
| 7   | AF    | 113 | PHE  |
| 7   | AF    | 159 | ASN  |
| 7   | AF    | 235 | ILE  |
| 7   | AF    | 296 | GLN  |
| 12  | AZ    | 121 | LEU  |
| 12  | AZ    | 192 | GLU  |
| 12  | AZ    | 206 | ASP  |
| 13  | Aa    | 170 | GLU  |
| 13  | Aa    | 178 | THR  |
| 14  | Ab    | 79  | GLU  |
| 15  | Ac    | 46  | THR  |
| 15  | Ac    | 48  | ILE  |
| 15  | Ac    | 72  | VAL  |
| 15  | Ac    | 175 | VAL  |
| 18  | Af    | 190 | ARG  |
| 19  | Ag    | 18  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 19  | Ag    | 53   | VAL  |
| 19  | Ag    | 75   | ILE  |
| 19  | Ag    | 110  | THR  |
| 20  | Ah    | 46   | VAL  |
| 21  | Ai    | 55   | LYS  |
| 22  | Aj    | 40   | VAL  |
| 23  | Ak    | 24   | LEU  |
| 24  | Al    | 42   | LEU  |
| 24  | Al    | 75   | ASN  |
| 24  | Al    | 91   | LEU  |
| 24  | Al    | 104  | VAL  |
| 26  | An    | 113  | GLN  |
| 26  | An    | 138  | ASP  |
| 30  | Ar    | 59   | LEU  |
| 30  | Ar    | 94   | LYS  |
| 30  | Ar    | 103  | LEU  |
| 32  | At    | 54   | VAL  |
| 32  | At    | 68   | THR  |
| 33  | Au    | 42   | VAL  |
| 33  | Au    | 61   | ARG  |
| 35  | Aw    | 61   | GLN  |
| 35  | Aw    | 105  | PHE  |
| 35  | Aw    | 125  | VAL  |
| 36  | Ax    | 98   | GLU  |
| 37  | Ay    | 44   | LEU  |
| 42  | BA    | 14   | SER  |
| 43  | BB    | 90   | VAL  |
| 43  | BB    | 162  | VAL  |
| 46  | BE    | 223  | LYS  |
| 46  | BE    | 289  | LEU  |
| 47  | BF    | 85   | GLU  |
| 48  | BG    | 106  | THR  |
| 48  | BG    | 220  | GLU  |
| 50  | BI    | 163  | GLN  |
| 52  | BK    | 4400 | LEU  |
| 53  | BL    | 63   | THR  |
| 53  | BL    | 81   | LEU  |
| 53  | BL    | 115  | GLN  |
| 53  | BL    | 129  | ARG  |
| 54  | BM    | 126  | GLU  |
| 58  | BQ    | 14   | ARG  |
| 58  | BQ    | 82   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | BQ    | 87  | THR  |
| 58  | BQ    | 115 | LYS  |
| 60  | BS    | 82  | LEU  |
| 63  | BV    | 50  | ASN  |
| 64  | BW    | 67  | ILE  |
| 66  | BY    | 88  | GLU  |
| 71  | Bd    | 106 | VAL  |
| 76  | Bi    | 81  | ILE  |
| 77  | Bj    | 57  | ASN  |
| 78  | Bk    | 30  | ASP  |
| 78  | Bk    | 36  | VAL  |
| 79  | Bl    | 28  | TRP  |
| 82  | Bp    | 52  | VAL  |
| 84  | Bs    | 75  | LEU  |
| 85  | Bt    | 58  | ILE  |
| 85  | Bt    | 60  | VAL  |
| 85  | Bt    | 149 | HIS  |
| 86  | Bv    | 15  | ARG  |
| 86  | Bv    | 58  | THR  |
| 86  | Bv    | 60  | ARG  |
| 86  | Bv    | 96  | ASN  |
| 86  | Bv    | 99  | LEU  |
| 86  | Bv    | 159 | MET  |
| 87  | By    | 32  | THR  |
| 87  | By    | 44  | GLN  |
| 87  | By    | 87  | LYS  |
| 87  | By    | 88  | VAL  |
| 87  | By    | 93  | LEU  |
| 87  | By    | 101 | VAL  |
| 87  | By    | 102 | THR  |
| 87  | By    | 110 | VAL  |
| 87  | By    | 111 | ASN  |
| 87  | By    | 166 | ARG  |
| 87  | By    | 185 | GLN  |
| 87  | By    | 203 | ARG  |
| 87  | By    | 211 | GLN  |
| 87  | By    | 224 | LEU  |
| 87  | By    | 232 | PHE  |
| 87  | By    | 258 | TYR  |
| 87  | By    | 321 | ILE  |
| 87  | By    | 332 | VAL  |
| 87  | By    | 342 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | By    | 354 | LYS  |
| 87  | By    | 356 | HIS  |
| 88  | Bz    | 41  | VAL  |
| 88  | Bz    | 75  | LEU  |
| 88  | Bz    | 128 | LYS  |
| 88  | Bz    | 183 | THR  |
| 88  | Bz    | 211 | GLU  |
| 88  | Bz    | 232 | ILE  |
| 88  | Bz    | 359 | GLU  |
| 88  | Bz    | 427 | LEU  |
| 88  | Bz    | 484 | LEU  |
| 88  | Bz    | 493 | ASP  |
| 88  | Bz    | 508 | ILE  |
| 88  | Bz    | 524 | MET  |
| 88  | Bz    | 551 | LEU  |
| 88  | Bz    | 597 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AA    | 9   | HIS  |
| 2   | AA    | 29  | ASN  |
| 2   | AA    | 51  | GLN  |
| 4   | AC    | 139 | HIS  |
| 4   | AC    | 151 | ASN  |
| 5   | AD    | 89  | GLN  |
| 6   | AE    | 72  | HIS  |
| 7   | AF    | 62  | HIS  |
| 7   | AF    | 196 | ASN  |
| 7   | AF    | 296 | GLN  |
| 8   | AG    | 16  | GLN  |
| 8   | AG    | 28  | HIS  |
| 8   | AG    | 37  | ASN  |
| 13  | Aa    | 186 | ASN  |
| 14  | Ab    | 115 | GLN  |
| 14  | Ab    | 178 | HIS  |
| 15  | Ac    | 4   | GLN  |
| 15  | Ac    | 145 | GLN  |
| 15  | Ac    | 174 | HIS  |
| 16  | Ad    | 98  | ASN  |
| 16  | Ad    | 142 | HIS  |
| 16  | Ad    | 157 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Ae    | 65  | GLN  |
| 17  | Ae    | 83  | ASN  |
| 17  | Ae    | 101 | HIS  |
| 17  | Ae    | 110 | GLN  |
| 17  | Ae    | 118 | ASN  |
| 18  | Af    | 65  | GLN  |
| 20  | Ah    | 7   | ASN  |
| 20  | Ah    | 146 | GLN  |
| 20  | Ah    | 167 | GLN  |
| 22  | Aj    | 50  | GLN  |
| 22  | Aj    | 66  | HIS  |
| 22  | Aj    | 77  | GLN  |
| 23  | Ak    | 11  | GLN  |
| 23  | Ak    | 19  | ASN  |
| 23  | Ak    | 39  | ASN  |
| 24  | Al    | 28  | HIS  |
| 24  | Al    | 72  | HIS  |
| 25  | Am    | 13  | GLN  |
| 25  | Am    | 49  | GLN  |
| 27  | Ao    | 103 | ASN  |
| 28  | Ap    | 11  | GLN  |
| 28  | Ap    | 24  | HIS  |
| 28  | Ap    | 77  | HIS  |
| 28  | Ap    | 80  | GLN  |
| 28  | Ap    | 86  | GLN  |
| 28  | Ap    | 97  | GLN  |
| 29  | Aq    | 29  | HIS  |
| 30  | Ar    | 72  | GLN  |
| 31  | As    | 12  | GLN  |
| 33  | Au    | 2   | GLN  |
| 33  | Au    | 35  | ASN  |
| 34  | Av    | 90  | GLN  |
| 34  | Av    | 91  | ASN  |
| 34  | Av    | 120 | HIS  |
| 35  | Aw    | 23  | HIS  |
| 36  | Ax    | 19  | GLN  |
| 36  | Ax    | 85  | ASN  |
| 42  | BA    | 50  | HIS  |
| 42  | BA    | 140 | ASN  |
| 42  | BA    | 205 | ASN  |
| 42  | BA    | 253 | GLN  |
| 43  | BB    | 109 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BB    | 175 | GLN  |
| 43  | BB    | 184 | GLN  |
| 43  | BB    | 289 | GLN  |
| 43  | BB    | 354 | GLN  |
| 44  | BC    | 21  | ASN  |
| 44  | BC    | 50  | GLN  |
| 44  | BC    | 89  | GLN  |
| 44  | BC    | 119 | GLN  |
| 44  | BC    | 215 | ASN  |
| 44  | BC    | 276 | ASN  |
| 44  | BC    | 329 | ASN  |
| 44  | BC    | 347 | HIS  |
| 45  | BD    | 122 | GLN  |
| 45  | BD    | 202 | GLN  |
| 45  | BD    | 222 | GLN  |
| 45  | BD    | 225 | GLN  |
| 46  | BE    | 269 | GLN  |
| 47  | BF    | 57  | HIS  |
| 47  | BF    | 115 | GLN  |
| 47  | BF    | 118 | ASN  |
| 48  | BG    | 38  | ASN  |
| 48  | BG    | 64  | GLN  |
| 48  | BG    | 81  | ASN  |
| 49  | BH    | 106 | GLN  |
| 50  | BI    | 59  | GLN  |
| 50  | BI    | 73  | ASN  |
| 50  | BI    | 163 | GLN  |
| 53  | BL    | 188 | ASN  |
| 54  | BM    | 33  | GLN  |
| 54  | BM    | 48  | GLN  |
| 55  | BN    | 57  | GLN  |
| 56  | BO    | 143 | HIS  |
| 56  | BO    | 167 | HIS  |
| 56  | BO    | 173 | GLN  |
| 56  | BO    | 180 | GLN  |
| 57  | BP    | 34  | GLN  |
| 58  | BQ    | 7   | HIS  |
| 58  | BQ    | 45  | GLN  |
| 58  | BQ    | 160 | HIS  |
| 59  | BR    | 40  | GLN  |
| 59  | BR    | 75  | HIS  |
| 59  | BR    | 143 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 60  | BS    | 125 | GLN  |
| 61  | BT    | 131 | GLN  |
| 62  | BU    | 17  | GLN  |
| 62  | BU    | 44  | GLN  |
| 64  | BW    | 96  | GLN  |
| 64  | BW    | 120 | GLN  |
| 65  | BX    | 107 | HIS  |
| 65  | BX    | 111 | GLN  |
| 66  | BY    | 14  | ASN  |
| 66  | BY    | 56  | GLN  |
| 66  | BY    | 61  | HIS  |
| 67  | BZ    | 78  | ASN  |
| 68  | Ba    | 34  | ASN  |
| 68  | Ba    | 66  | ASN  |
| 69  | Bb    | 17  | HIS  |
| 72  | Be    | 23  | HIS  |
| 73  | Bf    | 91  | ASN  |
| 73  | Bf    | 99  | HIS  |
| 74  | Bg    | 114 | GLN  |
| 76  | Bi    | 15  | HIS  |
| 76  | Bi    | 36  | HIS  |
| 77  | Bj    | 13  | ASN  |
| 77  | Bj    | 66  | HIS  |
| 78  | Bk    | 58  | GLN  |
| 79  | Bl    | 4   | HIS  |
| 80  | Bm    | 117 | HIS  |
| 81  | Bo    | 45  | GLN  |
| 83  | Br    | 4   | HIS  |
| 83  | Br    | 6   | GLN  |
| 84  | Bs    | 39  | GLN  |
| 84  | Bs    | 41  | GLN  |
| 84  | Bs    | 190 | GLN  |
| 84  | Bs    | 191 | GLN  |
| 85  | Bt    | 97  | ASN  |
| 85  | Bt    | 137 | GLN  |
| 86  | Bv    | 96  | ASN  |
| 87  | By    | 44  | GLN  |
| 87  | By    | 67  | ASN  |
| 87  | By    | 79  | GLN  |
| 87  | By    | 80  | GLN  |
| 87  | By    | 111 | ASN  |
| 87  | By    | 162 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | By    | 170 | HIS  |
| 87  | By    | 185 | GLN  |
| 87  | By    | 211 | GLN  |
| 87  | By    | 238 | GLN  |
| 87  | By    | 334 | HIS  |
| 87  | By    | 350 | GLN  |
| 87  | By    | 380 | ASN  |
| 87  | By    | 401 | GLN  |
| 87  | By    | 420 | GLN  |
| 88  | Bz    | 85  | HIS  |
| 88  | Bz    | 127 | GLN  |
| 88  | Bz    | 153 | GLN  |
| 88  | Bz    | 429 | HIS  |
| 88  | Bz    | 440 | GLN  |
| 88  | Bz    | 460 | GLN  |
| 88  | Bz    | 549 | GLN  |
| 88  | Bz    | 588 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A2    | 1764/1870 (94%) | 234 (13%)         | 1 (0%)          |
| 10  | AI    | 2/76 (2%)       | 1 (50%)           | 0               |
| 11  | AT    | 85/86 (98%)     | 15 (17%)          | 0               |
| 39  | B5    | 3752/4808 (78%) | 471 (12%)         | 1 (0%)          |
| 40  | B7    | 118/119 (99%)   | 7 (5%)            | 0               |
| 41  | B8    | 155/158 (98%)   | 17 (10%)          | 0               |
| 9   | AH    | 23/217 (10%)    | 8 (34%)           | 0               |
| All | All   | 5899/7334 (80%) | 753 (12%)         | 2 (0%)          |

All (753) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A2    | 3   | C    |
| 1   | A2    | 17  | C    |
| 1   | A2    | 26  | U    |
| 1   | A2    | 33  | G    |
| 1   | A2    | 41  | G    |
| 1   | A2    | 44  | U    |
| 1   | A2    | 46  | A    |
| 1   | A2    | 56  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A2    | 58  | C    |
| 1   | A2    | 67  | C    |
| 1   | A2    | 68  | A    |
| 1   | A2    | 73  | C    |
| 1   | A2    | 74  | G    |
| 1   | A2    | 77  | A    |
| 1   | A2    | 79  | A    |
| 1   | A2    | 103 | A    |
| 1   | A2    | 113 | G    |
| 1   | A2    | 114 | G    |
| 1   | A2    | 115 | U    |
| 1   | A2    | 126 | G    |
| 1   | A2    | 130 | G    |
| 1   | A2    | 142 | C    |
| 1   | A2    | 143 | U    |
| 1   | A2    | 155 | G    |
| 1   | A2    | 159 | A2M  |
| 1   | A2    | 160 | U    |
| 1   | A2    | 162 | C    |
| 1   | A2    | 163 | U    |
| 1   | A2    | 168 | C    |
| 1   | A2    | 170 | A    |
| 1   | A2    | 178 | C    |
| 1   | A2    | 180 | G    |
| 1   | A2    | 184 | G    |
| 1   | A2    | 188 | C    |
| 1   | A2    | 192 | C    |
| 1   | A2    | 226 | A    |
| 1   | A2    | 228 | C    |
| 1   | A2    | 282 | C    |
| 1   | A2    | 298 | A    |
| 1   | A2    | 303 | A    |
| 1   | A2    | 306 | U    |
| 1   | A2    | 308 | G    |
| 1   | A2    | 310 | G    |
| 1   | A2    | 313 | G    |
| 1   | A2    | 320 | C    |
| 1   | A2    | 325 | U    |
| 1   | A2    | 327 | C    |
| 1   | A2    | 328 | G    |
| 1   | A2    | 329 | U    |
| 1   | A2    | 330 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A2    | 348 | G    |
| 1   | A2    | 365 | A    |
| 1   | A2    | 369 | U    |
| 1   | A2    | 370 | C    |
| 1   | A2    | 386 | G    |
| 1   | A2    | 387 | C    |
| 1   | A2    | 401 | C    |
| 1   | A2    | 410 | C    |
| 1   | A2    | 439 | G    |
| 1   | A2    | 449 | A    |
| 1   | A2    | 450 | A    |
| 1   | A2    | 451 | C    |
| 1   | A2    | 465 | A    |
| 1   | A2    | 466 | A    |
| 1   | A2    | 467 | G    |
| 1   | A2    | 472 | G    |
| 1   | A2    | 473 | C    |
| 1   | A2    | 474 | A    |
| 1   | A2    | 475 | G    |
| 1   | A2    | 483 | G    |
| 1   | A2    | 488 | U    |
| 1   | A2    | 493 | C    |
| 1   | A2    | 509 | A    |
| 1   | A2    | 513 | A2M  |
| 1   | A2    | 526 | A    |
| 1   | A2    | 542 | U    |
| 1   | A2    | 543 | U    |
| 1   | A2    | 544 | C    |
| 1   | A2    | 550 | C    |
| 1   | A2    | 556 | A    |
| 1   | A2    | 557 | U    |
| 1   | A2    | 565 | A    |
| 1   | A2    | 569 | C    |
| 1   | A2    | 584 | A    |
| 1   | A2    | 590 | G    |
| 1   | A2    | 592 | U    |
| 1   | A2    | 605 | A    |
| 1   | A2    | 607 | G    |
| 1   | A2    | 609 | C    |
| 1   | A2    | 615 | C    |
| 1   | A2    | 629 | A    |
| 1   | A2    | 632 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A2    | 644 | A    |
| 1   | A2    | 645 | OMG  |
| 1   | A2    | 656 | A    |
| 1   | A2    | 661 | C    |
| 1   | A2    | 669 | A2M  |
| 1   | A2    | 670 | A    |
| 1   | A2    | 672 | A    |
| 1   | A2    | 673 | A    |
| 1   | A2    | 698 | G    |
| 1   | A2    | 734 | C    |
| 1   | A2    | 747 | C    |
| 1   | A2    | 748 | U    |
| 1   | A2    | 749 | C    |
| 1   | A2    | 753 | G    |
| 1   | A2    | 755 | G    |
| 1   | A2    | 795 | A    |
| 1   | A2    | 796 | A    |
| 1   | A2    | 800 | U    |
| 1   | A2    | 812 | A    |
| 1   | A2    | 822 | G    |
| 1   | A2    | 823 | PSU  |
| 1   | A2    | 831 | A    |
| 1   | A2    | 832 | G    |
| 1   | A2    | 837 | G    |
| 1   | A2    | 838 | A    |
| 1   | A2    | 839 | G    |
| 1   | A2    | 840 | C    |
| 1   | A2    | 841 | C    |
| 1   | A2    | 842 | G    |
| 1   | A2    | 848 | A    |
| 1   | A2    | 870 | A    |
| 1   | A2    | 871 | A    |
| 1   | A2    | 872 | U    |
| 1   | A2    | 873 | A    |
| 1   | A2    | 892 | G    |
| 1   | A2    | 914 | A    |
| 1   | A2    | 915 | U    |
| 1   | A2    | 921 | A    |
| 1   | A2    | 923 | A    |
| 1   | A2    | 931 | C    |
| 1   | A2    | 934 | G    |
| 1   | A2    | 944 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A2    | 956  | A    |
| 1   | A2    | 964  | A    |
| 1   | A2    | 972  | G    |
| 1   | A2    | 991  | A    |
| 1   | A2    | 993  | A    |
| 1   | A2    | 1000 | G    |
| 1   | A2    | 1003 | U    |
| 1   | A2    | 1024 | A    |
| 1   | A2    | 1084 | A    |
| 1   | A2    | 1086 | C    |
| 1   | A2    | 1116 | U    |
| 1   | A2    | 1117 | C    |
| 1   | A2    | 1118 | C    |
| 1   | A2    | 1119 | C    |
| 1   | A2    | 1122 | G    |
| 1   | A2    | 1134 | A    |
| 1   | A2    | 1145 | A    |
| 1   | A2    | 1154 | C    |
| 1   | A2    | 1155 | U    |
| 1   | A2    | 1196 | A    |
| 1   | A2    | 1208 | G    |
| 1   | A2    | 1216 | C    |
| 1   | A2    | 1225 | G    |
| 1   | A2    | 1243 | U    |
| 1   | A2    | 1252 | A    |
| 1   | A2    | 1254 | A    |
| 1   | A2    | 1257 | G    |
| 1   | A2    | 1258 | G    |
| 1   | A2    | 1260 | A    |
| 1   | A2    | 1272 | C    |
| 1   | A2    | 1275 | G    |
| 1   | A2    | 1276 | G    |
| 1   | A2    | 1283 | A    |
| 1   | A2    | 1303 | G    |
| 1   | A2    | 1304 | C    |
| 1   | A2    | 1343 | U    |
| 1   | A2    | 1359 | U    |
| 1   | A2    | 1365 | U    |
| 1   | A2    | 1372 | U    |
| 1   | A2    | 1373 | U    |
| 1   | A2    | 1379 | A    |
| 1   | A2    | 1383 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A2    | 1398 | U    |
| 1   | A2    | 1406 | A    |
| 1   | A2    | 1407 | G    |
| 1   | A2    | 1419 | C    |
| 1   | A2    | 1420 | C    |
| 1   | A2    | 1422 | A    |
| 1   | A2    | 1424 | C    |
| 1   | A2    | 1436 | C    |
| 1   | A2    | 1447 | A    |
| 1   | A2    | 1455 | A    |
| 1   | A2    | 1463 | U    |
| 1   | A2    | 1464 | U    |
| 1   | A2    | 1481 | A    |
| 1   | A2    | 1490 | A    |
| 1   | A2    | 1491 | OMG  |
| 1   | A2    | 1498 | G    |
| 1   | A2    | 1508 | G    |
| 1   | A2    | 1510 | U    |
| 1   | A2    | 1522 | C    |
| 1   | A2    | 1523 | A    |
| 1   | A2    | 1545 | C    |
| 1   | A2    | 1553 | G    |
| 1   | A2    | 1554 | C    |
| 1   | A2    | 1571 | G    |
| 1   | A2    | 1580 | A    |
| 1   | A2    | 1581 | A    |
| 1   | A2    | 1589 | A    |
| 1   | A2    | 1602 | A    |
| 1   | A2    | 1622 | U    |
| 1   | A2    | 1624 | A    |
| 1   | A2    | 1655 | G    |
| 1   | A2    | 1662 | A    |
| 1   | A2    | 1666 | G    |
| 1   | A2    | 1681 | G    |
| 1   | A2    | 1699 | C    |
| 1   | A2    | 1722 | U    |
| 1   | A2    | 1723 | G    |
| 1   | A2    | 1745 | G    |
| 1   | A2    | 1759 | G    |
| 1   | A2    | 1766 | C    |
| 1   | A2    | 1768 | C    |
| 1   | A2    | 1769 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A2    | 1776 | U    |
| 1   | A2    | 1778 | G    |
| 1   | A2    | 1780 | G    |
| 1   | A2    | 1782 | A    |
| 1   | A2    | 1784 | C    |
| 1   | A2    | 1785 | G    |
| 1   | A2    | 1830 | G    |
| 1   | A2    | 1836 | A    |
| 1   | A2    | 1837 | G    |
| 1   | A2    | 1839 | U    |
| 1   | A2    | 1850 | G    |
| 1   | A2    | 1852 | MA6  |
| 1   | A2    | 1862 | G    |
| 1   | A2    | 1863 | G    |
| 1   | A2    | 1864 | A    |
| 1   | A2    | 1866 | C    |
| 9   | AH    | 3457 | U    |
| 9   | AH    | 3458 | C    |
| 9   | AH    | 3459 | G    |
| 9   | AH    | 3466 | U    |
| 9   | AH    | 3470 | G    |
| 9   | AH    | 3473 | U    |
| 9   | AH    | 3474 | U    |
| 9   | AH    | 3477 | G    |
| 10  | AI    | 76   | A    |
| 11  | AT    | 9    | G    |
| 11  | AT    | 10   | G    |
| 11  | AT    | 14   | A    |
| 11  | AT    | 16   | U    |
| 11  | AT    | 18   | G    |
| 11  | AT    | 19   | U    |
| 11  | AT    | 20   | U    |
| 11  | AT    | 21   | A    |
| 11  | AT    | 22   | A    |
| 11  | AT    | 45   | G    |
| 11  | AT    | 46   | G    |
| 11  | AT    | 50   | A    |
| 11  | AT    | 52   | U    |
| 11  | AT    | 59   | G    |
| 11  | AT    | 69   | A    |
| 39  | B5    | 25   | A    |
| 39  | B5    | 39   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | B5    | 42  | A    |
| 39  | B5    | 58  | G    |
| 39  | B5    | 59  | A    |
| 39  | B5    | 64  | A    |
| 39  | B5    | 65  | A    |
| 39  | B5    | 85  | G    |
| 39  | B5    | 91  | G    |
| 39  | B5    | 98  | A    |
| 39  | B5    | 109 | G    |
| 39  | B5    | 110 | C    |
| 39  | B5    | 119 | G    |
| 39  | B5    | 134 | G    |
| 39  | B5    | 135 | G    |
| 39  | B5    | 136 | U    |
| 39  | B5    | 142 | G    |
| 39  | B5    | 144 | G    |
| 39  | B5    | 159 | C    |
| 39  | B5    | 185 | C    |
| 39  | B5    | 187 | U    |
| 39  | B5    | 188 | G    |
| 39  | B5    | 189 | G    |
| 39  | B5    | 200 | U    |
| 39  | B5    | 201 | C    |
| 39  | B5    | 209 | U    |
| 39  | B5    | 210 | C    |
| 39  | B5    | 218 | A    |
| 39  | B5    | 219 | G    |
| 39  | B5    | 220 | C    |
| 39  | B5    | 234 | G    |
| 39  | B5    | 266 | C    |
| 39  | B5    | 297 | U    |
| 39  | B5    | 315 | G    |
| 39  | B5    | 316 | U    |
| 39  | B5    | 326 | C    |
| 39  | B5    | 334 | A    |
| 39  | B5    | 340 | C    |
| 39  | B5    | 363 | A    |
| 39  | B5    | 387 | G    |
| 39  | B5    | 401 | G    |
| 39  | B5    | 408 | A    |
| 39  | B5    | 409 | G    |
| 39  | B5    | 412 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | B5    | 446 | C    |
| 39  | B5    | 449 | C    |
| 39  | B5    | 450 | G    |
| 39  | B5    | 452 | A    |
| 39  | B5    | 453 | G    |
| 39  | B5    | 454 | U    |
| 39  | B5    | 463 | A    |
| 39  | B5    | 467 | U    |
| 39  | B5    | 468 | U    |
| 39  | B5    | 482 | U    |
| 39  | B5    | 483 | G    |
| 39  | B5    | 485 | U    |
| 39  | B5    | 486 | C    |
| 39  | B5    | 493 | U    |
| 39  | B5    | 497 | G    |
| 39  | B5    | 499 | C    |
| 39  | B5    | 502 | U    |
| 39  | B5    | 503 | C    |
| 39  | B5    | 504 | U    |
| 39  | B5    | 505 | C    |
| 39  | B5    | 506 | G    |
| 39  | B5    | 515 | U    |
| 39  | B5    | 516 | U    |
| 39  | B5    | 517 | C    |
| 39  | B5    | 628 | U    |
| 39  | B5    | 634 | C    |
| 39  | B5    | 635 | G    |
| 39  | B5    | 660 | G    |
| 39  | B5    | 691 | G    |
| 39  | B5    | 698 | C    |
| 39  | B5    | 699 | G    |
| 39  | B5    | 724 | G    |
| 39  | B5    | 725 | G    |
| 39  | B5    | 732 | C    |
| 39  | B5    | 734 | G    |
| 39  | B5    | 738 | G    |
| 39  | B5    | 758 | C    |
| 39  | B5    | 760 | C    |
| 39  | B5    | 790 | G    |
| 39  | B5    | 791 | C    |
| 39  | B5    | 792 | G    |
| 39  | B5    | 795 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 797  | C    |
| 39  | B5    | 798  | C    |
| 39  | B5    | 803  | C    |
| 39  | B5    | 810  | U    |
| 39  | B5    | 812  | A    |
| 39  | B5    | 814  | A    |
| 39  | B5    | 815  | G    |
| 39  | B5    | 824  | C    |
| 39  | B5    | 825  | G    |
| 39  | B5    | 831  | A    |
| 39  | B5    | 832  | G    |
| 39  | B5    | 835  | G    |
| 39  | B5    | 843  | A    |
| 39  | B5    | 844  | A    |
| 39  | B5    | 845  | U    |
| 39  | B5    | 856  | A    |
| 39  | B5    | 859  | G    |
| 39  | B5    | 860  | A    |
| 39  | B5    | 861  | G    |
| 39  | B5    | 866  | A    |
| 39  | B5    | 867  | C    |
| 39  | B5    | 868  | C    |
| 39  | B5    | 869  | U    |
| 39  | B5    | 870  | G    |
| 39  | B5    | 884  | U    |
| 39  | B5    | 983  | G    |
| 39  | B5    | 985  | G    |
| 39  | B5    | 987  | C    |
| 39  | B5    | 1072 | C    |
| 39  | B5    | 1073 | C    |
| 39  | B5    | 1074 | C    |
| 39  | B5    | 1084 | C    |
| 39  | B5    | 1091 | G    |
| 39  | B5    | 1102 | G    |
| 39  | B5    | 1105 | C    |
| 39  | B5    | 1106 | U    |
| 39  | B5    | 1124 | A    |
| 39  | B5    | 1127 | G    |
| 39  | B5    | 1129 | G    |
| 39  | B5    | 1133 | C    |
| 39  | B5    | 1136 | G    |
| 39  | B5    | 1202 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 1214 | A    |
| 39  | B5    | 1215 | G    |
| 39  | B5    | 1216 | C    |
| 39  | B5    | 1217 | G    |
| 39  | B5    | 1221 | G    |
| 39  | B5    | 1228 | G    |
| 39  | B5    | 1231 | G    |
| 39  | B5    | 1239 | U    |
| 39  | B5    | 1240 | G    |
| 39  | B5    | 1247 | A    |
| 39  | B5    | 1270 | A2M  |
| 39  | B5    | 1298 | A    |
| 39  | B5    | 1299 | G    |
| 39  | B5    | 1303 | G    |
| 39  | B5    | 1308 | U    |
| 39  | B5    | 1309 | C    |
| 39  | B5    | 1310 | G    |
| 39  | B5    | 1312 | A    |
| 39  | B5    | 1323 | C    |
| 39  | B5    | 1331 | A    |
| 39  | B5    | 1341 | A    |
| 39  | B5    | 1367 | G    |
| 39  | B5    | 1375 | A    |
| 39  | B5    | 1391 | C    |
| 39  | B5    | 1393 | C    |
| 39  | B5    | 1401 | C    |
| 39  | B5    | 1452 | A    |
| 39  | B5    | 1453 | G    |
| 39  | B5    | 1457 | G    |
| 39  | B5    | 1480 | A    |
| 39  | B5    | 1489 | A2M  |
| 39  | B5    | 1490 | C    |
| 39  | B5    | 1502 | A    |
| 39  | B5    | 1521 | C    |
| 39  | B5    | 1533 | U    |
| 39  | B5    | 1546 | U    |
| 39  | B5    | 1551 | U    |
| 39  | B5    | 1579 | G    |
| 39  | B5    | 1580 | OMG  |
| 39  | B5    | 1586 | A    |
| 39  | B5    | 1588 | G    |
| 39  | B5    | 1589 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 1593 | A    |
| 39  | B5    | 1596 | G    |
| 39  | B5    | 1609 | G    |
| 39  | B5    | 1616 | C    |
| 39  | B5    | 1631 | C    |
| 39  | B5    | 1632 | PSU  |
| 39  | B5    | 1633 | C    |
| 39  | B5    | 1646 | G    |
| 39  | B5    | 1653 | C    |
| 39  | B5    | 1657 | C    |
| 39  | B5    | 1658 | C    |
| 39  | B5    | 1673 | G    |
| 39  | B5    | 1694 | C    |
| 39  | B5    | 1704 | A    |
| 39  | B5    | 1705 | A    |
| 39  | B5    | 1726 | A    |
| 39  | B5    | 1743 | A    |
| 39  | B5    | 1745 | G    |
| 39  | B5    | 1754 | G    |
| 39  | B5    | 1767 | C    |
| 39  | B5    | 1774 | G    |
| 39  | B5    | 1775 | G    |
| 39  | B5    | 1776 | A    |
| 39  | B5    | 1781 | G    |
| 39  | B5    | 1794 | G    |
| 39  | B5    | 1808 | G    |
| 39  | B5    | 1830 | A    |
| 39  | B5    | 1832 | C    |
| 39  | B5    | 1836 | A    |
| 39  | B5    | 1857 | U    |
| 39  | B5    | 1859 | C    |
| 39  | B5    | 1860 | C    |
| 39  | B5    | 1861 | G    |
| 39  | B5    | 1870 | C    |
| 39  | B5    | 1871 | A    |
| 39  | B5    | 1879 | G    |
| 39  | B5    | 1887 | G    |
| 39  | B5    | 1890 | G    |
| 39  | B5    | 1898 | U    |
| 39  | B5    | 1900 | G    |
| 39  | B5    | 1913 | U    |
| 39  | B5    | 1914 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 1915 | G    |
| 39  | B5    | 1917 | C    |
| 39  | B5    | 1923 | A    |
| 39  | B5    | 1937 | A    |
| 39  | B5    | 1940 | G    |
| 39  | B5    | 1942 | G    |
| 39  | B5    | 1963 | G    |
| 39  | B5    | 1965 | A    |
| 39  | B5    | 1983 | U    |
| 39  | B5    | 1985 | G    |
| 39  | B5    | 1987 | U    |
| 39  | B5    | 1994 | G    |
| 39  | B5    | 1995 | G    |
| 39  | B5    | 2008 | A    |
| 39  | B5    | 2023 | U    |
| 39  | B5    | 2032 | G    |
| 39  | B5    | 2037 | G    |
| 39  | B5    | 2041 | G    |
| 39  | B5    | 2043 | A    |
| 39  | B5    | 2044 | A    |
| 39  | B5    | 2045 | G    |
| 39  | B5    | 2046 | A    |
| 39  | B5    | 2050 | U    |
| 39  | B5    | 2143 | A    |
| 39  | B5    | 2144 | G    |
| 39  | B5    | 2149 | G    |
| 39  | B5    | 2156 | A    |
| 39  | B5    | 2157 | G    |
| 39  | B5    | 2174 | G    |
| 39  | B5    | 2191 | G    |
| 39  | B5    | 2194 | OMC  |
| 39  | B5    | 2207 | OMG  |
| 39  | B5    | 2238 | A    |
| 39  | B5    | 2260 | A    |
| 39  | B5    | 2264 | G    |
| 39  | B5    | 2268 | U    |
| 39  | B5    | 2322 | G    |
| 39  | B5    | 2332 | C    |
| 39  | B5    | 2333 | U    |
| 39  | B5    | 2349 | G    |
| 39  | B5    | 2356 | A    |
| 39  | B5    | 2372 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 2380 | A    |
| 39  | B5    | 2386 | A    |
| 39  | B5    | 2387 | G    |
| 39  | B5    | 2388 | U    |
| 39  | B5    | 2390 | G    |
| 39  | B5    | 2397 | U    |
| 39  | B5    | 2409 | G    |
| 39  | B5    | 2429 | G    |
| 39  | B5    | 2430 | A    |
| 39  | B5    | 2432 | C    |
| 39  | B5    | 2444 | A    |
| 39  | B5    | 2496 | C    |
| 39  | B5    | 2503 | A    |
| 39  | B5    | 2504 | U    |
| 39  | B5    | 2512 | C    |
| 39  | B5    | 2530 | U    |
| 39  | B5    | 2537 | G    |
| 39  | B5    | 2538 | A    |
| 39  | B5    | 2539 | A    |
| 39  | B5    | 2551 | U    |
| 39  | B5    | 2552 | C    |
| 39  | B5    | 2553 | C    |
| 39  | B5    | 2554 | G    |
| 39  | B5    | 2564 | G    |
| 39  | B5    | 2586 | A    |
| 39  | B5    | 2606 | U    |
| 39  | B5    | 2612 | U    |
| 39  | B5    | 2630 | A2M  |
| 39  | B5    | 2631 | U    |
| 39  | B5    | 2633 | U    |
| 39  | B5    | 2641 | A    |
| 39  | B5    | 2657 | C    |
| 39  | B5    | 2658 | A2M  |
| 39  | B5    | 2669 | U    |
| 39  | B5    | 2670 | G    |
| 39  | B5    | 2672 | U    |
| 39  | B5    | 2698 | G    |
| 39  | B5    | 2745 | G    |
| 39  | B5    | 3329 | G    |
| 39  | B5    | 3350 | C    |
| 39  | B5    | 3358 | G    |
| 39  | B5    | 3362 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 3367 | A    |
| 39  | B5    | 3380 | A    |
| 39  | B5    | 3385 | A    |
| 39  | B5    | 3394 | A    |
| 39  | B5    | 3396 | G    |
| 39  | B5    | 3405 | C    |
| 39  | B5    | 3428 | C    |
| 39  | B5    | 3444 | A    |
| 39  | B5    | 3485 | G    |
| 39  | B5    | 3491 | A    |
| 39  | B5    | 3492 | A2M  |
| 39  | B5    | 3498 | A    |
| 39  | B5    | 3508 | G    |
| 39  | B5    | 3509 | G    |
| 39  | B5    | 3517 | A2M  |
| 39  | B5    | 3518 | U    |
| 39  | B5    | 3543 | G    |
| 39  | B5    | 3544 | C    |
| 39  | B5    | 3546 | U    |
| 39  | B5    | 3549 | A    |
| 39  | B5    | 3551 | G    |
| 39  | B5    | 3570 | U    |
| 39  | B5    | 3572 | U    |
| 39  | B5    | 3599 | A2M  |
| 39  | B5    | 3609 | A    |
| 39  | B5    | 3610 | C    |
| 39  | B5    | 3611 | G    |
| 39  | B5    | 3629 | G    |
| 39  | B5    | 3630 | G    |
| 39  | B5    | 3633 | A    |
| 39  | B5    | 3638 | A    |
| 39  | B5    | 3639 | G    |
| 39  | B5    | 3640 | A    |
| 39  | B5    | 3647 | U    |
| 39  | B5    | 3670 | G    |
| 39  | B5    | 3688 | G    |
| 39  | B5    | 3689 | U    |
| 39  | B5    | 3704 | A    |
| 39  | B5    | 3804 | G    |
| 39  | B5    | 3812 | G    |
| 39  | B5    | 3823 | G    |
| 39  | B5    | 3824 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 3825 | G    |
| 39  | B5    | 3832 | G    |
| 39  | B5    | 3833 | A    |
| 39  | B5    | 3834 | G    |
| 39  | B5    | 3847 | C    |
| 39  | B5    | 3850 | G    |
| 39  | B5    | 3855 | A    |
| 39  | B5    | 3869 | G    |
| 39  | B5    | 3874 | U    |
| 39  | B5    | 3875 | C    |
| 39  | B5    | 3891 | C    |
| 39  | B5    | 3892 | G    |
| 39  | B5    | 3904 | C    |
| 39  | B5    | 3908 | C    |
| 39  | B5    | 3909 | U    |
| 39  | B5    | 3916 | A    |
| 39  | B5    | 3929 | G    |
| 39  | B5    | 3930 | G    |
| 39  | B5    | 3937 | G    |
| 39  | B5    | 3949 | A    |
| 39  | B5    | 3971 | G    |
| 39  | B5    | 3975 | U    |
| 39  | B5    | 3979 | A    |
| 39  | B5    | 3997 | A    |
| 39  | B5    | 4000 | G    |
| 39  | B5    | 4012 | G    |
| 39  | B5    | 4014 | A    |
| 39  | B5    | 4017 | A    |
| 39  | B5    | 4019 | A    |
| 39  | B5    | 4027 | A    |
| 39  | B5    | 4037 | G    |
| 39  | B5    | 4051 | G    |
| 39  | B5    | 4052 | OMU  |
| 39  | B5    | 4060 | C    |
| 39  | B5    | 4075 | G    |
| 39  | B5    | 4076 | G    |
| 39  | B5    | 4078 | C    |
| 39  | B5    | 4096 | C    |
| 39  | B5    | 4100 | U    |
| 39  | B5    | 4119 | G    |
| 39  | B5    | 4123 | G    |
| 39  | B5    | 4124 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 4126 | A    |
| 39  | B5    | 4133 | C    |
| 39  | B5    | 4137 | G    |
| 39  | B5    | 4140 | A    |
| 39  | B5    | 4161 | A    |
| 39  | B5    | 4167 | C    |
| 39  | B5    | 4168 | A    |
| 39  | B5    | 4172 | C    |
| 39  | B5    | 4194 | G    |
| 39  | B5    | 4198 | U    |
| 39  | B5    | 4210 | A    |
| 39  | B5    | 4212 | C    |
| 39  | B5    | 4221 | G    |
| 39  | B5    | 4258 | U    |
| 39  | B5    | 4259 | A    |
| 39  | B5    | 4261 | G    |
| 39  | B5    | 4265 | C    |
| 39  | B5    | 4269 | A2M  |
| 39  | B5    | 4270 | G    |
| 39  | B5    | 4278 | PSU  |
| 39  | B5    | 4294 | A    |
| 39  | B5    | 4295 | G    |
| 39  | B5    | 4306 | C    |
| 39  | B5    | 4313 | G    |
| 39  | B5    | 4321 | G    |
| 39  | B5    | 4336 | A2M  |
| 39  | B5    | 4381 | A    |
| 39  | B5    | 4382 | PSU  |
| 39  | B5    | 4383 | OMG  |
| 39  | B5    | 4402 | A    |
| 39  | B5    | 4416 | C    |
| 39  | B5    | 4418 | A    |
| 39  | B5    | 4423 | U    |
| 39  | B5    | 4437 | A    |
| 39  | B5    | 4445 | U    |
| 39  | B5    | 4446 | A    |
| 39  | B5    | 4454 | A    |
| 39  | B5    | 4455 | U    |
| 39  | B5    | 4465 | G    |
| 39  | B5    | 4475 | A    |
| 39  | B5    | 4476 | C    |
| 39  | B5    | 4477 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 4478 | G    |
| 39  | B5    | 4486 | G    |
| 39  | B5    | 4487 | A    |
| 39  | B5    | 4488 | A    |
| 39  | B5    | 4489 | G    |
| 39  | B5    | 4490 | G    |
| 39  | B5    | 4492 | G    |
| 39  | B5    | 4498 | G    |
| 39  | B5    | 4501 | G    |
| 39  | B5    | 4504 | C    |
| 39  | B5    | 4506 | C    |
| 39  | B5    | 4508 | G    |
| 39  | B5    | 4512 | G    |
| 39  | B5    | 4518 | C    |
| 39  | B5    | 4609 | G    |
| 39  | B5    | 4610 | C    |
| 39  | B5    | 4614 | G    |
| 39  | B5    | 4621 | U    |
| 39  | B5    | 4622 | C    |
| 39  | B5    | 4634 | U    |
| 39  | B5    | 4638 | G    |
| 39  | B5    | 4639 | C    |
| 39  | B5    | 4640 | G    |
| 39  | B5    | 4642 | G    |
| 39  | B5    | 4644 | C    |
| 39  | B5    | 4645 | C    |
| 39  | B5    | 4646 | G    |
| 39  | B5    | 4647 | G    |
| 39  | B5    | 4649 | A    |
| 39  | B5    | 4651 | G    |
| 39  | B5    | 4655 | G    |
| 39  | B5    | 4658 | G    |
| 39  | B5    | 4674 | C    |
| 39  | B5    | 4682 | A    |
| 39  | B5    | 4686 | U    |
| 39  | B5    | 4705 | A    |
| 39  | B5    | 4715 | U    |
| 39  | B5    | 4728 | U    |
| 39  | B5    | 4729 | C    |
| 39  | B5    | 4753 | A    |
| 39  | B5    | 4756 | G    |
| 39  | B5    | 4762 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 39  | B5    | 4763 | C    |
| 39  | B5    | 4766 | C    |
| 39  | B5    | 4780 | G    |
| 39  | B5    | 4789 | C    |
| 39  | B5    | 4793 | C    |
| 39  | B5    | 4801 | G    |
| 39  | B5    | 4808 | U    |
| 40  | B7    | 7    | G    |
| 40  | B7    | 11   | A    |
| 40  | B7    | 53   | U    |
| 40  | B7    | 54   | A    |
| 40  | B7    | 64   | G    |
| 40  | B7    | 110  | G    |
| 40  | B7    | 120  | U    |
| 41  | B8    | 23   | C    |
| 41  | B8    | 34   | U    |
| 41  | B8    | 35   | C    |
| 41  | B8    | 59   | A    |
| 41  | B8    | 62   | A    |
| 41  | B8    | 63   | U    |
| 41  | B8    | 81   | C    |
| 41  | B8    | 84   | A    |
| 41  | B8    | 87   | G    |
| 41  | B8    | 94   | G    |
| 41  | B8    | 103  | A    |
| 41  | B8    | 105  | C    |
| 41  | B8    | 110  | U    |
| 41  | B8    | 114  | G    |
| 41  | B8    | 123  | U    |
| 41  | B8    | 127  | U    |
| 41  | B8    | 150  | C    |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A2    | 549  | C    |
| 39  | B5    | 4445 | U    |

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

224 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 |
| 39  | PSU  | B5    | 3500 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 1   | OMG  | A2    | 1448 | 1     | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 39  | PSU  | B5    | 4042 | 39    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.92 | 3 (13%)  |
| 39  | PSU  | B5    | 1491 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 1   | PSU  | A2    | 573  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | PSU  | B5    | 4045 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 39  | A2M  | B5    | 2206 | 39,90 | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.10 | 9 (29%)  |
| 39  | A2M  | B5    | 4269 | 39,90 | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.14 | 10 (32%) |
| 39  | PSU  | B5    | 4246 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.92 | 3 (13%)  |
| 39  | PSU  | B5    | 4322 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | A2M  | B5    | 1270 | 39    | 22,25,26     | 1.43 | 4 (18%)  | 31,36,39    | 2.13 | 10 (32%) |
| 39  | PSU  | B5    | 4711 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.89 | 4 (18%)  |
| 1   | OMC  | A2    | 1704 | 1     | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.84 | 1 (3%)   |
| 1   | OMU  | A2    | 116  | 1     | 19,22,23     | 1.19 | 2 (10%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 11  | PSU  | AT    | 65   | 11    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 39  | OMC  | B5    | 2704 | 39    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.77 | 0        |
| 39  | PSU  | B5    | 3585 | 39,90 | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 39  | OMG  | B5    | 4116 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 39  | A2M  | B5    | 3557 | 39    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.13 | 10 (32%) |
| 39  | OMG  | B5    | 4364 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 39  | PSU  | B5    | 4435 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.94 | 3 (13%)  |
| 39  | OMG  | B5    | 3631 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.92 | 6 (18%)  |
| 39  | PSU  | B5    | 3496 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.92 | 4 (18%)  |
| 39  | PSU  | B5    | 4099 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.91 | 3 (13%)  |
| 39  | PSU  | B5    | 3427 | 39    | 18,21,22     | 1.37 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 1   | OMC  | A2    | 174  | 1,90  | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.80 | 0        |
| 1   | PSU  | A2    | 652  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.92 | 4 (18%)  |
| 1   | OMG  | A2    | 645  | 1     | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 39  | OMC  | B5    | 3540 | 39    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.84 | 1 (3%)   |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | OMG  | B5    | 3359 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.96 | 6 (18%)  |
| 39  | PSU  | B5    | 4267 | 39,90 | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.94 | 4 (18%)  |
| 1   | OMC  | A2    | 518  | 1     | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.81 | 0        |
| 39  | OMC  | B5    | 3601 | 39    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.76 | 0        |
| 39  | A2M  | B5    | 3562 | 39    | 22,25,26     | 1.44 | 4 (18%)  | 31,36,39    | 2.13 | 10 (32%) |
| 1   | A2M  | A2    | 159  | 1     | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.19 | 10 (32%) |
| 39  | A2M  | B5    | 3517 | 39    | 22,25,26     | 1.41 | 4 (18%)  | 31,36,39    | 2.27 | 11 (35%) |
| 39  | PSU  | B5    | 4177 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | UR3  | B5    | 4276 | 39    | 19,22,23     | 0.99 | 0        | 26,32,35    | 1.43 | 1 (3%)   |
| 39  | OMG  | B5    | 2267 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.91 | 6 (18%)  |
| 39  | OMC  | B5    | 2208 | 39,90 | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.79 | 0        |
| 1   | OMU  | A2    | 1443 | 1,90  | 19,22,23     | 1.23 | 2 (10%)  | 26,31,34    | 1.70 | 4 (15%)  |
| 39  | PSU  | B5    | 4278 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | OMG  | A2    | 868  | 1     | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | PSU  | A2    | 687  | 1     | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | OMG  | B5    | 4383 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 39  | A2M  | B5    | 3599 | 39    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.10 | 8 (25%)  |
| 39  | OMG  | B5    | 4240 | 39    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 1   | OMU  | A2    | 172  | 1     | 19,22,23     | 1.19 | 2 (10%)  | 26,31,34    | 1.71 | 4 (15%)  |
| 1   | 4AC  | A2    | 1843 | 1     | 21,24,25     | 1.11 | 2 (9%)   | 29,34,37    | 1.21 | 3 (10%)  |
| 1   | PSU  | A2    | 823  | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.91 | 4 (18%)  |
| 39  | PSU  | B5    | 4107 | 39    | 18,21,22     | 1.37 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | PSU  | B5    | 1537 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | A2M  | B5    | 4336 | 39    | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.13 | 10 (32%) |
| 1   | PSU  | A2    | 36   | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | B8N  | A2    | 1249 | 1     | 24,29,30     | 1.28 | 3 (12%)  | 29,42,45    | 1.30 | 3 (10%)  |
| 1   | OMG  | A2    | 684  | 1     | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 30  | SAC  | Ar    | 2    | 30    | 7,8,9        | 0.54 | 0        | 8,9,11      | 0.92 | 1 (12%)  |
| 39  | PSU  | B5    | 3490 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | PSU  | A2    | 1233 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | A2M  | A2    | 513  | 1     | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.14 | 10 (32%) |
| 1   | A2M  | A2    | 27   | 1,90  | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.14 | 10 (32%) |
| 39  | A2M  | B5    | 2658 | 39    | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.13 | 9 (29%)  |
| 1   | PSU  | A2    | 816  | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | A2M  | B5    | 1479 | 39    | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.09 | 8 (25%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | A2M  | B5    | 2630 | 39,90 | 22,25,26     | 1.44 | 4 (18%)  | 31,36,39    | 2.15 | 9 (29%)  |
| 39  | OMC  | B5    | 1820 | 39,90 | 19,22,23     | 0.80 | 0        | 26,31,34    | 0.83 | 0        |
| 39  | PSU  | B5    | 4298 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.92 | 3 (13%)  |
| 39  | OMC  | B5    | 2194 | 39,90 | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.92 | 2 (7%)   |
| 39  | A2M  | B5    | 2244 | 39,90 | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.13 | 10 (32%) |
| 39  | PSU  | B5    | 4325 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | UY1  | B5    | 3550 | 39    | 19,22,23     | 1.36 | 3 (15%)  | 22,31,34    | 1.96 | 5 (22%)  |
| 39  | 5MC  | B5    | 3514 | 39,90 | 18,22,23     | 0.96 | 2 (11%)  | 26,32,35    | 1.20 | 3 (11%)  |
| 1   | G7M  | A2    | 1640 | 11,1  | 23,26,27     | 2.31 | 5 (21%)  | 35,39,42    | 2.98 | 10 (28%) |
| 39  | PSU  | B5    | 2351 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | PSU  | A2    | 109  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | PSU  | A2    | 1245 | 1     | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.90 | 3 (13%)  |
| 39  | A2M  | B5    | 3456 | 39    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.09 | 10 (32%) |
| 39  | OMG  | B5    | 3524 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.91 | 6 (18%)  |
| 39  | PSU  | B5    | 4374 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.92 | 3 (13%)  |
| 39  | PSU  | B5    | 4749 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.91 | 3 (13%)  |
| 1   | PSU  | A2    | 610  | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 39  | PSU  | B5    | 1720 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | PSU  | A2    | 864  | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 39  | OMC  | B5    | 3433 | 39    | 19,22,23     | 0.80 | 0        | 26,31,34    | 0.80 | 0        |
| 1   | A2M  | A2    | 485  | 1     | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.08 | 9 (29%)  |
| 39  | OMC  | B5    | 4282 | 39    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.82 | 0        |
| 11  | 5MU  | AT    | 64   | 11    | 19,22,23     | 1.42 | 5 (26%)  | 28,32,35    | 2.02 | 5 (17%)  |
| 39  | PSU  | B5    | 1721 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.90 | 4 (18%)  |
| 39  | PSU  | B5    | 1638 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.94 | 3 (13%)  |
| 1   | A2M  | A2    | 1679 | 1     | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.17 | 10 (32%) |
| 1   | PSU  | A2    | 105  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | A2M  | A2    | 669  | 1,90  | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.11 | 10 (32%) |
| 35  | HY3  | Aw    | 62   | 35    | 6,8,9        | 2.13 | 1 (16%)  | 5,10,12     | 1.12 | 1 (20%)  |
| 1   | A2M  | A2    | 469  | 1     | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.09 | 9 (29%)  |
| 1   | OMG  | A2    | 602  | 1     | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 1   | OMU  | A2    | 1289 | 1     | 19,22,23     | 1.22 | 3 (15%)  | 26,31,34    | 1.66 | 4 (15%)  |
| 39  | PSU  | B5    | 3583 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.91 | 3 (13%)  |
| 68  | V5N  | Ba    | 39   | 68    | 9,11,12      | 2.14 | 2 (22%)  | 9,14,16     | 1.71 | 2 (22%)  |
| 39  | PSU  | B5    | 4169 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 69  | MLZ  | Bb    | 5    | 69    | 8,9,10       | 0.49 | 0        | 4,9,11      | 0.24 | 0        |
| 39  | OMG  | B5    | 2207 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 39  | PSU  | B5    | 3494 | 39    | 18,21,22     | 1.38 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | OMU  | B5    | 3973 | 39    | 19,22,23     | 1.24 | 3 (15%)  | 26,31,34    | 1.69 | 4 (15%)  |
| 39  | 5MC  | B5    | 4193 | 39    | 18,22,23     | 0.98 | 2 (11%)  | 26,32,35    | 1.19 | 2 (7%)   |
| 1   | OMU  | A2    | 121  | 1     | 19,22,23     | 1.23 | 3 (15%)  | 26,31,34    | 1.70 | 4 (15%)  |
| 1   | PSU  | A2    | 867  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 1   | A2M  | A2    | 1032 | 1     | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.14 | 10 (32%) |
| 1   | OMG  | A2    | 1491 | 1,90  | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | PSU  | A2    | 1626 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 39  | PSU  | B5    | 4149 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.94 | 4 (18%)  |
| 39  | OMG  | B5    | 3676 | 39    | 23,26,27     | 1.18 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 1   | PSU  | A2    | 1175 | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.93 | 3 (13%)  |
| 39  | A2M  | B5    | 400  | 39    | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.09 | 10 (32%) |
| 1   | OMG  | A2    | 510  | 1,90  | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 39  | OMG  | B5    | 3974 | 39    | 23,26,27     | 1.18 | 3 (13%)  | 33,38,41    | 1.91 | 6 (18%)  |
| 39  | OMU  | B5    | 4366 | 39    | 19,22,23     | 1.24 | 4 (21%)  | 26,31,34    | 1.75 | 4 (15%)  |
| 39  | PSU  | B5    | 1718 | 39    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | PSU  | A2    | 407  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | PSU  | B5    | 1799 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.93 | 3 (13%)  |
| 39  | A2M  | B5    | 3450 | 39    | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.07 | 9 (29%)  |
| 39  | OMG  | B5    | 3942 | 11,39 | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 1   | PSU  | A2    | 1446 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.91 | 4 (18%)  |
| 39  | A2M  | B5    | 398  | 39    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.16 | 10 (32%) |
| 31  | NMM  | As    | 67   | 31    | 9,11,12      | 0.59 | 0        | 6,12,14     | 0.39 | 0        |
| 1   | PSU  | A2    | 815  | 1     | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 39  | PSU  | B5    | 1683 | 39    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.90 | 3 (13%)  |
| 39  | A2M  | B5    | 3492 | 39    | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.12 | 8 (25%)  |
| 39  | PSU  | B5    | 4166 | 39    | 18,21,22     | 1.37 | 2 (11%)  | 22,30,33    | 1.81 | 3 (13%)  |
| 1   | 6MZ  | A2    | 1833 | 1,90  | 22,25,26     | 1.45 | 4 (18%)  | 30,36,39    | 2.12 | 9 (30%)  |
| 1   | PSU  | A2    | 967  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | PSU  | B5    | 4203 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | A2M  | A2    | 591  | 1     | 22,25,26     | 1.48 | 4 (18%)  | 31,36,39    | 2.20 | 7 (22%)  |
| 39  | OMC  | B5    | 3619 | 39    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.78 | 0        |
| 42  | V5N  | BA    | 216  | 42    | 9,11,12      | 2.11 | 2 (22%)  | 9,14,16     | 1.73 | 2 (22%)  |



| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PSU  | A2    | 682  | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | OMU  | B5    | 2258 | 39    | 19,22,23     | 1.21 | 3 (15%)  | 26,31,34    | 1.68 | 4 (15%)  |
| 1   | OMU  | A2    | 429  | 1     | 19,22,23     | 1.19 | 2 (10%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 39  | OMC  | B5    | 3573 | 39    | 19,22,23     | 0.80 | 0        | 26,31,34    | 0.82 | 0        |
| 1   | A2M  | A2    | 577  | 1     | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.12 | 9 (29%)  |
| 1   | PSU  | A2    | 1046 | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.90 | 3 (13%)  |
| 1   | PSU  | A2    | 1368 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.90 | 3 (13%)  |
| 1   | OMU  | A2    | 1327 | 1,90  | 19,22,23     | 1.20 | 2 (10%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 39  | PSU  | B5    | 4039 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | OMC  | A2    | 463  | 1     | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.82 | 0        |
| 1   | PSU  | A2    | 1239 | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | OMC  | B5    | 1284 | 39    | 19,22,23     | 0.83 | 0        | 26,31,34    | 0.80 | 0        |
| 1   | OMU  | A2    | 355  | 1     | 19,22,23     | 1.22 | 2 (10%)  | 26,31,34    | 1.73 | 4 (15%)  |
| 39  | OMG  | B5    | 1260 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.97 | 6 (18%)  |
| 39  | A2M  | B5    | 1489 | 39,90 | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.07 | 9 (29%)  |
| 39  | OMG  | B5    | 3476 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | PSU  | A2    | 34   | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | PSU  | B5    | 3502 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | OMU  | B5    | 4052 | 39    | 19,22,23     | 1.24 | 3 (15%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 1   | PSU  | A2    | 1348 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | PSU  | A2    | 1644 | 1,90  | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 39  | PSU  | B5    | 3466 | 39    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.89 | 4 (18%)  |
| 81  | MLZ  | Bo    | 53   | 81    | 8,9,10       | 0.48 | 0        | 4,9,11      | 0.09 | 0        |
| 1   | OMU  | A2    | 628  | 1     | 19,22,23     | 1.18 | 2 (10%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 1   | PSU  | A2    | 802  | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | OMG  | B5    | 2719 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.96 | 6 (18%)  |
| 39  | OMG  | B5    | 4245 | 39    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.92 | 6 (18%)  |
| 1   | MA6  | A2    | 1852 | 1     | 23,26,27     | 1.51 | 5 (21%)  | 34,38,41    | 2.21 | 10 (29%) |
| 39  | PSU  | B5    | 3369 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.90 | 4 (18%)  |
| 39  | OMG  | B5    | 4369 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 39  | PSU  | B5    | 4740 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 1   | 4AC  | A2    | 1338 | 1     | 21,24,25     | 1.06 | 1 (4%)   | 29,34,37    | 1.27 | 3 (10%)  |
| 39  | PSU  | B5    | 3554 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 1   | PSU  | A2    | 1693 | 1     | 18,21,22     | 1.37 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | PSU  | B5    | 4217 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | PSU  | B5    | 3371 | 39    | 18,21,22     | 1.37 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | PSU  | B5    | 3616 | 39    | 18,21,22     | 1.38 | 2 (11%)  | 22,30,33    | 1.93 | 3 (13%)  |
| 39  | A2M  | B5    | 4317 | 39    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.13 | 10 (32%) |
| 41  | PSU  | B8    | 55   | 41    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.91 | 4 (18%)  |
| 39  | OMC  | B5    | 2667 | 39    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.84 | 1 (3%)   |
| 39  | A2M  | B5    | 1810 | 39,90 | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.15 | 10 (32%) |
| 1   | PSU  | A2    | 1082 | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 41  | OMG  | B8    | 75   | 41    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 1   | OMU  | A2    | 1805 | 1     | 19,22,23     | 1.23 | 3 (15%)  | 26,31,34    | 1.71 | 4 (15%)  |
| 39  | PSU  | B5    | 4188 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.92 | 3 (13%)  |
| 39  | PSU  | B5    | 2475 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | OMG  | B5    | 1580 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.92 | 6 (18%)  |
| 39  | PSU  | B5    | 4382 | 39    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | OMU  | B5    | 4244 | 39    | 19,22,23     | 1.21 | 2 (10%)  | 26,31,34    | 1.74 | 5 (19%)  |
| 39  | PSU  | B5    | 3447 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.91 | 3 (13%)  |
| 1   | PSU  | A2    | 93   | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | A2M  | A2    | 1384 | 1     | 22,25,26     | 1.45 | 4 (18%)  | 31,36,39    | 2.09 | 10 (32%) |
| 39  | OMG  | B5    | 4138 | 39    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 43  | HIC  | BB    | 245  | 43    | 10,11,12     | 0.61 | 0        | 8,14,16     | 0.43 | 0        |
| 39  | OMU  | B5    | 3657 | 39    | 19,22,23     | 1.23 | 2 (10%)  | 26,31,34    | 1.74 | 5 (19%)  |
| 39  | OMC  | B5    | 2265 | 39,90 | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.88 | 1 (3%)   |
| 1   | PSU  | A2    | 650  | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.90 | 4 (18%)  |
| 39  | OMG  | B5    | 1477 | 39    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.96 | 6 (18%)  |
| 39  | 6MZ  | B5    | 3966 | 39    | 22,25,26     | 1.43 | 4 (18%)  | 30,36,39    | 2.27 | 9 (30%)  |
| 80  | M3L  | Bm    | 98   | 80    | 10,11,12     | 0.82 | 0        | 9,14,16     | 0.47 | 0        |
| 1   | PSU  | A2    | 210  | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.85 | 3 (13%)  |
| 39  | PSU  | B5    | 1632 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 4 (18%)  |
| 39  | PSU  | B5    | 4058 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.91 | 3 (13%)  |
| 1   | OMC  | A2    | 1392 | 1     | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.88 | 1 (3%)   |
| 1   | PSU  | A2    | 1057 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 1   | PSU  | A2    | 218  | 1     | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | OMG  | A2    | 437  | 1     | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 12  | SAC  | AZ    | 2    | 12    | 7,8,9        | 0.53 | 0        | 8,9,11      | 0.86 | 1 (12%)  |
| 41  | PSU  | B8    | 69   | 41    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.92 | 3 (13%)  |
| 39  | PSU  | B5    | 3576 | 39    | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | A2    | 1329 | 1     | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 44  | AYA  | BC    | 2    | 44    | 6,7,8        | 0.76 | 0        | 5,8,10      | 0.28 | 0        |
| 1   | MA6  | A2    | 1851 | 1     | 23,26,27     | 1.72 | 7 (30%)  | 34,38,41    | 2.45 | 12 (35%) |
| 39  | PSU  | B5    | 4419 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.90 | 3 (13%)  |
| 39  | OMC  | B5    | 2647 | 39    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.81 | 0        |
| 1   | PSU  | A2    | 1005 | 1     | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 39  | PSU  | B5    | 3462 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.91 | 3 (13%)  |
| 1   | PSU  | A2    | 1178 | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.90 | 3 (13%)  |
| 83  | SAC  | Br    | 2    | 83    | 7,8,9        | 0.53 | 0        | 8,9,11      | 0.82 | 1 (12%)  |
| 1   | A2M  | A2    | 99   | 1,90  | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.12 | 9 (29%)  |
| 39  | 1MA  | B5    | 1266 | 39,90 | 21,25,26     | 1.37 | 4 (19%)  | 31,37,40    | 1.68 | 5 (16%)  |
| 33  | AME  | Au    | 1    | 33    | 9,10,11      | 0.48 | 0        | 9,11,13     | 0.85 | 1 (11%)  |
| 1   | A2M  | A2    | 166  | 1     | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.14 | 9 (29%)  |
| 1   | PSU  | A2    | 1047 | 1     | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | PSU  | B5    | 1801 | 39    | 18,21,22     | 1.34 | 2 (11%)  | 22,30,33    | 1.92 | 4 (18%)  |
| 39  | PSU  | B5    | 1731 | 39    | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.89 | 3 (13%)  |
| 39  | PSU  | B5    | 3652 | 39,90 | 18,21,22     | 1.36 | 2 (11%)  | 22,30,33    | 1.88 | 3 (13%)  |
| 39  | OMC  | B5    | 4202 | 39    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.80 | 0        |
| 1   | PSU  | A2    | 119  | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.86 | 3 (13%)  |
| 39  | OMU  | B5    | 2680 | 39    | 19,22,23     | 1.23 | 2 (10%)  | 26,31,34    | 1.75 | 5 (19%)  |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 39  | PSU  | B5    | 3500 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | A2    | 1448 | 1     | -       | 3/9/27/28 | 0/3/3/3 |
| 39  | PSU  | B5    | 4042 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 1491 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | A2    | 573  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 4045 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | A2M  | B5    | 2206 | 39,90 | -       | 0/9/27/28 | 0/3/3/3 |
| 39  | A2M  | B5    | 4269 | 39,90 | -       | 2/9/27/28 | 0/3/3/3 |
| 39  | PSU  | B5    | 4246 | 39    | -       | 1/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 4322 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | A2M  | B5    | 1270 | 39    | -       | 0/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 39  | PSU  | B5    | 4711 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | A2    | 1704 | 1     | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMU  | A2    | 116  | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 11  | PSU  | AT    | 65   | 11    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMC  | B5    | 2704 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | PSU  | B5    | 3585 | 39,90 | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 4116 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | A2M  | B5    | 3557 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | OMG  | B5    | 4364 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4435 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 3631 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 3496 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 4099 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3427 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | A2    | 174  | 1,90  | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 652  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | A2    | 645  | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 39  | OMC  | B5    | 3540 | 39    | -       | 1/9/27/28  | 0/2/2/2 |
| 39  | OMG  | B5    | 3359 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4267 | 39,90 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | A2    | 518  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | OMC  | B5    | 3601 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | A2M  | B5    | 3562 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | A2    | 159  | 1     | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | A2M  | B5    | 3517 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4177 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | UR3  | B5    | 4276 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 2267 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | OMC  | B5    | 2208 | 39,90 | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | A2    | 1443 | 1,90  | -       | 2/9/27/28  | 0/2/2/2 |
| 39  | PSU  | B5    | 4278 | 39    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | OMG  | A2    | 868  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 687  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 4383 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | A2M  | B5    | 3599 | 39    | -       | 2/9/27/28  | 0/3/3/3 |
| 39  | OMG  | B5    | 4240 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMU  | A2    | 172  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | A2    | 1843 | 1     | -       | 2/11/29/30 | 0/2/2/2 |
| 1   | PSU  | A2    | 823  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 4107 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 1537 | 39    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 39  | A2M  | B5    | 4336 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 36   | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | B8N  | A2    | 1249 | 1     | -       | 4/16/34/35 | 0/2/2/2 |
| 1   | OMG  | A2    | 684  | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 30  | SAC  | Ar    | 2    | 30    | -       | 0/7/8/10   | -       |
| 39  | PSU  | B5    | 3490 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 1233 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | A2    | 513  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | A2M  | A2    | 27   | 1,90  | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | A2M  | B5    | 2658 | 39    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 816  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | A2M  | B5    | 1479 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | A2M  | B5    | 2630 | 39,90 | -       | 3/9/27/28  | 0/3/3/3 |
| 39  | OMC  | B5    | 1820 | 39,90 | -       | 1/9/27/28  | 0/2/2/2 |
| 39  | PSU  | B5    | 4298 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMC  | B5    | 2194 | 39,90 | -       | 2/9/27/28  | 0/2/2/2 |
| 39  | A2M  | B5    | 2244 | 39,90 | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4325 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | UY1  | B5    | 3550 | 39    | -       | 1/9/27/28  | 0/2/2/2 |
| 39  | 5MC  | B5    | 3514 | 39,90 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | G7M  | A2    | 1640 | 11,1  | -       | 0/7/25/26  | 0/3/3/3 |
| 39  | PSU  | B5    | 2351 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 109  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 1245 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | A2M  | B5    | 3456 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | OMG  | B5    | 3524 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4374 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 4749 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 610  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 1720 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 864  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMC  | B5    | 3433 | 39    | -       | 4/9/27/28  | 0/2/2/2 |
| 1   | A2M  | A2    | 485  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | OMC  | B5    | 4282 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | 5MU  | AT    | 64   | 11    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 1721 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 1638 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | A2    | 1679 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 105  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | A2    | 669  | 1,90  | -       | 2/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 35  | HY3  | Aw    | 62   | 35    | -       | 1/1/12/14 | 0/1/1/1 |
| 1   | A2M  | A2    | 469  | 1     | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | OMG  | A2    | 602  | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMU  | A2    | 1289 | 1     | -       | 2/9/27/28 | 0/2/2/2 |
| 39  | PSU  | B5    | 3583 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 68  | V5N  | Ba    | 39   | 68    | -       | 1/9/10/12 | 0/1/1/1 |
| 39  | PSU  | B5    | 4169 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 69  | MLZ  | Bb    | 5    | 69    | -       | 2/7/8/10  | -       |
| 39  | OMG  | B5    | 2207 | 39    | -       | 2/9/27/28 | 0/3/3/3 |
| 39  | PSU  | B5    | 3494 | 39    | -       | 2/7/25/26 | 0/2/2/2 |
| 39  | OMU  | B5    | 3973 | 39    | -       | 1/9/27/28 | 0/2/2/2 |
| 39  | 5MC  | B5    | 4193 | 39    | -       | 4/7/25/26 | 0/2/2/2 |
| 1   | OMU  | A2    | 121  | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | PSU  | A2    | 867  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | A2M  | A2    | 1032 | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMG  | A2    | 1491 | 1,90  | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | PSU  | A2    | 1626 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 4149 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | OMG  | B5    | 3676 | 39    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | A2    | 1175 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | A2M  | B5    | 400  | 39    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMG  | A2    | 510  | 1,90  | -       | 1/9/27/28 | 0/3/3/3 |
| 39  | OMG  | B5    | 3974 | 39    | -       | 0/9/27/28 | 0/3/3/3 |
| 39  | OMU  | B5    | 4366 | 39    | -       | 0/9/27/28 | 0/2/2/2 |
| 39  | PSU  | B5    | 1718 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | A2    | 407  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 1799 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | A2M  | B5    | 3450 | 39    | -       | 1/9/27/28 | 0/3/3/3 |
| 39  | OMG  | B5    | 3942 | 11,39 | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | A2    | 1446 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | A2M  | B5    | 398  | 39    | -       | 2/9/27/28 | 0/3/3/3 |
| 31  | NMM  | As    | 67   | 31    | -       | 0/9/11/13 | -       |
| 1   | PSU  | A2    | 815  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 1683 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | A2M  | B5    | 3492 | 39    | -       | 0/9/27/28 | 0/3/3/3 |
| 39  | PSU  | B5    | 4166 | 39    | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | 6MZ  | A2    | 1833 | 1,90  | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | PSU  | A2    | 967  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 4203 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | A2M  | A2    | 591  | 1     | -       | 3/9/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 39  | OMC  | B5    | 3619 | 39    | -       | 2/9/27/28  | 0/2/2/2 |
| 42  | V5N  | BA    | 216  | 42    | -       | 3/9/10/12  | 0/1/1/1 |
| 1   | PSU  | A2    | 682  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMU  | B5    | 2258 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | A2    | 429  | 1     | -       | 6/9/27/28  | 0/2/2/2 |
| 39  | OMC  | B5    | 3573 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | A2M  | A2    | 577  | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 1046 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 1368 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | A2    | 1327 | 1,90  | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | PSU  | B5    | 4039 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | A2    | 463  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 1239 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMC  | B5    | 1284 | 39    | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMU  | A2    | 355  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | OMG  | B5    | 1260 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | A2M  | B5    | 1489 | 39,90 | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | OMG  | B5    | 3476 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 34   | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3502 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMU  | B5    | 4052 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 1348 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 1644 | 1,90  | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3466 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 81  | MLZ  | Bo    | 53   | 81    | -       | 0/7/8/10   | -       |
| 1   | OMU  | A2    | 628  | 1     | -       | 3/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 802  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 2719 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | OMG  | B5    | 4245 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | MA6  | A2    | 1852 | 1     | -       | 1/11/29/30 | 0/3/3/3 |
| 39  | PSU  | B5    | 3369 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 4369 | 39    | -       | 1/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4740 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | A2    | 1338 | 1     | -       | 4/11/29/30 | 0/2/2/2 |
| 39  | PSU  | B5    | 3554 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 1693 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 4217 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3371 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3616 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | A2M  | B5    | 4317 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 41  | PSU  | B8    | 55   | 41    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 39  | OMC  | B5    | 2667 | 39    | -       | 1/9/27/28  | 0/2/2/2 |
| 39  | A2M  | B5    | 1810 | 39,90 | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | A2    | 1082 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 41  | OMG  | B8    | 75   | 41    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | OMU  | A2    | 1805 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | PSU  | B5    | 4188 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 2475 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 1580 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | PSU  | B5    | 4382 | 39    | -       | 4/7/25/26  | 0/2/2/2 |
| 39  | OMU  | B5    | 4244 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | PSU  | B5    | 3447 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 93   | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | A2    | 1384 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | OMG  | B5    | 4138 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 43  | HIC  | BB    | 245  | 43    | -       | 2/5/6/8    | 0/1/1/1 |
| 39  | OMU  | B5    | 3657 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 39  | OMC  | B5    | 2265 | 39,90 | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 650  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMG  | B5    | 1477 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 39  | 6MZ  | B5    | 3966 | 39    | -       | 0/9/27/28  | 0/3/3/3 |
| 80  | M3L  | Bm    | 98   | 80    | -       | 0/9/10/12  | -       |
| 1   | PSU  | A2    | 210  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 1632 | 39    | -       | 3/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 4058 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | A2    | 1392 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 1057 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 218  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | A2    | 437  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 12  | SAC  | AZ    | 2    | 12    | -       | 1/7/8/10   | -       |
| 41  | PSU  | B8    | 69   | 41    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3576 | 39    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | OMG  | A2    | 1329 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 44  | AYA  | BC    | 2    | 44    | -       | 3/4/6/8    | -       |
| 1   | MA6  | A2    | 1851 | 1     | -       | 0/11/29/30 | 0/3/3/3 |
| 39  | PSU  | B5    | 4419 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | OMC  | B5    | 2647 | 39    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | A2    | 1005 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 39  | PSU  | B5    | 3462 | 39    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A2    | 1178 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 83  | SAC  | Br    | 2    | 83    | -       | 0/7/8/10   | -       |
| 1   | A2M  | A2    | 99   | 1,90  | -       | 2/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 39  | 1MA  | B5    | 1266 | 39,90 | -       | 1/7/25/26 | 0/3/3/3 |
| 33  | AME  | Au    | 1    | 33    | -       | 2/9/10/12 | -       |
| 1   | A2M  | A2    | 166  | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | PSU  | A2    | 1047 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 1801 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 1731 | 39    | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | PSU  | B5    | 3652 | 39,90 | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | OMC  | B5    | 4202 | 39    | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | PSU  | A2    | 119  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 39  | OMU  | B5    | 2680 | 39    | -       | 1/9/27/28 | 0/2/2/2 |

All (510) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A2    | 1640 | G7M  | C8-N7  | 7.29  | 1.46        | 1.33     |
| 68  | Ba    | 39   | V5N  | CG-ND1 | -5.08 | 1.32        | 1.37     |
| 42  | BA    | 216  | V5N  | CG-ND1 | -4.99 | 1.32        | 1.37     |
| 35  | Aw    | 62   | HY3  | C3-CA  | -4.91 | 1.50        | 1.55     |
| 1   | A2    | 1640 | G7M  | C5-N7  | -4.68 | 1.33        | 1.39     |
| 1   | A2    | 591  | A2M  | C5-C4  | 4.63  | 1.47        | 1.39     |
| 1   | A2    | 166  | A2M  | C5-C4  | 4.56  | 1.47        | 1.39     |
| 39  | B5    | 3492 | A2M  | C5-C4  | 4.56  | 1.47        | 1.39     |
| 1   | A2    | 159  | A2M  | C5-C4  | 4.53  | 1.47        | 1.39     |
| 1   | A2    | 469  | A2M  | C5-C4  | 4.53  | 1.47        | 1.39     |
| 39  | B5    | 1479 | A2M  | C5-C4  | 4.52  | 1.47        | 1.39     |
| 1   | A2    | 577  | A2M  | C5-C4  | 4.52  | 1.47        | 1.39     |
| 39  | B5    | 3450 | A2M  | C5-C4  | 4.52  | 1.47        | 1.39     |
| 1   | A2    | 1851 | MA6  | C5-C4  | 4.51  | 1.47        | 1.39     |
| 1   | A2    | 1852 | MA6  | C5-C4  | 4.50  | 1.47        | 1.39     |
| 1   | A2    | 485  | A2M  | C5-C4  | 4.50  | 1.47        | 1.39     |
| 39  | B5    | 3599 | A2M  | C5-C4  | 4.48  | 1.47        | 1.39     |
| 1   | A2    | 1679 | A2M  | C5-C4  | 4.48  | 1.47        | 1.39     |
| 39  | B5    | 398  | A2M  | C5-C4  | 4.48  | 1.47        | 1.39     |
| 39  | B5    | 2206 | A2M  | C5-C4  | 4.47  | 1.47        | 1.39     |
| 39  | B5    | 2630 | A2M  | C5-C4  | 4.47  | 1.47        | 1.39     |
| 39  | B5    | 400  | A2M  | C5-C4  | 4.47  | 1.47        | 1.39     |
| 39  | B5    | 2244 | A2M  | C5-C4  | 4.47  | 1.47        | 1.39     |
| 1   | A2    | 99   | A2M  | C5-C4  | 4.46  | 1.47        | 1.39     |
| 1   | A2    | 513  | A2M  | C5-C4  | 4.46  | 1.47        | 1.39     |
| 39  | B5    | 3557 | A2M  | C5-C4  | 4.45  | 1.47        | 1.39     |
| 1   | A2    | 27   | A2M  | C5-C4  | 4.45  | 1.47        | 1.39     |
| 39  | B5    | 4336 | A2M  | C5-C4  | 4.45  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 39  | B5    | 3456 | A2M  | C5-C4 | 4.45  | 1.47        | 1.39     |
| 39  | B5    | 3966 | 6MZ  | C5-C4 | 4.45  | 1.47        | 1.39     |
| 1   | A2    | 1384 | A2M  | C5-C4 | 4.44  | 1.47        | 1.39     |
| 1   | A2    | 1032 | A2M  | C5-C4 | 4.43  | 1.47        | 1.39     |
| 39  | B5    | 2658 | A2M  | C5-C4 | 4.42  | 1.47        | 1.39     |
| 39  | B5    | 4317 | A2M  | C5-C4 | 4.42  | 1.47        | 1.39     |
| 1   | A2    | 669  | A2M  | C5-C4 | 4.42  | 1.47        | 1.39     |
| 39  | B5    | 1489 | A2M  | C5-C4 | 4.38  | 1.47        | 1.39     |
| 39  | B5    | 4269 | A2M  | C5-C4 | 4.38  | 1.47        | 1.39     |
| 39  | B5    | 1810 | A2M  | C5-C4 | 4.37  | 1.47        | 1.39     |
| 39  | B5    | 3562 | A2M  | C5-C4 | 4.35  | 1.47        | 1.39     |
| 1   | A2    | 1833 | 6MZ  | C5-C4 | 4.30  | 1.47        | 1.39     |
| 39  | B5    | 1270 | A2M  | C5-C4 | 4.30  | 1.47        | 1.39     |
| 39  | B5    | 3517 | A2M  | C5-C4 | 4.22  | 1.46        | 1.39     |
| 1   | A2    | 1640 | G7M  | C8-N9 | 3.96  | 1.46        | 1.35     |
| 1   | A2    | 1640 | G7M  | C5-C4 | 3.72  | 1.47        | 1.38     |
| 39  | B5    | 3550 | UY1  | C6-C5 | 3.59  | 1.39        | 1.35     |
| 1   | A2    | 1851 | MA6  | C8-N9 | -3.29 | 1.31        | 1.37     |
| 1   | A2    | 1175 | PSU  | C6-C5 | 3.27  | 1.39        | 1.35     |
| 1   | A2    | 210  | PSU  | C6-C5 | 3.22  | 1.39        | 1.35     |
| 39  | B5    | 3447 | PSU  | C6-C5 | 3.21  | 1.39        | 1.35     |
| 11  | AT    | 65   | PSU  | C6-C5 | 3.20  | 1.39        | 1.35     |
| 39  | B5    | 4166 | PSU  | C6-C5 | 3.19  | 1.39        | 1.35     |
| 39  | B5    | 3500 | PSU  | C6-C5 | 3.16  | 1.39        | 1.35     |
| 1   | A2    | 1239 | PSU  | C6-C5 | 3.16  | 1.39        | 1.35     |
| 1   | A2    | 407  | PSU  | C6-C5 | 3.16  | 1.39        | 1.35     |
| 1   | A2    | 610  | PSU  | C6-C5 | 3.15  | 1.39        | 1.35     |
| 1   | A2    | 573  | PSU  | C6-C5 | 3.15  | 1.39        | 1.35     |
| 39  | B5    | 3494 | PSU  | C6-C5 | 3.15  | 1.39        | 1.35     |
| 39  | B5    | 3462 | PSU  | C6-C5 | 3.14  | 1.39        | 1.35     |
| 39  | B5    | 1266 | 1MA  | C6-N6 | 3.14  | 1.35        | 1.28     |
| 1   | A2    | 802  | PSU  | C6-C5 | 3.14  | 1.39        | 1.35     |
| 1   | A2    | 868  | OMG  | C5-C4 | 3.14  | 1.47        | 1.38     |
| 1   | A2    | 967  | PSU  | C6-C5 | 3.13  | 1.39        | 1.35     |
| 39  | B5    | 4107 | PSU  | C6-C5 | 3.13  | 1.39        | 1.35     |
| 39  | B5    | 4740 | PSU  | C6-C5 | 3.13  | 1.39        | 1.35     |
| 1   | A2    | 1178 | PSU  | C6-C5 | 3.13  | 1.39        | 1.35     |
| 39  | B5    | 1799 | PSU  | C6-C5 | 3.12  | 1.39        | 1.35     |
| 1   | A2    | 1047 | PSU  | C6-C5 | 3.12  | 1.39        | 1.35     |
| 1   | A2    | 652  | PSU  | C6-C5 | 3.12  | 1.39        | 1.35     |
| 1   | A2    | 109  | PSU  | C6-C5 | 3.12  | 1.39        | 1.35     |
| 39  | B5    | 3496 | PSU  | C6-C5 | 3.11  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A2    | 1046 | PSU  | C6-C5 | 3.11  | 1.38        | 1.35     |
| 1   | A2    | 93   | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 1   | A2    | 823  | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 1   | A2    | 1005 | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 39  | B5    | 1731 | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 39  | B5    | 1721 | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 39  | B5    | 4322 | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 39  | B5    | 3502 | PSU  | C6-C5 | 3.10  | 1.38        | 1.35     |
| 39  | B5    | 4278 | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 1   | A2    | 119  | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 39  | B5    | 1266 | 1MA  | C5-C4 | 3.09  | 1.47        | 1.38     |
| 1   | A2    | 1693 | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 39  | B5    | 2475 | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 1   | A2    | 1249 | B8N  | C4-N3 | -3.09 | 1.34        | 1.40     |
| 39  | B5    | 4711 | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 39  | B5    | 4169 | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 1   | A2    | 815  | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 39  | B5    | 4217 | PSU  | C6-C5 | 3.09  | 1.38        | 1.35     |
| 1   | A2    | 105  | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 1   | A2    | 1446 | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 1   | A2    | 218  | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 1   | A2    | 36   | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 1   | A2    | 867  | PSU  | C6-C5 | 3.08  | 1.38        | 1.35     |
| 39  | B5    | 4364 | OMG  | C5-C4 | 3.07  | 1.47        | 1.38     |
| 1   | A2    | 34   | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 1   | A2    | 650  | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 1   | A2    | 816  | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 1   | A2    | 510  | OMG  | C5-C4 | 3.07  | 1.47        | 1.38     |
| 1   | A2    | 864  | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 41  | B8    | 75   | OMG  | C5-C4 | 3.07  | 1.47        | 1.38     |
| 39  | B5    | 3427 | PSU  | C6-C5 | 3.07  | 1.38        | 1.35     |
| 1   | A2    | 1368 | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 39  | B5    | 2719 | OMG  | C5-C4 | 3.06  | 1.47        | 1.38     |
| 39  | B5    | 1718 | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 39  | B5    | 4749 | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 1   | A2    | 1626 | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 39  | B5    | 1683 | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 41  | B8    | 69   | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 41  | B8    | 55   | PSU  | C6-C5 | 3.06  | 1.38        | 1.35     |
| 39  | B5    | 1580 | OMG  | C5-C4 | 3.05  | 1.47        | 1.38     |
| 1   | A2    | 1329 | OMG  | C5-C4 | 3.05  | 1.47        | 1.38     |
| 1   | A2    | 682  | PSU  | C6-C5 | 3.05  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 39  | B5    | 4099 | PSU  | C6-C5 | 3.05 | 1.38        | 1.35     |
| 39  | B5    | 4240 | OMG  | C5-C4 | 3.05 | 1.47        | 1.38     |
| 39  | B5    | 4245 | OMG  | C5-C4 | 3.05 | 1.47        | 1.38     |
| 39  | B5    | 4325 | PSU  | C6-C5 | 3.05 | 1.38        | 1.35     |
| 39  | B5    | 4435 | PSU  | C6-C5 | 3.05 | 1.38        | 1.35     |
| 1   | A2    | 1233 | PSU  | C6-C5 | 3.05 | 1.38        | 1.35     |
| 1   | A2    | 1644 | PSU  | C6-C5 | 3.05 | 1.38        | 1.35     |
| 1   | A2    | 1348 | PSU  | C6-C5 | 3.05 | 1.38        | 1.35     |
| 39  | B5    | 4419 | PSU  | C6-C5 | 3.04 | 1.38        | 1.35     |
| 1   | A2    | 1491 | OMG  | C5-C4 | 3.04 | 1.47        | 1.38     |
| 39  | B5    | 4045 | PSU  | C6-C5 | 3.04 | 1.38        | 1.35     |
| 1   | A2    | 437  | OMG  | C5-C4 | 3.04 | 1.47        | 1.38     |
| 39  | B5    | 4039 | PSU  | C6-C5 | 3.04 | 1.38        | 1.35     |
| 39  | B5    | 3466 | PSU  | C6-C5 | 3.04 | 1.38        | 1.35     |
| 39  | B5    | 4382 | PSU  | C6-C5 | 3.04 | 1.38        | 1.35     |
| 39  | B5    | 1720 | PSU  | C6-C5 | 3.04 | 1.38        | 1.35     |
| 39  | B5    | 3676 | OMG  | C5-C4 | 3.04 | 1.47        | 1.38     |
| 1   | A2    | 1448 | OMG  | C5-C4 | 3.03 | 1.47        | 1.38     |
| 1   | A2    | 602  | OMG  | C5-C4 | 3.03 | 1.47        | 1.38     |
| 1   | A2    | 1082 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 3359 | OMG  | C5-C4 | 3.03 | 1.47        | 1.38     |
| 39  | B5    | 4116 | OMG  | C5-C4 | 3.03 | 1.47        | 1.38     |
| 39  | B5    | 3576 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 4246 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 4267 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 1638 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 1   | A2    | 1057 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 3490 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 1632 | PSU  | C6-C5 | 3.03 | 1.38        | 1.35     |
| 39  | B5    | 2267 | OMG  | C5-C4 | 3.02 | 1.47        | 1.38     |
| 1   | A2    | 645  | OMG  | C5-C4 | 3.02 | 1.47        | 1.38     |
| 1   | A2    | 687  | PSU  | C6-C5 | 3.02 | 1.38        | 1.35     |
| 39  | B5    | 3616 | PSU  | C6-C5 | 3.02 | 1.38        | 1.35     |
| 39  | B5    | 3554 | PSU  | C6-C5 | 3.02 | 1.38        | 1.35     |
| 39  | B5    | 1537 | PSU  | C6-C5 | 3.02 | 1.38        | 1.35     |
| 39  | B5    | 3476 | OMG  | C5-C4 | 3.02 | 1.47        | 1.38     |
| 39  | B5    | 3942 | OMG  | C5-C4 | 3.02 | 1.47        | 1.38     |
| 39  | B5    | 3371 | PSU  | C6-C5 | 3.01 | 1.38        | 1.35     |
| 1   | A2    | 1245 | PSU  | C6-C5 | 3.01 | 1.38        | 1.35     |
| 39  | B5    | 3524 | OMG  | C5-C4 | 3.01 | 1.47        | 1.38     |
| 1   | A2    | 684  | OMG  | C5-C4 | 3.01 | 1.47        | 1.38     |
| 39  | B5    | 4383 | OMG  | C5-C4 | 3.01 | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 39  | B5    | 4058 | PSU  | C6-C5   | 3.01  | 1.38        | 1.35     |
| 39  | B5    | 3631 | OMG  | C5-C4   | 3.00  | 1.47        | 1.38     |
| 39  | B5    | 4042 | PSU  | C6-C5   | 3.00  | 1.38        | 1.35     |
| 39  | B5    | 4188 | PSU  | C6-C5   | 3.00  | 1.38        | 1.35     |
| 39  | B5    | 4203 | PSU  | C6-C5   | 3.00  | 1.38        | 1.35     |
| 39  | B5    | 4138 | OMG  | C5-C4   | 2.99  | 1.47        | 1.38     |
| 39  | B5    | 2207 | OMG  | C5-C4   | 2.99  | 1.47        | 1.38     |
| 39  | B5    | 2351 | PSU  | C6-C5   | 2.99  | 1.38        | 1.35     |
| 39  | B5    | 1491 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 39  | B5    | 4369 | OMG  | C5-C4   | 2.98  | 1.47        | 1.38     |
| 39  | B5    | 1801 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 39  | B5    | 3369 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 39  | B5    | 4177 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 39  | B5    | 4298 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 39  | B5    | 3583 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 39  | B5    | 4374 | PSU  | C6-C5   | 2.98  | 1.38        | 1.35     |
| 1   | A2    | 1249 | B8N  | C6-C5   | 2.97  | 1.39        | 1.34     |
| 39  | B5    | 3974 | OMG  | C5-C4   | 2.97  | 1.47        | 1.38     |
| 39  | B5    | 1477 | OMG  | C5-C4   | 2.97  | 1.47        | 1.38     |
| 39  | B5    | 3585 | PSU  | C6-C5   | 2.97  | 1.38        | 1.35     |
| 39  | B5    | 3652 | PSU  | C6-C5   | 2.95  | 1.38        | 1.35     |
| 1   | A2    | 1843 | 4AC  | C4-N4   | -2.95 | 1.35        | 1.39     |
| 39  | B5    | 1260 | OMG  | C5-C4   | 2.93  | 1.46        | 1.38     |
| 39  | B5    | 4149 | PSU  | C6-C5   | 2.92  | 1.38        | 1.35     |
| 68  | Ba    | 39   | V5N  | CD2-NE2 | -2.89 | 1.33        | 1.37     |
| 42  | BA    | 216  | V5N  | CD2-NE2 | -2.86 | 1.33        | 1.37     |
| 1   | A2    | 1338 | 4AC  | C4-N4   | -2.85 | 1.35        | 1.39     |
| 39  | B5    | 3652 | PSU  | C4-N3   | -2.84 | 1.33        | 1.38     |
| 39  | B5    | 3616 | PSU  | C4-N3   | -2.82 | 1.33        | 1.38     |
| 39  | B5    | 3369 | PSU  | C4-N3   | -2.81 | 1.33        | 1.38     |
| 39  | B5    | 3371 | PSU  | C4-N3   | -2.81 | 1.33        | 1.38     |
| 1   | A2    | 1851 | MA6  | C5-C6   | 2.80  | 1.48        | 1.41     |
| 39  | B5    | 4149 | PSU  | C4-N3   | -2.80 | 1.33        | 1.38     |
| 39  | B5    | 3427 | PSU  | C4-N3   | -2.78 | 1.33        | 1.38     |
| 39  | B5    | 1491 | PSU  | C4-N3   | -2.78 | 1.33        | 1.38     |
| 41  | B8    | 69   | PSU  | C4-N3   | -2.77 | 1.33        | 1.38     |
| 39  | B5    | 1801 | PSU  | C4-N3   | -2.77 | 1.33        | 1.38     |
| 39  | B5    | 4267 | PSU  | C4-N3   | -2.77 | 1.33        | 1.38     |
| 39  | B5    | 3576 | PSU  | C4-N3   | -2.77 | 1.33        | 1.38     |
| 39  | B5    | 4203 | PSU  | C4-N3   | -2.77 | 1.33        | 1.38     |
| 1   | A2    | 1082 | PSU  | C4-N3   | -2.76 | 1.33        | 1.38     |
| 39  | B5    | 3585 | PSU  | C4-N3   | -2.76 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 39  | B5    | 4039 | PSU  | C4-N3 | -2.76 | 1.33        | 1.38     |
| 39  | B5    | 4435 | PSU  | C4-N3 | -2.75 | 1.33        | 1.38     |
| 39  | B5    | 4177 | PSU  | C4-N3 | -2.75 | 1.33        | 1.38     |
| 39  | B5    | 2351 | PSU  | C4-N3 | -2.75 | 1.33        | 1.38     |
| 39  | B5    | 4298 | PSU  | C4-N3 | -2.75 | 1.33        | 1.38     |
| 1   | A2    | 867  | PSU  | C4-N3 | -2.74 | 1.33        | 1.38     |
| 39  | B5    | 4188 | PSU  | C4-N3 | -2.74 | 1.33        | 1.38     |
| 1   | A2    | 105  | PSU  | C4-N3 | -2.74 | 1.33        | 1.38     |
| 39  | B5    | 1721 | PSU  | C4-N3 | -2.74 | 1.33        | 1.38     |
| 1   | A2    | 1693 | PSU  | C4-N3 | -2.74 | 1.33        | 1.38     |
| 39  | B5    | 4107 | PSU  | C4-N3 | -2.74 | 1.33        | 1.38     |
| 39  | B5    | 1638 | PSU  | C4-N3 | -2.73 | 1.33        | 1.38     |
| 1   | A2    | 1046 | PSU  | C4-N3 | -2.73 | 1.33        | 1.38     |
| 39  | B5    | 3500 | PSU  | C4-N3 | -2.73 | 1.33        | 1.38     |
| 39  | B5    | 4058 | PSU  | C4-N3 | -2.73 | 1.33        | 1.38     |
| 1   | A2    | 652  | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 11  | AT    | 64   | 5MU  | C6-C5 | 2.72  | 1.39        | 1.34     |
| 1   | A2    | 610  | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 39  | B5    | 1720 | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 39  | B5    | 1731 | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 1   | A2    | 407  | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 39  | B5    | 4193 | 5MC  | C6-C5 | 2.72  | 1.39        | 1.34     |
| 39  | B5    | 4740 | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 39  | B5    | 1799 | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 1   | A2    | 682  | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 39  | B5    | 4322 | PSU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 39  | B5    | 3492 | A2M  | C5-C6 | 2.71  | 1.48        | 1.41     |
| 1   | A2    | 1852 | MA6  | C5-C6 | 2.71  | 1.48        | 1.41     |
| 39  | B5    | 3456 | A2M  | C5-C6 | 2.71  | 1.48        | 1.41     |
| 39  | B5    | 3496 | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 1   | A2    | 93   | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 39  | B5    | 2475 | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 39  | B5    | 4382 | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 41  | B8    | 55   | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 1   | A2    | 1368 | PSU  | C4-N3 | -2.71 | 1.33        | 1.38     |
| 1   | A2    | 218  | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 1   | A2    | 864  | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 3583 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 4419 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 1   | A2    | 469  | A2M  | C5-C6 | 2.70  | 1.48        | 1.41     |
| 1   | A2    | 591  | A2M  | C5-C6 | 2.70  | 1.48        | 1.41     |
| 39  | B5    | 4099 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A2    | 1245 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 3466 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 1537 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 1   | A2    | 1047 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 1   | A2    | 650  | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 1489 | A2M  | C5-C6 | 2.70  | 1.48        | 1.41     |
| 1   | A2    | 1233 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 4217 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 39  | B5    | 3554 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 1   | A2    | 166  | A2M  | C5-C6 | 2.69  | 1.48        | 1.41     |
| 1   | A2    | 1446 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 39  | B5    | 4711 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 39  | B5    | 4374 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 39  | B5    | 4042 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 39  | B5    | 4325 | PSU  | C4-N3 | -2.69 | 1.33        | 1.38     |
| 1   | A2    | 34   | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 1   | A2    | 815  | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 1   | A2    | 1057 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 11  | AT    | 65   | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 1   | A2    | 1644 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 1   | A2    | 159  | A2M  | C5-C6 | 2.68  | 1.48        | 1.41     |
| 1   | A2    | 816  | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 1   | A2    | 1005 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 39  | B5    | 3462 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 39  | B5    | 4246 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 39  | B5    | 3657 | OMU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 1   | A2    | 1178 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 39  | B5    | 3490 | PSU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 39  | B5    | 3447 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 1   | A2    | 687  | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 1   | A2    | 1239 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 39  | B5    | 3599 | A2M  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 1   | A2    | 119  | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 1   | A2    | 485  | A2M  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 1   | A2    | 513  | A2M  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 39  | B5    | 4317 | A2M  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 1   | A2    | 1348 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 39  | B5    | 3450 | A2M  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 39  | B5    | 1718 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 1   | A2    | 1626 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 1   | A2    | 1175 | PSU  | C4-N3 | -2.66 | 1.33        | 1.38     |
| 39  | B5    | 3550 | UY1  | C2-N1 | 2.66  | 1.40        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A2    | 27   | A2M  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 1   | A2    | 1032 | A2M  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 1   | A2    | 109  | PSU  | C4-N3 | -2.66 | 1.33        | 1.38     |
| 1   | A2    | 967  | PSU  | C4-N3 | -2.66 | 1.33        | 1.38     |
| 1   | A2    | 1384 | A2M  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 39  | B5    | 2658 | A2M  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 39  | B5    | 4169 | PSU  | C4-N3 | -2.65 | 1.33        | 1.38     |
| 39  | B5    | 4045 | PSU  | C4-N3 | -2.65 | 1.33        | 1.38     |
| 39  | B5    | 4278 | PSU  | C4-N3 | -2.65 | 1.33        | 1.38     |
| 39  | B5    | 4269 | A2M  | C5-C6 | 2.65  | 1.48        | 1.41     |
| 39  | B5    | 2244 | A2M  | C5-C6 | 2.64  | 1.48        | 1.41     |
| 1   | A2    | 573  | PSU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 39  | B5    | 3502 | PSU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 39  | B5    | 4749 | PSU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 1   | A2    | 823  | PSU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 1   | A2    | 1833 | 6MZ  | C8-N7 | 2.64  | 1.36        | 1.31     |
| 1   | A2    | 1679 | A2M  | C5-C6 | 2.64  | 1.48        | 1.41     |
| 39  | B5    | 398  | A2M  | C5-C6 | 2.64  | 1.48        | 1.41     |
| 39  | B5    | 4052 | OMU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 39  | B5    | 3557 | A2M  | C5-C6 | 2.64  | 1.48        | 1.41     |
| 39  | B5    | 3562 | A2M  | C5-C6 | 2.64  | 1.48        | 1.41     |
| 1   | A2    | 669  | A2M  | C5-C6 | 2.64  | 1.48        | 1.41     |
| 39  | B5    | 1683 | PSU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 39  | B5    | 4366 | OMU  | C4-N3 | -2.64 | 1.33        | 1.38     |
| 39  | B5    | 3494 | PSU  | C4-N3 | -2.63 | 1.33        | 1.38     |
| 39  | B5    | 4336 | A2M  | C5-C6 | 2.63  | 1.48        | 1.41     |
| 39  | B5    | 1632 | PSU  | C4-N3 | -2.63 | 1.34        | 1.38     |
| 39  | B5    | 400  | A2M  | C5-C6 | 2.62  | 1.48        | 1.41     |
| 1   | A2    | 577  | A2M  | C5-C6 | 2.62  | 1.48        | 1.41     |
| 39  | B5    | 2206 | A2M  | C5-C6 | 2.62  | 1.48        | 1.41     |
| 1   | A2    | 36   | PSU  | C4-N3 | -2.61 | 1.34        | 1.38     |
| 39  | B5    | 3514 | 5MC  | C6-C5 | 2.61  | 1.38        | 1.34     |
| 39  | B5    | 1479 | A2M  | C5-C6 | 2.61  | 1.48        | 1.41     |
| 1   | A2    | 802  | PSU  | C4-N3 | -2.60 | 1.34        | 1.38     |
| 1   | A2    | 1851 | MA6  | C6-N6 | 2.60  | 1.44        | 1.36     |
| 11  | AT    | 64   | 5MU  | C4-N3 | -2.60 | 1.34        | 1.38     |
| 39  | B5    | 3973 | OMU  | C4-N3 | -2.59 | 1.33        | 1.38     |
| 1   | A2    | 99   | A2M  | C5-C6 | 2.59  | 1.48        | 1.41     |
| 39  | B5    | 3524 | OMG  | C6-N1 | -2.59 | 1.34        | 1.38     |
| 39  | B5    | 1810 | A2M  | C5-C6 | 2.59  | 1.48        | 1.41     |
| 1   | A2    | 210  | PSU  | C4-N3 | -2.59 | 1.34        | 1.38     |
| 39  | B5    | 2630 | A2M  | C5-C6 | 2.59  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 39  | B5    | 4244 | OMU  | C4-N3 | -2.58 | 1.33        | 1.38     |
| 39  | B5    | 4116 | OMG  | C6-N1 | -2.58 | 1.34        | 1.38     |
| 39  | B5    | 3966 | 6MZ  | C5-C6 | 2.58  | 1.48        | 1.41     |
| 39  | B5    | 2207 | OMG  | C6-N1 | -2.58 | 1.34        | 1.38     |
| 1   | A2    | 355  | OMU  | C4-N3 | -2.57 | 1.33        | 1.38     |
| 1   | A2    | 121  | OMU  | C4-N3 | -2.57 | 1.34        | 1.38     |
| 39  | B5    | 1260 | OMG  | C6-N1 | -2.57 | 1.34        | 1.38     |
| 39  | B5    | 4138 | OMG  | C6-N1 | -2.57 | 1.34        | 1.38     |
| 1   | A2    | 1443 | OMU  | C4-N3 | -2.57 | 1.34        | 1.38     |
| 39  | B5    | 1477 | OMG  | C6-N1 | -2.57 | 1.34        | 1.38     |
| 39  | B5    | 2267 | OMG  | C6-N1 | -2.56 | 1.34        | 1.38     |
| 39  | B5    | 3631 | OMG  | C6-N1 | -2.56 | 1.34        | 1.38     |
| 39  | B5    | 4166 | PSU  | C4-N3 | -2.56 | 1.34        | 1.38     |
| 39  | B5    | 2680 | OMU  | C4-N3 | -2.56 | 1.34        | 1.38     |
| 39  | B5    | 4240 | OMG  | C6-N1 | -2.55 | 1.34        | 1.38     |
| 1   | A2    | 510  | OMG  | C6-N1 | -2.55 | 1.34        | 1.38     |
| 39  | B5    | 3517 | A2M  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 1   | A2    | 1852 | MA6  | C6-N6 | 2.54  | 1.44        | 1.36     |
| 39  | B5    | 2258 | OMU  | C4-N3 | -2.54 | 1.34        | 1.38     |
| 39  | B5    | 1270 | A2M  | C5-C6 | 2.54  | 1.48        | 1.41     |
| 39  | B5    | 1580 | OMG  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 39  | B5    | 3942 | OMG  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 39  | B5    | 4245 | OMG  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 1   | A2    | 1327 | OMU  | C4-N3 | -2.53 | 1.34        | 1.38     |
| 39  | B5    | 4383 | OMG  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 41  | B8    | 75   | OMG  | C6-N1 | -2.52 | 1.34        | 1.38     |
| 1   | A2    | 1491 | OMG  | C6-N1 | -2.52 | 1.34        | 1.38     |
| 39  | B5    | 4364 | OMG  | C6-N1 | -2.52 | 1.34        | 1.38     |
| 1   | A2    | 602  | OMG  | C6-N1 | -2.51 | 1.34        | 1.38     |
| 1   | A2    | 1805 | OMU  | C4-N3 | -2.51 | 1.34        | 1.38     |
| 39  | B5    | 4369 | OMG  | C6-N1 | -2.51 | 1.34        | 1.38     |
| 39  | B5    | 3476 | OMG  | C6-N1 | -2.49 | 1.34        | 1.38     |
| 39  | B5    | 2719 | OMG  | C6-N1 | -2.49 | 1.34        | 1.38     |
| 1   | A2    | 645  | OMG  | C6-N1 | -2.49 | 1.34        | 1.38     |
| 39  | B5    | 3359 | OMG  | C6-N1 | -2.49 | 1.34        | 1.38     |
| 1   | A2    | 1329 | OMG  | C6-N1 | -2.49 | 1.34        | 1.38     |
| 1   | A2    | 437  | OMG  | C6-N1 | -2.48 | 1.34        | 1.38     |
| 1   | A2    | 868  | OMG  | C6-N1 | -2.48 | 1.34        | 1.38     |
| 1   | A2    | 116  | OMU  | C4-N3 | -2.48 | 1.34        | 1.38     |
| 1   | A2    | 429  | OMU  | C4-N3 | -2.48 | 1.34        | 1.38     |
| 1   | A2    | 1249 | B8N  | C2-N3 | -2.46 | 1.34        | 1.38     |
| 1   | A2    | 684  | OMG  | C6-N1 | -2.46 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A2    | 1448 | OMG  | C6-N1 | -2.45 | 1.34        | 1.38     |
| 1   | A2    | 172  | OMU  | C4-N3 | -2.45 | 1.34        | 1.38     |
| 1   | A2    | 1289 | OMU  | C4-N3 | -2.44 | 1.34        | 1.38     |
| 39  | B5    | 3974 | OMG  | C6-N1 | -2.44 | 1.34        | 1.38     |
| 39  | B5    | 3456 | A2M  | C8-N7 | 2.42  | 1.36        | 1.31     |
| 1   | A2    | 628  | OMU  | C4-N3 | -2.42 | 1.34        | 1.38     |
| 39  | B5    | 398  | A2M  | C8-N7 | 2.42  | 1.36        | 1.31     |
| 1   | A2    | 166  | A2M  | C8-N7 | 2.42  | 1.36        | 1.31     |
| 39  | B5    | 3450 | A2M  | C8-N7 | 2.42  | 1.36        | 1.31     |
| 39  | B5    | 3514 | 5MC  | C6-N1 | -2.42 | 1.33        | 1.38     |
| 1   | A2    | 1851 | MA6  | C4-N9 | -2.41 | 1.32        | 1.37     |
| 1   | A2    | 99   | A2M  | C8-N7 | 2.41  | 1.36        | 1.31     |
| 1   | A2    | 1679 | A2M  | C8-N7 | 2.41  | 1.36        | 1.31     |
| 39  | B5    | 3676 | OMG  | C6-N1 | -2.40 | 1.34        | 1.38     |
| 39  | B5    | 1489 | A2M  | C8-N7 | 2.40  | 1.36        | 1.31     |
| 1   | A2    | 513  | A2M  | C8-N7 | 2.40  | 1.36        | 1.31     |
| 1   | A2    | 469  | A2M  | C8-N7 | 2.40  | 1.36        | 1.31     |
| 1   | A2    | 1032 | A2M  | C8-N7 | 2.40  | 1.36        | 1.31     |
| 39  | B5    | 3492 | A2M  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 1   | A2    | 669  | A2M  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 1   | A2    | 27   | A2M  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 1   | A2    | 485  | A2M  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 1   | A2    | 1384 | A2M  | C8-N7 | 2.38  | 1.36        | 1.31     |
| 1   | A2    | 159  | A2M  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 1   | A2    | 577  | A2M  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 39  | B5    | 1479 | A2M  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 39  | B5    | 3557 | A2M  | C8-N7 | 2.36  | 1.36        | 1.31     |
| 39  | B5    | 4317 | A2M  | C8-N7 | 2.36  | 1.36        | 1.31     |
| 1   | A2    | 1640 | G7M  | C6-N1 | -2.36 | 1.34        | 1.38     |
| 39  | B5    | 2658 | A2M  | C8-N7 | 2.36  | 1.36        | 1.31     |
| 39  | B5    | 400  | A2M  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 39  | B5    | 3562 | A2M  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 39  | B5    | 3599 | A2M  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 39  | B5    | 4336 | A2M  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 39  | B5    | 3966 | 6MZ  | C8-N7 | 2.34  | 1.36        | 1.31     |
| 1   | A2    | 1851 | MA6  | C8-N7 | 2.34  | 1.36        | 1.31     |
| 1   | A2    | 591  | A2M  | C8-N7 | 2.34  | 1.36        | 1.31     |
| 39  | B5    | 3517 | A2M  | C8-N7 | 2.33  | 1.36        | 1.31     |
| 11  | AT    | 64   | 5MU  | C2-N1 | 2.33  | 1.42        | 1.38     |
| 39  | B5    | 2244 | A2M  | C8-N7 | 2.33  | 1.36        | 1.31     |
| 11  | AT    | 64   | 5MU  | C4-C5 | 2.32  | 1.48        | 1.44     |
| 39  | B5    | 4269 | A2M  | C8-N7 | 2.31  | 1.36        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 39  | B5    | 4193 | 5MC  | C6-N1 | -2.31 | 1.34        | 1.38     |
| 1   | A2    | 1833 | 6MZ  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 39  | B5    | 1266 | 1MA  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 39  | B5    | 1270 | A2M  | C8-N7 | 2.29  | 1.35        | 1.31     |
| 39  | B5    | 1810 | A2M  | C8-N7 | 2.29  | 1.35        | 1.31     |
| 39  | B5    | 2206 | A2M  | C8-N7 | 2.29  | 1.35        | 1.31     |
| 1   | A2    | 591  | A2M  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 39  | B5    | 2206 | A2M  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 39  | B5    | 1810 | A2M  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 39  | B5    | 1479 | A2M  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 39  | B5    | 3657 | OMU  | C2-N3 | -2.27 | 1.33        | 1.38     |
| 39  | B5    | 3973 | OMU  | C2-N3 | -2.27 | 1.33        | 1.38     |
| 39  | B5    | 4240 | OMG  | C5-N7 | -2.27 | 1.34        | 1.39     |
| 11  | AT    | 64   | 5MU  | C6-N1 | -2.26 | 1.34        | 1.38     |
| 39  | B5    | 1270 | A2M  | C5-N7 | -2.26 | 1.34        | 1.39     |
| 1   | A2    | 1833 | 6MZ  | C5-C6 | 2.26  | 1.47        | 1.41     |
| 39  | B5    | 2680 | OMU  | C2-N3 | -2.25 | 1.34        | 1.38     |
| 39  | B5    | 4366 | OMU  | C2-N3 | -2.25 | 1.34        | 1.38     |
| 39  | B5    | 2630 | A2M  | C8-N7 | 2.25  | 1.35        | 1.31     |
| 39  | B5    | 3550 | UY1  | C6-N1 | -2.24 | 1.32        | 1.36     |
| 1   | A2    | 1443 | OMU  | C2-N3 | -2.24 | 1.34        | 1.38     |
| 39  | B5    | 2719 | OMG  | C5-N7 | -2.24 | 1.34        | 1.39     |
| 1   | A2    | 1843 | 4AC  | C7-N4 | -2.24 | 1.33        | 1.37     |
| 1   | A2    | 1491 | OMG  | C5-N7 | -2.23 | 1.34        | 1.39     |
| 39  | B5    | 3942 | OMG  | C5-N7 | -2.23 | 1.34        | 1.39     |
| 39  | B5    | 1489 | A2M  | C5-N7 | -2.23 | 1.34        | 1.39     |
| 1   | A2    | 121  | OMU  | C2-N3 | -2.23 | 1.34        | 1.38     |
| 1   | A2    | 1805 | OMU  | C2-N3 | -2.23 | 1.34        | 1.38     |
| 1   | A2    | 99   | A2M  | C5-N7 | -2.23 | 1.34        | 1.39     |
| 1   | A2    | 1852 | MA6  | C8-N7 | 2.23  | 1.35        | 1.31     |
| 1   | A2    | 485  | A2M  | C5-N7 | -2.23 | 1.34        | 1.39     |
| 39  | B5    | 2658 | A2M  | C5-N7 | -2.23 | 1.34        | 1.39     |
| 39  | B5    | 4336 | A2M  | C5-N7 | -2.22 | 1.34        | 1.39     |
| 1   | A2    | 1852 | MA6  | C5-N7 | -2.22 | 1.34        | 1.39     |
| 39  | B5    | 3599 | A2M  | C5-N7 | -2.22 | 1.34        | 1.39     |
| 1   | A2    | 602  | OMG  | C5-N7 | -2.22 | 1.34        | 1.39     |
| 39  | B5    | 2267 | OMG  | C5-N7 | -2.21 | 1.34        | 1.39     |
| 1   | A2    | 27   | A2M  | C5-N7 | -2.21 | 1.34        | 1.39     |
| 39  | B5    | 3557 | A2M  | C5-N7 | -2.21 | 1.34        | 1.39     |
| 39  | B5    | 4052 | OMU  | C2-N3 | -2.21 | 1.34        | 1.38     |
| 39  | B5    | 4138 | OMG  | C5-N7 | -2.21 | 1.34        | 1.39     |
| 1   | A2    | 1032 | A2M  | C5-N7 | -2.21 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 39  | B5    | 3562 | A2M  | C5-N7 | -2.21 | 1.34        | 1.39     |
| 39  | B5    | 3966 | 6MZ  | C5-N7 | -2.21 | 1.34        | 1.39     |
| 39  | B5    | 1580 | OMG  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 39  | B5    | 4269 | A2M  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 39  | B5    | 1260 | OMG  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 39  | B5    | 2630 | A2M  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 39  | B5    | 4245 | OMG  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 1   | A2    | 513  | A2M  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 39  | B5    | 400  | A2M  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 1   | A2    | 1329 | OMG  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 39  | B5    | 3517 | A2M  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 39  | B5    | 1266 | 1MA  | C2-N3 | 2.19  | 1.34        | 1.30     |
| 1   | A2    | 355  | OMU  | C2-N3 | -2.19 | 1.34        | 1.38     |
| 1   | A2    | 669  | A2M  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 39  | B5    | 2207 | OMG  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 39  | B5    | 4383 | OMG  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 39  | B5    | 4244 | OMU  | C2-N3 | -2.18 | 1.34        | 1.38     |
| 39  | B5    | 4317 | A2M  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 1   | A2    | 645  | OMG  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 39  | B5    | 3476 | OMG  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 1   | A2    | 1384 | A2M  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 39  | B5    | 398  | A2M  | C5-N7 | -2.17 | 1.34        | 1.39     |
| 39  | B5    | 4364 | OMG  | C5-N7 | -2.17 | 1.34        | 1.39     |
| 1   | A2    | 159  | A2M  | C5-N7 | -2.17 | 1.34        | 1.39     |
| 39  | B5    | 2258 | OMU  | C2-N3 | -2.17 | 1.34        | 1.38     |
| 1   | A2    | 868  | OMG  | C5-N7 | -2.17 | 1.34        | 1.39     |
| 39  | B5    | 3974 | OMG  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 39  | B5    | 3456 | A2M  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 1   | A2    | 437  | OMG  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 1   | A2    | 1327 | OMU  | C2-N3 | -2.16 | 1.34        | 1.38     |
| 41  | B8    | 75   | OMG  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 39  | B5    | 3450 | A2M  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 39  | B5    | 2244 | A2M  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 39  | B5    | 3524 | OMG  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 1   | A2    | 429  | OMU  | C2-N3 | -2.15 | 1.34        | 1.38     |
| 1   | A2    | 510  | OMG  | C5-N7 | -2.15 | 1.34        | 1.39     |
| 1   | A2    | 172  | OMU  | C2-N3 | -2.15 | 1.34        | 1.38     |
| 1   | A2    | 628  | OMU  | C2-N3 | -2.15 | 1.34        | 1.38     |
| 39  | B5    | 3359 | OMG  | C5-N7 | -2.14 | 1.34        | 1.39     |
| 39  | B5    | 3631 | OMG  | C5-N7 | -2.14 | 1.34        | 1.39     |
| 1   | A2    | 469  | A2M  | C5-N7 | -2.14 | 1.35        | 1.39     |
| 39  | B5    | 4369 | OMG  | C5-N7 | -2.14 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A2    | 1289 | OMU  | C2-N3 | -2.14 | 1.34        | 1.38     |
| 1   | A2    | 1679 | A2M  | C5-N7 | -2.13 | 1.35        | 1.39     |
| 39  | B5    | 1477 | OMG  | C5-N7 | -2.13 | 1.35        | 1.39     |
| 39  | B5    | 3492 | A2M  | C5-N7 | -2.13 | 1.35        | 1.39     |
| 39  | B5    | 4116 | OMG  | C5-N7 | -2.12 | 1.35        | 1.39     |
| 1   | A2    | 684  | OMG  | C5-N7 | -2.12 | 1.35        | 1.39     |
| 1   | A2    | 577  | A2M  | C5-N7 | -2.11 | 1.35        | 1.39     |
| 1   | A2    | 1851 | MA6  | C5-N7 | -2.11 | 1.35        | 1.39     |
| 1   | A2    | 166  | A2M  | C5-N7 | -2.11 | 1.35        | 1.39     |
| 1   | A2    | 116  | OMU  | C2-N3 | -2.11 | 1.34        | 1.38     |
| 1   | A2    | 1448 | OMG  | C5-N7 | -2.10 | 1.35        | 1.39     |
| 1   | A2    | 1289 | OMU  | C2-N1 | 2.10  | 1.41        | 1.38     |
| 39  | B5    | 3676 | OMG  | C5-N7 | -2.09 | 1.35        | 1.39     |
| 39  | B5    | 3973 | OMU  | C2-N1 | 2.08  | 1.41        | 1.38     |
| 1   | A2    | 1805 | OMU  | C2-N1 | 2.07  | 1.41        | 1.38     |
| 39  | B5    | 4052 | OMU  | C5-C4 | -2.03 | 1.39        | 1.43     |
| 39  | B5    | 4366 | OMU  | C5-C4 | -2.02 | 1.39        | 1.43     |
| 1   | A2    | 121  | OMU  | C5-C4 | -2.02 | 1.39        | 1.43     |
| 39  | B5    | 2258 | OMU  | C5-C4 | -2.00 | 1.39        | 1.43     |
| 39  | B5    | 4366 | OMU  | C2-N1 | 2.00  | 1.41        | 1.38     |

All (969) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A2    | 1640 | G7M  | CN7-N7-C8 | -7.96 | 112.56      | 124.84   |
| 1   | A2    | 591  | A2M  | C5-C4-N3  | -6.89 | 117.76      | 126.75   |
| 1   | A2    | 1640 | G7M  | N9-C8-N7  | -6.59 | 95.91       | 112.21   |
| 1   | A2    | 1640 | G7M  | C8-N7-C5  | 6.54  | 115.96      | 107.78   |
| 1   | A2    | 1640 | G7M  | N9-C4-N3  | 6.49  | 138.98      | 125.94   |
| 39  | B5    | 2658 | A2M  | C5-C4-N3  | -6.36 | 118.45      | 126.75   |
| 1   | A2    | 166  | A2M  | C5-C4-N3  | -6.36 | 118.45      | 126.75   |
| 1   | A2    | 1833 | 6MZ  | C5-C4-N3  | -6.32 | 118.50      | 126.75   |
| 39  | B5    | 3599 | A2M  | C5-C4-N3  | -6.29 | 118.54      | 126.75   |
| 39  | B5    | 2719 | OMG  | C5-C4-N3  | -6.28 | 118.27      | 128.46   |
| 39  | B5    | 2206 | A2M  | C5-C4-N3  | -6.26 | 118.58      | 126.75   |
| 39  | B5    | 4240 | OMG  | C5-C4-N3  | -6.24 | 118.34      | 128.46   |
| 39  | B5    | 3557 | A2M  | C5-C4-N3  | -6.23 | 118.63      | 126.75   |
| 39  | B5    | 3492 | A2M  | C5-C4-N3  | -6.21 | 118.64      | 126.75   |
| 1   | A2    | 485  | A2M  | C5-C4-N3  | -6.21 | 118.65      | 126.75   |
| 39  | B5    | 398  | A2M  | C5-C4-N3  | -6.19 | 118.67      | 126.75   |
| 1   | A2    | 469  | A2M  | C5-C4-N3  | -6.19 | 118.67      | 126.75   |
| 39  | B5    | 1479 | A2M  | C5-C4-N3  | -6.19 | 118.68      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A2    | 513  | A2M  | C5-C4-N3 | -6.18 | 118.68      | 126.75   |
| 39  | B5    | 4336 | A2M  | C5-C4-N3 | -6.18 | 118.68      | 126.75   |
| 1   | A2    | 868  | OMG  | C5-C4-N3 | -6.16 | 118.47      | 128.46   |
| 1   | A2    | 1852 | MA6  | C5-C4-N3 | -6.16 | 118.72      | 126.75   |
| 39  | B5    | 4138 | OMG  | C5-C4-N3 | -6.16 | 118.47      | 128.46   |
| 39  | B5    | 3966 | 6MZ  | C5-C4-N3 | -6.16 | 118.72      | 126.75   |
| 1   | A2    | 27   | A2M  | C5-C4-N3 | -6.15 | 118.72      | 126.75   |
| 39  | B5    | 1638 | PSU  | N1-C2-N3 | 6.15  | 122.10      | 115.13   |
| 41  | B8    | 69   | PSU  | N1-C2-N3 | 6.15  | 122.10      | 115.13   |
| 39  | B5    | 4149 | PSU  | N1-C2-N3 | 6.15  | 122.09      | 115.13   |
| 1   | A2    | 99   | A2M  | C5-C4-N3 | -6.14 | 118.73      | 126.75   |
| 39  | B5    | 400  | A2M  | C5-C4-N3 | -6.14 | 118.74      | 126.75   |
| 1   | A2    | 1679 | A2M  | C5-C4-N3 | -6.14 | 118.74      | 126.75   |
| 1   | A2    | 1491 | OMG  | C5-C4-N3 | -6.14 | 118.50      | 128.46   |
| 1   | A2    | 1032 | A2M  | C5-C4-N3 | -6.14 | 118.74      | 126.75   |
| 1   | A2    | 1384 | A2M  | C5-C4-N3 | -6.14 | 118.74      | 126.75   |
| 39  | B5    | 3494 | PSU  | N1-C2-N3 | 6.14  | 122.08      | 115.13   |
| 1   | A2    | 159  | A2M  | C5-C4-N3 | -6.13 | 118.76      | 126.75   |
| 39  | B5    | 4246 | PSU  | N1-C2-N3 | 6.13  | 122.07      | 115.13   |
| 39  | B5    | 1270 | A2M  | C5-C4-N3 | -6.13 | 118.76      | 126.75   |
| 39  | B5    | 4435 | PSU  | N1-C2-N3 | 6.13  | 122.07      | 115.13   |
| 39  | B5    | 3562 | A2M  | C5-C4-N3 | -6.12 | 118.76      | 126.75   |
| 1   | A2    | 652  | PSU  | N1-C2-N3 | 6.12  | 122.06      | 115.13   |
| 39  | B5    | 2244 | A2M  | C5-C4-N3 | -6.12 | 118.77      | 126.75   |
| 1   | A2    | 510  | OMG  | C5-C4-N3 | -6.12 | 118.54      | 128.46   |
| 39  | B5    | 1632 | PSU  | N1-C2-N3 | 6.12  | 122.06      | 115.13   |
| 41  | B8    | 75   | OMG  | C5-C4-N3 | -6.12 | 118.54      | 128.46   |
| 39  | B5    | 4188 | PSU  | N1-C2-N3 | 6.11  | 122.06      | 115.13   |
| 39  | B5    | 4383 | OMG  | C5-C4-N3 | -6.11 | 118.55      | 128.46   |
| 39  | B5    | 3583 | PSU  | N1-C2-N3 | 6.11  | 122.05      | 115.13   |
| 1   | A2    | 645  | OMG  | C5-C4-N3 | -6.11 | 118.55      | 128.46   |
| 39  | B5    | 4267 | PSU  | N1-C2-N3 | 6.11  | 122.05      | 115.13   |
| 1   | A2    | 602  | OMG  | C5-C4-N3 | -6.10 | 118.56      | 128.46   |
| 1   | A2    | 437  | OMG  | C5-C4-N3 | -6.10 | 118.56      | 128.46   |
| 39  | B5    | 1799 | PSU  | N1-C2-N3 | 6.10  | 122.04      | 115.13   |
| 1   | A2    | 1329 | OMG  | C5-C4-N3 | -6.10 | 118.57      | 128.46   |
| 1   | A2    | 669  | A2M  | C5-C4-N3 | -6.10 | 118.79      | 126.75   |
| 39  | B5    | 3616 | PSU  | N1-C2-N3 | 6.09  | 122.03      | 115.13   |
| 39  | B5    | 4099 | PSU  | N1-C2-N3 | 6.09  | 122.03      | 115.13   |
| 39  | B5    | 1489 | A2M  | C5-C4-N3 | -6.09 | 118.81      | 126.75   |
| 39  | B5    | 3456 | A2M  | C5-C4-N3 | -6.09 | 118.81      | 126.75   |
| 39  | B5    | 4317 | A2M  | C5-C4-N3 | -6.09 | 118.81      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 39  | B5    | 1260 | OMG  | C5-C4-N3 | -6.09 | 118.59      | 128.46   |
| 39  | B5    | 4749 | PSU  | N1-C2-N3 | 6.08  | 122.02      | 115.13   |
| 1   | A2    | 577  | A2M  | C5-C4-N3 | -6.08 | 118.82      | 126.75   |
| 39  | B5    | 4374 | PSU  | N1-C2-N3 | 6.08  | 122.02      | 115.13   |
| 39  | B5    | 4042 | PSU  | N1-C2-N3 | 6.08  | 122.02      | 115.13   |
| 39  | B5    | 3359 | OMG  | C5-C4-N3 | -6.08 | 118.60      | 128.46   |
| 39  | B5    | 3447 | PSU  | N1-C2-N3 | 6.08  | 122.01      | 115.13   |
| 39  | B5    | 1477 | OMG  | C5-C4-N3 | -6.07 | 118.61      | 128.46   |
| 39  | B5    | 4269 | A2M  | C5-C4-N3 | -6.07 | 118.83      | 126.75   |
| 39  | B5    | 3496 | PSU  | N1-C2-N3 | 6.07  | 122.01      | 115.13   |
| 1   | A2    | 682  | PSU  | N1-C2-N3 | 6.07  | 122.00      | 115.13   |
| 39  | B5    | 4245 | OMG  | C5-C4-N3 | -6.06 | 118.63      | 128.46   |
| 39  | B5    | 1801 | PSU  | N1-C2-N3 | 6.06  | 122.00      | 115.13   |
| 41  | B8    | 55   | PSU  | N1-C2-N3 | 6.06  | 122.00      | 115.13   |
| 39  | B5    | 4364 | OMG  | C5-C4-N3 | -6.06 | 118.64      | 128.46   |
| 1   | A2    | 1175 | PSU  | N1-C2-N3 | 6.05  | 121.99      | 115.13   |
| 39  | B5    | 3462 | PSU  | N1-C2-N3 | 6.05  | 121.99      | 115.13   |
| 39  | B5    | 1810 | A2M  | C5-C4-N3 | -6.05 | 118.86      | 126.75   |
| 39  | B5    | 3450 | A2M  | C5-C4-N3 | -6.05 | 118.86      | 126.75   |
| 39  | B5    | 4058 | PSU  | N1-C2-N3 | 6.05  | 121.99      | 115.13   |
| 1   | A2    | 1446 | PSU  | N1-C2-N3 | 6.05  | 121.98      | 115.13   |
| 1   | A2    | 1448 | OMG  | C5-C4-N3 | -6.05 | 118.65      | 128.46   |
| 1   | A2    | 823  | PSU  | N1-C2-N3 | 6.05  | 121.98      | 115.13   |
| 39  | B5    | 1580 | OMG  | C5-C4-N3 | -6.05 | 118.65      | 128.46   |
| 1   | A2    | 802  | PSU  | N1-C2-N3 | 6.05  | 121.98      | 115.13   |
| 39  | B5    | 2267 | OMG  | C5-C4-N3 | -6.04 | 118.66      | 128.46   |
| 1   | A2    | 967  | PSU  | N1-C2-N3 | 6.04  | 121.98      | 115.13   |
| 39  | B5    | 3369 | PSU  | N1-C2-N3 | 6.04  | 121.97      | 115.13   |
| 39  | B5    | 3524 | OMG  | C5-C4-N3 | -6.03 | 118.67      | 128.46   |
| 39  | B5    | 4298 | PSU  | N1-C2-N3 | 6.03  | 121.97      | 115.13   |
| 39  | B5    | 3476 | OMG  | C5-C4-N3 | -6.03 | 118.67      | 128.46   |
| 1   | A2    | 1057 | PSU  | N1-C2-N3 | 6.03  | 121.96      | 115.13   |
| 39  | B5    | 4322 | PSU  | N1-C2-N3 | 6.03  | 121.96      | 115.13   |
| 39  | B5    | 4419 | PSU  | N1-C2-N3 | 6.03  | 121.96      | 115.13   |
| 1   | A2    | 1693 | PSU  | N1-C2-N3 | 6.02  | 121.96      | 115.13   |
| 39  | B5    | 3371 | PSU  | N1-C2-N3 | 6.02  | 121.95      | 115.13   |
| 39  | B5    | 2207 | OMG  | C5-C4-N3 | -6.02 | 118.69      | 128.46   |
| 1   | A2    | 1245 | PSU  | N1-C2-N3 | 6.02  | 121.95      | 115.13   |
| 1   | A2    | 687  | PSU  | N1-C2-N3 | 6.02  | 121.95      | 115.13   |
| 1   | A2    | 1046 | PSU  | N1-C2-N3 | 6.02  | 121.95      | 115.13   |
| 39  | B5    | 4325 | PSU  | N1-C2-N3 | 6.01  | 121.94      | 115.13   |
| 1   | A2    | 34   | PSU  | N1-C2-N3 | 6.01  | 121.94      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 39  | B5    | 1683 | PSU  | N1-C2-N3 | 6.01  | 121.94      | 115.13   |
| 39  | B5    | 3576 | PSU  | N1-C2-N3 | 6.01  | 121.94      | 115.13   |
| 39  | B5    | 4177 | PSU  | N1-C2-N3 | 6.01  | 121.94      | 115.13   |
| 1   | A2    | 1239 | PSU  | N1-C2-N3 | 6.00  | 121.93      | 115.13   |
| 1   | A2    | 1368 | PSU  | N1-C2-N3 | 6.00  | 121.93      | 115.13   |
| 1   | A2    | 816  | PSU  | N1-C2-N3 | 6.00  | 121.93      | 115.13   |
| 39  | B5    | 4369 | OMG  | C5-C4-N3 | -6.00 | 118.73      | 128.46   |
| 39  | B5    | 3554 | PSU  | N1-C2-N3 | 6.00  | 121.93      | 115.13   |
| 1   | A2    | 1047 | PSU  | N1-C2-N3 | 6.00  | 121.92      | 115.13   |
| 39  | B5    | 2630 | A2M  | C5-C4-N3 | -6.00 | 118.93      | 126.75   |
| 39  | B5    | 4740 | PSU  | N1-C2-N3 | 6.00  | 121.92      | 115.13   |
| 1   | A2    | 1178 | PSU  | N1-C2-N3 | 5.99  | 121.92      | 115.13   |
| 39  | B5    | 3652 | PSU  | N1-C2-N3 | 5.99  | 121.92      | 115.13   |
| 39  | B5    | 4107 | PSU  | N1-C2-N3 | 5.99  | 121.92      | 115.13   |
| 39  | B5    | 3427 | PSU  | N1-C2-N3 | 5.99  | 121.92      | 115.13   |
| 39  | B5    | 3942 | OMG  | C5-C4-N3 | -5.99 | 118.75      | 128.46   |
| 39  | B5    | 1537 | PSU  | N1-C2-N3 | 5.99  | 121.92      | 115.13   |
| 1   | A2    | 650  | PSU  | N1-C2-N3 | 5.99  | 121.91      | 115.13   |
| 39  | B5    | 3676 | OMG  | C5-C4-N3 | -5.99 | 118.75      | 128.46   |
| 39  | B5    | 1721 | PSU  | N1-C2-N3 | 5.98  | 121.91      | 115.13   |
| 39  | B5    | 1720 | PSU  | N1-C2-N3 | 5.98  | 121.91      | 115.13   |
| 1   | A2    | 105  | PSU  | N1-C2-N3 | 5.98  | 121.90      | 115.13   |
| 1   | A2    | 1851 | MA6  | C5-C4-N3 | -5.98 | 118.95      | 126.75   |
| 39  | B5    | 4217 | PSU  | N1-C2-N3 | 5.98  | 121.90      | 115.13   |
| 39  | B5    | 2475 | PSU  | N1-C2-N3 | 5.98  | 121.90      | 115.13   |
| 39  | B5    | 4382 | PSU  | N1-C2-N3 | 5.97  | 121.90      | 115.13   |
| 39  | B5    | 4116 | OMG  | C5-C4-N3 | -5.97 | 118.77      | 128.46   |
| 1   | A2    | 684  | OMG  | C5-C4-N3 | -5.97 | 118.78      | 128.46   |
| 39  | B5    | 3517 | A2M  | C5-C4-N3 | -5.97 | 118.97      | 126.75   |
| 1   | A2    | 36   | PSU  | N1-C2-N3 | 5.96  | 121.89      | 115.13   |
| 1   | A2    | 867  | PSU  | N1-C2-N3 | 5.96  | 121.89      | 115.13   |
| 39  | B5    | 1731 | PSU  | N1-C2-N3 | 5.96  | 121.89      | 115.13   |
| 39  | B5    | 3466 | PSU  | N1-C2-N3 | 5.96  | 121.88      | 115.13   |
| 39  | B5    | 3500 | PSU  | N1-C2-N3 | 5.96  | 121.88      | 115.13   |
| 39  | B5    | 3502 | PSU  | N1-C2-N3 | 5.96  | 121.88      | 115.13   |
| 39  | B5    | 4711 | PSU  | N1-C2-N3 | 5.96  | 121.88      | 115.13   |
| 1   | A2    | 109  | PSU  | N1-C2-N3 | 5.96  | 121.88      | 115.13   |
| 39  | B5    | 1491 | PSU  | N1-C2-N3 | 5.96  | 121.88      | 115.13   |
| 1   | A2    | 864  | PSU  | N1-C2-N3 | 5.95  | 121.88      | 115.13   |
| 1   | A2    | 93   | PSU  | N1-C2-N3 | 5.95  | 121.88      | 115.13   |
| 1   | A2    | 573  | PSU  | N1-C2-N3 | 5.95  | 121.88      | 115.13   |
| 1   | A2    | 407  | PSU  | N1-C2-N3 | 5.95  | 121.87      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 39  | B5    | 4045 | PSU  | N1-C2-N3 | 5.95  | 121.87      | 115.13   |
| 39  | B5    | 4278 | PSU  | N1-C2-N3 | 5.95  | 121.87      | 115.13   |
| 39  | B5    | 4039 | PSU  | N1-C2-N3 | 5.95  | 121.87      | 115.13   |
| 39  | B5    | 4203 | PSU  | N1-C2-N3 | 5.95  | 121.87      | 115.13   |
| 39  | B5    | 1718 | PSU  | N1-C2-N3 | 5.94  | 121.86      | 115.13   |
| 39  | B5    | 2351 | PSU  | N1-C2-N3 | 5.94  | 121.86      | 115.13   |
| 39  | B5    | 3631 | OMG  | C5-C4-N3 | -5.94 | 118.83      | 128.46   |
| 1   | A2    | 1626 | PSU  | N1-C2-N3 | 5.94  | 121.86      | 115.13   |
| 1   | A2    | 815  | PSU  | N1-C2-N3 | 5.93  | 121.85      | 115.13   |
| 1   | A2    | 1348 | PSU  | N1-C2-N3 | 5.93  | 121.85      | 115.13   |
| 1   | A2    | 1644 | PSU  | N1-C2-N3 | 5.93  | 121.85      | 115.13   |
| 11  | AT    | 65   | PSU  | N1-C2-N3 | 5.93  | 121.85      | 115.13   |
| 1   | A2    | 119  | PSU  | N1-C2-N3 | 5.92  | 121.84      | 115.13   |
| 39  | B5    | 3490 | PSU  | N1-C2-N3 | 5.92  | 121.84      | 115.13   |
| 39  | B5    | 4169 | PSU  | N1-C2-N3 | 5.92  | 121.84      | 115.13   |
| 1   | A2    | 1005 | PSU  | N1-C2-N3 | 5.91  | 121.83      | 115.13   |
| 1   | A2    | 1233 | PSU  | N1-C2-N3 | 5.91  | 121.83      | 115.13   |
| 1   | A2    | 1082 | PSU  | N1-C2-N3 | 5.91  | 121.82      | 115.13   |
| 39  | B5    | 3585 | PSU  | N1-C2-N3 | 5.90  | 121.82      | 115.13   |
| 1   | A2    | 210  | PSU  | N1-C2-N3 | 5.90  | 121.82      | 115.13   |
| 39  | B5    | 4276 | UR3  | C4-N3-C2 | -5.90 | 119.00      | 124.56   |
| 1   | A2    | 218  | PSU  | N1-C2-N3 | 5.89  | 121.81      | 115.13   |
| 1   | A2    | 610  | PSU  | N1-C2-N3 | 5.88  | 121.80      | 115.13   |
| 39  | B5    | 3974 | OMG  | C5-C4-N3 | -5.82 | 119.02      | 128.46   |
| 39  | B5    | 4166 | PSU  | N1-C2-N3 | 5.72  | 121.61      | 115.13   |
| 1   | A2    | 1851 | MA6  | N3-C4-N9 | 5.53  | 136.19      | 127.08   |
| 1   | A2    | 591  | A2M  | N3-C4-N9 | 5.45  | 136.06      | 127.08   |
| 1   | A2    | 1640 | G7M  | C5-C4-N3 | -5.45 | 117.70      | 128.15   |
| 39  | B5    | 3550 | UY1  | C4-N3-C2 | -5.39 | 118.57      | 126.34   |
| 39  | B5    | 1266 | 1MA  | C5-C4-N3 | -5.36 | 119.27      | 127.26   |
| 1   | A2    | 1851 | MA6  | C4-N9-C8 | 5.19  | 111.35      | 105.73   |
| 1   | A2    | 1833 | 6MZ  | N3-C4-N9 | 5.10  | 135.49      | 127.08   |
| 39  | B5    | 2719 | OMG  | C2-N3-C4 | 5.00  | 121.22      | 112.30   |
| 11  | AT    | 64   | 5MU  | C4-N3-C2 | -4.93 | 120.97      | 127.35   |
| 1   | A2    | 1491 | OMG  | C2-N3-C4 | 4.92  | 121.07      | 112.30   |
| 39  | B5    | 3359 | OMG  | C2-N3-C4 | 4.92  | 121.06      | 112.30   |
| 39  | B5    | 4138 | OMG  | C2-N3-C4 | 4.92  | 121.06      | 112.30   |
| 39  | B5    | 2658 | A2M  | N3-C4-N9 | 4.92  | 135.18      | 127.08   |
| 41  | B8    | 75   | OMG  | C2-N3-C4 | 4.92  | 121.06      | 112.30   |
| 39  | B5    | 4336 | A2M  | N3-C4-N9 | 4.91  | 135.18      | 127.08   |
| 39  | B5    | 3599 | A2M  | N3-C4-N9 | 4.91  | 135.17      | 127.08   |
| 39  | B5    | 2207 | OMG  | C2-N3-C4 | 4.90  | 121.04      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1   | A2    | 684  | OMG  | C2-N3-C4 | 4.90 | 121.03      | 112.30   |
| 39  | B5    | 4383 | OMG  | C2-N3-C4 | 4.90 | 121.03      | 112.30   |
| 39  | B5    | 1260 | OMG  | C2-N3-C4 | 4.90 | 121.03      | 112.30   |
| 39  | B5    | 4364 | OMG  | C2-N3-C4 | 4.89 | 121.02      | 112.30   |
| 1   | A2    | 437  | OMG  | C2-N3-C4 | 4.89 | 121.02      | 112.30   |
| 39  | B5    | 1477 | OMG  | C2-N3-C4 | 4.89 | 121.01      | 112.30   |
| 39  | B5    | 4240 | OMG  | C2-N3-C4 | 4.88 | 121.00      | 112.30   |
| 39  | B5    | 3476 | OMG  | C2-N3-C4 | 4.88 | 121.00      | 112.30   |
| 1   | A2    | 645  | OMG  | C2-N3-C4 | 4.88 | 120.99      | 112.30   |
| 1   | A2    | 1329 | OMG  | C2-N3-C4 | 4.87 | 120.98      | 112.30   |
| 39  | B5    | 3557 | A2M  | N3-C4-N9 | 4.87 | 135.11      | 127.08   |
| 1   | A2    | 602  | OMG  | C2-N3-C4 | 4.87 | 120.98      | 112.30   |
| 39  | B5    | 3942 | OMG  | C2-N3-C4 | 4.87 | 120.98      | 112.30   |
| 39  | B5    | 4245 | OMG  | C2-N3-C4 | 4.87 | 120.97      | 112.30   |
| 1   | A2    | 510  | OMG  | C2-N3-C4 | 4.87 | 120.97      | 112.30   |
| 1   | A2    | 868  | OMG  | C2-N3-C4 | 4.86 | 120.97      | 112.30   |
| 39  | B5    | 3676 | OMG  | C2-N3-C4 | 4.86 | 120.96      | 112.30   |
| 1   | A2    | 1448 | OMG  | C2-N3-C4 | 4.85 | 120.94      | 112.30   |
| 39  | B5    | 2206 | A2M  | N3-C4-N9 | 4.85 | 135.07      | 127.08   |
| 1   | A2    | 166  | A2M  | N3-C4-N9 | 4.84 | 135.05      | 127.08   |
| 1   | A2    | 1679 | A2M  | N3-C4-N9 | 4.84 | 135.05      | 127.08   |
| 39  | B5    | 4116 | OMG  | C2-N3-C4 | 4.84 | 120.92      | 112.30   |
| 39  | B5    | 2267 | OMG  | C2-N3-C4 | 4.83 | 120.91      | 112.30   |
| 39  | B5    | 3631 | OMG  | C2-N3-C4 | 4.83 | 120.91      | 112.30   |
| 39  | B5    | 4369 | OMG  | C2-N3-C4 | 4.83 | 120.91      | 112.30   |
| 39  | B5    | 1479 | A2M  | N3-C4-N9 | 4.82 | 135.03      | 127.08   |
| 39  | B5    | 1580 | OMG  | C2-N3-C4 | 4.81 | 120.88      | 112.30   |
| 1   | A2    | 159  | A2M  | N3-C4-N9 | 4.81 | 135.01      | 127.08   |
| 39  | B5    | 400  | A2M  | N3-C4-N9 | 4.81 | 135.01      | 127.08   |
| 39  | B5    | 3492 | A2M  | N3-C4-N9 | 4.81 | 135.01      | 127.08   |
| 39  | B5    | 398  | A2M  | N3-C4-N9 | 4.81 | 135.00      | 127.08   |
| 1   | A2    | 99   | A2M  | N3-C4-N9 | 4.80 | 134.99      | 127.08   |
| 1   | A2    | 485  | A2M  | N3-C4-N9 | 4.80 | 134.99      | 127.08   |
| 39  | B5    | 3524 | OMG  | C2-N3-C4 | 4.80 | 120.85      | 112.30   |
| 39  | B5    | 1270 | A2M  | N3-C4-N9 | 4.79 | 134.97      | 127.08   |
| 39  | B5    | 3974 | OMG  | C2-N3-C4 | 4.77 | 120.81      | 112.30   |
| 11  | AT    | 64   | 5MU  | N3-C2-N1 | 4.76 | 121.21      | 114.89   |
| 1   | A2    | 1384 | A2M  | N3-C4-N9 | 4.76 | 134.93      | 127.08   |
| 39  | B5    | 3517 | A2M  | N3-C4-N9 | 4.76 | 134.92      | 127.08   |
| 39  | B5    | 4269 | A2M  | N3-C4-N9 | 4.76 | 134.92      | 127.08   |
| 39  | B5    | 2630 | A2M  | N3-C4-N9 | 4.75 | 134.91      | 127.08   |
| 1   | A2    | 513  | A2M  | N3-C4-N9 | 4.75 | 134.91      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 39  | B5    | 1810 | A2M  | N3-C4-N9 | 4.75  | 134.90      | 127.08   |
| 39  | B5    | 2244 | A2M  | N3-C4-N9 | 4.74  | 134.90      | 127.08   |
| 1   | A2    | 27   | A2M  | N3-C4-N9 | 4.74  | 134.89      | 127.08   |
| 1   | A2    | 669  | A2M  | N3-C4-N9 | 4.74  | 134.88      | 127.08   |
| 1   | A2    | 469  | A2M  | N3-C4-N9 | 4.73  | 134.88      | 127.08   |
| 1   | A2    | 1852 | MA6  | N3-C4-N9 | 4.73  | 134.88      | 127.08   |
| 39  | B5    | 3562 | A2M  | N3-C4-N9 | 4.73  | 134.87      | 127.08   |
| 39  | B5    | 4317 | A2M  | N3-C4-N9 | 4.73  | 134.87      | 127.08   |
| 1   | A2    | 1032 | A2M  | N3-C4-N9 | 4.72  | 134.86      | 127.08   |
| 1   | A2    | 577  | A2M  | N3-C4-N9 | 4.72  | 134.85      | 127.08   |
| 39  | B5    | 3966 | 6MZ  | N3-C4-N9 | 4.71  | 134.85      | 127.08   |
| 39  | B5    | 4240 | OMG  | N9-C4-N3 | 4.71  | 135.40      | 125.94   |
| 39  | B5    | 2719 | OMG  | N9-C4-N3 | 4.70  | 135.37      | 125.94   |
| 39  | B5    | 1266 | 1MA  | C2-N3-C4 | 4.68  | 121.61      | 112.41   |
| 1   | A2    | 1338 | 4AC  | N4-C4-N3 | 4.67  | 121.70      | 113.85   |
| 39  | B5    | 1489 | A2M  | N3-C4-N9 | 4.66  | 134.76      | 127.08   |
| 1   | A2    | 868  | OMG  | N9-C4-N3 | 4.65  | 135.29      | 125.94   |
| 39  | B5    | 3456 | A2M  | N3-C4-N9 | 4.65  | 134.75      | 127.08   |
| 39  | B5    | 3450 | A2M  | N3-C4-N9 | 4.65  | 134.75      | 127.08   |
| 39  | B5    | 3942 | OMG  | N9-C4-N3 | 4.63  | 135.24      | 125.94   |
| 39  | B5    | 1260 | OMG  | N9-C4-N3 | 4.62  | 135.22      | 125.94   |
| 39  | B5    | 2267 | OMG  | N9-C4-N3 | 4.61  | 135.20      | 125.94   |
| 39  | B5    | 4244 | OMU  | C4-N3-C2 | -4.61 | 120.50      | 126.58   |
| 39  | B5    | 3657 | OMU  | C4-N3-C2 | -4.60 | 120.51      | 126.58   |
| 1   | A2    | 1491 | OMG  | N9-C4-N3 | 4.59  | 135.16      | 125.94   |
| 41  | B8    | 75   | OMG  | N9-C4-N3 | 4.59  | 135.15      | 125.94   |
| 1   | A2    | 602  | OMG  | N9-C4-N3 | 4.59  | 135.15      | 125.94   |
| 39  | B5    | 4138 | OMG  | N9-C4-N3 | 4.59  | 135.15      | 125.94   |
| 1   | A2    | 510  | OMG  | N9-C4-N3 | 4.58  | 135.14      | 125.94   |
| 1   | A2    | 645  | OMG  | N9-C4-N3 | 4.57  | 135.12      | 125.94   |
| 39  | B5    | 2680 | OMU  | C4-N3-C2 | -4.57 | 120.55      | 126.58   |
| 39  | B5    | 4383 | OMG  | N9-C4-N3 | 4.57  | 135.11      | 125.94   |
| 39  | B5    | 1580 | OMG  | N9-C4-N3 | 4.56  | 135.09      | 125.94   |
| 39  | B5    | 4364 | OMG  | N9-C4-N3 | 4.56  | 135.09      | 125.94   |
| 1   | A2    | 437  | OMG  | N9-C4-N3 | 4.54  | 135.06      | 125.94   |
| 1   | A2    | 1327 | OMU  | C4-N3-C2 | -4.54 | 120.59      | 126.58   |
| 39  | B5    | 3359 | OMG  | N9-C4-N3 | 4.53  | 135.04      | 125.94   |
| 39  | B5    | 3524 | OMG  | N9-C4-N3 | 4.53  | 135.03      | 125.94   |
| 1   | A2    | 429  | OMU  | C4-N3-C2 | -4.53 | 120.61      | 126.58   |
| 1   | A2    | 1329 | OMG  | N9-C4-N3 | 4.52  | 135.02      | 125.94   |
| 1   | A2    | 628  | OMU  | C4-N3-C2 | -4.52 | 120.62      | 126.58   |
| 39  | B5    | 3966 | 6MZ  | C9-N6-C6 | -4.52 | 118.98      | 122.87   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 39  | B5    | 3476 | OMG  | N9-C4-N3  | 4.50  | 134.97      | 125.94   |
| 39  | B5    | 4366 | OMU  | C4-N3-C2  | -4.49 | 120.66      | 126.58   |
| 1   | A2    | 1448 | OMG  | N9-C4-N3  | 4.48  | 134.93      | 125.94   |
| 1   | A2    | 1443 | OMU  | C4-N3-C2  | -4.48 | 120.68      | 126.58   |
| 1   | A2    | 355  | OMU  | C4-N3-C2  | -4.47 | 120.68      | 126.58   |
| 39  | B5    | 4245 | OMG  | N9-C4-N3  | 4.46  | 134.90      | 125.94   |
| 39  | B5    | 3973 | OMU  | C4-N3-C2  | -4.46 | 120.70      | 126.58   |
| 39  | B5    | 3550 | UY1  | N1-C2-N3  | 4.45  | 120.17      | 115.13   |
| 1   | A2    | 172  | OMU  | C4-N3-C2  | -4.45 | 120.71      | 126.58   |
| 1   | A2    | 121  | OMU  | C4-N3-C2  | -4.45 | 120.71      | 126.58   |
| 39  | B5    | 4116 | OMG  | N9-C4-N3  | 4.44  | 134.86      | 125.94   |
| 39  | B5    | 4369 | OMG  | N9-C4-N3  | 4.44  | 134.85      | 125.94   |
| 39  | B5    | 3676 | OMG  | N9-C4-N3  | 4.42  | 134.82      | 125.94   |
| 39  | B5    | 2207 | OMG  | N9-C4-N3  | 4.42  | 134.82      | 125.94   |
| 39  | B5    | 1477 | OMG  | N9-C4-N3  | 4.42  | 134.81      | 125.94   |
| 39  | B5    | 2258 | OMU  | C4-N3-C2  | -4.39 | 120.80      | 126.58   |
| 1   | A2    | 116  | OMU  | C4-N3-C2  | -4.38 | 120.80      | 126.58   |
| 1   | A2    | 684  | OMG  | N9-C4-N3  | 4.37  | 134.71      | 125.94   |
| 1   | A2    | 1640 | G7M  | C2-N3-C4  | 4.35  | 120.04      | 112.30   |
| 1   | A2    | 1852 | MA6  | C2-N1-C6  | 4.34  | 122.00      | 111.75   |
| 39  | B5    | 3631 | OMG  | N9-C4-N3  | 4.34  | 134.65      | 125.94   |
| 39  | B5    | 4244 | OMU  | N3-C2-N1  | 4.32  | 120.62      | 114.89   |
| 1   | A2    | 1851 | MA6  | C2-N1-C6  | 4.32  | 121.95      | 111.75   |
| 39  | B5    | 3974 | OMG  | N9-C4-N3  | 4.31  | 134.59      | 125.94   |
| 1   | A2    | 1805 | OMU  | C4-N3-C2  | -4.30 | 120.91      | 126.58   |
| 39  | B5    | 4052 | OMU  | C4-N3-C2  | -4.28 | 120.94      | 126.58   |
| 11  | AT    | 64   | 5MU  | C5-C4-N3  | 4.28  | 118.96      | 115.31   |
| 1   | A2    | 1289 | OMU  | C4-N3-C2  | -4.26 | 120.96      | 126.58   |
| 1   | A2    | 1640 | G7M  | C8-N9-C4  | 4.25  | 117.91      | 107.16   |
| 1   | A2    | 1843 | 4AC  | N4-C4-N3  | 4.24  | 120.96      | 113.85   |
| 39  | B5    | 4366 | OMU  | N3-C2-N1  | 4.23  | 120.50      | 114.89   |
| 39  | B5    | 2680 | OMU  | N3-C2-N1  | 4.19  | 120.45      | 114.89   |
| 39  | B5    | 3657 | OMU  | N3-C2-N1  | 4.18  | 120.44      | 114.89   |
| 1   | A2    | 1640 | G7M  | C1'-N9-C8 | -4.18 | 112.63      | 126.74   |
| 1   | A2    | 1851 | MA6  | N1-C6-N6  | 4.16  | 121.64      | 117.08   |
| 1   | A2    | 355  | OMU  | N3-C2-N1  | 4.16  | 120.42      | 114.89   |
| 1   | A2    | 172  | OMU  | N3-C2-N1  | 4.15  | 120.40      | 114.89   |
| 1   | A2    | 591  | A2M  | C2-N3-C4  | 4.15  | 121.55      | 111.75   |
| 39  | B5    | 3973 | OMU  | N3-C2-N1  | 4.11  | 120.34      | 114.89   |
| 1   | A2    | 628  | OMU  | N3-C2-N1  | 4.10  | 120.34      | 114.89   |
| 1   | A2    | 429  | OMU  | N3-C2-N1  | 4.10  | 120.33      | 114.89   |
| 39  | B5    | 4267 | PSU  | C4-N3-C2  | -4.09 | 120.44      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 39  | B5    | 1632 | PSU  | C4-N3-C2 | -4.09 | 120.45      | 126.34   |
| 39  | B5    | 4149 | PSU  | C4-N3-C2 | -4.06 | 120.48      | 126.34   |
| 39  | B5    | 3369 | PSU  | C4-N3-C2 | -4.06 | 120.50      | 126.34   |
| 1   | A2    | 1327 | OMU  | N3-C2-N1 | 4.05  | 120.27      | 114.89   |
| 39  | B5    | 1801 | PSU  | C4-N3-C2 | -4.05 | 120.50      | 126.34   |
| 1   | A2    | 116  | OMU  | N3-C2-N1 | 4.04  | 120.25      | 114.89   |
| 39  | B5    | 1638 | PSU  | C4-N3-C2 | -4.04 | 120.52      | 126.34   |
| 39  | B5    | 3496 | PSU  | C4-N3-C2 | -4.03 | 120.53      | 126.34   |
| 39  | B5    | 4298 | PSU  | C4-N3-C2 | -4.03 | 120.53      | 126.34   |
| 39  | B5    | 4052 | OMU  | N3-C2-N1 | 4.03  | 120.24      | 114.89   |
| 39  | B5    | 4042 | PSU  | C4-N3-C2 | -4.03 | 120.53      | 126.34   |
| 1   | A2    | 1805 | OMU  | N3-C2-N1 | 4.02  | 120.22      | 114.89   |
| 1   | A2    | 1175 | PSU  | C4-N3-C2 | -4.01 | 120.56      | 126.34   |
| 41  | B8    | 69   | PSU  | C4-N3-C2 | -4.01 | 120.57      | 126.34   |
| 39  | B5    | 3583 | PSU  | C4-N3-C2 | -3.99 | 120.58      | 126.34   |
| 39  | B5    | 1721 | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 39  | B5    | 3616 | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 1   | A2    | 650  | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 1   | A2    | 1446 | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 39  | B5    | 4749 | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 41  | B8    | 55   | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 39  | B5    | 4374 | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 39  | B5    | 4188 | PSU  | C4-N3-C2 | -3.99 | 120.59      | 126.34   |
| 1   | A2    | 1178 | PSU  | C4-N3-C2 | -3.99 | 120.60      | 126.34   |
| 1   | A2    | 652  | PSU  | C4-N3-C2 | -3.98 | 120.60      | 126.34   |
| 1   | A2    | 121  | OMU  | N3-C2-N1 | 3.98  | 120.17      | 114.89   |
| 39  | B5    | 1491 | PSU  | C4-N3-C2 | -3.98 | 120.61      | 126.34   |
| 1   | A2    | 687  | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 39  | B5    | 1799 | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 1   | A2    | 867  | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 39  | B5    | 3462 | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 39  | B5    | 3502 | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 1   | A2    | 1245 | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 1   | A2    | 1368 | PSU  | C4-N3-C2 | -3.97 | 120.62      | 126.34   |
| 39  | B5    | 4711 | PSU  | C4-N3-C2 | -3.96 | 120.63      | 126.34   |
| 39  | B5    | 4058 | PSU  | C4-N3-C2 | -3.96 | 120.63      | 126.34   |
| 39  | B5    | 4246 | PSU  | C4-N3-C2 | -3.96 | 120.63      | 126.34   |
| 39  | B5    | 4435 | PSU  | C4-N3-C2 | -3.96 | 120.63      | 126.34   |
| 39  | B5    | 3466 | PSU  | C4-N3-C2 | -3.96 | 120.64      | 126.34   |
| 1   | A2    | 816  | PSU  | C4-N3-C2 | -3.95 | 120.65      | 126.34   |
| 39  | B5    | 4419 | PSU  | C4-N3-C2 | -3.95 | 120.65      | 126.34   |
| 39  | B5    | 2658 | A2M  | C2-N3-C4 | 3.95  | 121.07      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A2    | 166  | A2M  | C2-N3-C4   | 3.94  | 121.07      | 111.75   |
| 1   | A2    | 1233 | PSU  | C4-N3-C2   | -3.94 | 120.66      | 126.34   |
| 39  | B5    | 4099 | PSU  | C4-N3-C2   | -3.94 | 120.66      | 126.34   |
| 1   | A2    | 1057 | PSU  | C4-N3-C2   | -3.94 | 120.66      | 126.34   |
| 39  | B5    | 1810 | A2M  | C2'-C1'-N9 | -3.94 | 106.90      | 113.53   |
| 1   | A2    | 1046 | PSU  | C4-N3-C2   | -3.94 | 120.67      | 126.34   |
| 39  | B5    | 4039 | PSU  | C4-N3-C2   | -3.93 | 120.67      | 126.34   |
| 1   | A2    | 1239 | PSU  | C4-N3-C2   | -3.93 | 120.67      | 126.34   |
| 1   | A2    | 1443 | OMU  | N3-C2-N1   | 3.93  | 120.11      | 114.89   |
| 39  | B5    | 4740 | PSU  | C4-N3-C2   | -3.93 | 120.68      | 126.34   |
| 39  | B5    | 1731 | PSU  | C4-N3-C2   | -3.93 | 120.68      | 126.34   |
| 39  | B5    | 3966 | 6MZ  | C2-N3-C4   | 3.92  | 121.02      | 111.75   |
| 39  | B5    | 4045 | PSU  | C4-N3-C2   | -3.92 | 120.69      | 126.34   |
| 1   | A2    | 1289 | OMU  | N3-C2-N1   | 3.92  | 120.09      | 114.89   |
| 39  | B5    | 3447 | PSU  | C4-N3-C2   | -3.92 | 120.69      | 126.34   |
| 39  | B5    | 4177 | PSU  | C4-N3-C2   | -3.92 | 120.69      | 126.34   |
| 39  | B5    | 1683 | PSU  | C4-N3-C2   | -3.91 | 120.70      | 126.34   |
| 39  | B5    | 3652 | PSU  | C4-N3-C2   | -3.91 | 120.70      | 126.34   |
| 1   | A2    | 823  | PSU  | C4-N3-C2   | -3.91 | 120.70      | 126.34   |
| 39  | B5    | 2351 | PSU  | C4-N3-C2   | -3.91 | 120.70      | 126.34   |
| 11  | AT    | 64   | 5MU  | O4-C4-C5   | -3.91 | 120.37      | 124.90   |
| 1   | A2    | 407  | PSU  | C4-N3-C2   | -3.91 | 120.71      | 126.34   |
| 1   | A2    | 573  | PSU  | C4-N3-C2   | -3.91 | 120.71      | 126.34   |
| 39  | B5    | 3554 | PSU  | C4-N3-C2   | -3.91 | 120.71      | 126.34   |
| 39  | B5    | 4107 | PSU  | C4-N3-C2   | -3.90 | 120.71      | 126.34   |
| 11  | AT    | 65   | PSU  | C4-N3-C2   | -3.90 | 120.71      | 126.34   |
| 39  | B5    | 4193 | 5MC  | C5-C6-N1   | -3.90 | 119.32      | 123.34   |
| 1   | A2    | 109  | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 1   | A2    | 218  | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 1   | A2    | 1693 | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 1   | A2    | 802  | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 1   | A2    | 1348 | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 1   | A2    | 34   | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 39  | B5    | 3492 | A2M  | C2-N3-C4   | 3.90  | 120.96      | 111.75   |
| 39  | B5    | 3427 | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 39  | B5    | 4203 | PSU  | C4-N3-C2   | -3.90 | 120.72      | 126.34   |
| 39  | B5    | 3599 | A2M  | C2-N3-C4   | 3.90  | 120.95      | 111.75   |
| 1   | A2    | 1047 | PSU  | C4-N3-C2   | -3.90 | 120.73      | 126.34   |
| 39  | B5    | 3371 | PSU  | C4-N3-C2   | -3.89 | 120.73      | 126.34   |
| 1   | A2    | 682  | PSU  | C4-N3-C2   | -3.89 | 120.73      | 126.34   |
| 39  | B5    | 3557 | A2M  | C2-N3-C4   | 3.89  | 120.94      | 111.75   |
| 1   | A2    | 815  | PSU  | C4-N3-C2   | -3.89 | 120.74      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A2    | 1626 | PSU  | C4-N3-C2 | -3.89 | 120.74      | 126.34   |
| 39  | B5    | 4278 | PSU  | C4-N3-C2 | -3.88 | 120.75      | 126.34   |
| 1   | A2    | 1005 | PSU  | C4-N3-C2 | -3.88 | 120.75      | 126.34   |
| 39  | B5    | 1718 | PSU  | C4-N3-C2 | -3.88 | 120.75      | 126.34   |
| 39  | B5    | 3576 | PSU  | C4-N3-C2 | -3.88 | 120.75      | 126.34   |
| 39  | B5    | 2206 | A2M  | C2-N3-C4 | 3.88  | 120.91      | 111.75   |
| 39  | B5    | 1720 | PSU  | C4-N3-C2 | -3.88 | 120.75      | 126.34   |
| 39  | B5    | 3517 | A2M  | C2-N3-C4 | 3.88  | 120.91      | 111.75   |
| 39  | B5    | 2258 | OMU  | N3-C2-N1 | 3.87  | 120.03      | 114.89   |
| 39  | B5    | 4322 | PSU  | C4-N3-C2 | -3.87 | 120.76      | 126.34   |
| 1   | A2    | 1032 | A2M  | C2-N3-C4 | 3.87  | 120.89      | 111.75   |
| 39  | B5    | 2475 | PSU  | C4-N3-C2 | -3.87 | 120.76      | 126.34   |
| 1   | A2    | 967  | PSU  | C4-N3-C2 | -3.87 | 120.77      | 126.34   |
| 1   | A2    | 27   | A2M  | C2-N3-C4 | 3.87  | 120.88      | 111.75   |
| 39  | B5    | 4325 | PSU  | C4-N3-C2 | -3.86 | 120.77      | 126.34   |
| 39  | B5    | 1270 | A2M  | C2-N3-C4 | 3.86  | 120.88      | 111.75   |
| 39  | B5    | 4269 | A2M  | C2-N3-C4 | 3.86  | 120.87      | 111.75   |
| 39  | B5    | 398  | A2M  | C2-N3-C4 | 3.86  | 120.87      | 111.75   |
| 39  | B5    | 4336 | A2M  | C2-N3-C4 | 3.86  | 120.87      | 111.75   |
| 39  | B5    | 1489 | A2M  | C2-N3-C4 | 3.86  | 120.87      | 111.75   |
| 39  | B5    | 1537 | PSU  | C4-N3-C2 | -3.86 | 120.78      | 126.34   |
| 1   | A2    | 105  | PSU  | C4-N3-C2 | -3.85 | 120.78      | 126.34   |
| 39  | B5    | 3456 | A2M  | C2-N3-C4 | 3.85  | 120.85      | 111.75   |
| 39  | B5    | 4317 | A2M  | C2-N3-C4 | 3.85  | 120.85      | 111.75   |
| 1   | A2    | 485  | A2M  | C2-N3-C4 | 3.85  | 120.84      | 111.75   |
| 1   | A2    | 469  | A2M  | C2-N3-C4 | 3.85  | 120.84      | 111.75   |
| 39  | B5    | 1479 | A2M  | C2-N3-C4 | 3.85  | 120.84      | 111.75   |
| 39  | B5    | 4169 | PSU  | C4-N3-C2 | -3.85 | 120.80      | 126.34   |
| 39  | B5    | 3490 | PSU  | C4-N3-C2 | -3.85 | 120.80      | 126.34   |
| 1   | A2    | 1679 | A2M  | C2-N3-C4 | 3.85  | 120.83      | 111.75   |
| 1   | A2    | 36   | PSU  | C4-N3-C2 | -3.84 | 120.80      | 126.34   |
| 1   | A2    | 99   | A2M  | C2-N3-C4 | 3.84  | 120.83      | 111.75   |
| 39  | B5    | 3562 | A2M  | C2-N3-C4 | 3.84  | 120.83      | 111.75   |
| 1   | A2    | 513  | A2M  | C2-N3-C4 | 3.84  | 120.83      | 111.75   |
| 1   | A2    | 93   | PSU  | C4-N3-C2 | -3.84 | 120.81      | 126.34   |
| 1   | A2    | 1833 | 6MZ  | C2-N3-C4 | 3.84  | 120.82      | 111.75   |
| 1   | A2    | 119  | PSU  | C4-N3-C2 | -3.84 | 120.81      | 126.34   |
| 39  | B5    | 400  | A2M  | C2-N3-C4 | 3.83  | 120.80      | 111.75   |
| 39  | B5    | 3585 | PSU  | C4-N3-C2 | -3.83 | 120.82      | 126.34   |
| 1   | A2    | 669  | A2M  | C2-N3-C4 | 3.83  | 120.79      | 111.75   |
| 1   | A2    | 1852 | MA6  | C2-N3-C4 | 3.83  | 120.79      | 111.75   |
| 1   | A2    | 1082 | PSU  | C4-N3-C2 | -3.83 | 120.83      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 2244 | A2M  | C2-N3-C4   | 3.82  | 120.78      | 111.75   |
| 1   | A2    | 159  | A2M  | C2-N3-C4   | 3.82  | 120.78      | 111.75   |
| 1   | A2    | 864  | PSU  | C4-N3-C2   | -3.82 | 120.83      | 126.34   |
| 1   | A2    | 1384 | A2M  | C2-N3-C4   | 3.82  | 120.78      | 111.75   |
| 1   | A2    | 210  | PSU  | C4-N3-C2   | -3.81 | 120.84      | 126.34   |
| 1   | A2    | 610  | PSU  | C4-N3-C2   | -3.81 | 120.84      | 126.34   |
| 39  | B5    | 4382 | PSU  | C4-N3-C2   | -3.81 | 120.85      | 126.34   |
| 39  | B5    | 3450 | A2M  | C2-N3-C4   | 3.81  | 120.75      | 111.75   |
| 39  | B5    | 4217 | PSU  | C4-N3-C2   | -3.81 | 120.85      | 126.34   |
| 39  | B5    | 3500 | PSU  | C4-N3-C2   | -3.80 | 120.86      | 126.34   |
| 1   | A2    | 1644 | PSU  | C4-N3-C2   | -3.80 | 120.86      | 126.34   |
| 1   | A2    | 1851 | MA6  | C2-N3-C4   | 3.80  | 120.73      | 111.75   |
| 1   | A2    | 577  | A2M  | C2-N3-C4   | 3.79  | 120.71      | 111.75   |
| 39  | B5    | 1810 | A2M  | C2-N3-C4   | 3.79  | 120.71      | 111.75   |
| 1   | A2    | 1640 | G7M  | CN7-N7-C5  | 3.79  | 131.48      | 126.77   |
| 39  | B5    | 3494 | PSU  | C4-N3-C2   | -3.78 | 120.90      | 126.34   |
| 39  | B5    | 2630 | A2M  | C2-N3-C4   | 3.77  | 120.65      | 111.75   |
| 1   | A2    | 1443 | OMU  | C5-C4-N3   | 3.76  | 120.46      | 114.84   |
| 39  | B5    | 4435 | PSU  | O2-C2-N1   | -3.71 | 118.70      | 122.79   |
| 39  | B5    | 3657 | OMU  | C5-C4-N3   | 3.69  | 120.35      | 114.84   |
| 39  | B5    | 2258 | OMU  | C5-C4-N3   | 3.67  | 120.33      | 114.84   |
| 39  | B5    | 3966 | 6MZ  | C6-C5-N7   | 3.67  | 136.36      | 132.39   |
| 1   | A2    | 1175 | PSU  | O2-C2-N1   | -3.66 | 118.76      | 122.79   |
| 39  | B5    | 2680 | OMU  | C5-C4-N3   | 3.65  | 120.30      | 114.84   |
| 1   | A2    | 1851 | MA6  | C4-C5-N7   | -3.65 | 106.18      | 110.62   |
| 1   | A2    | 121  | OMU  | C5-C4-N3   | 3.63  | 120.28      | 114.84   |
| 39  | B5    | 3494 | PSU  | O2-C2-N1   | -3.63 | 118.79      | 122.79   |
| 39  | B5    | 1799 | PSU  | O2-C2-N1   | -3.62 | 118.81      | 122.79   |
| 1   | A2    | 1679 | A2M  | C2'-C1'-N9 | -3.61 | 107.45      | 113.53   |
| 1   | A2    | 1327 | OMU  | C5-C4-N3   | 3.61  | 120.24      | 114.84   |
| 1   | A2    | 429  | OMU  | C5-C4-N3   | 3.61  | 120.23      | 114.84   |
| 1   | A2    | 628  | OMU  | C5-C4-N3   | 3.60  | 120.23      | 114.84   |
| 39  | B5    | 3973 | OMU  | C5-C4-N3   | 3.59  | 120.22      | 114.84   |
| 1   | A2    | 1852 | MA6  | N1-C6-N6   | 3.59  | 121.01      | 117.08   |
| 1   | A2    | 1805 | OMU  | C5-C4-N3   | 3.59  | 120.20      | 114.84   |
| 39  | B5    | 4366 | OMU  | C5-C4-N3   | 3.58  | 120.19      | 114.84   |
| 1   | A2    | 355  | OMU  | C5-C4-N3   | 3.57  | 120.19      | 114.84   |
| 39  | B5    | 3517 | A2M  | O4'-C1'-N9 | 3.57  | 115.10      | 108.06   |
| 1   | A2    | 116  | OMU  | C5-C4-N3   | 3.57  | 120.18      | 114.84   |
| 39  | B5    | 4244 | OMU  | C5-C4-N3   | 3.57  | 120.18      | 114.84   |
| 39  | B5    | 1638 | PSU  | O2-C2-N1   | -3.57 | 118.86      | 122.79   |
| 39  | B5    | 4325 | PSU  | O2-C2-N1   | -3.56 | 118.87      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 4166 | PSU  | C4-N3-C2   | -3.56 | 121.22      | 126.34   |
| 1   | A2    | 1289 | OMU  | C5-C4-N3   | 3.55  | 120.15      | 114.84   |
| 39  | B5    | 3462 | PSU  | O2-C2-N1   | -3.54 | 118.89      | 122.79   |
| 1   | A2    | 513  | A2M  | C2'-C1'-N9 | -3.54 | 107.57      | 113.53   |
| 39  | B5    | 4149 | PSU  | O2-C2-N1   | -3.54 | 118.90      | 122.79   |
| 39  | B5    | 1537 | PSU  | O2-C2-N1   | -3.53 | 118.90      | 122.79   |
| 39  | B5    | 3616 | PSU  | O2-C2-N1   | -3.53 | 118.91      | 122.79   |
| 39  | B5    | 3447 | PSU  | O2-C2-N1   | -3.53 | 118.91      | 122.79   |
| 39  | B5    | 4298 | PSU  | O2-C2-N1   | -3.52 | 118.92      | 122.79   |
| 39  | B5    | 3490 | PSU  | O2-C2-N1   | -3.52 | 118.92      | 122.79   |
| 39  | B5    | 4374 | PSU  | O2-C2-N1   | -3.51 | 118.92      | 122.79   |
| 1   | A2    | 1852 | MA6  | C4-C5-N7   | -3.51 | 106.35      | 110.62   |
| 39  | B5    | 4052 | OMU  | C5-C4-N3   | 3.50  | 120.08      | 114.84   |
| 1   | A2    | 1368 | PSU  | O2-C2-N1   | -3.49 | 118.94      | 122.79   |
| 39  | B5    | 4058 | PSU  | O2-C2-N1   | -3.49 | 118.95      | 122.79   |
| 1   | A2    | 172  | OMU  | C5-C4-N3   | 3.48  | 120.05      | 114.84   |
| 1   | A2    | 577  | A2M  | C2'-C1'-N9 | -3.47 | 107.68      | 113.53   |
| 39  | B5    | 1683 | PSU  | O2-C2-N1   | -3.47 | 118.97      | 122.79   |
| 1   | A2    | 823  | PSU  | O2-C2-N1   | -3.47 | 118.97      | 122.79   |
| 39  | B5    | 3514 | 5MC  | C5-C6-N1   | -3.47 | 119.77      | 123.34   |
| 39  | B5    | 3562 | A2M  | C2'-C1'-N9 | -3.47 | 107.70      | 113.53   |
| 1   | A2    | 1046 | PSU  | O2-C2-N1   | -3.46 | 118.98      | 122.79   |
| 39  | B5    | 3554 | PSU  | O2-C2-N1   | -3.46 | 118.99      | 122.79   |
| 41  | B8    | 69   | PSU  | O2-C2-N1   | -3.46 | 118.99      | 122.79   |
| 1   | A2    | 1047 | PSU  | O2-C2-N1   | -3.45 | 118.99      | 122.79   |
| 39  | B5    | 4382 | PSU  | O2-C2-N1   | -3.45 | 118.99      | 122.79   |
| 39  | B5    | 1718 | PSU  | O2-C2-N1   | -3.45 | 118.99      | 122.79   |
| 1   | A2    | 802  | PSU  | O2-C2-N1   | -3.45 | 119.00      | 122.79   |
| 39  | B5    | 4322 | PSU  | O2-C2-N1   | -3.45 | 119.00      | 122.79   |
| 39  | B5    | 4246 | PSU  | O2-C2-N1   | -3.44 | 119.00      | 122.79   |
| 42  | BA    | 216  | V5N  | CD2-CG-ND1 | 3.44  | 110.23      | 105.71   |
| 1   | A2    | 109  | PSU  | O2-C2-N1   | -3.44 | 119.00      | 122.79   |
| 39  | B5    | 1632 | PSU  | O2-C2-N1   | -3.44 | 119.01      | 122.79   |
| 1   | A2    | 652  | PSU  | O2-C2-N1   | -3.43 | 119.01      | 122.79   |
| 39  | B5    | 3371 | PSU  | O2-C2-N1   | -3.43 | 119.01      | 122.79   |
| 39  | B5    | 3502 | PSU  | O2-C2-N1   | -3.43 | 119.02      | 122.79   |
| 39  | B5    | 4278 | PSU  | O2-C2-N1   | -3.43 | 119.02      | 122.79   |
| 1   | A2    | 1245 | PSU  | O2-C2-N1   | -3.42 | 119.02      | 122.79   |
| 41  | B8    | 55   | PSU  | O2-C2-N1   | -3.42 | 119.02      | 122.79   |
| 1   | A2    | 36   | PSU  | O2-C2-N1   | -3.42 | 119.03      | 122.79   |
| 39  | B5    | 4419 | PSU  | O2-C2-N1   | -3.42 | 119.03      | 122.79   |
| 1   | A2    | 650  | PSU  | O2-C2-N1   | -3.42 | 119.03      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 1491 | PSU  | O2-C2-N1   | -3.42 | 119.03      | 122.79   |
| 1   | A2    | 573  | PSU  | O2-C2-N1   | -3.41 | 119.03      | 122.79   |
| 1   | A2    | 166  | A2M  | C4-C5-N7   | -3.41 | 106.46      | 110.62   |
| 1   | A2    | 1005 | PSU  | O2-C2-N1   | -3.41 | 119.03      | 122.79   |
| 39  | B5    | 4188 | PSU  | O2-C2-N1   | -3.41 | 119.04      | 122.79   |
| 1   | A2    | 867  | PSU  | O2-C2-N1   | -3.41 | 119.04      | 122.79   |
| 39  | B5    | 1801 | PSU  | O2-C2-N1   | -3.41 | 119.04      | 122.79   |
| 39  | B5    | 4749 | PSU  | O2-C2-N1   | -3.41 | 119.04      | 122.79   |
| 1   | A2    | 1348 | PSU  | O2-C2-N1   | -3.41 | 119.04      | 122.79   |
| 1   | A2    | 93   | PSU  | O2-C2-N1   | -3.40 | 119.04      | 122.79   |
| 1   | A2    | 682  | PSU  | O2-C2-N1   | -3.40 | 119.04      | 122.79   |
| 39  | B5    | 4711 | PSU  | O2-C2-N1   | -3.40 | 119.04      | 122.79   |
| 39  | B5    | 1720 | PSU  | O2-C2-N1   | -3.40 | 119.05      | 122.79   |
| 39  | B5    | 3466 | PSU  | O2-C2-N1   | -3.40 | 119.05      | 122.79   |
| 1   | A2    | 1057 | PSU  | O2-C2-N1   | -3.40 | 119.05      | 122.79   |
| 39  | B5    | 4099 | PSU  | O2-C2-N1   | -3.40 | 119.05      | 122.79   |
| 39  | B5    | 3427 | PSU  | O2-C2-N1   | -3.40 | 119.05      | 122.79   |
| 39  | B5    | 4267 | PSU  | O2-C2-N1   | -3.39 | 119.05      | 122.79   |
| 39  | B5    | 4740 | PSU  | O2-C2-N1   | -3.39 | 119.05      | 122.79   |
| 39  | B5    | 398  | A2M  | C2'-C1'-N9 | -3.39 | 107.82      | 113.53   |
| 1   | A2    | 684  | OMG  | C6-C5-N7   | 3.39  | 136.55      | 130.25   |
| 1   | A2    | 610  | PSU  | O2-C2-N1   | -3.39 | 119.06      | 122.79   |
| 1   | A2    | 816  | PSU  | O2-C2-N1   | -3.39 | 119.06      | 122.79   |
| 11  | AT    | 64   | 5MU  | C5-C6-N1   | -3.39 | 119.86      | 123.34   |
| 1   | A2    | 967  | PSU  | O2-C2-N1   | -3.39 | 119.06      | 122.79   |
| 39  | B5    | 1489 | A2M  | C4-C5-N7   | -3.39 | 106.50      | 110.62   |
| 39  | B5    | 3500 | PSU  | O2-C2-N1   | -3.38 | 119.06      | 122.79   |
| 39  | B5    | 3576 | PSU  | O2-C2-N1   | -3.38 | 119.06      | 122.79   |
| 1   | A2    | 1032 | A2M  | C4-C5-N7   | -3.38 | 106.50      | 110.62   |
| 39  | B5    | 3583 | PSU  | O2-C2-N1   | -3.38 | 119.07      | 122.79   |
| 39  | B5    | 4177 | PSU  | O2-C2-N1   | -3.38 | 119.07      | 122.79   |
| 1   | A2    | 687  | PSU  | O2-C2-N1   | -3.37 | 119.08      | 122.79   |
| 1   | A2    | 1178 | PSU  | O2-C2-N1   | -3.37 | 119.08      | 122.79   |
| 1   | A2    | 1249 | B8N  | C4-N3-C2   | -3.37 | 121.20      | 125.46   |
| 1   | A2    | 1626 | PSU  | O2-C2-N1   | -3.37 | 119.08      | 122.79   |
| 39  | B5    | 3585 | PSU  | O2-C2-N1   | -3.37 | 119.08      | 122.79   |
| 39  | B5    | 2244 | A2M  | C4-C5-N7   | -3.37 | 106.52      | 110.62   |
| 39  | B5    | 3496 | PSU  | O2-C2-N1   | -3.36 | 119.09      | 122.79   |
| 1   | A2    | 407  | PSU  | O2-C2-N1   | -3.36 | 119.09      | 122.79   |
| 68  | Ba    | 39   | V5N  | CD2-CG-ND1 | 3.36  | 110.12      | 105.71   |
| 39  | B5    | 4166 | PSU  | O2-C2-N1   | -3.36 | 119.09      | 122.79   |
| 39  | B5    | 1477 | OMG  | C6-C5-N7   | 3.36  | 136.49      | 130.25   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A2    | 513  | A2M  | C4-C5-N7   | -3.36 | 106.53      | 110.62   |
| 1   | A2    | 1644 | PSU  | O2-C2-N1   | -3.35 | 119.10      | 122.79   |
| 39  | B5    | 2475 | PSU  | O2-C2-N1   | -3.35 | 119.10      | 122.79   |
| 39  | B5    | 1731 | PSU  | O2-C2-N1   | -3.35 | 119.10      | 122.79   |
| 1   | A2    | 469  | A2M  | C4-C5-N7   | -3.34 | 106.55      | 110.62   |
| 39  | B5    | 3492 | A2M  | C4-C5-N7   | -3.34 | 106.55      | 110.62   |
| 39  | B5    | 4042 | PSU  | O2-C2-N1   | -3.34 | 119.11      | 122.79   |
| 1   | A2    | 159  | A2M  | C4-C5-N7   | -3.34 | 106.55      | 110.62   |
| 1   | A2    | 27   | A2M  | C4-C5-N7   | -3.33 | 106.56      | 110.62   |
| 1   | A2    | 119  | PSU  | O2-C2-N1   | -3.33 | 119.12      | 122.79   |
| 1   | A2    | 210  | PSU  | O2-C2-N1   | -3.33 | 119.12      | 122.79   |
| 1   | A2    | 864  | PSU  | O2-C2-N1   | -3.33 | 119.12      | 122.79   |
| 1   | A2    | 218  | PSU  | O2-C2-N1   | -3.33 | 119.12      | 122.79   |
| 39  | B5    | 3456 | A2M  | C4-C5-N7   | -3.33 | 106.56      | 110.62   |
| 39  | B5    | 4039 | PSU  | O2-C2-N1   | -3.33 | 119.13      | 122.79   |
| 39  | B5    | 4116 | OMG  | C6-C5-N7   | 3.33  | 136.44      | 130.25   |
| 1   | A2    | 1446 | PSU  | O2-C2-N1   | -3.33 | 119.13      | 122.79   |
| 39  | B5    | 1721 | PSU  | O2-C2-N1   | -3.32 | 119.13      | 122.79   |
| 39  | B5    | 4169 | PSU  | O2-C2-N1   | -3.32 | 119.14      | 122.79   |
| 1   | A2    | 1233 | PSU  | O2-C2-N1   | -3.32 | 119.14      | 122.79   |
| 1   | A2    | 1239 | PSU  | O2-C2-N1   | -3.31 | 119.14      | 122.79   |
| 1   | A2    | 34   | PSU  | O2-C2-N1   | -3.31 | 119.14      | 122.79   |
| 1   | A2    | 1693 | PSU  | O2-C2-N1   | -3.31 | 119.14      | 122.79   |
| 39  | B5    | 3974 | OMG  | C6-C5-N7   | 3.31  | 136.41      | 130.25   |
| 1   | A2    | 105  | PSU  | O2-C2-N1   | -3.30 | 119.15      | 122.79   |
| 39  | B5    | 4317 | A2M  | C4-C5-N7   | -3.30 | 106.59      | 110.62   |
| 39  | B5    | 3517 | A2M  | N3-C2-N1   | -3.30 | 123.44      | 128.60   |
| 39  | B5    | 4217 | PSU  | O2-C2-N1   | -3.30 | 119.16      | 122.79   |
| 39  | B5    | 3966 | 6MZ  | C4-C5-N7   | -3.30 | 106.60      | 110.62   |
| 39  | B5    | 4045 | PSU  | O2-C2-N1   | -3.30 | 119.16      | 122.79   |
| 39  | B5    | 1266 | 1MA  | N9-C4-N3   | 3.30  | 134.63      | 126.94   |
| 39  | B5    | 2206 | A2M  | C4-C5-N7   | -3.30 | 106.60      | 110.62   |
| 1   | A2    | 27   | A2M  | C2'-C1'-N9 | -3.30 | 107.98      | 113.53   |
| 1   | A2    | 577  | A2M  | C4-C5-N7   | -3.29 | 106.61      | 110.62   |
| 39  | B5    | 3631 | OMG  | C6-C5-N7   | 3.29  | 136.37      | 130.25   |
| 39  | B5    | 3562 | A2M  | C4-C5-N7   | -3.29 | 106.62      | 110.62   |
| 1   | A2    | 485  | A2M  | C4-C5-N7   | -3.28 | 106.62      | 110.62   |
| 39  | B5    | 3599 | A2M  | C4-C5-N7   | -3.28 | 106.62      | 110.62   |
| 39  | B5    | 3450 | A2M  | C4-C5-N7   | -3.28 | 106.63      | 110.62   |
| 39  | B5    | 398  | A2M  | C4-C5-N7   | -3.27 | 106.63      | 110.62   |
| 1   | A2    | 669  | A2M  | C4-C5-N7   | -3.27 | 106.64      | 110.62   |
| 39  | B5    | 2658 | A2M  | C4-C5-N7   | -3.26 | 106.64      | 110.62   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 4269 | A2M  | C4-C5-N7   | -3.26 | 106.65      | 110.62   |
| 39  | B5    | 2351 | PSU  | O2-C2-N1   | -3.26 | 119.20      | 122.79   |
| 1   | A2    | 1679 | A2M  | C4-C5-N7   | -3.26 | 106.65      | 110.62   |
| 39  | B5    | 3652 | PSU  | O2-C2-N1   | -3.26 | 119.20      | 122.79   |
| 39  | B5    | 2207 | OMG  | C6-C5-N7   | 3.26  | 136.30      | 130.25   |
| 1   | A2    | 1384 | A2M  | C4-C5-N7   | -3.25 | 106.66      | 110.62   |
| 1   | A2    | 815  | PSU  | O2-C2-N1   | -3.25 | 119.22      | 122.79   |
| 39  | B5    | 400  | A2M  | C4-C5-N7   | -3.24 | 106.67      | 110.62   |
| 39  | B5    | 2630 | A2M  | C2'-C1'-N9 | -3.24 | 108.07      | 113.53   |
| 39  | B5    | 4369 | OMG  | C6-C5-N7   | 3.24  | 136.27      | 130.25   |
| 39  | B5    | 4203 | PSU  | O2-C2-N1   | -3.24 | 119.23      | 122.79   |
| 39  | B5    | 1479 | A2M  | C4-C5-N7   | -3.24 | 106.68      | 110.62   |
| 39  | B5    | 1270 | A2M  | C4-C5-N7   | -3.23 | 106.68      | 110.62   |
| 39  | B5    | 3557 | A2M  | C4-C5-N7   | -3.23 | 106.68      | 110.62   |
| 39  | B5    | 1270 | A2M  | N3-C2-N1   | -3.23 | 123.55      | 128.60   |
| 1   | A2    | 1032 | A2M  | N3-C2-N1   | -3.23 | 123.56      | 128.60   |
| 11  | AT    | 65   | PSU  | O2-C2-N1   | -3.22 | 119.24      | 122.79   |
| 39  | B5    | 3359 | OMG  | C6-C5-N7   | 3.22  | 136.23      | 130.25   |
| 39  | B5    | 3966 | 6MZ  | N1-C2-N3   | -3.22 | 123.57      | 128.60   |
| 39  | B5    | 3476 | OMG  | C6-C5-N7   | 3.22  | 136.23      | 130.25   |
| 39  | B5    | 3676 | OMG  | C6-C5-N7   | 3.22  | 136.23      | 130.25   |
| 39  | B5    | 4107 | PSU  | O2-C2-N1   | -3.21 | 119.26      | 122.79   |
| 39  | B5    | 4245 | OMG  | C6-C5-N7   | 3.21  | 136.22      | 130.25   |
| 39  | B5    | 1810 | A2M  | C4-C5-N7   | -3.20 | 106.72      | 110.62   |
| 39  | B5    | 4336 | A2M  | C4-C5-N7   | -3.20 | 106.72      | 110.62   |
| 39  | B5    | 4269 | A2M  | N3-C2-N1   | -3.19 | 123.61      | 128.60   |
| 39  | B5    | 3557 | A2M  | C2'-C1'-N9 | -3.19 | 108.16      | 113.53   |
| 41  | B8    | 75   | OMG  | C6-C5-N7   | 3.19  | 136.18      | 130.25   |
| 39  | B5    | 1489 | A2M  | N3-C2-N1   | -3.19 | 123.61      | 128.60   |
| 39  | B5    | 2244 | A2M  | C2'-C1'-N9 | -3.19 | 108.16      | 113.53   |
| 1   | A2    | 99   | A2M  | C4-C5-N7   | -3.19 | 106.74      | 110.62   |
| 39  | B5    | 4317 | A2M  | N3-C2-N1   | -3.19 | 123.62      | 128.60   |
| 1   | A2    | 27   | A2M  | N3-C2-N1   | -3.18 | 123.62      | 128.60   |
| 1   | A2    | 437  | OMG  | C6-C5-N7   | 3.18  | 136.16      | 130.25   |
| 1   | A2    | 591  | A2M  | N3-C2-N1   | -3.18 | 123.63      | 128.60   |
| 39  | B5    | 2658 | A2M  | N3-C2-N1   | -3.18 | 123.63      | 128.60   |
| 1   | A2    | 99   | A2M  | N3-C2-N1   | -3.18 | 123.64      | 128.60   |
| 39  | B5    | 3369 | PSU  | O2-C2-N1   | -3.17 | 119.30      | 122.79   |
| 39  | B5    | 2630 | A2M  | C4-C5-N7   | -3.17 | 106.76      | 110.62   |
| 39  | B5    | 4364 | OMG  | C6-C5-N7   | 3.17  | 136.14      | 130.25   |
| 1   | A2    | 1329 | OMG  | C6-C5-N7   | 3.17  | 136.14      | 130.25   |
| 39  | B5    | 3557 | A2M  | N3-C2-N1   | -3.16 | 123.66      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 4383 | OMG  | C6-C5-N7   | 3.16  | 136.13      | 130.25   |
| 1   | A2    | 591  | A2M  | C4-C5-N7   | -3.16 | 106.77      | 110.62   |
| 39  | B5    | 3456 | A2M  | N3-C2-N1   | -3.16 | 123.66      | 128.60   |
| 39  | B5    | 3492 | A2M  | N3-C2-N1   | -3.15 | 123.67      | 128.60   |
| 1   | A2    | 1679 | A2M  | N3-C2-N1   | -3.15 | 123.67      | 128.60   |
| 39  | B5    | 4138 | OMG  | C6-C5-N7   | 3.15  | 136.11      | 130.25   |
| 1   | A2    | 645  | OMG  | C6-C5-N7   | 3.15  | 136.10      | 130.25   |
| 39  | B5    | 398  | A2M  | N3-C2-N1   | -3.15 | 123.68      | 128.60   |
| 39  | B5    | 3517 | A2M  | C4-C5-N7   | -3.14 | 106.79      | 110.62   |
| 39  | B5    | 1260 | OMG  | C6-C5-N7   | 3.14  | 136.09      | 130.25   |
| 1   | A2    | 166  | A2M  | N3-C2-N1   | -3.14 | 123.69      | 128.60   |
| 1   | A2    | 1448 | OMG  | C6-C5-N7   | 3.14  | 136.09      | 130.25   |
| 39  | B5    | 4336 | A2M  | N3-C2-N1   | -3.14 | 123.69      | 128.60   |
| 39  | B5    | 2244 | A2M  | N3-C2-N1   | -3.14 | 123.70      | 128.60   |
| 39  | B5    | 2630 | A2M  | N3-C2-N1   | -3.13 | 123.70      | 128.60   |
| 39  | B5    | 3562 | A2M  | N3-C2-N1   | -3.13 | 123.70      | 128.60   |
| 39  | B5    | 1810 | A2M  | N3-C2-N1   | -3.13 | 123.71      | 128.60   |
| 39  | B5    | 3450 | A2M  | N3-C2-N1   | -3.13 | 123.71      | 128.60   |
| 39  | B5    | 1479 | A2M  | N3-C2-N1   | -3.13 | 123.71      | 128.60   |
| 1   | A2    | 669  | A2M  | N3-C2-N1   | -3.12 | 123.72      | 128.60   |
| 1   | A2    | 577  | A2M  | N3-C2-N1   | -3.12 | 123.72      | 128.60   |
| 39  | B5    | 3942 | OMG  | C6-C5-N7   | 3.12  | 136.05      | 130.25   |
| 1   | A2    | 1082 | PSU  | O2-C2-N1   | -3.12 | 119.36      | 122.79   |
| 39  | B5    | 2206 | A2M  | N3-C2-N1   | -3.12 | 123.72      | 128.60   |
| 1   | A2    | 1491 | OMG  | C6-C5-N7   | 3.12  | 136.04      | 130.25   |
| 1   | A2    | 1852 | MA6  | N1-C2-N3   | -3.11 | 123.73      | 128.60   |
| 39  | B5    | 1580 | OMG  | C6-C5-N7   | 3.11  | 136.03      | 130.25   |
| 39  | B5    | 3599 | A2M  | N3-C2-N1   | -3.11 | 123.74      | 128.60   |
| 1   | A2    | 510  | OMG  | C6-C5-N7   | 3.11  | 136.03      | 130.25   |
| 1   | A2    | 159  | A2M  | N3-C2-N1   | -3.11 | 123.74      | 128.60   |
| 1   | A2    | 469  | A2M  | N3-C2-N1   | -3.11 | 123.74      | 128.60   |
| 39  | B5    | 400  | A2M  | N3-C2-N1   | -3.11 | 123.74      | 128.60   |
| 1   | A2    | 1249 | B8N  | N3-C2-N1   | 3.11  | 121.14      | 116.76   |
| 1   | A2    | 602  | OMG  | C6-C5-N7   | 3.10  | 136.02      | 130.25   |
| 1   | A2    | 99   | A2M  | C2'-C1'-N9 | -3.10 | 108.31      | 113.53   |
| 1   | A2    | 485  | A2M  | N3-C2-N1   | -3.09 | 123.76      | 128.60   |
| 1   | A2    | 1384 | A2M  | N3-C2-N1   | -3.09 | 123.76      | 128.60   |
| 1   | A2    | 868  | OMG  | C6-C5-N7   | 3.09  | 136.00      | 130.25   |
| 1   | A2    | 1851 | MA6  | N1-C2-N3   | -3.09 | 123.77      | 128.60   |
| 39  | B5    | 4269 | A2M  | C2'-C1'-N9 | -3.09 | 108.33      | 113.53   |
| 39  | B5    | 3524 | OMG  | C6-C5-N7   | 3.09  | 135.99      | 130.25   |
| 39  | B5    | 2719 | OMG  | C6-C5-N7   | 3.08  | 135.98      | 130.25   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 2258 | OMU  | O4-C4-C5   | -3.08 | 119.75      | 125.16   |
| 1   | A2    | 1805 | OMU  | O4-C4-C5   | -3.07 | 119.77      | 125.16   |
| 1   | A2    | 1032 | A2M  | C2'-C1'-N9 | -3.06 | 108.37      | 113.53   |
| 1   | A2    | 1833 | 6MZ  | N1-C2-N3   | -3.06 | 123.81      | 128.60   |
| 1   | A2    | 513  | A2M  | N3-C2-N1   | -3.06 | 123.82      | 128.60   |
| 1   | A2    | 116  | OMU  | O4-C4-C5   | -3.06 | 119.79      | 125.16   |
| 1   | A2    | 429  | OMU  | O4-C4-C5   | -3.05 | 119.79      | 125.16   |
| 39  | B5    | 3517 | A2M  | C2'-C1'-N9 | -3.05 | 108.39      | 113.53   |
| 39  | B5    | 4336 | A2M  | C2'-C1'-N9 | -3.04 | 108.41      | 113.53   |
| 1   | A2    | 121  | OMU  | O4-C4-C5   | -3.04 | 119.81      | 125.16   |
| 39  | B5    | 2267 | OMG  | C6-C5-N7   | 3.03  | 135.89      | 130.25   |
| 39  | B5    | 2680 | OMU  | O4-C4-C5   | -3.03 | 119.83      | 125.16   |
| 1   | A2    | 1443 | OMU  | O4-C4-C5   | -3.03 | 119.84      | 125.16   |
| 39  | B5    | 4317 | A2M  | C2'-C1'-N9 | -3.02 | 108.44      | 113.53   |
| 39  | B5    | 3657 | OMU  | O4-C4-C5   | -3.02 | 119.85      | 125.16   |
| 39  | B5    | 4240 | OMG  | C6-C5-N7   | 3.02  | 135.86      | 130.25   |
| 1   | A2    | 1327 | OMU  | O4-C4-C5   | -3.01 | 119.86      | 125.16   |
| 1   | A2    | 1851 | MA6  | C5-N7-C8   | 3.00  | 107.77      | 103.51   |
| 39  | B5    | 4244 | OMU  | O4-C4-C5   | -3.00 | 119.89      | 125.16   |
| 1   | A2    | 628  | OMU  | O4-C4-C5   | -2.99 | 119.89      | 125.16   |
| 1   | A2    | 355  | OMU  | O4-C4-C5   | -2.99 | 119.90      | 125.16   |
| 1   | A2    | 1851 | MA6  | N9-C8-N7   | -2.98 | 109.84      | 113.91   |
| 39  | B5    | 4052 | OMU  | O4-C4-C5   | -2.98 | 119.92      | 125.16   |
| 1   | A2    | 172  | OMU  | O4-C4-C5   | -2.97 | 119.94      | 125.16   |
| 39  | B5    | 3550 | UY1  | C6-C5-C4   | 2.96  | 120.27      | 118.20   |
| 39  | B5    | 4366 | OMU  | O4-C4-C5   | -2.95 | 119.98      | 125.16   |
| 39  | B5    | 3517 | A2M  | C4-N9-C8   | 2.93  | 108.90      | 105.73   |
| 1   | A2    | 1289 | OMU  | O4-C4-C5   | -2.92 | 120.03      | 125.16   |
| 1   | A2    | 1852 | MA6  | C5-N7-C8   | 2.90  | 107.63      | 103.51   |
| 39  | B5    | 3973 | OMU  | O4-C4-C5   | -2.87 | 120.12      | 125.16   |
| 1   | A2    | 159  | A2M  | C5-N7-C8   | 2.86  | 107.57      | 103.51   |
| 1   | A2    | 1032 | A2M  | C5-N7-C8   | 2.86  | 107.57      | 103.51   |
| 1   | A2    | 159  | A2M  | C2'-C1'-N9 | -2.85 | 108.74      | 113.53   |
| 39  | B5    | 1270 | A2M  | C2'-C1'-N9 | -2.84 | 108.74      | 113.53   |
| 1   | A2    | 1833 | 6MZ  | C4-C5-N7   | -2.84 | 107.16      | 110.62   |
| 1   | A2    | 513  | A2M  | C5-N7-C8   | 2.83  | 107.52      | 103.51   |
| 1   | A2    | 27   | A2M  | C5-N7-C8   | 2.82  | 107.52      | 103.51   |
| 39  | B5    | 1489 | A2M  | C5-N7-C8   | 2.82  | 107.52      | 103.51   |
| 39  | B5    | 2244 | A2M  | C5-N7-C8   | 2.82  | 107.52      | 103.51   |
| 1   | A2    | 166  | A2M  | C5-N7-C8   | 2.81  | 107.50      | 103.51   |
| 1   | A2    | 1833 | 6MZ  | C4-N9-C8   | 2.80  | 108.77      | 105.73   |
| 39  | B5    | 3456 | A2M  | C5-N7-C8   | 2.78  | 107.46      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 39  | B5    | 1477 | OMG  | C4-C5-N7   | -2.78 | 106.32      | 110.72   |
| 39  | B5    | 3492 | A2M  | C5-N7-C8   | 2.78  | 107.46      | 103.51   |
| 39  | B5    | 4336 | A2M  | C5-N7-C8   | 2.77  | 107.44      | 103.51   |
| 39  | B5    | 1270 | A2M  | C5-N7-C8   | 2.76  | 107.44      | 103.51   |
| 39  | B5    | 4317 | A2M  | C5-N7-C8   | 2.76  | 107.44      | 103.51   |
| 1   | A2    | 1679 | A2M  | C5-N7-C8   | 2.76  | 107.43      | 103.51   |
| 39  | B5    | 3599 | A2M  | C5-N7-C8   | 2.76  | 107.42      | 103.51   |
| 39  | B5    | 3562 | A2M  | C5-N7-C8   | 2.75  | 107.42      | 103.51   |
| 1   | A2    | 1384 | A2M  | C2'-C1'-N9 | -2.75 | 108.89      | 113.53   |
| 1   | A2    | 591  | A2M  | C5-N7-C8   | 2.75  | 107.42      | 103.51   |
| 39  | B5    | 4269 | A2M  | C5-N7-C8   | 2.75  | 107.41      | 103.51   |
| 1   | A2    | 469  | A2M  | C5-N7-C8   | 2.75  | 107.41      | 103.51   |
| 39  | B5    | 400  | A2M  | C5-N7-C8   | 2.74  | 107.40      | 103.51   |
| 39  | B5    | 3517 | A2M  | C5-N7-C8   | 2.73  | 107.39      | 103.51   |
| 39  | B5    | 398  | A2M  | C5-N7-C8   | 2.73  | 107.39      | 103.51   |
| 1   | A2    | 1384 | A2M  | C5-N7-C8   | 2.73  | 107.39      | 103.51   |
| 39  | B5    | 3557 | A2M  | C5-N7-C8   | 2.72  | 107.38      | 103.51   |
| 39  | B5    | 3966 | 6MZ  | C5-N7-C8   | 2.72  | 107.37      | 103.51   |
| 39  | B5    | 1810 | A2M  | C5-N7-C8   | 2.72  | 107.37      | 103.51   |
| 1   | A2    | 485  | A2M  | C5-N7-C8   | 2.71  | 107.36      | 103.51   |
| 1   | A2    | 684  | OMG  | C4-C5-N7   | -2.71 | 106.43      | 110.72   |
| 1   | A2    | 669  | A2M  | C5-N7-C8   | 2.71  | 107.36      | 103.51   |
| 39  | B5    | 2658 | A2M  | C5-N7-C8   | 2.71  | 107.36      | 103.51   |
| 1   | A2    | 577  | A2M  | C5-N7-C8   | 2.71  | 107.36      | 103.51   |
| 39  | B5    | 4336 | A2M  | C4-N9-C8   | 2.70  | 108.65      | 105.73   |
| 39  | B5    | 1479 | A2M  | C5-N7-C8   | 2.70  | 107.34      | 103.51   |
| 1   | A2    | 159  | A2M  | C4-N9-C8   | 2.69  | 108.65      | 105.73   |
| 39  | B5    | 2206 | A2M  | C5-N7-C8   | 2.69  | 107.33      | 103.51   |
| 39  | B5    | 3456 | A2M  | C2'-C1'-N9 | -2.69 | 109.00      | 113.53   |
| 1   | A2    | 469  | A2M  | C2'-C1'-N9 | -2.69 | 109.00      | 113.53   |
| 1   | A2    | 99   | A2M  | C5-N7-C8   | 2.68  | 107.32      | 103.51   |
| 1   | A2    | 1833 | 6MZ  | C6-C5-N7   | 2.68  | 135.29      | 132.39   |
| 1   | A2    | 1679 | A2M  | C4-N9-C8   | 2.68  | 108.63      | 105.73   |
| 39  | B5    | 3450 | A2M  | C5-N7-C8   | 2.68  | 107.31      | 103.51   |
| 39  | B5    | 3450 | A2M  | C2'-C1'-N9 | -2.67 | 109.03      | 113.53   |
| 39  | B5    | 4245 | OMG  | C4-C5-N7   | -2.65 | 106.52      | 110.72   |
| 39  | B5    | 2630 | A2M  | C5-N7-C8   | 2.65  | 107.28      | 103.51   |
| 39  | B5    | 3631 | OMG  | C4-C5-N7   | -2.64 | 106.54      | 110.72   |
| 39  | B5    | 2207 | OMG  | C4-C5-N7   | -2.64 | 106.55      | 110.72   |
| 39  | B5    | 2630 | A2M  | C4-N9-C8   | 2.63  | 108.58      | 105.73   |
| 39  | B5    | 4116 | OMG  | C4-C5-N7   | -2.63 | 106.56      | 110.72   |
| 39  | B5    | 4369 | OMG  | C4-C5-N7   | -2.63 | 106.56      | 110.72   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A2    | 669  | A2M  | C4-N9-C8   | 2.62  | 108.57      | 105.73   |
| 39  | B5    | 2244 | A2M  | C4-N9-C8   | 2.62  | 108.56      | 105.73   |
| 39  | B5    | 2658 | A2M  | C2'-C1'-N9 | -2.62 | 109.12      | 113.53   |
| 39  | B5    | 3676 | OMG  | C4-C5-N7   | -2.62 | 106.58      | 110.72   |
| 39  | B5    | 3974 | OMG  | C4-C5-N7   | -2.62 | 106.58      | 110.72   |
| 39  | B5    | 1270 | A2M  | C4-N9-C8   | 2.61  | 108.56      | 105.73   |
| 39  | B5    | 3476 | OMG  | C4-C5-N7   | -2.61 | 106.58      | 110.72   |
| 39  | B5    | 3359 | OMG  | C4-C5-N7   | -2.61 | 106.59      | 110.72   |
| 1   | A2    | 437  | OMG  | C4-C5-N7   | -2.61 | 106.59      | 110.72   |
| 39  | B5    | 4269 | A2M  | C4-N9-C8   | 2.60  | 108.55      | 105.73   |
| 1   | A2    | 1032 | A2M  | C4-N9-C8   | 2.60  | 108.55      | 105.73   |
| 1   | A2    | 1329 | OMG  | C4-C5-N7   | -2.60 | 106.60      | 110.72   |
| 41  | B8    | 75   | OMG  | C4-C5-N7   | -2.60 | 106.61      | 110.72   |
| 39  | B5    | 4317 | A2M  | C4-N9-C8   | 2.60  | 108.55      | 105.73   |
| 39  | B5    | 4383 | OMG  | C4-C5-N7   | -2.60 | 106.61      | 110.72   |
| 1   | A2    | 645  | OMG  | C4-C5-N7   | -2.60 | 106.61      | 110.72   |
| 39  | B5    | 3514 | 5MC  | C5-C4-N3   | -2.60 | 118.87      | 121.67   |
| 1   | A2    | 1448 | OMG  | C4-C5-N7   | -2.59 | 106.61      | 110.72   |
| 39  | B5    | 4138 | OMG  | C4-C5-N7   | -2.59 | 106.63      | 110.72   |
| 1   | A2    | 513  | A2M  | C4-N9-C8   | 2.59  | 108.53      | 105.73   |
| 39  | B5    | 2719 | OMG  | C4-C5-N7   | -2.58 | 106.64      | 110.72   |
| 1   | A2    | 510  | OMG  | C4-C5-N7   | -2.57 | 106.65      | 110.72   |
| 39  | B5    | 400  | A2M  | C4-N9-C8   | 2.57  | 108.52      | 105.73   |
| 39  | B5    | 1810 | A2M  | C4-N9-C8   | 2.57  | 108.51      | 105.73   |
| 39  | B5    | 3557 | A2M  | C4-N9-C8   | 2.56  | 108.51      | 105.73   |
| 1   | A2    | 577  | A2M  | C4-N9-C8   | 2.56  | 108.50      | 105.73   |
| 39  | B5    | 4240 | OMG  | C4-C5-N7   | -2.56 | 106.67      | 110.72   |
| 1   | A2    | 868  | OMG  | C4-C5-N7   | -2.56 | 106.68      | 110.72   |
| 39  | B5    | 4364 | OMG  | C4-C5-N7   | -2.55 | 106.68      | 110.72   |
| 39  | B5    | 1489 | A2M  | C4-N9-C8   | 2.54  | 108.49      | 105.73   |
| 1   | A2    | 602  | OMG  | C4-C5-N7   | -2.54 | 106.69      | 110.72   |
| 39  | B5    | 1580 | OMG  | C4-C5-N7   | -2.54 | 106.69      | 110.72   |
| 39  | B5    | 4193 | 5MC  | C5-C4-N3   | -2.54 | 118.93      | 121.67   |
| 1   | A2    | 1640 | G7M  | O6-C6-C5   | -2.54 | 122.33      | 128.06   |
| 39  | B5    | 1260 | OMG  | C4-C5-N7   | -2.53 | 106.71      | 110.72   |
| 39  | B5    | 2206 | A2M  | C2'-C1'-N9 | -2.53 | 109.27      | 113.53   |
| 1   | A2    | 1384 | A2M  | C4-N9-C8   | 2.53  | 108.47      | 105.73   |
| 39  | B5    | 398  | A2M  | C4-N9-C8   | 2.53  | 108.47      | 105.73   |
| 39  | B5    | 3599 | A2M  | C4-N9-C8   | 2.52  | 108.46      | 105.73   |
| 1   | A2    | 99   | A2M  | C4-N9-C8   | 2.52  | 108.46      | 105.73   |
| 1   | A2    | 27   | A2M  | C4-N9-C8   | 2.52  | 108.46      | 105.73   |
| 1   | A2    | 1491 | OMG  | C4-C5-N7   | -2.52 | 106.74      | 110.72   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A2    | 1851 | MA6  | C5-C6-N6   | -2.52 | 120.92      | 125.30   |
| 1   | A2    | 166  | A2M  | C2'-C1'-N9 | -2.51 | 109.30      | 113.53   |
| 39  | B5    | 3524 | OMG  | C4-C5-N7   | -2.50 | 106.76      | 110.72   |
| 39  | B5    | 3492 | A2M  | C4-N9-C8   | 2.50  | 108.44      | 105.73   |
| 39  | B5    | 3562 | A2M  | C4-N9-C8   | 2.50  | 108.44      | 105.73   |
| 39  | B5    | 1479 | A2M  | C4-N9-C8   | 2.49  | 108.43      | 105.73   |
| 39  | B5    | 3456 | A2M  | C4-N9-C8   | 2.49  | 108.43      | 105.73   |
| 39  | B5    | 400  | A2M  | C2'-C1'-N9 | -2.49 | 109.34      | 113.53   |
| 1   | A2    | 1852 | MA6  | C4-N9-C8   | 2.48  | 108.42      | 105.73   |
| 42  | BA    | 216  | V5N  | O-C-CA     | -2.47 | 118.30      | 124.78   |
| 1   | A2    | 1338 | 4AC  | C5-C4-N4   | -2.47 | 118.64      | 122.92   |
| 39  | B5    | 1266 | 1MA  | C4-C5-N7   | -2.46 | 106.83      | 110.72   |
| 30  | Ar    | 2    | SAC  | O-C-CA     | -2.46 | 118.34      | 124.78   |
| 1   | A2    | 1843 | 4AC  | C6-C5-C4   | 2.45  | 119.96      | 116.96   |
| 68  | Ba    | 39   | V5N  | O-C-CA     | -2.45 | 118.36      | 124.78   |
| 39  | B5    | 3450 | A2M  | C4-N9-C8   | 2.45  | 108.38      | 105.73   |
| 33  | Au    | 1    | AME  | O-C-CA     | -2.45 | 118.36      | 124.78   |
| 39  | B5    | 2267 | OMG  | C4-C5-N7   | -2.43 | 106.87      | 110.72   |
| 39  | B5    | 3550 | UY1  | O2-C2-N1   | -2.43 | 120.12      | 122.79   |
| 1   | A2    | 485  | A2M  | C4-N9-C8   | 2.42  | 108.35      | 105.73   |
| 39  | B5    | 2206 | A2M  | C4-N9-C8   | 2.42  | 108.35      | 105.73   |
| 39  | B5    | 3966 | 6MZ  | C4-N9-C8   | 2.41  | 108.34      | 105.73   |
| 39  | B5    | 3942 | OMG  | C4-C5-N7   | -2.40 | 106.93      | 110.72   |
| 1   | A2    | 469  | A2M  | C4-N9-C8   | 2.39  | 108.32      | 105.73   |
| 1   | A2    | 1338 | 4AC  | C6-C5-C4   | 2.38  | 119.88      | 116.96   |
| 39  | B5    | 2658 | A2M  | C4-N9-C8   | 2.38  | 108.30      | 105.73   |
| 1   | A2    | 1833 | 6MZ  | C5-N7-C8   | 2.36  | 106.86      | 103.51   |
| 1   | A2    | 166  | A2M  | C4-N9-C8   | 2.36  | 108.28      | 105.73   |
| 12  | AZ    | 2    | SAC  | O-C-CA     | -2.32 | 118.69      | 124.78   |
| 39  | B5    | 3942 | OMG  | O6-C6-C5   | -2.32 | 120.44      | 126.60   |
| 39  | B5    | 1489 | A2M  | C6-C5-N7   | 2.29  | 136.29      | 132.02   |
| 39  | B5    | 1260 | OMG  | O6-C6-C5   | -2.29 | 120.54      | 126.60   |
| 1   | A2    | 1327 | OMU  | O2-C2-N1   | -2.28 | 119.76      | 122.79   |
| 1   | A2    | 429  | OMU  | O2-C2-N1   | -2.28 | 119.76      | 122.79   |
| 39  | B5    | 3517 | A2M  | N9-C8-N7   | -2.27 | 110.80      | 113.91   |
| 1   | A2    | 1032 | A2M  | C6-C5-N7   | 2.27  | 136.26      | 132.02   |
| 39  | B5    | 2244 | A2M  | C6-C5-N7   | 2.27  | 136.25      | 132.02   |
| 39  | B5    | 3517 | A2M  | C6-C5-N7   | 2.27  | 136.24      | 132.02   |
| 39  | B5    | 2265 | OMC  | O2-C2-N3   | -2.26 | 118.65      | 122.33   |
| 39  | B5    | 3456 | A2M  | C6-C5-N7   | 2.26  | 136.23      | 132.02   |
| 39  | B5    | 2194 | OMC  | O2-C2-N3   | -2.25 | 118.67      | 122.33   |
| 1   | A2    | 1491 | OMG  | O6-C6-C5   | -2.25 | 120.63      | 126.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A2    | 513  | A2M  | C6-C5-N7    | 2.25  | 136.21      | 132.02   |
| 39  | B5    | 3514 | 5MC  | O2-C2-N3    | -2.25 | 118.67      | 122.33   |
| 39  | B5    | 4244 | OMU  | O2-C2-N1    | -2.24 | 119.81      | 122.79   |
| 39  | B5    | 4317 | A2M  | C6-C5-N7    | 2.23  | 136.17      | 132.02   |
| 1   | A2    | 27   | A2M  | C6-C5-N7    | 2.23  | 136.17      | 132.02   |
| 39  | B5    | 3492 | A2M  | C6-C5-N7    | 2.23  | 136.17      | 132.02   |
| 35  | Aw    | 62   | HY3  | O-C-CA      | -2.22 | 118.63      | 124.83   |
| 39  | B5    | 3450 | A2M  | C6-C5-N7    | 2.22  | 136.16      | 132.02   |
| 39  | B5    | 4269 | A2M  | C6-C5-N7    | 2.22  | 136.16      | 132.02   |
| 1   | A2    | 159  | A2M  | C6-C5-N7    | 2.22  | 136.16      | 132.02   |
| 1   | A2    | 469  | A2M  | C6-C5-N7    | 2.21  | 136.15      | 132.02   |
| 39  | B5    | 3562 | A2M  | C6-C5-N7    | 2.21  | 136.13      | 132.02   |
| 1   | A2    | 166  | A2M  | C6-C5-N7    | 2.20  | 136.12      | 132.02   |
| 1   | A2    | 669  | A2M  | C6-C5-N7    | 2.20  | 136.11      | 132.02   |
| 1   | A2    | 1679 | A2M  | C6-C5-N7    | 2.20  | 136.11      | 132.02   |
| 83  | Br    | 2    | SAC  | O-C-CA      | -2.19 | 119.03      | 124.78   |
| 39  | B5    | 3524 | OMG  | O6-C6-C5    | -2.19 | 120.80      | 126.60   |
| 1   | A2    | 591  | A2M  | C4-N9-C8    | 2.19  | 108.10      | 105.73   |
| 39  | B5    | 3359 | OMG  | O6-C6-C5    | -2.18 | 120.81      | 126.60   |
| 39  | B5    | 2267 | OMG  | O6-C6-C5    | -2.18 | 120.81      | 126.60   |
| 39  | B5    | 4138 | OMG  | O6-C6-C5    | -2.18 | 120.82      | 126.60   |
| 1   | A2    | 577  | A2M  | C6-C5-N7    | 2.18  | 136.08      | 132.02   |
| 39  | B5    | 1270 | A2M  | C6-C5-N7    | 2.18  | 136.07      | 132.02   |
| 39  | B5    | 398  | A2M  | C6-C5-N7    | 2.17  | 136.07      | 132.02   |
| 39  | B5    | 4369 | OMG  | O6-C6-C5    | -2.17 | 120.83      | 126.60   |
| 39  | B5    | 400  | A2M  | C6-C5-N7    | 2.17  | 136.06      | 132.02   |
| 1   | A2    | 1448 | OMG  | O6-C6-C5    | -2.17 | 120.84      | 126.60   |
| 39  | B5    | 3550 | UY1  | CM2-O2'-C2' | -2.17 | 108.83      | 114.52   |
| 39  | B5    | 4364 | OMG  | O6-C6-C5    | -2.17 | 120.85      | 126.60   |
| 39  | B5    | 2206 | A2M  | C6-C5-N7    | 2.17  | 136.06      | 132.02   |
| 39  | B5    | 1580 | OMG  | O6-C6-C5    | -2.16 | 120.86      | 126.60   |
| 1   | A2    | 437  | OMG  | O6-C6-C5    | -2.16 | 120.87      | 126.60   |
| 1   | A2    | 510  | OMG  | O6-C6-C5    | -2.16 | 120.87      | 126.60   |
| 39  | B5    | 2680 | OMU  | O2-C2-N1    | -2.16 | 119.92      | 122.79   |
| 1   | A2    | 1384 | A2M  | C6-C5-N7    | 2.15  | 136.03      | 132.02   |
| 39  | B5    | 3599 | A2M  | C6-C5-N7    | 2.15  | 136.03      | 132.02   |
| 39  | B5    | 4267 | PSU  | C5-C6-N1    | -2.15 | 118.89      | 122.11   |
| 1   | A2    | 485  | A2M  | C6-C5-N7    | 2.15  | 136.02      | 132.02   |
| 1   | A2    | 1704 | OMC  | O2-C2-N3    | -2.14 | 118.84      | 122.33   |
| 39  | B5    | 3557 | A2M  | C6-C5-N7    | 2.14  | 136.01      | 132.02   |
| 39  | B5    | 2630 | A2M  | C6-C5-N7    | 2.14  | 136.01      | 132.02   |
| 1   | A2    | 1032 | A2M  | N9-C8-N7    | -2.14 | 110.99      | 113.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | B5    | 2719 | OMG  | O6-C6-C5    | -2.14 | 120.93      | 126.60   |
| 1   | A2    | 159  | A2M  | N9-C8-N7    | -2.14 | 110.99      | 113.91   |
| 39  | B5    | 1810 | A2M  | C6-C5-N7    | 2.13  | 135.99      | 132.02   |
| 39  | B5    | 4336 | A2M  | C6-C5-N7    | 2.13  | 135.99      | 132.02   |
| 39  | B5    | 3974 | OMG  | O6-C6-C5    | -2.13 | 120.95      | 126.60   |
| 1   | A2    | 1329 | OMG  | O6-C6-C5    | -2.13 | 120.96      | 126.60   |
| 1   | A2    | 602  | OMG  | O6-C6-C5    | -2.12 | 120.97      | 126.60   |
| 1   | A2    | 99   | A2M  | C6-C5-N7    | 2.12  | 135.98      | 132.02   |
| 1   | A2    | 628  | OMU  | O2-C2-N1    | -2.12 | 119.97      | 122.79   |
| 1   | A2    | 513  | A2M  | N9-C8-N7    | -2.12 | 111.01      | 113.91   |
| 39  | B5    | 4240 | OMG  | O6-C6-C5    | -2.12 | 120.98      | 126.60   |
| 39  | B5    | 3676 | OMG  | O6-C6-C5    | -2.11 | 120.99      | 126.60   |
| 39  | B5    | 1479 | A2M  | C6-C5-N7    | 2.11  | 135.96      | 132.02   |
| 1   | A2    | 684  | OMG  | O6-C6-C5    | -2.11 | 121.00      | 126.60   |
| 1   | A2    | 669  | A2M  | C2'-C1'-N9  | -2.11 | 109.98      | 113.53   |
| 1   | A2    | 645  | OMG  | O6-C6-C5    | -2.11 | 121.00      | 126.60   |
| 39  | B5    | 2658 | A2M  | C6-C5-N7    | 2.11  | 135.95      | 132.02   |
| 39  | B5    | 3476 | OMG  | O6-C6-C5    | -2.11 | 121.01      | 126.60   |
| 1   | A2    | 868  | OMG  | O6-C6-C5    | -2.11 | 121.01      | 126.60   |
| 41  | B8    | 75   | OMG  | O6-C6-C5    | -2.11 | 121.01      | 126.60   |
| 1   | A2    | 485  | A2M  | C2'-C1'-N9  | -2.10 | 109.99      | 113.53   |
| 39  | B5    | 3631 | OMG  | O6-C6-C5    | -2.10 | 121.02      | 126.60   |
| 1   | A2    | 1392 | OMC  | O2-C2-N3    | -2.10 | 118.91      | 122.33   |
| 39  | B5    | 4336 | A2M  | N9-C8-N7    | -2.10 | 111.05      | 113.91   |
| 1   | A2    | 1843 | 4AC  | C5-C4-N4    | -2.09 | 119.29      | 122.92   |
| 39  | B5    | 1270 | A2M  | N9-C8-N7    | -2.09 | 111.06      | 113.91   |
| 1   | A2    | 1249 | B8N  | C5-C4-N3    | 2.09  | 120.04      | 116.17   |
| 1   | A2    | 1852 | MA6  | C5-C6-N6    | -2.09 | 121.67      | 125.30   |
| 39  | B5    | 1489 | A2M  | N9-C8-N7    | -2.08 | 111.06      | 113.91   |
| 39  | B5    | 2244 | A2M  | N9-C8-N7    | -2.08 | 111.06      | 113.91   |
| 1   | A2    | 1833 | 6MZ  | C9-N6-C6    | -2.08 | 121.08      | 122.87   |
| 39  | B5    | 4383 | OMG  | O6-C6-C5    | -2.08 | 121.09      | 126.60   |
| 1   | A2    | 27   | A2M  | N9-C8-N7    | -2.08 | 111.08      | 113.91   |
| 39  | B5    | 2207 | OMG  | O6-C6-C5    | -2.08 | 121.09      | 126.60   |
| 1   | A2    | 1679 | A2M  | N9-C8-N7    | -2.07 | 111.08      | 113.91   |
| 1   | A2    | 823  | PSU  | O4'-C1'-C2' | 2.07  | 108.06      | 105.14   |
| 39  | B5    | 1632 | PSU  | C5-C6-N1    | -2.07 | 119.01      | 122.11   |
| 39  | B5    | 4317 | A2M  | N9-C8-N7    | -2.06 | 111.10      | 113.91   |
| 39  | B5    | 4116 | OMG  | O6-C6-C5    | -2.05 | 121.15      | 126.60   |
| 39  | B5    | 3456 | A2M  | N9-C8-N7    | -2.05 | 111.11      | 113.91   |
| 39  | B5    | 3369 | PSU  | C5-C6-N1    | -2.05 | 119.03      | 122.11   |
| 39  | B5    | 3657 | OMU  | O2-C2-N1    | -2.05 | 120.06      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A2    | 669  | A2M  | N9-C8-N7  | -2.05 | 111.11      | 113.91   |
| 39  | B5    | 1477 | OMG  | O6-C6-C5  | -2.04 | 121.18      | 126.60   |
| 39  | B5    | 1801 | PSU  | C5-C6-N1  | -2.04 | 119.04      | 122.11   |
| 39  | B5    | 1266 | 1MA  | C6-C5-N7  | 2.04  | 135.91      | 132.20   |
| 39  | B5    | 4245 | OMG  | O6-C6-C5  | -2.04 | 121.20      | 126.60   |
| 39  | B5    | 4269 | A2M  | N9-C8-N7  | -2.03 | 111.13      | 113.91   |
| 1   | A2    | 652  | PSU  | C5-C6-N1  | -2.03 | 119.06      | 122.11   |
| 39  | B5    | 1721 | PSU  | C5-C6-N1  | -2.03 | 119.07      | 122.11   |
| 1   | A2    | 1446 | PSU  | C5-C6-N1  | -2.03 | 119.07      | 122.11   |
| 1   | A2    | 116  | OMU  | O2-C2-N1  | -2.03 | 120.09      | 122.79   |
| 1   | A2    | 650  | PSU  | C5-C6-N1  | -2.02 | 119.07      | 122.11   |
| 39  | B5    | 3540 | OMC  | O2-C2-N3  | -2.02 | 119.04      | 122.33   |
| 39  | B5    | 4149 | PSU  | C5-C6-N1  | -2.02 | 119.07      | 122.11   |
| 39  | B5    | 4052 | OMU  | C1'-N1-C2 | 2.02  | 121.23      | 117.57   |
| 39  | B5    | 3562 | A2M  | N9-C8-N7  | -2.02 | 111.15      | 113.91   |
| 39  | B5    | 1810 | A2M  | N9-C8-N7  | -2.02 | 111.15      | 113.91   |
| 1   | A2    | 1851 | MA6  | C6-C5-N7  | 2.01  | 136.66      | 133.28   |
| 39  | B5    | 2194 | OMC  | C1'-N1-C2 | 2.01  | 122.92      | 118.42   |
| 39  | B5    | 4711 | PSU  | C5-C6-N1  | -2.01 | 119.09      | 122.11   |
| 1   | A2    | 1384 | A2M  | N9-C8-N7  | -2.01 | 111.16      | 113.91   |
| 39  | B5    | 3466 | PSU  | C5-C6-N1  | -2.01 | 119.09      | 122.11   |
| 39  | B5    | 400  | A2M  | N9-C8-N7  | -2.01 | 111.16      | 113.91   |
| 39  | B5    | 2667 | OMC  | O2-C2-N3  | -2.01 | 119.07      | 122.33   |
| 39  | B5    | 3557 | A2M  | N9-C8-N7  | -2.01 | 111.17      | 113.91   |
| 39  | B5    | 3496 | PSU  | C5-C6-N1  | -2.00 | 119.10      | 122.11   |
| 39  | B5    | 398  | A2M  | N9-C8-N7  | -2.00 | 111.17      | 113.91   |
| 41  | B8    | 55   | PSU  | C5-C6-N1  | -2.00 | 119.11      | 122.11   |

There are no chirality outliers.

All (129) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A2    | 159  | A2M  | C1'-C2'-O2'-CM' |
| 1   | A2    | 429  | OMU  | C2'-C1'-N1-C2   |
| 1   | A2    | 429  | OMU  | C2'-C1'-N1-C6   |
| 1   | A2    | 513  | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 645  | OMG  | O4'-C4'-C5'-O5' |
| 1   | A2    | 645  | OMG  | C3'-C4'-C5'-O5' |
| 39  | B5    | 2207 | OMG  | O4'-C4'-C5'-O5' |
| 39  | B5    | 3433 | OMC  | C2'-C1'-N1-C2   |
| 39  | B5    | 3433 | OMC  | C2'-C1'-N1-C6   |
| 39  | B5    | 4166 | PSU  | C2'-C1'-C5-C4   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 39  | B5    | 4382 | PSU  | O4'-C1'-C5-C4   |
| 39  | B5    | 4382 | PSU  | O4'-C1'-C5-C6   |
| 39  | B5    | 4382 | PSU  | C3'-C4'-C5'-O5' |
| 1   | A2    | 1249 | B8N  | N34-C33-C34-O35 |
| 1   | A2    | 1338 | 4AC  | N3-C4-N4-C7     |
| 1   | A2    | 1338 | 4AC  | C5-C4-N4-C7     |
| 1   | A2    | 1338 | 4AC  | O7-C7-N4-C4     |
| 1   | A2    | 1338 | 4AC  | CM7-C7-N4-C4    |
| 1   | A2    | 1843 | 4AC  | N3-C4-N4-C7     |
| 1   | A2    | 1843 | 4AC  | C5-C4-N4-C7     |
| 42  | BA    | 216  | V5N  | O-C-CA-CB       |
| 39  | B5    | 4336 | A2M  | C4'-C5'-O5'-P   |
| 1   | A2    | 99   | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 669  | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 669  | A2M  | C3'-C4'-C5'-O5' |
| 39  | B5    | 2207 | OMG  | C3'-C4'-C5'-O5' |
| 39  | B5    | 2658 | A2M  | O4'-C4'-C5'-O5' |
| 39  | B5    | 2658 | A2M  | C3'-C4'-C5'-O5' |
| 44  | BC    | 2    | AYA  | CM-CT-N-CA      |
| 44  | BC    | 2    | AYA  | OT-CT-N-CA      |
| 33  | Au    | 1    | AME  | CT2-CT1-N-CA    |
| 33  | Au    | 1    | AME  | OT-CT1-N-CA     |
| 1   | A2    | 1249 | B8N  | N34-C33-C34-O36 |
| 1   | A2    | 513  | A2M  | C3'-C4'-C5'-O5' |
| 1   | A2    | 684  | OMG  | O4'-C4'-C5'-O5' |
| 1   | A2    | 1448 | OMG  | C3'-C4'-C5'-O5' |
| 39  | B5    | 398  | A2M  | O4'-C4'-C5'-O5' |
| 39  | B5    | 4382 | PSU  | O4'-C4'-C5'-O5' |
| 39  | B5    | 4193 | 5MC  | C2'-C1'-N1-C6   |
| 1   | A2    | 577  | A2M  | C3'-C4'-C5'-O5' |
| 39  | B5    | 1632 | PSU  | C3'-C4'-C5'-O5' |
| 39  | B5    | 1632 | PSU  | O4'-C4'-C5'-O5' |
| 39  | B5    | 3599 | A2M  | C3'-C4'-C5'-O5' |
| 1   | A2    | 577  | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 1448 | OMG  | O4'-C4'-C5'-O5' |
| 1   | A2    | 1704 | OMC  | O4'-C4'-C5'-O5' |
| 39  | B5    | 398  | A2M  | C3'-C4'-C5'-O5' |
| 39  | B5    | 3494 | PSU  | C3'-C4'-C5'-O5' |
| 1   | A2    | 684  | OMG  | C3'-C4'-C5'-O5' |
| 39  | B5    | 4269 | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 99   | A2M  | C3'-C4'-C5'-O5' |
| 1   | A2    | 1443 | OMU  | C1'-C2'-O2'-CM2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | BB    | 245  | HIC  | CA-CB-CG-ND1    |
| 44  | BC    | 2    | AYA  | C-CA-N-CT       |
| 1   | A2    | 1852 | MA6  | C4'-C5'-O5'-P   |
| 39  | B5    | 3576 | PSU  | C4'-C5'-O5'-P   |
| 39  | B5    | 4246 | PSU  | C4'-C5'-O5'-P   |
| 39  | B5    | 3550 | UY1  | C4'-C5'-O5'-P   |
| 39  | B5    | 2630 | A2M  | C2'-C1'-N9-C8   |
| 12  | AZ    | 2    | SAC  | C-CA-N-C1A      |
| 39  | B5    | 4193 | 5MC  | C2'-C1'-N1-C2   |
| 39  | B5    | 1260 | OMG  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 1820 | OMC  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 3540 | OMC  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 3631 | OMG  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 3973 | OMU  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 4193 | 5MC  | O4'-C1'-N1-C6   |
| 69  | Bb    | 5    | MLZ  | N-CA-CB-CG      |
| 1   | A2    | 1249 | B8N  | C32-C33-C34-O36 |
| 69  | Bb    | 5    | MLZ  | C-CA-CB-CG      |
| 1   | A2    | 645  | OMG  | C4'-C5'-O5'-P   |
| 39  | B5    | 4193 | 5MC  | O4'-C1'-N1-C2   |
| 39  | B5    | 3494 | PSU  | O4'-C4'-C5'-O5' |
| 39  | B5    | 3433 | OMC  | O4'-C1'-N1-C6   |
| 1   | A2    | 591  | A2M  | C2'-C1'-N9-C4   |
| 1   | A2    | 1249 | B8N  | C32-C33-C34-O35 |
| 1   | A2    | 628  | OMU  | C2'-C1'-N1-C6   |
| 68  | Ba    | 39   | V5N  | O2-CB-CG-CD2    |
| 42  | BA    | 216  | V5N  | O2-CB-CG-CD2    |
| 1   | A2    | 429  | OMU  | O4'-C4'-C5'-O5' |
| 1   | A2    | 684  | OMG  | C3'-C2'-O2'-CM2 |
| 1   | A2    | 1448 | OMG  | C3'-C2'-O2'-CM2 |
| 1   | A2    | 1491 | OMG  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 2680 | OMU  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 3619 | OMC  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 4369 | OMG  | C3'-C2'-O2'-CM2 |
| 42  | BA    | 216  | V5N  | O2-CB-CG-ND1    |
| 1   | A2    | 429  | OMU  | O4'-C1'-N1-C6   |
| 1   | A2    | 116  | OMU  | C3'-C2'-O2'-CM2 |
| 1   | A2    | 1289 | OMU  | C3'-C2'-O2'-CM2 |
| 1   | A2    | 1443 | OMU  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 1810 | A2M  | C3'-C2'-O2'-CM' |
| 39  | B5    | 2667 | OMC  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 3557 | A2M  | C3'-C2'-O2'-CM' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 39  | B5    | 1489 | A2M  | O4'-C4'-C5'-O5' |
| 39  | B5    | 3599 | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 1833 | 6MZ  | N1-C6-N6-C9     |
| 39  | B5    | 2630 | A2M  | O4'-C1'-N9-C8   |
| 39  | B5    | 3433 | OMC  | O4'-C1'-N1-C2   |
| 1   | A2    | 628  | OMU  | O4'-C1'-N1-C6   |
| 1   | A2    | 510  | OMG  | O4'-C4'-C5'-O5' |
| 39  | B5    | 4278 | PSU  | C3'-C4'-C5'-O5' |
| 1   | A2    | 591  | A2M  | C2'-C1'-N9-C8   |
| 1   | A2    | 1704 | OMC  | C3'-C4'-C5'-O5' |
| 39  | B5    | 1284 | OMC  | C1'-C2'-O2'-CM2 |
| 39  | B5    | 1810 | A2M  | C1'-C2'-O2'-CM' |
| 39  | B5    | 1284 | OMC  | C3'-C2'-O2'-CM2 |
| 43  | BB    | 245  | HIC  | CA-CB-CG-CD2    |
| 39  | B5    | 3619 | OMC  | C4'-C5'-O5'-P   |
| 39  | B5    | 4278 | PSU  | O4'-C4'-C5'-O5' |
| 35  | Aw    | 62   | HY3  | O-C-CA-C3       |
| 39  | B5    | 1632 | PSU  | O4'-C1'-C5-C6   |
| 39  | B5    | 2194 | OMC  | C2'-C1'-N1-C2   |
| 1   | A2    | 429  | OMU  | O4'-C1'-N1-C2   |
| 1   | A2    | 628  | OMU  | O4'-C1'-N1-C2   |
| 1   | A2    | 1289 | OMU  | C4'-C5'-O5'-P   |
| 39  | B5    | 2194 | OMC  | O4'-C4'-C5'-O5' |
| 39  | B5    | 3517 | A2M  | O4'-C4'-C5'-O5' |
| 1   | A2    | 469  | A2M  | C3'-C2'-O2'-CM' |
| 39  | B5    | 2265 | OMC  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 3476 | OMG  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 4383 | OMG  | C3'-C2'-O2'-CM2 |
| 41  | B8    | 75   | OMG  | C3'-C2'-O2'-CM2 |
| 39  | B5    | 4269 | A2M  | C3'-C4'-C5'-O5' |
| 1   | A2    | 591  | A2M  | O4'-C1'-N9-C8   |
| 39  | B5    | 1266 | 1MA  | C2'-C1'-N9-C8   |
| 1   | A2    | 429  | OMU  | C3'-C4'-C5'-O5' |
| 39  | B5    | 3450 | A2M  | O4'-C4'-C5'-O5' |
| 39  | B5    | 2630 | A2M  | C2'-C1'-N9-C4   |

There are no ring outliers.

94 monomers are involved in 118 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A2    | 1448 | OMG  | 2       | 0            |
| 39  | B5    | 2206 | A2M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 39  | B5    | 4269 | A2M  | 1       | 0            |
| 39  | B5    | 1270 | A2M  | 2       | 0            |
| 1   | A2    | 1704 | OMC  | 2       | 0            |
| 1   | A2    | 116  | OMU  | 1       | 0            |
| 11  | AT    | 65   | PSU  | 1       | 0            |
| 39  | B5    | 2704 | OMC  | 1       | 0            |
| 39  | B5    | 3557 | A2M  | 1       | 0            |
| 39  | B5    | 4364 | OMG  | 1       | 0            |
| 39  | B5    | 3631 | OMG  | 1       | 0            |
| 39  | B5    | 3540 | OMC  | 1       | 0            |
| 1   | A2    | 518  | OMC  | 1       | 0            |
| 39  | B5    | 3562 | A2M  | 1       | 0            |
| 39  | B5    | 3517 | A2M  | 1       | 0            |
| 39  | B5    | 2267 | OMG  | 1       | 0            |
| 39  | B5    | 2208 | OMC  | 2       | 0            |
| 1   | A2    | 868  | OMG  | 1       | 0            |
| 39  | B5    | 4383 | OMG  | 1       | 0            |
| 39  | B5    | 3599 | A2M  | 2       | 0            |
| 1   | A2    | 172  | OMU  | 2       | 0            |
| 1   | A2    | 1843 | 4AC  | 2       | 0            |
| 39  | B5    | 4336 | A2M  | 1       | 0            |
| 1   | A2    | 36   | PSU  | 1       | 0            |
| 1   | A2    | 1249 | B8N  | 1       | 0            |
| 1   | A2    | 684  | OMG  | 1       | 0            |
| 1   | A2    | 1233 | PSU  | 2       | 0            |
| 1   | A2    | 513  | A2M  | 1       | 0            |
| 1   | A2    | 27   | A2M  | 1       | 0            |
| 39  | B5    | 2658 | A2M  | 1       | 0            |
| 39  | B5    | 1820 | OMC  | 1       | 0            |
| 39  | B5    | 2194 | OMC  | 1       | 0            |
| 39  | B5    | 4325 | PSU  | 1       | 0            |
| 39  | B5    | 3550 | UY1  | 2       | 0            |
| 1   | A2    | 1640 | G7M  | 1       | 0            |
| 1   | A2    | 109  | PSU  | 1       | 0            |
| 39  | B5    | 3456 | A2M  | 1       | 0            |
| 39  | B5    | 3524 | OMG  | 1       | 0            |
| 1   | A2    | 864  | PSU  | 1       | 0            |
| 1   | A2    | 485  | A2M  | 1       | 0            |
| 39  | B5    | 4282 | OMC  | 1       | 0            |
| 39  | B5    | 1638 | PSU  | 1       | 0            |
| 1   | A2    | 1679 | A2M  | 2       | 0            |
| 1   | A2    | 469  | A2M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A2    | 602  | OMG  | 1       | 0            |
| 1   | A2    | 1289 | OMU  | 2       | 0            |
| 39  | B5    | 2207 | OMG  | 1       | 0            |
| 39  | B5    | 3494 | PSU  | 1       | 0            |
| 39  | B5    | 4193 | 5MC  | 2       | 0            |
| 1   | A2    | 121  | OMU  | 1       | 0            |
| 1   | A2    | 1032 | A2M  | 2       | 0            |
| 1   | A2    | 1491 | OMG  | 1       | 0            |
| 39  | B5    | 3974 | OMG  | 1       | 0            |
| 39  | B5    | 4366 | OMU  | 2       | 0            |
| 39  | B5    | 3450 | A2M  | 2       | 0            |
| 39  | B5    | 3942 | OMG  | 1       | 0            |
| 1   | A2    | 1446 | PSU  | 3       | 0            |
| 39  | B5    | 398  | A2M  | 1       | 0            |
| 1   | A2    | 1833 | 6MZ  | 1       | 0            |
| 39  | B5    | 4203 | PSU  | 1       | 0            |
| 39  | B5    | 3619 | OMC  | 1       | 0            |
| 39  | B5    | 2258 | OMU  | 2       | 0            |
| 1   | A2    | 577  | A2M  | 1       | 0            |
| 1   | A2    | 463  | OMC  | 1       | 0            |
| 39  | B5    | 1284 | OMC  | 1       | 0            |
| 1   | A2    | 355  | OMU  | 1       | 0            |
| 39  | B5    | 1260 | OMG  | 1       | 0            |
| 39  | B5    | 3476 | OMG  | 1       | 0            |
| 39  | B5    | 3502 | PSU  | 2       | 0            |
| 39  | B5    | 4052 | OMU  | 1       | 0            |
| 1   | A2    | 1348 | PSU  | 2       | 0            |
| 1   | A2    | 1644 | PSU  | 1       | 0            |
| 39  | B5    | 3466 | PSU  | 1       | 0            |
| 81  | Bo    | 53   | MLZ  | 1       | 0            |
| 39  | B5    | 2719 | OMG  | 1       | 0            |
| 1   | A2    | 1852 | MA6  | 1       | 0            |
| 1   | A2    | 1338 | 4AC  | 3       | 0            |
| 39  | B5    | 4317 | A2M  | 1       | 0            |
| 39  | B5    | 2667 | OMC  | 1       | 0            |
| 39  | B5    | 1810 | A2M  | 2       | 0            |
| 1   | A2    | 1805 | OMU  | 2       | 0            |
| 39  | B5    | 1580 | OMG  | 1       | 0            |
| 39  | B5    | 4382 | PSU  | 2       | 0            |
| 39  | B5    | 4138 | OMG  | 2       | 0            |
| 39  | B5    | 1632 | PSU  | 1       | 0            |
| 1   | A2    | 1392 | OMC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A2    | 437  | OMG  | 1       | 0            |
| 1   | A2    | 1329 | OMG  | 1       | 0            |
| 1   | A2    | 1851 | MA6  | 1       | 0            |
| 39  | B5    | 2647 | OMC  | 1       | 0            |
| 1   | A2    | 99   | A2M  | 1       | 0            |
| 33  | Au    | 1    | AME  | 2       | 0            |
| 1   | A2    | 166  | A2M  | 2       | 0            |
| 39  | B5    | 4202 | OMC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 741 ligands modelled in this entry, 363 are monoatomic and 374 are unknown - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 93  | GTP  | B7    | 201  | 40   | 30,34,34     | 0.50 | 0           | 46,54,54    | 0.57 | 0           |
| 94  | SF4  | Bz    | 1001 | 88   | 0,12,12      | -    | -           | -           |      |             |
| 89  | SPD  | A2    | 1901 | -    | 9,9,9        | 0.16 | 0           | 8,8,8       | 0.16 | 0           |
| 94  | SF4  | Bz    | 1000 | 88   | 0,12,12      | -    | -           | -           |      |             |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 93  | GTP  | B7    | 201  | 40   | -       | 0/22/38/38 | 0/3/3/3 |
| 94  | SF4  | Bz    | 1001 | 88   | -       | -          | 0/6/5/5 |
| 89  | SPD  | A2    | 1901 | -    | -       | 0/7/7/7    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 94  | SF4  | Bz    | 1000 | 88   | -       | -        | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 89  | A2    | 1901 | SPD  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

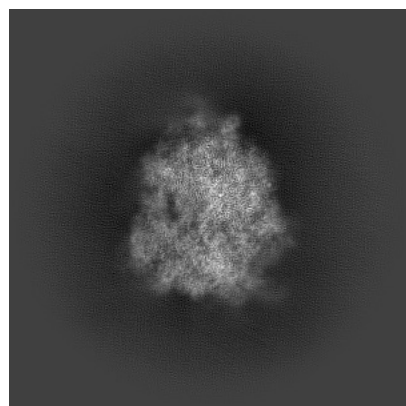
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12758. These allow visual inspection of the internal detail of the map and identification of artifacts.

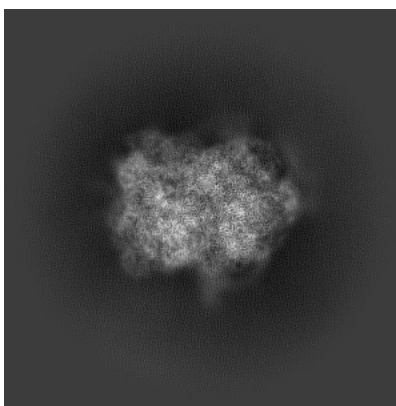
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

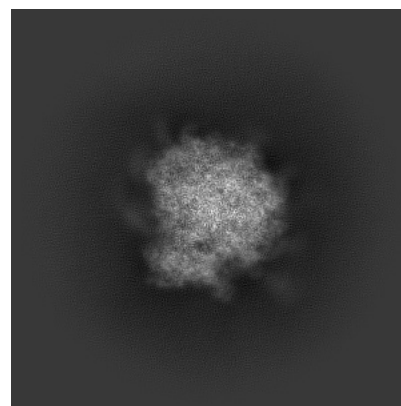
#### 6.1.1 Primary map



X

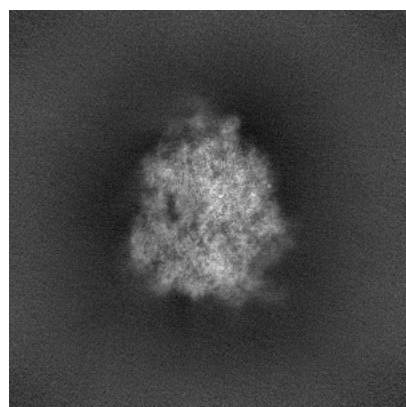


Y

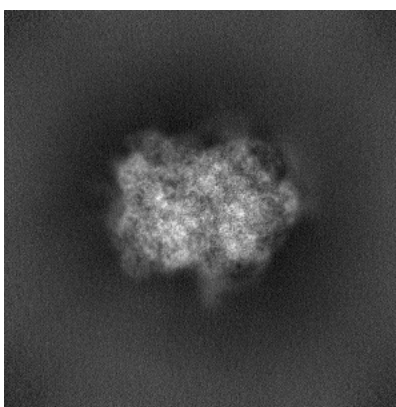


Z

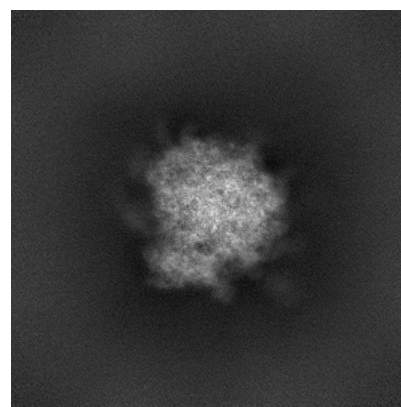
#### 6.1.2 Raw map



X



Y

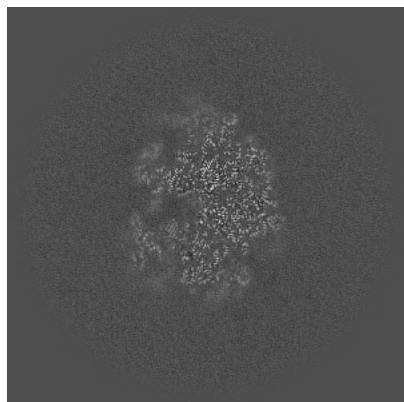


Z

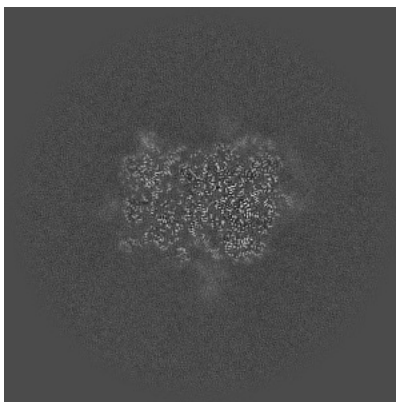
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

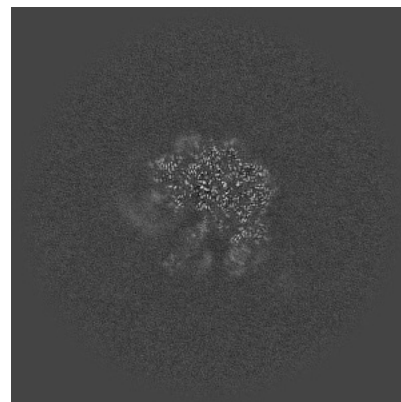
### 6.2.1 Primary map



X Index: 280

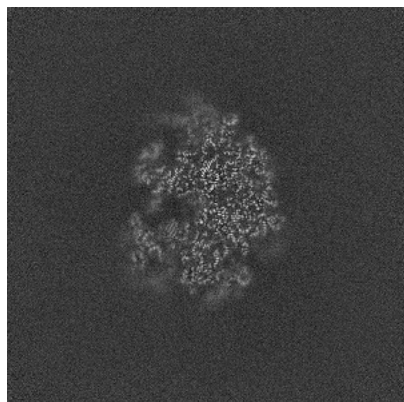


Y Index: 280

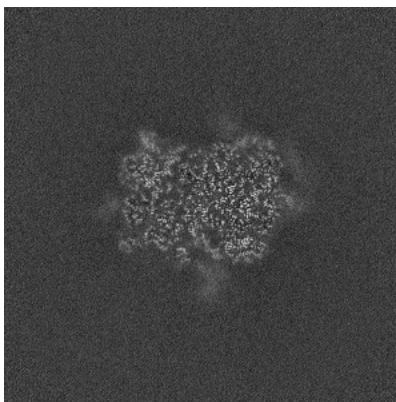


Z Index: 280

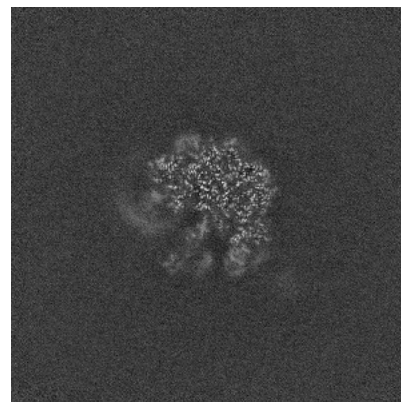
### 6.2.2 Raw map



X Index: 280



Y Index: 280



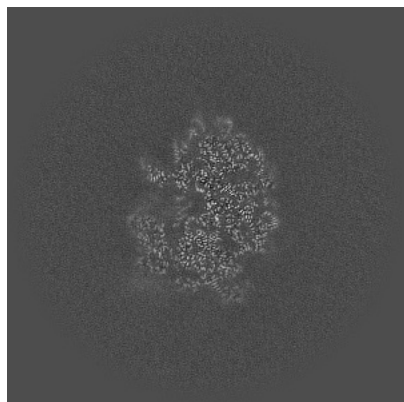
Z Index: 280

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

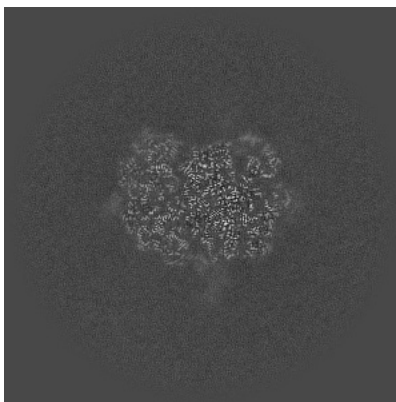


## 6.3 Largest variance slices [i](#)

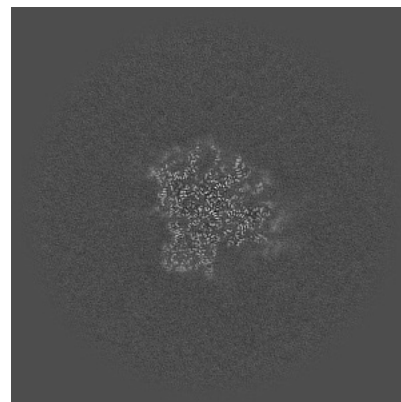
### 6.3.1 Primary map



X Index: 263

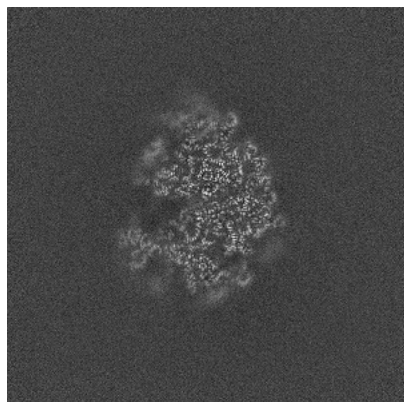


Y Index: 289

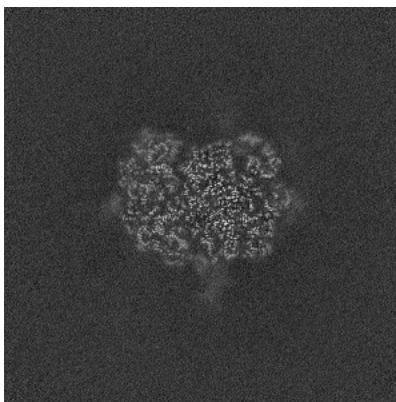


Z Index: 323

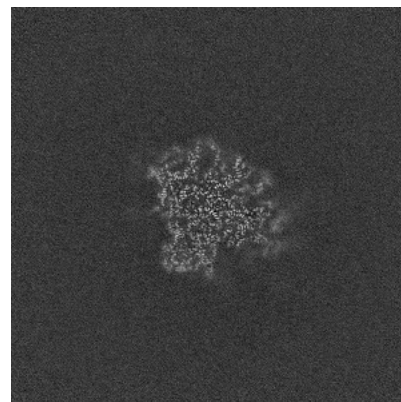
### 6.3.2 Raw map



X Index: 285



Y Index: 289

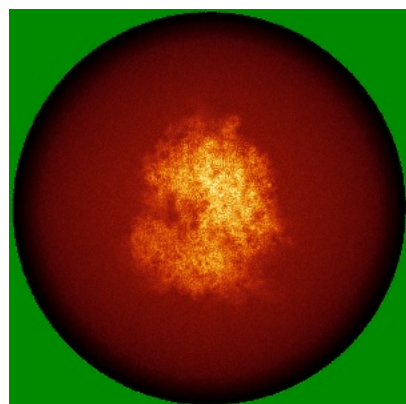


Z Index: 323

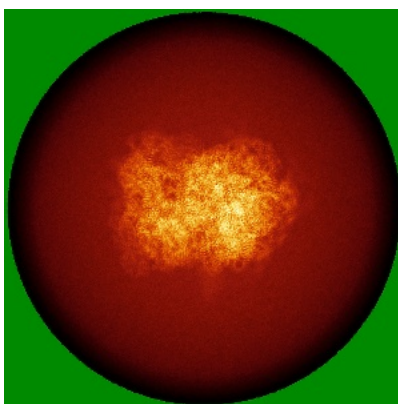
The images above show the largest variance slices of the map in three orthogonal directions.

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

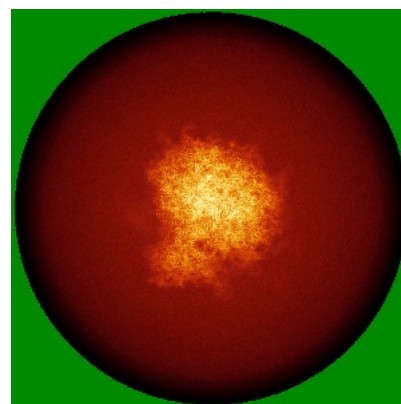
### 6.4.1 Primary map



X

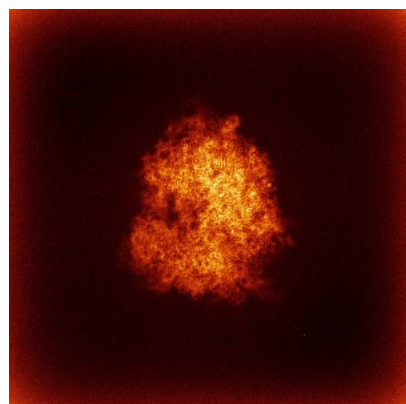


Y

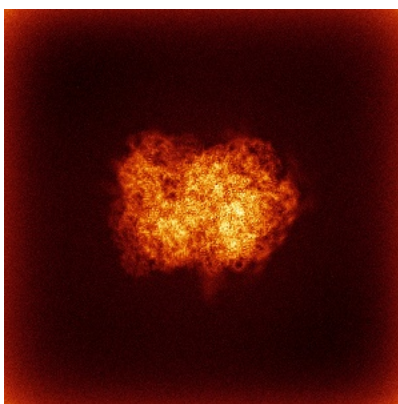


Z

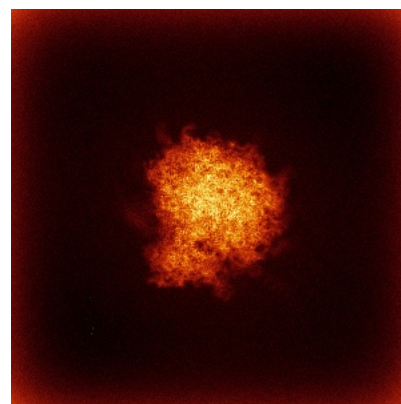
### 6.4.2 Raw map



X



Y

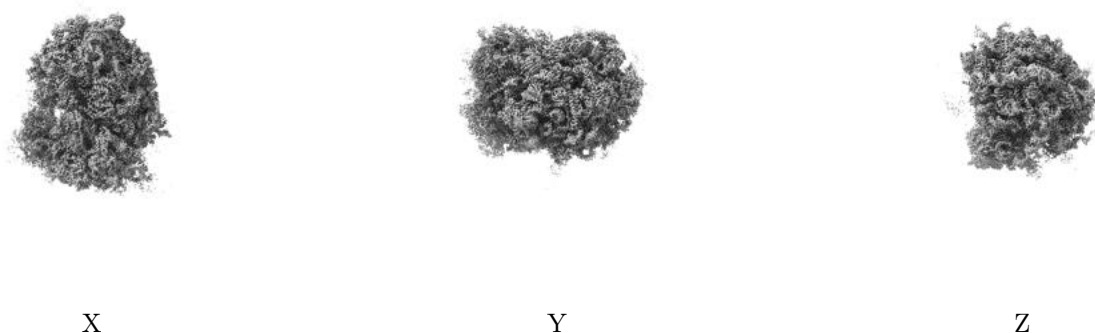


Z

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.

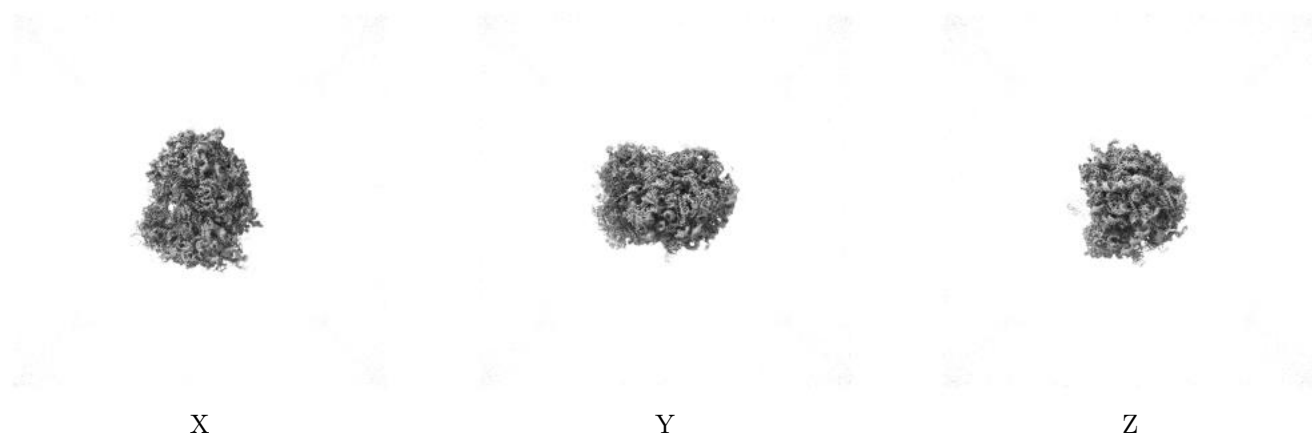
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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



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.



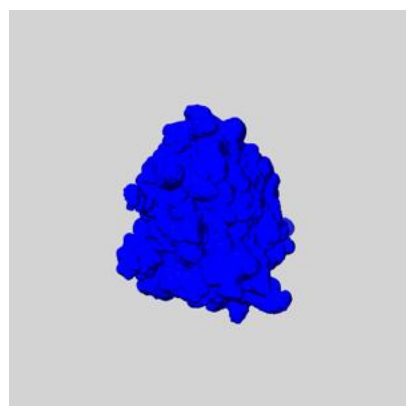
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

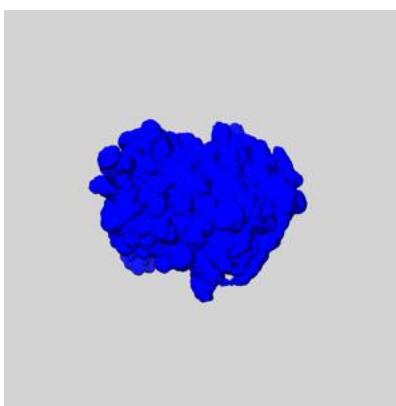
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

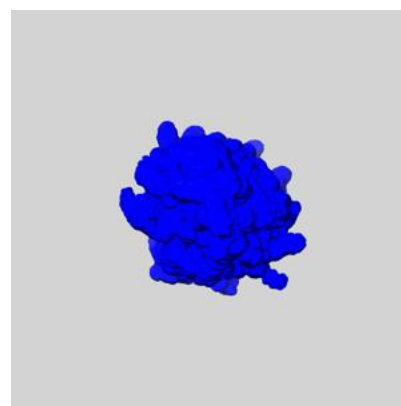
### 6.6.1 emd\_12758\_msk\_1.map [i](#)



X

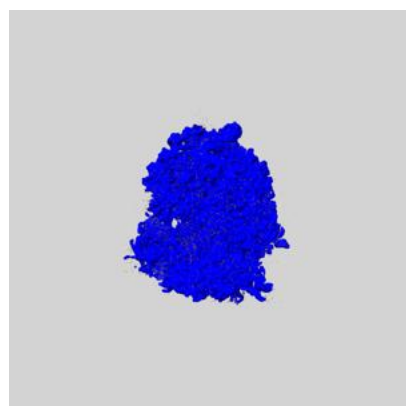


Y

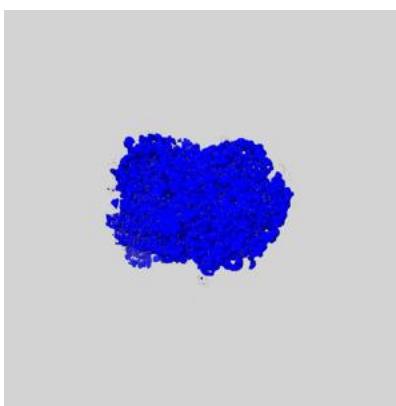


Z

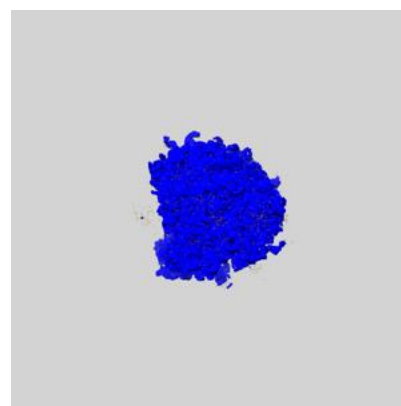
### 6.6.2 emd\_12758\_msk\_2.map [i](#)



X



Y

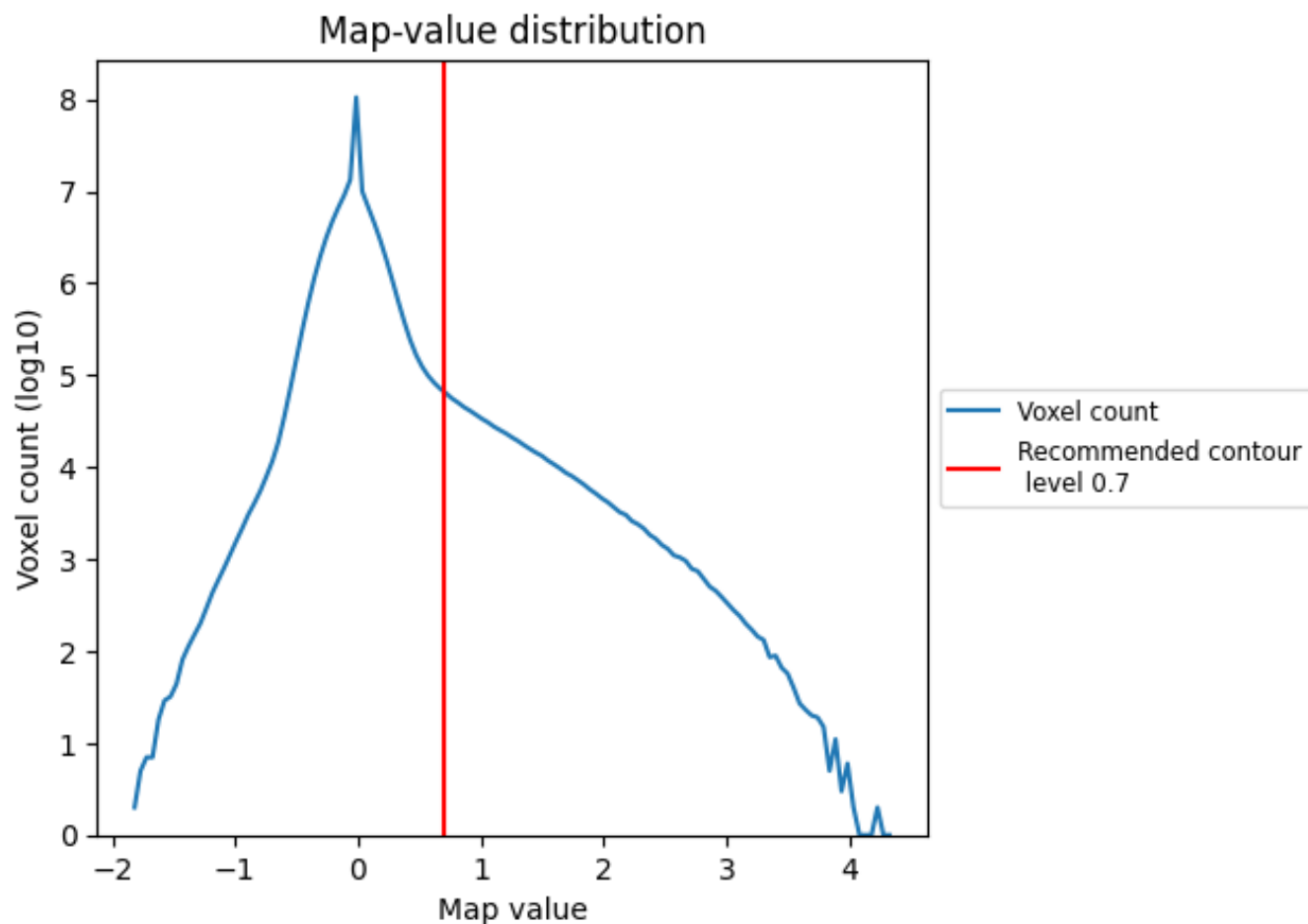


Z

## 7 Map analysis [i](#)

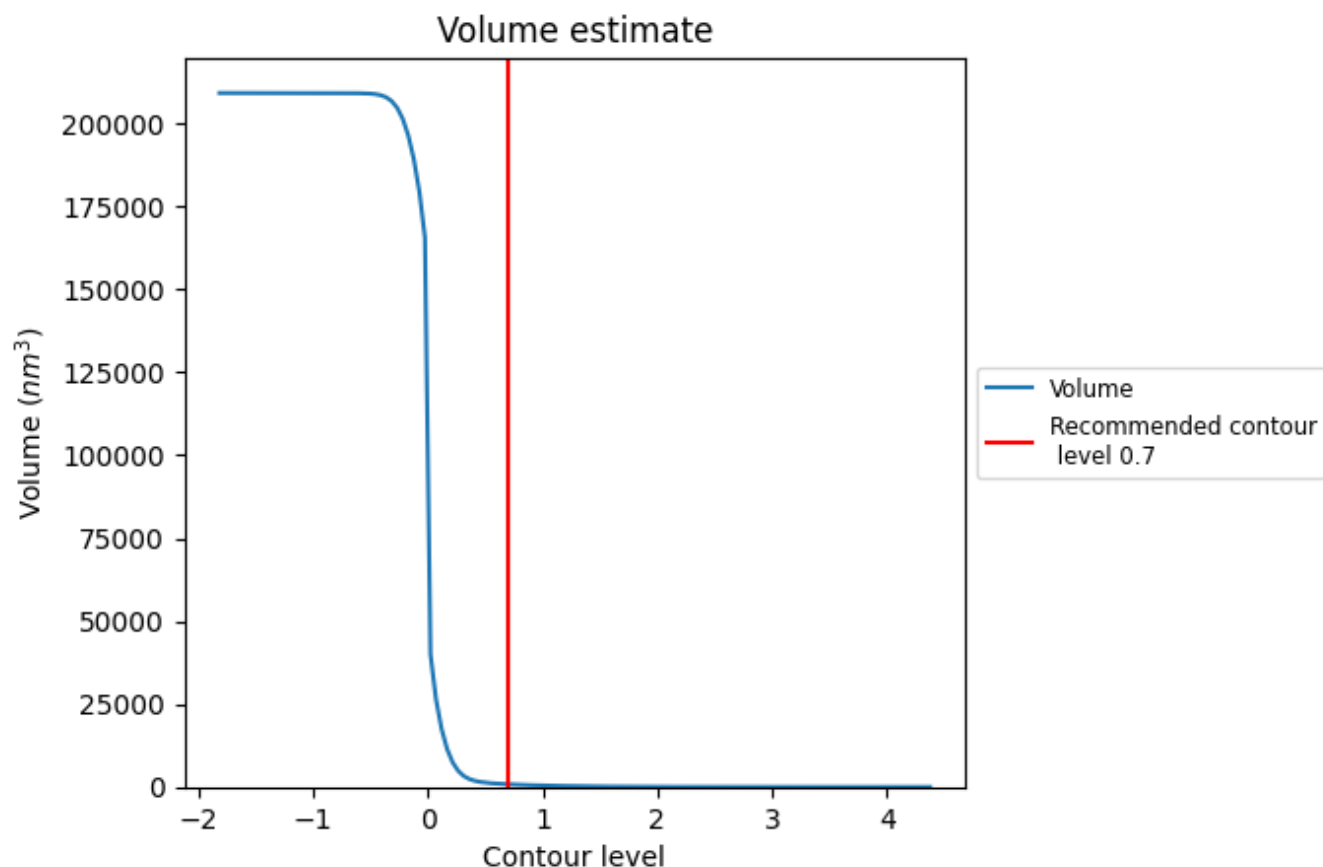
This section contains the results of statistical analysis of the map.

### 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.

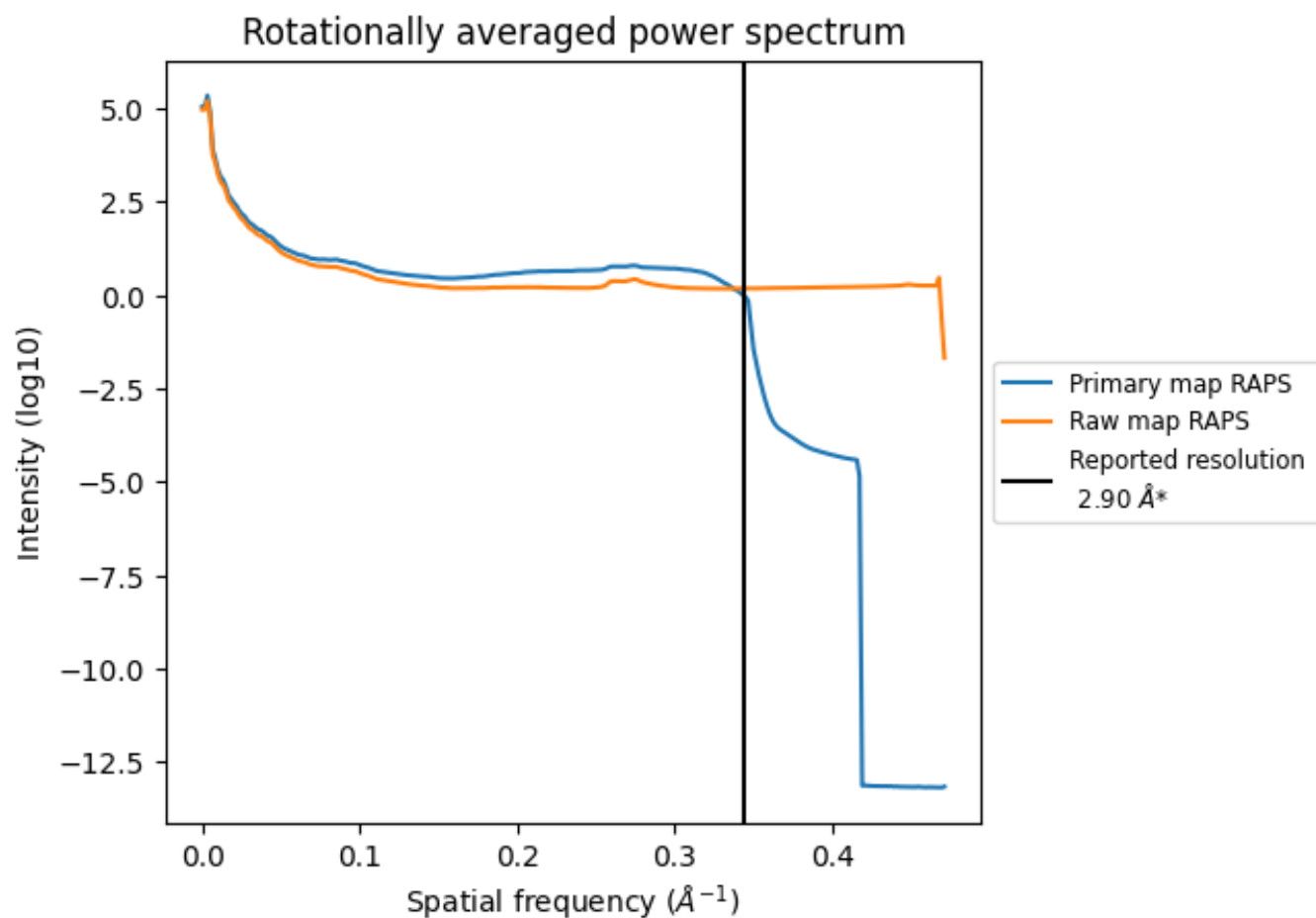
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 803  $\text{nm}^3$ ; this corresponds to an approximate mass of 726 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 ⓘ

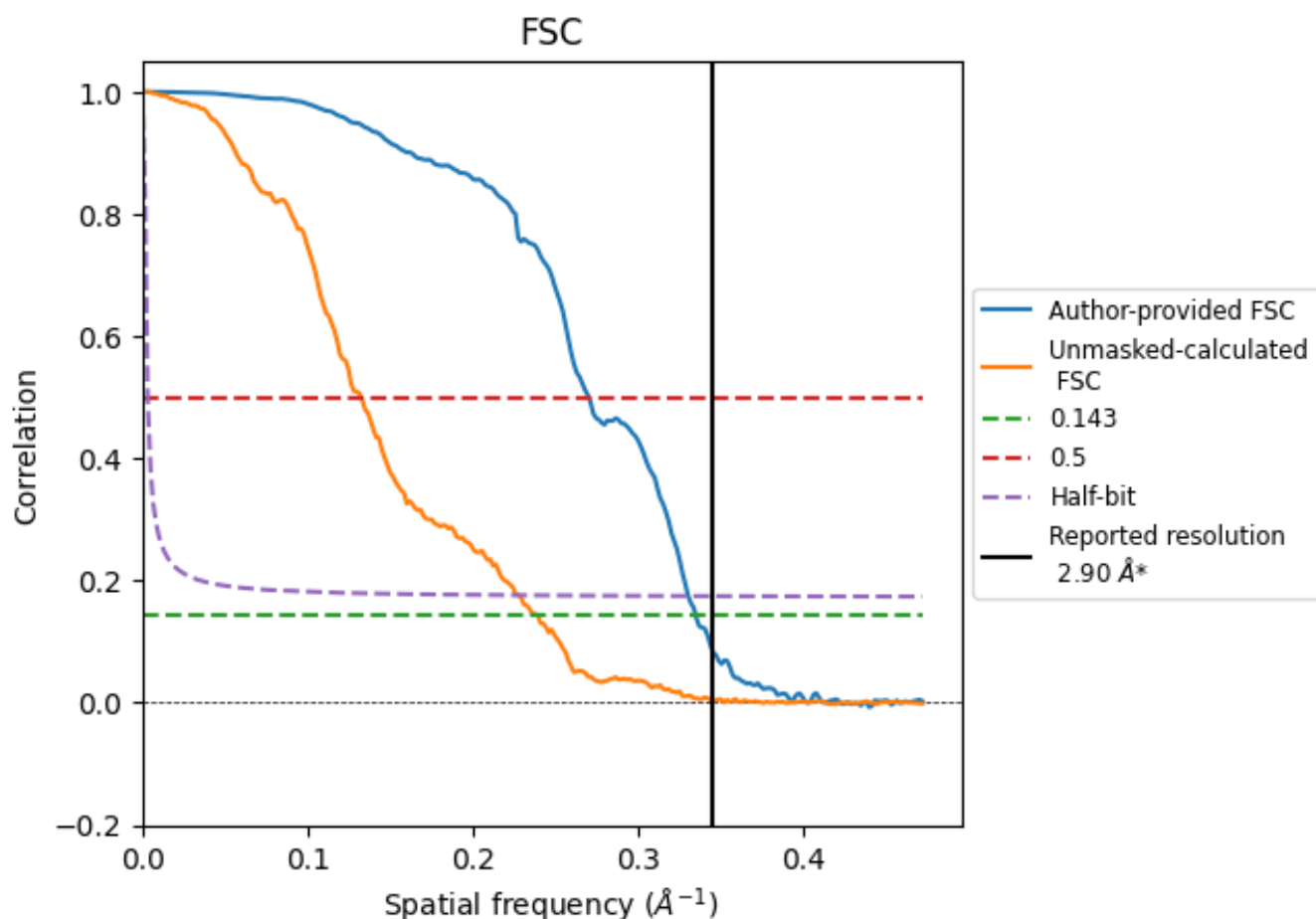


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

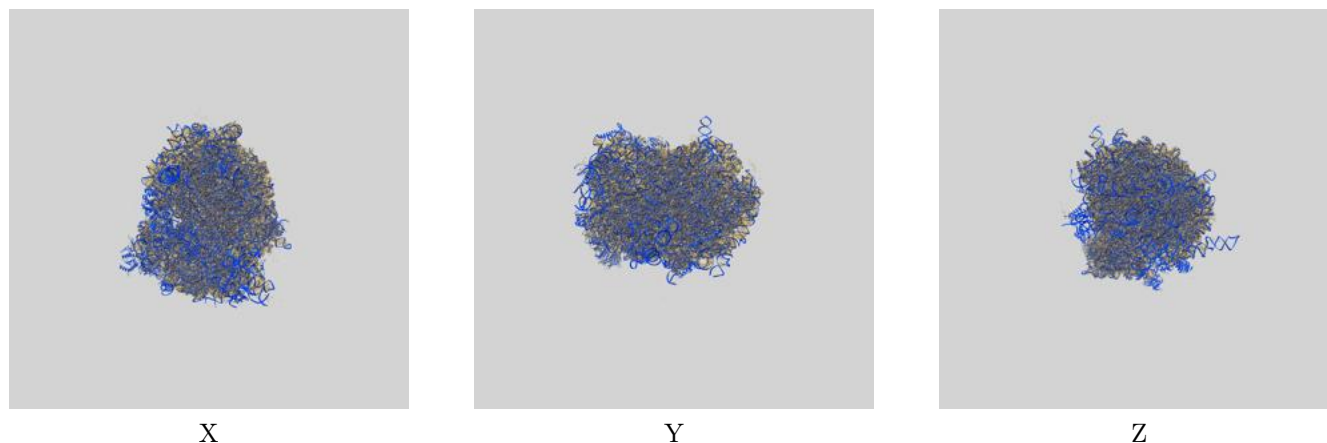
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.99                               | 3.70 | 3.03     |
| Unmasked-calculated*      | 4.18                               | 7.56 | 4.39     |

\*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 4.18 differs from the reported value 2.9 by more than 10 %

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

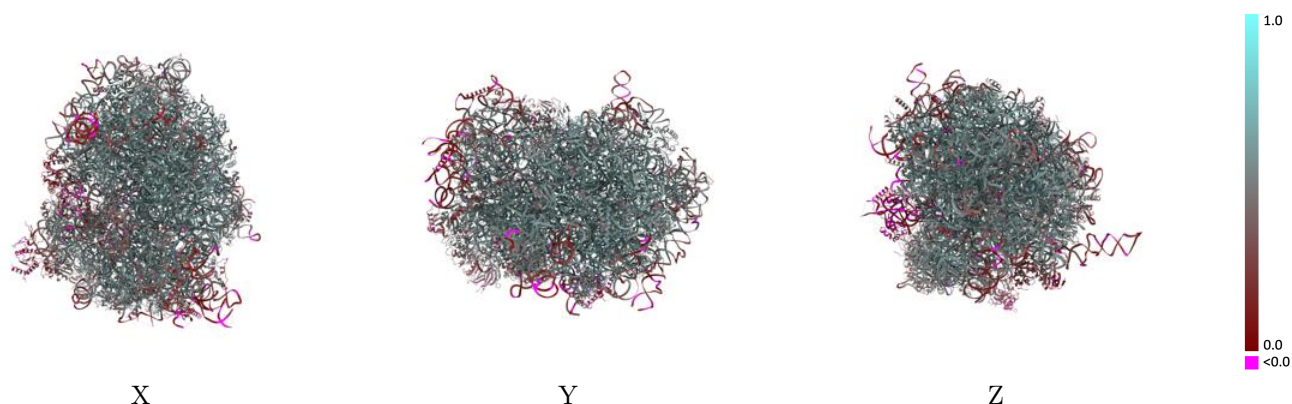
This section contains information regarding the fit between EMDB map EMD-12758 and PDB model 7O80. Per-residue inclusion information can be found in section [3](#) on page [27](#).

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



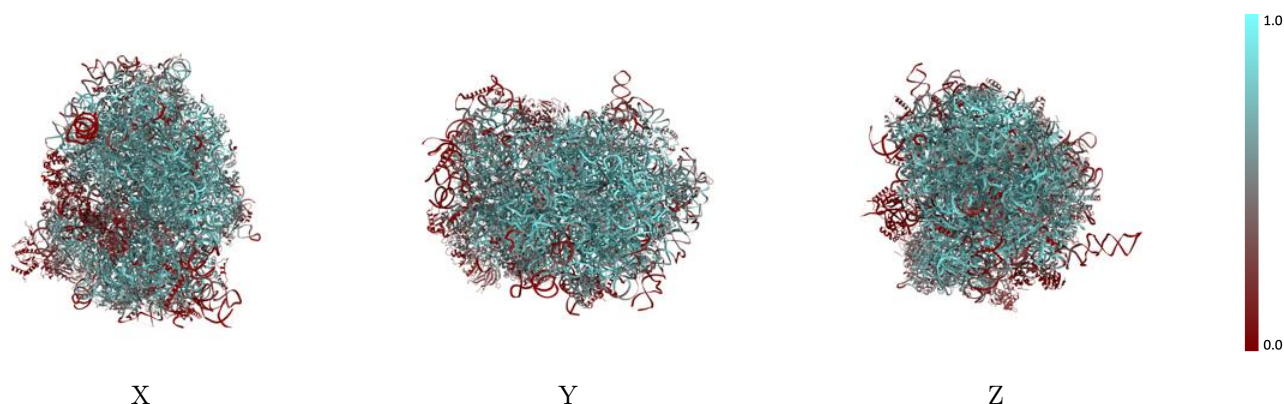
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

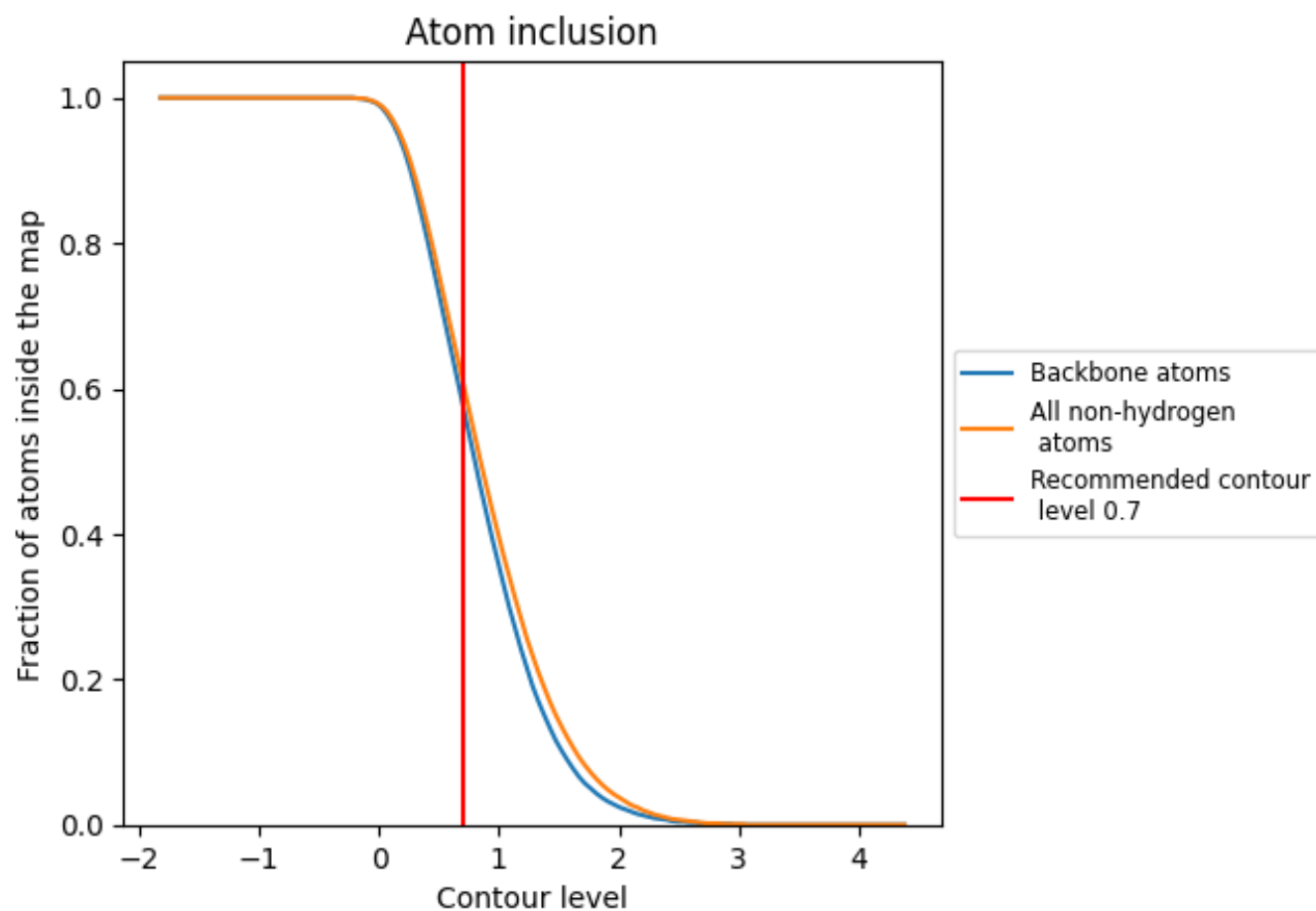
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.7).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 61% 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 (0.7) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6080   |  0.4970   |
| A2    |  0.6790   |  0.5030   |
| AA    |  0.4100   |  0.4750   |
| AB    |  0.3560   |  0.4680   |
| AC    |  0.0210   |  0.1980   |
| AD    |  0.3750   |  0.4330   |
| AE    |  0.5790   |  0.5190   |
| AF    |  0.1850   |  0.3450   |
| AG    |  0.5770   |  0.5200   |
| AH    |  0.2650   |  0.3280   |
| AI    |  0.0100   |  0.1090   |
| AT    |  0.4490   |  0.4340   |
| AZ    |  0.3900   |  0.4760   |
| Aa    |  0.4740   |  0.4800   |
| Ab    |  0.5260  |  0.5200  |
| Ac    |  0.3110 |  0.4240 |
| Ad    |  0.5380 |  0.5060 |
| Ae    |  0.4370 |  0.4700 |
| Af    |  0.3580 |  0.4040 |
| Ag    |  0.2480 |  0.3870 |
| Ah    |  0.5340 |  0.4990 |
| Ai    |  0.5500 |  0.4970 |
| Aj    |  0.2920 |  0.3860 |
| Ak    |  0.5510 |  0.4940 |
| Al    |  0.0050 |  0.1510 |
| Am    |  0.5410 |  0.5240 |
| An    |  0.5540 |  0.5200 |
| Ao    |  0.3470 |  0.4200 |
| Ap    |  0.4680 |  0.4910 |
| Aq    |  0.2680 |  0.4070 |
| Ar    |  0.4010 |  0.4430 |
| As    |  0.4600 |  0.4640 |
| At    |  0.2810 |  0.4000 |
| Au    |  0.3950 |  0.4780 |
| Av    |  0.6090 |  0.5500 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Aw    |  0.5870   |  0.5400   |
| Ax    |  0.4820   |  0.4650   |
| Ay    |  0.3210   |  0.3960   |
| Az    |  0.6560   |  0.5610   |
| B5    |  0.7290   |  0.5210   |
| B7    |  0.8580   |  0.5750   |
| B8    |  0.7860   |  0.5590   |
| BA    |  0.6980   |  0.5770   |
| BB    |  0.6900   |  0.5660   |
| BC    |  0.6970   |  0.5660   |
| BD    |  0.5950   |  0.5100   |
| BE    |  0.5100   |  0.4810   |
| BF    |  0.7020   |  0.5670   |
| BG    |  0.5180   |  0.4780   |
| BH    |  0.5760   |  0.5180   |
| BI    |  0.6030   |  0.5400   |
| BJ    |  0.5070   |  0.4870   |
| BK    |  0.0630   |  0.3010   |
| BL    |  0.6260   |  0.5240   |
| BM    |  0.6440  |  0.5360  |
| BN    |  0.7770 |  0.5980 |
| BO    |  0.7010 |  0.5720 |
| BP    |  0.6800 |  0.5580 |
| BQ    |  0.7070 |  0.5770 |
| BR    |  0.6150 |  0.5190 |
| BS    |  0.7060 |  0.5750 |
| BT    |  0.6320 |  0.5470 |
| BU    |  0.4380 |  0.4460 |
| BV    |  0.6240 |  0.5550 |
| BW    |  0.3690 |  0.3850 |
| BX    |  0.6150 |  0.5370 |
| BY    |  0.6650 |  0.5360 |
| BZ    |  0.6100 |  0.5200 |
| Ba    |  0.7550 |  0.5890 |
| Bb    |  0.4760 |  0.4780 |
| Bc    |  0.5350 |  0.4880 |
| Bd    |  0.6380 |  0.5390 |
| Be    |  0.7040 |  0.5740 |
| Bf    |  0.7320 |  0.5880 |
| Bg    |  0.6360 |  0.5480 |
| Bh    |  0.6060 |  0.5260 |
| Bi    |  0.5850 |  0.5210 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Bj    |  0.7770 |  0.5920 |
| Bk    |  0.4340 |  0.4540 |
| Bl    |  0.7070 |  0.5710 |
| Bm    |  0.6160 |  0.5460 |
| Bo    |  0.5960 |  0.5370 |
| Bp    |  0.6310 |  0.5550 |
| Br    |  0.6530 |  0.5640 |
| Bs    |  0.0200 |  0.1640 |
| Bt    |  0.0330 |  0.2220 |
| Bv    |  0.0000 |  0.0600 |
| By    |  0.2280 |  0.4100 |
| Bz    |  0.2530 |  0.3940 |