



# Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 10:42 AM JST

PDB ID : 6LSR / pdb\_00006lsr  
EMDB ID : EMD-0963  
Title : Cryo-EM structure of a pre-60S ribosomal subunit - state B  
Authors : Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.  
Deposited on : 2020-01-20  
Resolution : 3.13 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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

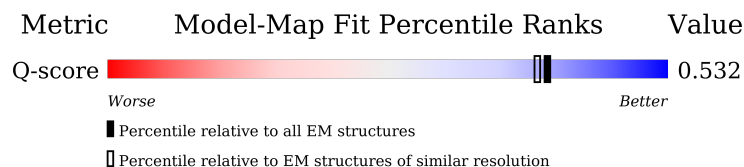
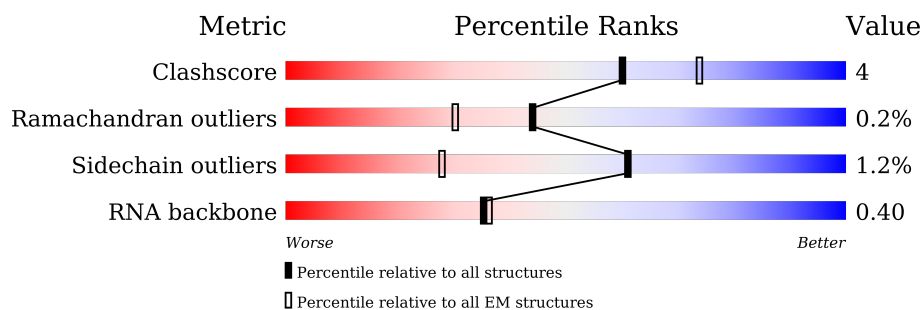
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.13 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.



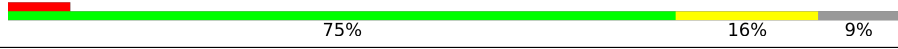
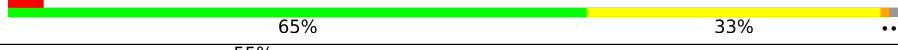
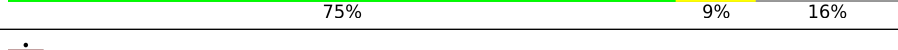
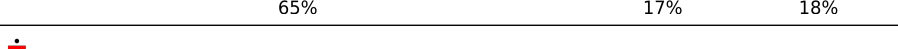
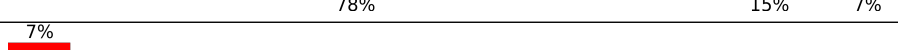
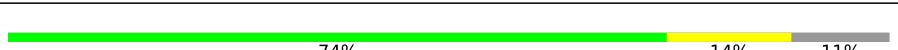
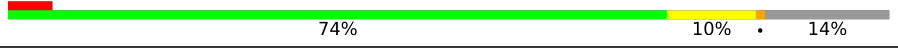
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14478 ( 2.63 - 3.63 )                                    |

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   | 0     | 477    |                  |
| 2   | 1     | 658    |                  |
| 3   | 2     | 5070   |                  |

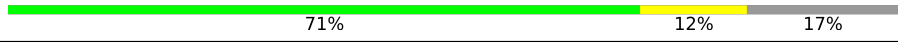
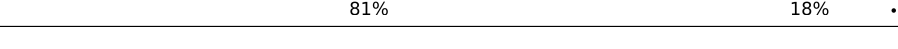
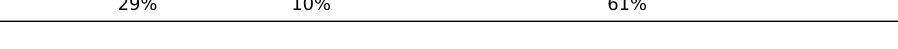
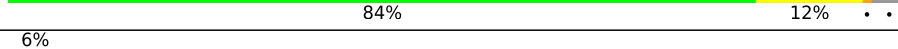
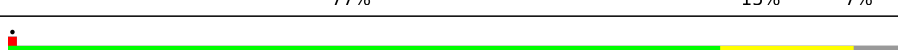
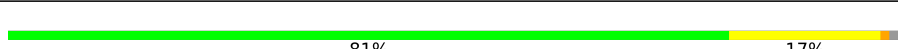
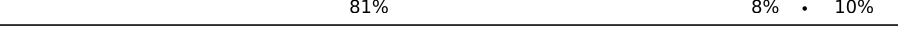
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 534    |    |
| 5   | 5     | 120    |    |
| 6   | 6     | 245    |    |
| 7   | 8     | 156    |    |
| 8   | A     | 217    |    |
| 9   | B     | 403    |    |
| 10  | C     | 159    |    |
| 11  | D     | 427    |    |
| 12  | E     | 115    |    |
| 13  | F     | 117    |    |
| 14  | G     | 266    |    |
| 15  | H     | 123    |  |
| 16  | I     | 192    |  |
| 17  | K     | 105    |  |
| 18  | L     | 148    |  |
| 19  | M     | 97     |  |
| 20  | N     | 178    |  |
| 21  | O     | 70     |  |
| 22  | P     | 51     |  |
| 23  | Q     | 211    |  |
| 24  | S     | 215    |  |
| 25  | T     | 125    |  |
| 26  | U     | 204    |  |
| 27  | V     | 203    |  |
| 28  | W     | 106    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | X     | 92     |    |
| 30  | Y     | 184    |    |
| 31  | Z     | 188    |    |
| 32  | a     | 196    |    |
| 33  | b     | 176    |    |
| 34  | c     | 160    |    |
| 35  | d     | 128    |    |
| 36  | e     | 140    |    |
| 37  | f     | 157    |    |
| 38  | g     | 156    |   |
| 39  | h     | 145    |  |
| 40  | i     | 136    |  |
| 41  | l     | 137    |  |
| 42  | m     | 257    |  |
| 43  | r     | 297    |  |
| 44  | t     | 135    |  |
| 45  | u     | 110    |  |
| 46  | v     | 288    |  |
| 47  | w     | 248    |  |
| 48  | z     | 394    |  |

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 141172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Zinc finger protein 622.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | 0     | 190      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1537  | 968 | 266 | 287 | 16 |         |       |

- Molecule 2 is a protein called Large subunit GTPase 1 homolog.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | 1     | 247      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 988   | 494 | 247 | 247 |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | 2     | 3482     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 74786 | 33362 | 13689 | 24254 | 3481 |         |       |

- Molecule 4 is a protein called 60S ribosomal export protein NMD3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 3     | 255      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2053  | 1305 | 358 | 373 | 17 |         |       |

There are 31 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 3     | 504     | GLY      | -      | expression tag | UNP Q96D46 |
| 3     | 505     | SER      | -      | expression tag | UNP Q96D46 |
| 3     | 506     | GLU      | -      | expression tag | UNP Q96D46 |
| 3     | 507     | ASN      | -      | expression tag | UNP Q96D46 |
| 3     | 508     | LEU      | -      | expression tag | UNP Q96D46 |
| 3     | 509     | TYR      | -      | expression tag | UNP Q96D46 |
| 3     | 510     | PHE      | -      | expression tag | UNP Q96D46 |
| 3     | 511     | GLN      | -      | expression tag | UNP Q96D46 |
| 3     | 512     | GLY      | -      | expression tag | UNP Q96D46 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 3     | 513     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 514     | TYR      | -      | expression tag | UNP Q96D46 |
| 3     | 515     | LYS      | -      | expression tag | UNP Q96D46 |
| 3     | 516     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 517     | HIS      | -      | expression tag | UNP Q96D46 |
| 3     | 518     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 519     | GLY      | -      | expression tag | UNP Q96D46 |
| 3     | 520     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 521     | TYR      | -      | expression tag | UNP Q96D46 |
| 3     | 522     | LYS      | -      | expression tag | UNP Q96D46 |
| 3     | 523     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 524     | HIS      | -      | expression tag | UNP Q96D46 |
| 3     | 525     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 526     | ILE      | -      | expression tag | UNP Q96D46 |
| 3     | 527     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 528     | TYR      | -      | expression tag | UNP Q96D46 |
| 3     | 529     | LYS      | -      | expression tag | UNP Q96D46 |
| 3     | 530     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 531     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 532     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 533     | ASP      | -      | expression tag | UNP Q96D46 |
| 3     | 534     | LYS      | -      | expression tag | UNP Q96D46 |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | 5     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 6 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 6     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1704  | 1060 | 294 | 339 | 11 |         |       |

- Molecule 7 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 7   | 8     | 155      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3294  | 1471 | 583 | 1086 | 154 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | A     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1708  | 1092 | 308 | 300 | 8 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | B     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3238  | 2060 | 608 | 556 | 14 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | C     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 757   | 471 | 166 | 117 | 3 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | D     | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2846  | 1791 | 569 | 472 | 14 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | E     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 732   | 465 | 130 | 131 | 6 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | F     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 544 | 179 | 139 | 6 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | G     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1853  | 1180 | 359 | 310 | 4 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | H     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | I     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | K     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | L     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | M     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | N     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1302  | 823 | 244 | 230 | 5 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21  | O     | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 559   | 360 | 101 | 97 | 1 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | P     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | Q     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | S     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1103  | 707 | 212 | 177 | 7 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | T     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | U     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | V     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1634  | 1053 | 319 | 257 | 5 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | W     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | X     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Y     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Z     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | a     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1217  | 759 | 262 | 187 | 9 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 33  | b     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | c     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1284  | 815 | 250 | 214 | 5 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | d     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 518 | 141 | 147 | 2 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | e     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 613 | 182 | 169 | 5 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 37  | f     | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 519   | 332 | 101 | 83 | 3 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | g     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 612 | 179 | 166 | 1 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | h     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | i     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | l     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | m     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | r     | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2237  | 1414 | 405 | 404 | 14 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | t     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | u     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | v     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1897  | 1217 | 360 | 316 | 4 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | w     | 225      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1878  | 1207 | 361 | 301 | 9 |         |       |

- Molecule 48 is a protein called Proliferation-associated protein 2G4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | z     | 354      | Total | C    | N   | O   | S  | 13      | 0     |
|     |       |          | 2837  | 1792 | 483 | 543 | 19 |         |       |

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 49  | 2     | 236      | Total | Mg  | 0       |
|     |       |          | 236   | 236 |         |
| 49  | 5     | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |
| 49  | 8     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

*Continued on next page...*

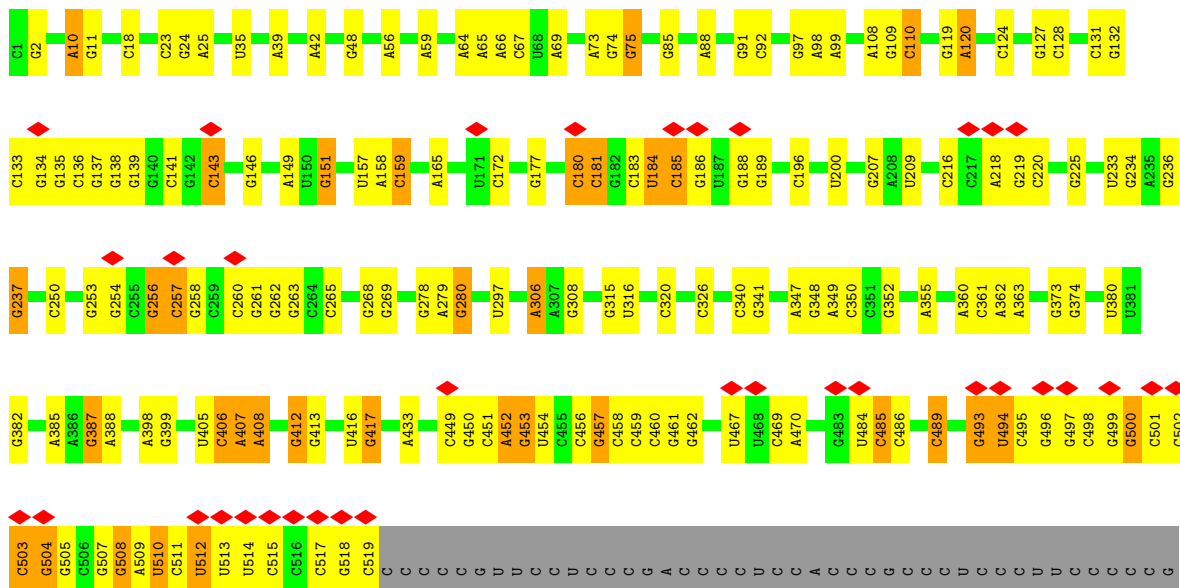
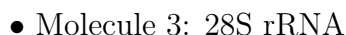
*Continued from previous page...*

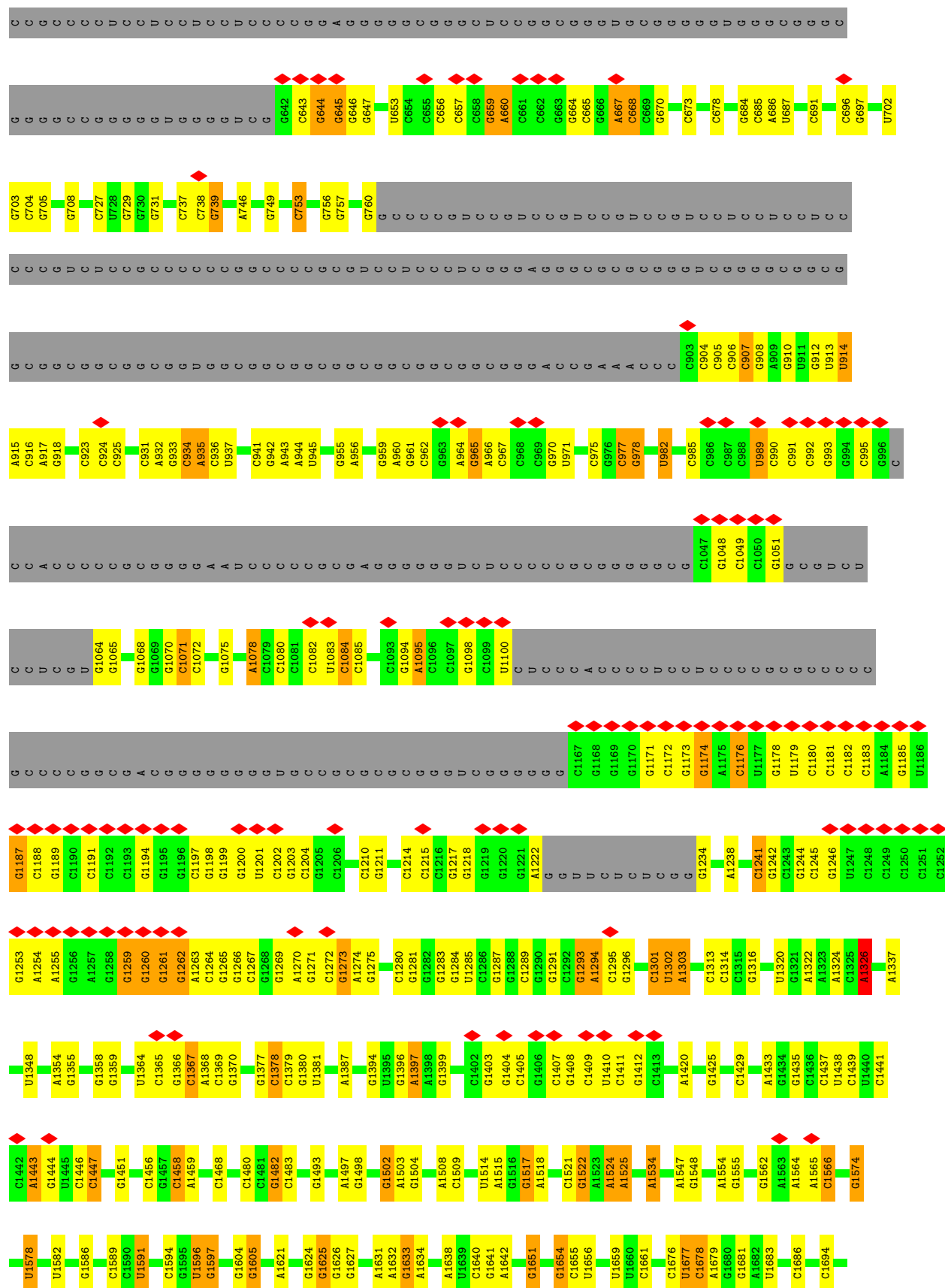
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 49  | F     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 49  | a     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 49  | c     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 49  | m     | 2        | Total<br>2 | Mg<br>2 | 0       |
| 49  | w     | 1        | Total<br>1 | Mg<br>1 | 0       |

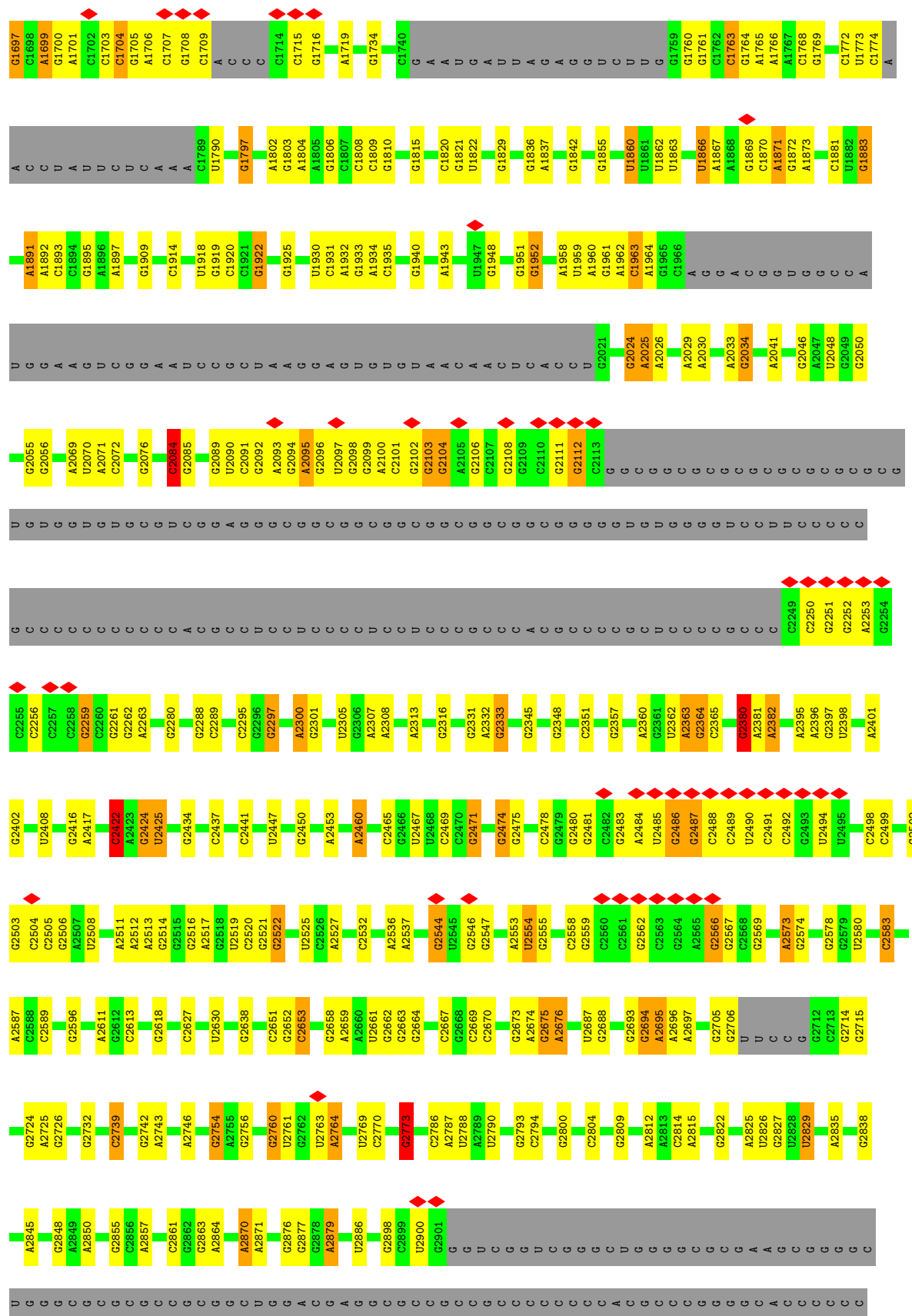
- Molecule 50 is water.

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 50  | 2     | 7        | Total<br>7 | O<br>7 | 0       |

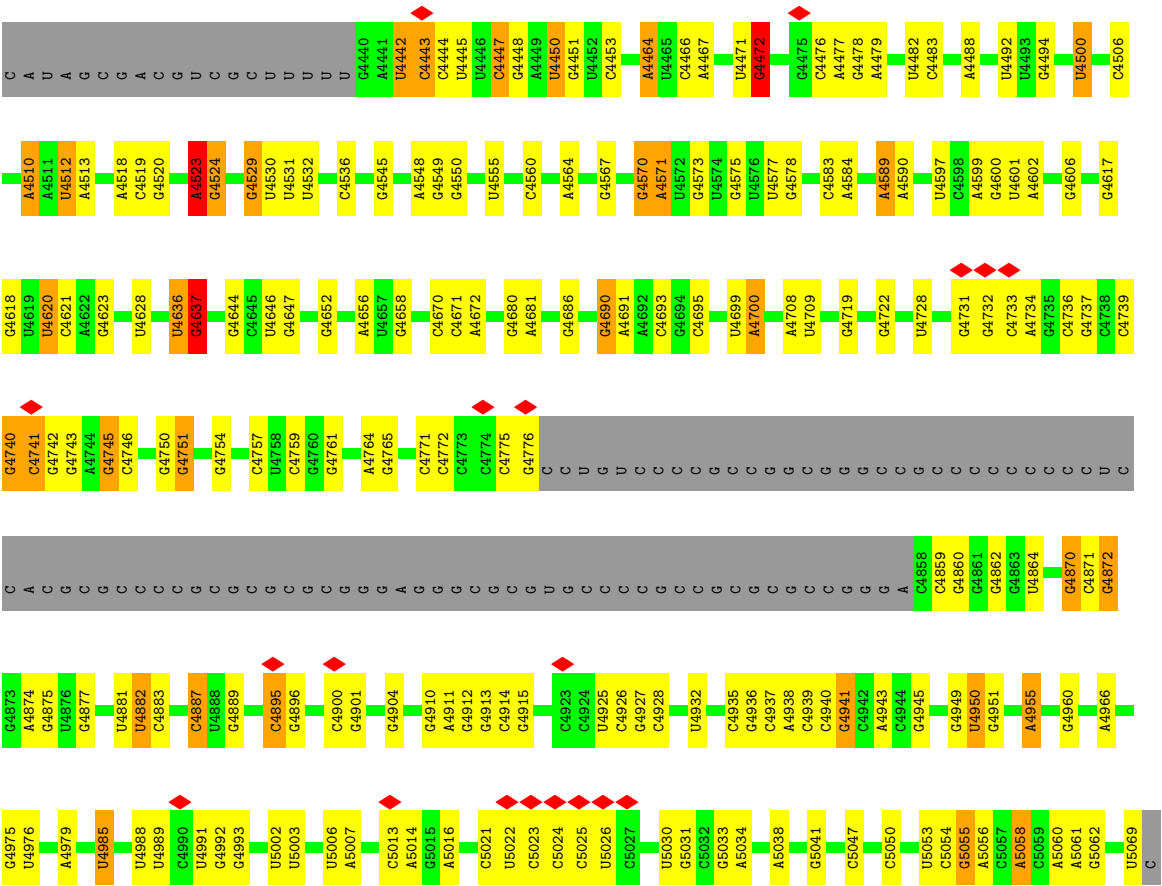




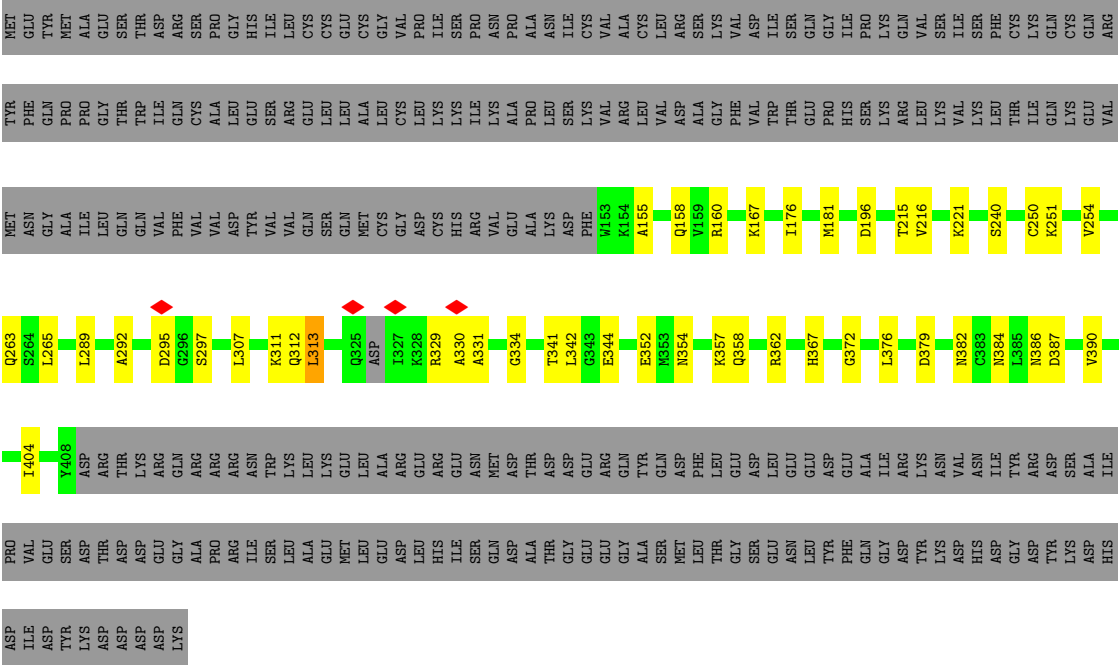
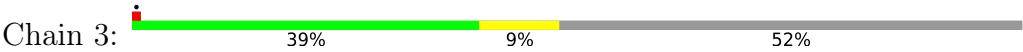








● Molecule 4: 60S ribosomal export protein NMD3



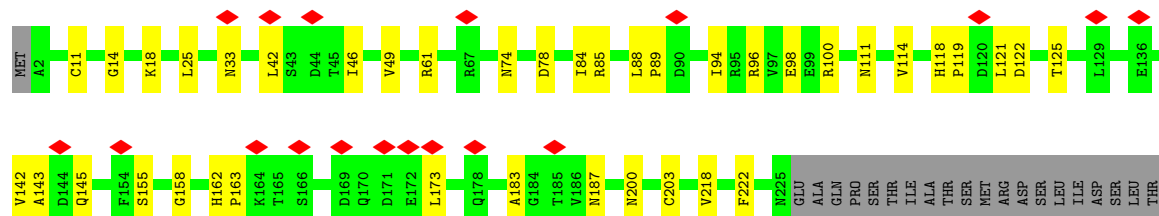
- Molecule 5: 5S rRNA

Chain 5: 



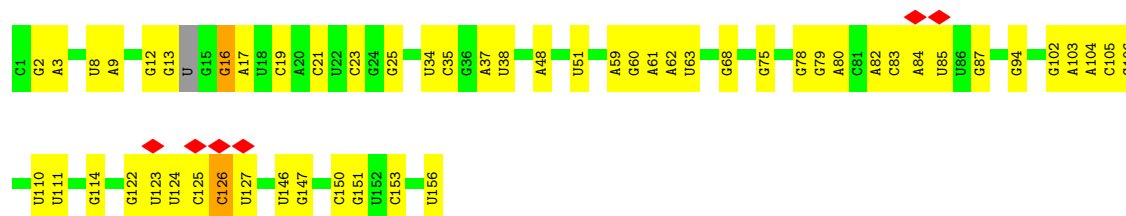
- Molecule 6: Eukaryotic translation initiation factor 6

Chain 6: 



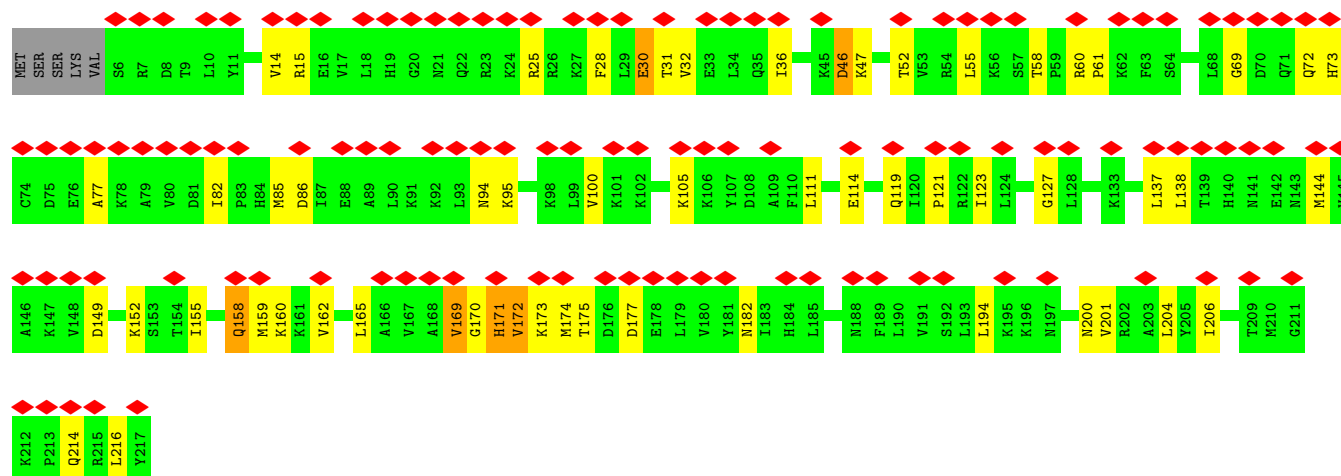
- Molecule 7: 5.8S rRNA

Chain 8: 



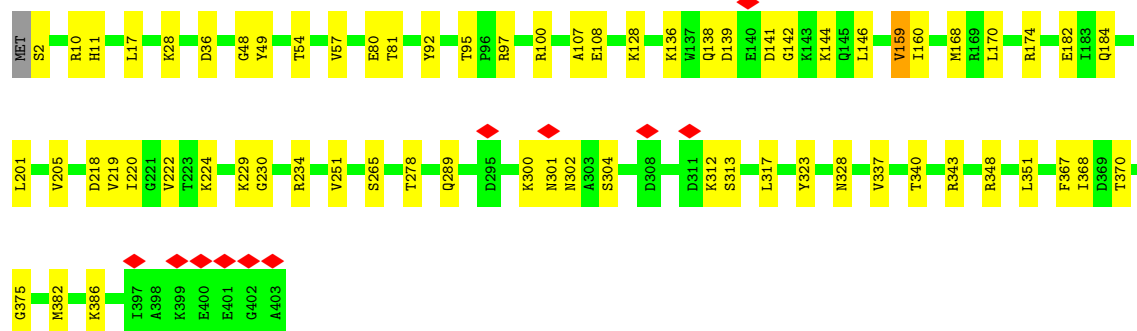
- Molecule 8: 60S ribosomal protein L10a

Chain A: 



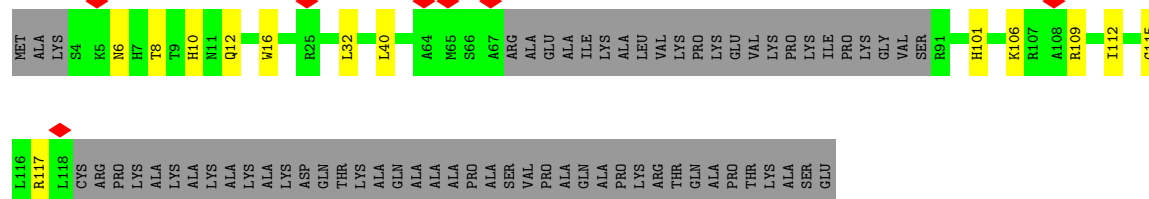
- Molecule 9: 60S ribosomal protein L3

Chain B:  83% 16%



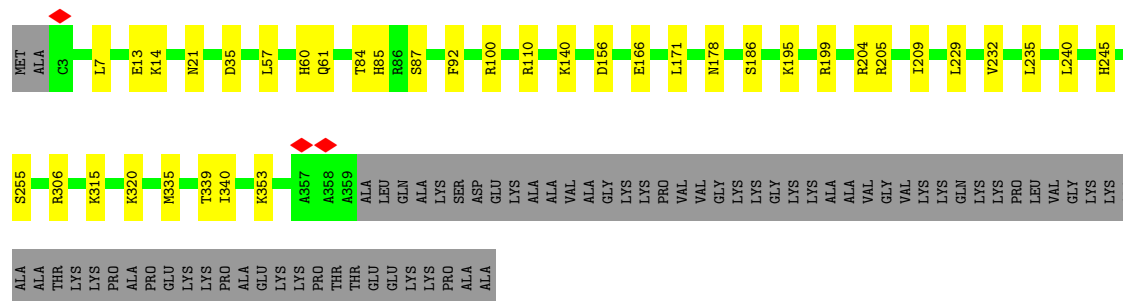
- Molecule 10: 60S ribosomal protein L29

Chain C:  50% 8% 42%



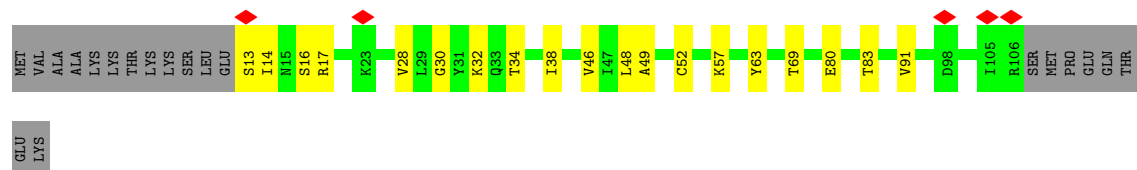
- Molecule 11: 60S ribosomal protein L4

Chain D:  75% 9% 16%



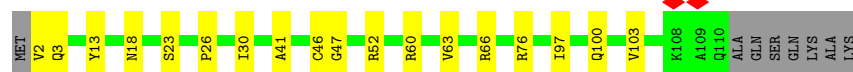
- Molecule 12: 60S ribosomal protein L30

Chain E:  65% 17% 18%



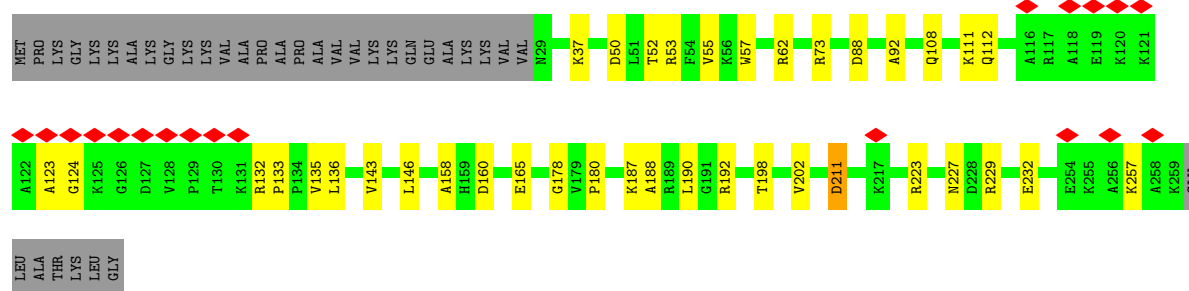
- Molecule 13: 60S ribosomal protein L34

Chain F: 



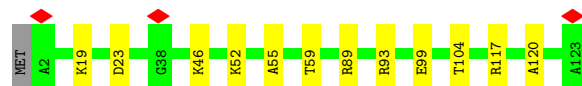
- Molecule 14: 60S ribosomal protein L7a

Chain G: 



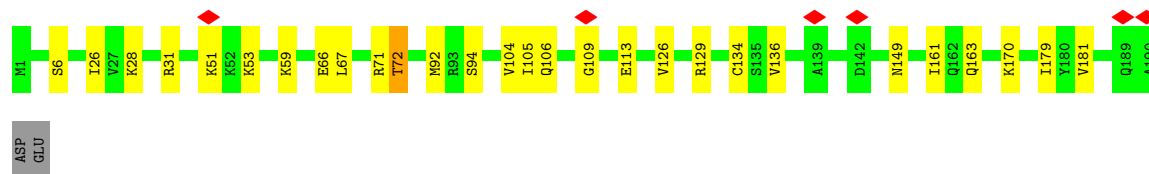
- Molecule 15: 60S ribosomal protein L35

Chain H: 



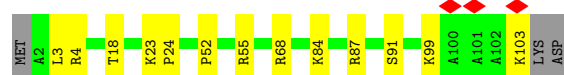
- Molecule 16: 60S ribosomal protein L9

Chain I: 



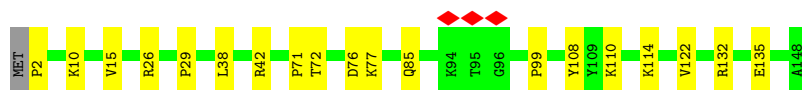
- Molecule 17: 60S ribosomal protein L36

Chain K: 



- Molecule 18: 60S ribosomal protein L27a

Chain L: 



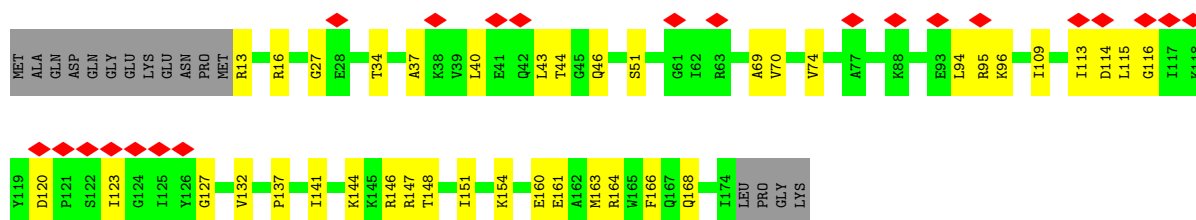
- Molecule 19: 60S ribosomal protein L37

Chain M: 74% 14% 11%



- Molecule 20: 60S ribosomal protein L11

Chain N: 12% 69% 22% 9%



- Molecule 21: 60S ribosomal protein L38

Chain O: 71% 26% 3%



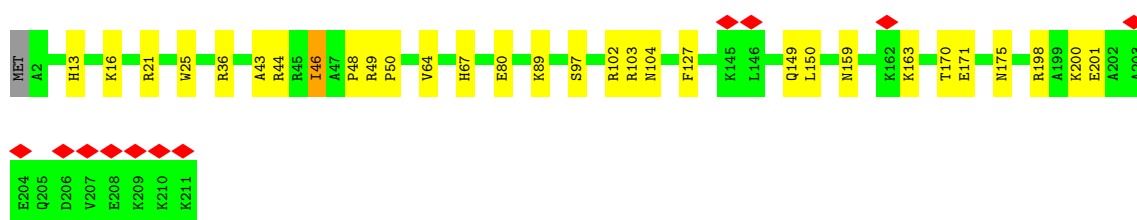
- Molecule 22: 60S ribosomal protein L39

Chain P: 86% 12% 2%



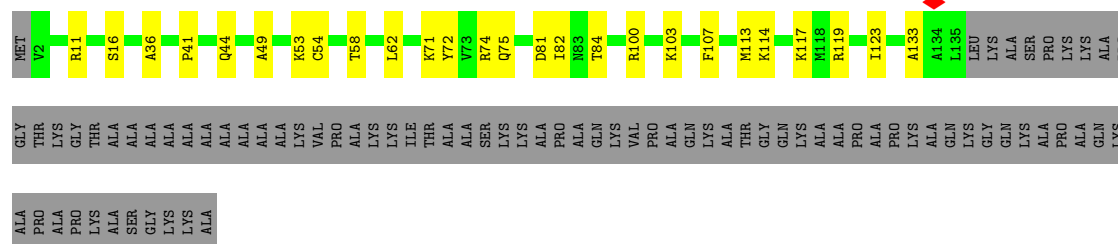
- Molecule 23: 60S ribosomal protein L13

Chain Q: 5% 85% 14%



- Molecule 24: 60S ribosomal protein L14

Chain S:  50% 12% 38%



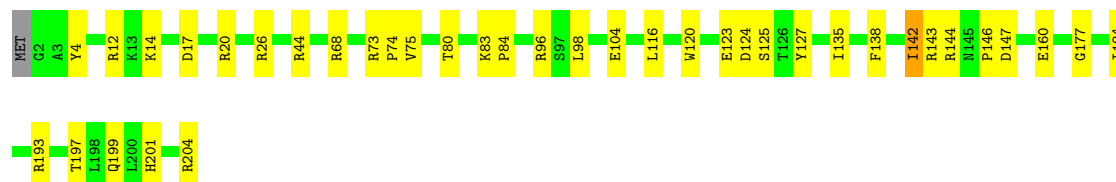
- Molecule 25: 60S ribosomal protein L31

Chain T:  5% 74% 10% 14%



- Molecule 26: 60S ribosomal protein L15

Chain U:  81% 18%



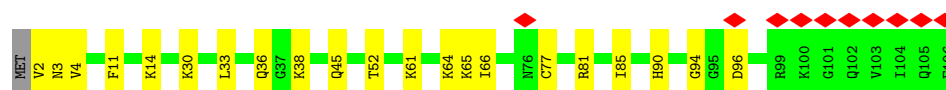
- Molecule 27: 60S ribosomal protein L13a

Chain V:  86% 11%



- Molecule 28: 60S ribosomal protein L36a

Chain W:  9% 79% 20%

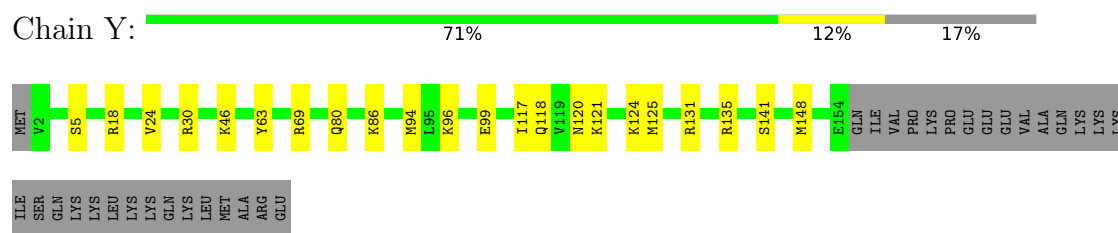


- Molecule 29: 60S ribosomal protein L37a

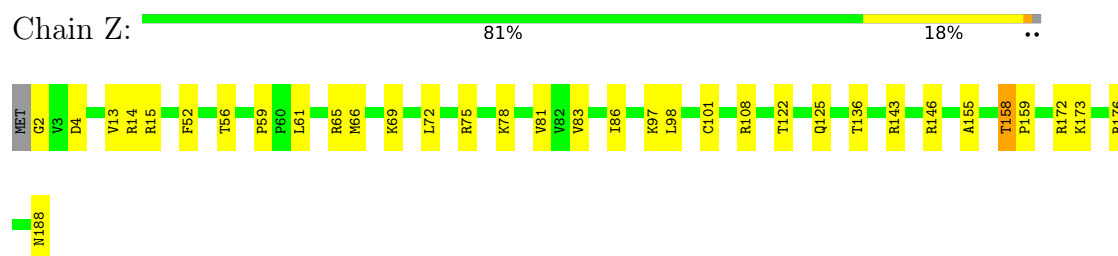
Chain X:  80% 18%



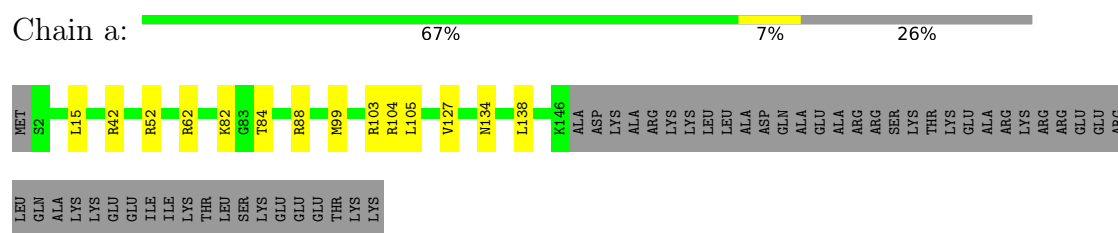
- Molecule 30: 60S ribosomal protein L17



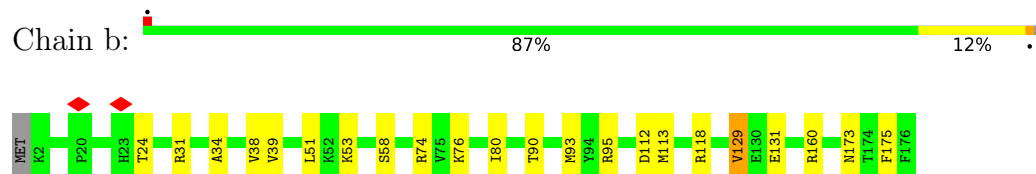
- Molecule 31: 60S ribosomal protein L18



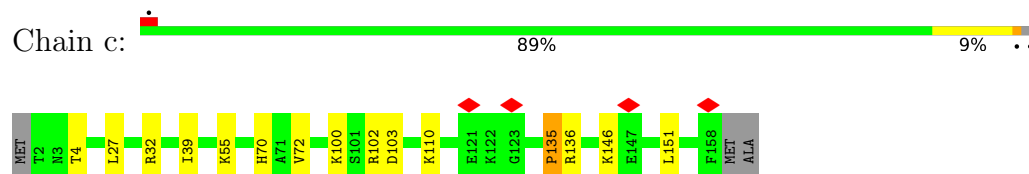
- Molecule 32: 60S ribosomal protein L19



- Molecule 33: 60S ribosomal protein L18a



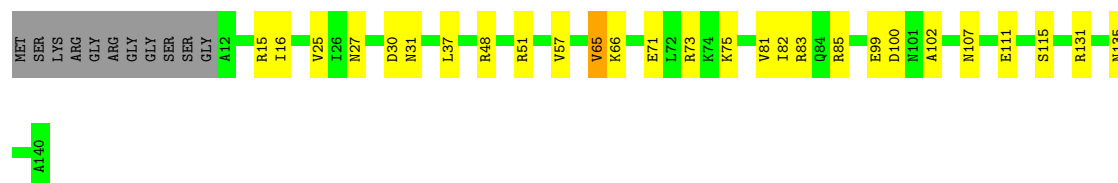
- Molecule 34: 60S ribosomal protein L21



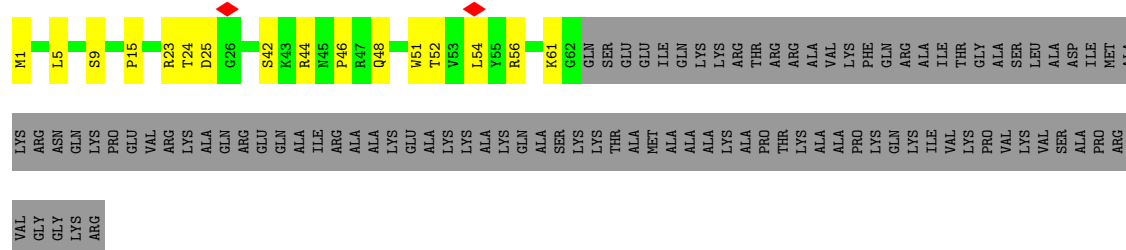
- Molecule 35: 60S ribosomal protein L22



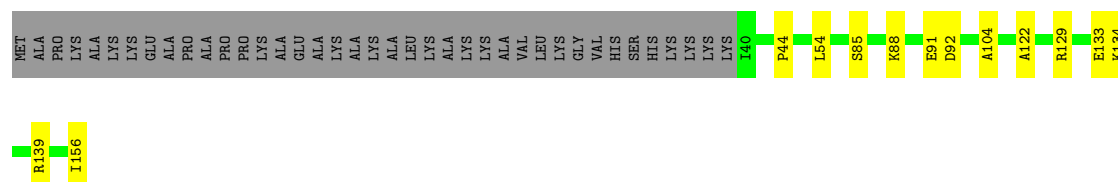
- Molecule 36: 60S ribosomal protein L23



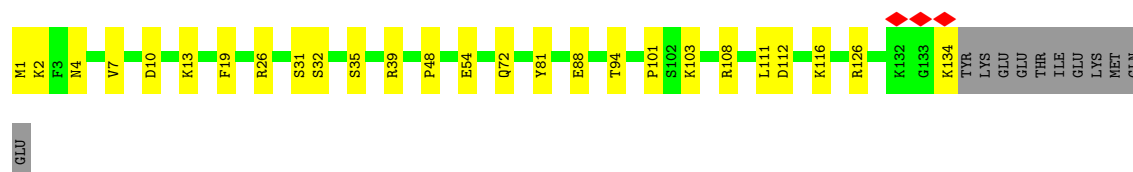
- Molecule 37: 60S ribosomal protein L24



- Molecule 38: 60S ribosomal protein L23a

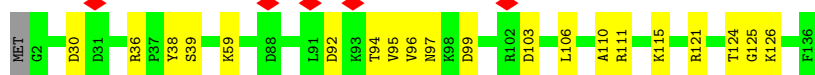


- Molecule 39: 60S ribosomal protein L26



- Molecule 40: 60S ribosomal protein L27

Chain i:  85% 15%



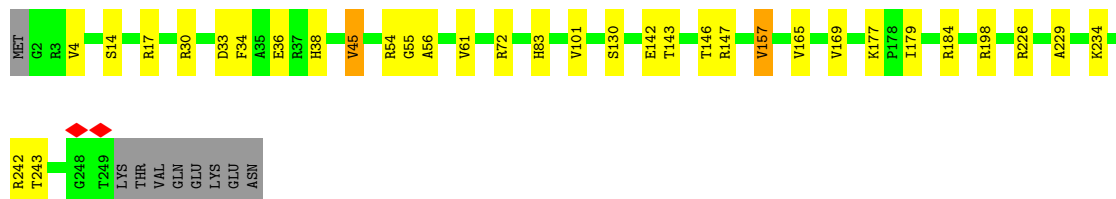
- Molecule 41: 60S ribosomal protein L28

Chain l:  79% 12% 9%



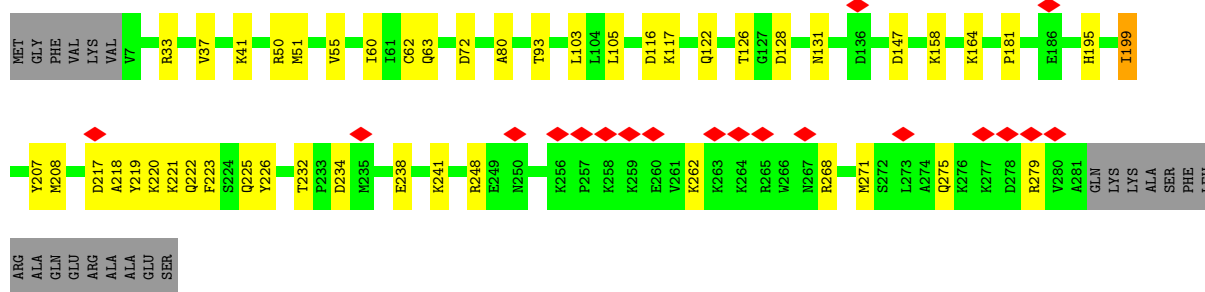
- Molecule 42: 60S ribosomal protein L8

Chain m:  84% 12%



- Molecule 43: 60S ribosomal protein L5

Chain r:  6% 77% 15% 7%



- Molecule 44: 60S ribosomal protein L32

Chain t:  80% 15% 5%

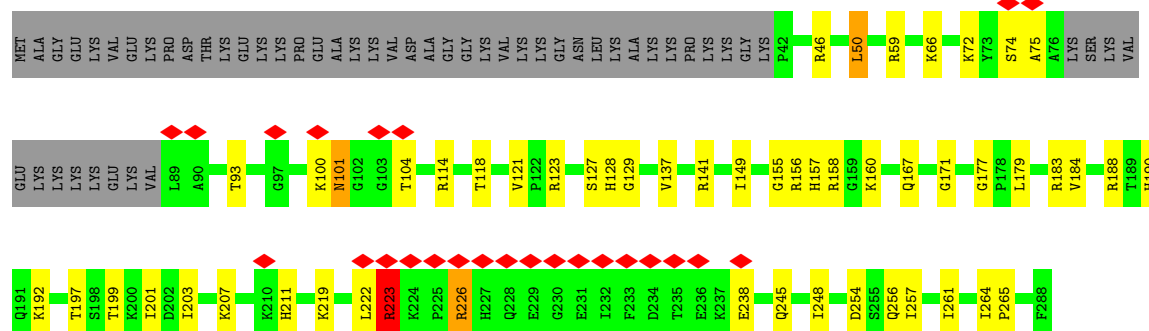


- Molecule 45: 60S ribosomal protein L35a

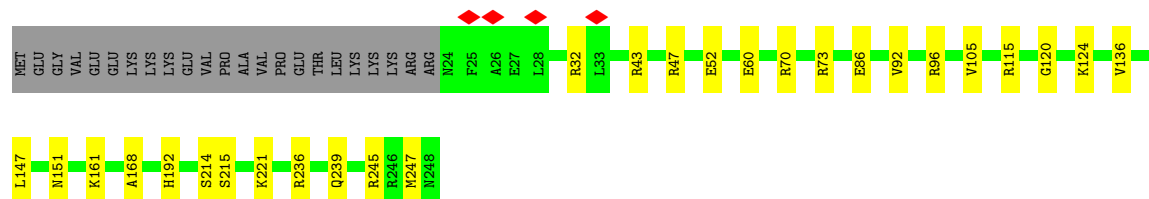
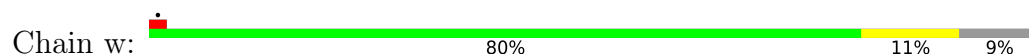
Chain u:  81% 17%



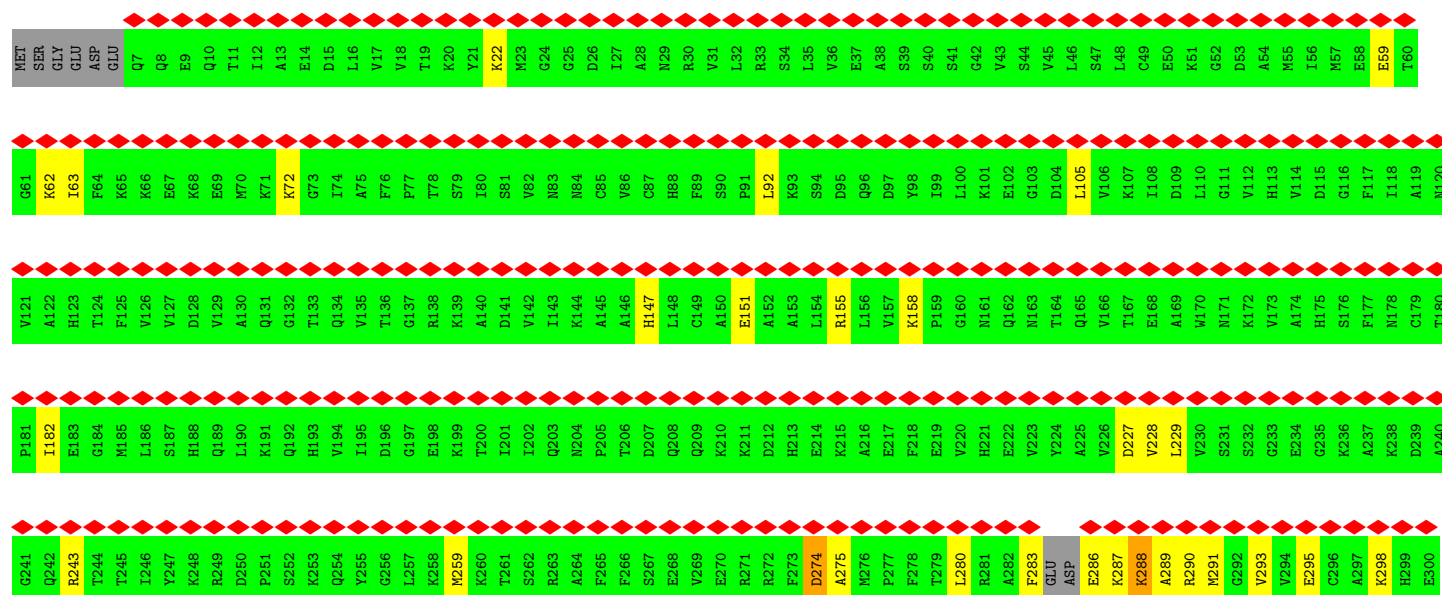
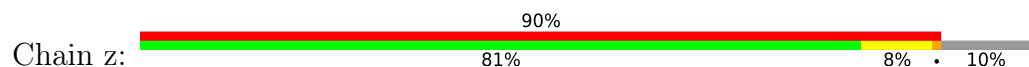
- Molecule 46: 60S ribosomal protein L6



- Molecule 47: 60S ribosomal protein L7



- Molecule 48: Proliferation-associated protein 2G4





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 18819                                   | 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 ( $e^-/\text{\AA}^2$ ) | 64                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.551                                   | Depositor |
| Minimum map value                    | -0.234                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.014                                   | Depositor |
| Recommended contour level            | 0.07                                    | Depositor |
| Map size (Å)                         | 507.84, 507.84, 507.84                  | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.058, 1.058, 1.058                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8Q, B8W, OMG, 7MG, E7G, OMC, 5MC, A2M, PSU, B9B, UR3, MG, M7A, 2MG, B9H, MHG, 1MA, B8K, B8H, 6MZ, BGH, P4U, P7G, 5MU, B8T, E6G, I4U, OMU

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   | 0     | 0.36         | 0/1569         | 0.76        | 3/2098 (0.1%)    |
| 2   | 1     | 0.49         | 0/976          | 1.01        | 1/1199 (0.1%)    |
| 3   | 2     | 0.56         | 2/81127 (0.0%) | 0.52        | 10/126475 (0.0%) |
| 4   | 3     | 0.40         | 0/2096         | 0.68        | 2/2832 (0.1%)    |
| 5   | 5     | 0.44         | 0/2858         | 0.47        | 0/4455           |
| 6   | 6     | 0.37         | 0/1728         | 0.69        | 0/2352           |
| 7   | 8     | 1.58         | 6/3678 (0.2%)  | 0.55        | 3/5728 (0.1%)    |
| 8   | A     | 0.41         | 0/1736         | 0.90        | 4/2328 (0.2%)    |
| 9   | B     | 0.50         | 0/3306         | 0.74        | 0/4424           |
| 10  | C     | 0.36         | 0/769          | 0.62        | 0/1014           |
| 11  | D     | 0.54         | 0/2900         | 0.70        | 0/3895           |
| 12  | E     | 0.46         | 0/742          | 0.68        | 0/996            |
| 13  | F     | 0.50         | 0/878          | 0.68        | 0/1170           |
| 14  | G     | 0.44         | 0/1886         | 0.67        | 0/2539           |
| 15  | H     | 0.45         | 0/1023         | 0.66        | 0/1351           |
| 16  | I     | 0.41         | 0/1537         | 0.66        | 0/2066           |
| 17  | K     | 0.41         | 0/843          | 0.65        | 0/1115           |
| 18  | L     | 0.54         | 0/1191         | 0.61        | 0/1591           |
| 19  | M     | 0.57         | 0/720          | 0.81        | 0/952            |
| 20  | N     | 0.35         | 0/1323         | 0.75        | 0/1768           |
| 21  | O     | 0.38         | 0/565          | 0.62        | 0/750            |
| 22  | P     | 0.57         | 0/454          | 0.75        | 0/599            |
| 23  | Q     | 0.48         | 0/1732         | 0.67        | 0/2315           |
| 24  | S     | 0.46         | 0/1125         | 0.65        | 0/1505           |
| 25  | T     | 0.48         | 0/903          | 0.66        | 0/1216           |
| 26  | U     | 0.56         | 0/1746         | 0.70        | 2/2338 (0.1%)    |
| 27  | V     | 0.52         | 0/1666         | 0.65        | 1/2228 (0.0%)    |
| 28  | W     | 0.46         | 0/876          | 0.71        | 0/1156           |
| 29  | X     | 0.50         | 0/718          | 0.69        | 0/953            |
| 30  | Y     | 0.52         | 0/1268         | 0.65        | 0/1701           |
| 31  | Z     | 0.56         | 0/1537         | 0.75        | 2/2052 (0.1%)    |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 32  | a     | 0.46         | 0/1233          | 0.62        | 0/1633           |
| 33  | b     | 0.48         | 0/1493          | 0.60        | 0/2003           |
| 34  | c     | 0.47         | 0/1312          | 0.65        | 0/1753           |
| 35  | d     | 0.41         | 0/822           | 0.76        | 0/1103           |
| 36  | e     | 0.46         | 0/983           | 0.70        | 0/1319           |
| 37  | f     | 0.40         | 0/532           | 0.65        | 1/708 (0.1%)     |
| 38  | g     | 0.47         | 0/975           | 0.63        | 0/1312           |
| 39  | h     | 0.49         | 0/1132          | 0.69        | 0/1504           |
| 40  | i     | 0.45         | 0/1130          | 0.73        | 0/1507           |
| 41  | l     | 0.50         | 0/1017          | 0.66        | 0/1364           |
| 42  | m     | 0.55         | 0/1936          | 0.77        | 2/2596 (0.1%)    |
| 43  | r     | 0.40         | 0/2281          | 0.66        | 0/3058           |
| 44  | t     | 0.55         | 0/1071          | 0.70        | 0/1429           |
| 45  | u     | 0.55         | 0/895           | 0.72        | 0/1198           |
| 46  | v     | 0.42         | 0/1935          | 0.76        | 2/2596 (0.1%)    |
| 47  | w     | 0.51         | 0/1916          | 0.69        | 0/2553           |
| 48  | z     | 0.66         | 0/2911          | 0.77        | 0/3913           |
| All | All   | 0.58         | 8/149050 (0.0%) | 0.60        | 33/218710 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | 1     | 0                   | 2                   |
| 8   | A     | 0                   | 3                   |
| 9   | B     | 0                   | 1                   |
| 12  | E     | 0                   | 1                   |
| 20  | N     | 0                   | 1                   |
| 21  | O     | 0                   | 1                   |
| 23  | Q     | 0                   | 1                   |
| 26  | U     | 0                   | 1                   |
| 30  | Y     | 0                   | 1                   |
| 34  | c     | 0                   | 1                   |
| 35  | d     | 0                   | 1                   |
| 40  | i     | 0                   | 1                   |
| 41  | l     | 0                   | 1                   |
| 42  | m     | 0                   | 1                   |
| 45  | u     | 0                   | 2                   |
| 46  | v     | 0                   | 2                   |
| 47  | w     | 0                   | 1                   |
| All | All   | 0                   | 22                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | 2     | 417  | G    | C2-N2 | 66.47 | 2.67        | 1.34     |
| 7   | 8     | 16   | G    | N3-C4 | 43.38 | 2.22        | 1.35     |
| 7   | 8     | 16   | G    | C2-N3 | 42.76 | 2.18        | 1.32     |
| 7   | 8     | 16   | G    | C6-N1 | 35.44 | 2.10        | 1.39     |
| 7   | 8     | 16   | G    | N1-C2 | 34.78 | 2.07        | 1.37     |
| 7   | 8     | 16   | G    | C5-C6 | 32.91 | 2.08        | 1.42     |
| 7   | 8     | 16   | G    | C5-C4 | 28.45 | 1.95        | 1.38     |
| 3   | 2     | 3785 | A2M  | O3'-P | 5.07  | 1.61        | 1.56     |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | A     | 170  | GLY  | N-CA-C      | 11.45 | 128.02      | 110.96   |
| 8   | A     | 172  | VAL  | N-CA-C      | 8.19  | 118.25      | 110.30   |
| 8   | A     | 171  | HIS  | N-CA-C      | 8.03  | 120.88      | 110.53   |
| 3   | 2     | 417  | G    | N1-C2-N3    | -7.38 | 101.76      | 123.90   |
| 8   | A     | 14   | VAL  | N-CA-C      | -7.02 | 105.88      | 112.83   |
| 2   | 1     | 447  | VAL  | N-CA-C      | -6.59 | 107.07      | 113.53   |
| 3   | 2     | 417  | G    | C2-N3-C4    | 6.43  | 131.19      | 111.90   |
| 7   | 8     | 16   | G    | C2-N3-C4    | 6.28  | 130.75      | 111.90   |
| 7   | 8     | 16   | G    | N1-C2-N3    | -6.04 | 105.76      | 123.90   |
| 1   | 0     | 251  | ILE  | N-CA-C      | -5.91 | 104.98      | 113.07   |
| 26  | U     | 177  | GLY  | N-CA-C      | 5.80  | 118.76      | 110.46   |
| 1   | 0     | 238  | GLU  | CA-C-N      | 5.77  | 132.09      | 121.70   |
| 1   | 0     | 238  | GLU  | C-N-CA      | 5.77  | 132.09      | 121.70   |
| 4   | 3     | 330  | ALA  | CA-C-N      | 5.75  | 132.53      | 121.54   |
| 4   | 3     | 330  | ALA  | C-N-CA      | 5.75  | 132.53      | 121.54   |
| 3   | 2     | 417  | G    | N1-C2-N2    | 5.71  | 133.32      | 116.20   |
| 46  | v     | 223  | ARG  | N-CA-C      | 5.58  | 117.36      | 111.28   |
| 27  | V     | 110  | PRO  | N-CA-C      | 5.47  | 117.38      | 110.70   |
| 31  | Z     | 158  | THR  | CA-C-N      | 5.47  | 125.12      | 119.05   |
| 31  | Z     | 158  | THR  | C-N-CA      | 5.47  | 125.12      | 119.05   |
| 3   | 2     | 1763 | C    | P-O3'-C3'   | 5.43  | 128.35      | 120.20   |
| 42  | m     | 142  | GLU  | CA-C-N      | 5.36  | 131.78      | 121.54   |
| 42  | m     | 142  | GLU  | C-N-CA      | 5.36  | 131.78      | 121.54   |
| 37  | f     | 25   | ASP  | N-CA-C      | -5.35 | 107.76      | 114.56   |
| 3   | 2     | 485  | C    | C2-N1-C1'   | 5.34  | 134.82      | 118.80   |
| 3   | 2     | 406  | C    | C2'-C3'-O3' | 5.34  | 121.71      | 113.70   |
| 3   | 2     | 914  | U    | P-O3'-C3'   | 5.31  | 128.16      | 120.20   |
| 26  | U     | 142  | ILE  | N-CA-C      | -5.31 | 107.66      | 112.12   |
| 46  | v     | 101  | ASN  | N-CA-C      | -5.30 | 104.46      | 112.99   |
| 3   | 2     | 1633 | G    | P-O3'-C3'   | 5.18  | 127.97      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 7   | 8     | 16   | G    | N3-C4-C5  | -5.17 | 113.08      | 128.60   |
| 3   | 2     | 2675 | G    | P-O3'-C3' | 5.17  | 127.95      | 120.20   |
| 3   | 2     | 2084 | C    | P-O3'-C3' | 5.03  | 127.75      | 120.20   |

There are no chirality outliers.

All (22) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | 1     | 502 | ARG  | Peptide |
| 2   | 1     | 503 | PRO  | Peptide |
| 8   | A     | 158 | GLN  | Peptide |
| 8   | A     | 46  | ASP  | Peptide |
| 8   | A     | 82  | ILE  | Peptide |
| 9   | B     | 17  | LEU  | Peptide |
| 12  | E     | 52  | CYS  | Peptide |
| 20  | N     | 94  | LEU  | Peptide |
| 21  | O     | 10  | ASP  | Peptide |
| 23  | Q     | 46  | ILE  | Peptide |
| 26  | U     | 147 | ASP  | Peptide |
| 30  | Y     | 131 | ARG  | Peptide |
| 34  | c     | 135 | PRO  | Peptide |
| 35  | d     | 20  | LYS  | Peptide |
| 40  | i     | 124 | THR  | Peptide |
| 41  | l     | 20  | ARG  | Peptide |
| 42  | m     | 54  | ARG  | Peptide |
| 45  | u     | 103 | VAL  | Peptide |
| 45  | u     | 106 | TYR  | Peptide |
| 46  | v     | 129 | GLY  | Peptide |
| 46  | v     | 203 | ILE  | Peptide |
| 47  | w     | 221 | LYS  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1537  | 0        | 1491     | 21      | 0            |
| 2   | 1     | 988   | 0        | 236      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 2     | 74786 | 0        | 37567    | 384     | 0            |
| 4   | 3     | 2053  | 0        | 2058     | 41      | 0            |
| 5   | 5     | 2558  | 0        | 1296     | 13      | 0            |
| 6   | 6     | 1704  | 0        | 1677     | 25      | 0            |
| 7   | 8     | 3294  | 0        | 1674     | 38      | 0            |
| 8   | A     | 1708  | 0        | 1815     | 43      | 0            |
| 9   | B     | 3238  | 0        | 3376     | 36      | 0            |
| 10  | C     | 757   | 0        | 818      | 10      | 0            |
| 11  | D     | 2846  | 0        | 3017     | 25      | 0            |
| 12  | E     | 732   | 0        | 767      | 9       | 0            |
| 13  | F     | 868   | 0        | 963      | 12      | 0            |
| 14  | G     | 1853  | 0        | 1987     | 24      | 0            |
| 15  | H     | 1015  | 0        | 1148     | 11      | 0            |
| 16  | I     | 1518  | 0        | 1601     | 19      | 0            |
| 17  | K     | 832   | 0        | 917      | 7       | 0            |
| 18  | L     | 1162  | 0        | 1213     | 13      | 0            |
| 19  | M     | 705   | 0        | 739      | 11      | 0            |
| 20  | N     | 1302  | 0        | 1337     | 20      | 0            |
| 21  | O     | 559   | 0        | 624      | 12      | 0            |
| 22  | P     | 444   | 0        | 483      | 5       | 0            |
| 23  | Q     | 1701  | 0        | 1818     | 24      | 0            |
| 24  | S     | 1103  | 0        | 1160     | 18      | 0            |
| 25  | T     | 888   | 0        | 930      | 8       | 0            |
| 26  | U     | 1701  | 0        | 1749     | 26      | 0            |
| 27  | V     | 1634  | 0        | 1778     | 14      | 0            |
| 28  | W     | 862   | 0        | 933      | 14      | 0            |
| 29  | X     | 708   | 0        | 757      | 13      | 0            |
| 30  | Y     | 1242  | 0        | 1268     | 14      | 0            |
| 31  | Z     | 1513  | 0        | 1628     | 24      | 0            |
| 32  | a     | 1217  | 0        | 1339     | 11      | 0            |
| 33  | b     | 1453  | 0        | 1490     | 14      | 0            |
| 34  | c     | 1284  | 0        | 1352     | 11      | 0            |
| 35  | d     | 808   | 0        | 831      | 13      | 0            |
| 36  | e     | 969   | 0        | 1031     | 18      | 0            |
| 37  | f     | 519   | 0        | 533      | 10      | 0            |
| 38  | g     | 958   | 0        | 1027     | 16      | 0            |
| 39  | h     | 1115  | 0        | 1205     | 18      | 0            |
| 40  | i     | 1107  | 0        | 1182     | 12      | 0            |
| 41  | l     | 1002  | 0        | 1068     | 11      | 0            |
| 42  | m     | 1898  | 0        | 1993     | 17      | 0            |
| 43  | r     | 2237  | 0        | 2253     | 33      | 0            |
| 44  | t     | 1053  | 0        | 1147     | 13      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 45  | u     | 876    | 0        | 912      | 9       | 0            |
| 46  | v     | 1897   | 0        | 2046     | 44      | 0            |
| 47  | w     | 1878   | 0        | 2009     | 19      | 0            |
| 48  | z     | 2837   | 0        | 2868     | 47      | 0            |
| 49  | 2     | 236    | 0        | 0        | 0       | 0            |
| 49  | 5     | 3      | 0        | 0        | 0       | 0            |
| 49  | 8     | 1      | 0        | 0        | 0       | 0            |
| 49  | F     | 1      | 0        | 0        | 0       | 0            |
| 49  | a     | 1      | 0        | 0        | 0       | 0            |
| 49  | c     | 1      | 0        | 0        | 0       | 0            |
| 49  | m     | 2      | 0        | 0        | 0       | 0            |
| 49  | w     | 1      | 0        | 0        | 0       | 0            |
| 50  | 2     | 7      | 0        | 0        | 0       | 0            |
| All | All   | 141172 | 0        | 103111   | 1031    | 0            |

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

All (1031) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:2:1860:B8H:C5   | 3:2:1860:B8H:C4  | 1.81                     | 1.59              |
| 3:2:4296:B8H:C5   | 3:2:4296:B8H:C4  | 1.80                     | 1.56              |
| 7:8:16:G:C4       | 7:8:16:G:C5      | 1.95                     | 1.43              |
| 7:8:16:G:C5       | 7:8:16:G:C6      | 2.08                     | 1.41              |
| 8:A:171:HIS:CD2   | 8:A:174:MET:HG3  | 1.53                     | 1.41              |
| 4:3:329:ARG:NH1   | 4:3:334:GLY:HA3  | 1.43                     | 1.30              |
| 3:2:417:G:N2      | 7:8:16:G:N3      | 1.81                     | 1.27              |
| 4:3:329:ARG:NH1   | 4:3:334:GLY:CA   | 1.98                     | 1.25              |
| 7:8:16:G:C2       | 7:8:16:G:N1      | 2.07                     | 1.23              |
| 3:2:4529:B8W:O4'  | 3:2:4529:B8W:C1' | 1.65                     | 1.23              |
| 3:2:4185:B8W:O4'  | 3:2:4185:B8W:C1' | 1.65                     | 1.19              |
| 3:2:4129:B8W:O4'  | 3:2:4129:B8W:C1' | 1.65                     | 1.19              |
| 3:2:2380:B8W:O4'  | 3:2:2380:B8W:C1' | 1.65                     | 1.18              |
| 7:8:16:G:C6       | 7:8:16:G:N1      | 2.10                     | 1.18              |
| 3:2:4472:B8W:O4'  | 3:2:4472:B8W:C1' | 1.65                     | 1.17              |
| 3:2:3897:B8K:O4'  | 3:2:3897:B8K:C4' | 1.67                     | 1.15              |
| 3:2:4690:B8K:O4'  | 3:2:4690:B8K:C4' | 1.66                     | 1.14              |
| 3:2:3899:BGH:O4'  | 3:2:3899:BGH:C4' | 1.65                     | 1.14              |
| 7:8:16:G:N3       | 7:8:16:G:C2      | 2.18                     | 1.11              |
| 38:g:156:ILE:HD12 | 48:z:291:MET:HE1 | 1.27                     | 1.11              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 7:8:16:G:C4         | 7:8:16:G:N3       | 2.22                     | 1.07              |
| 48:z:283:PHE:O      | 48:z:286:GLU:HA   | 1.54                     | 1.05              |
| 3:2:5016:A:C2       | 3:2:5033:G:N2     | 2.26                     | 1.03              |
| 48:z:92:LEU:CD1     | 48:z:290:ARG:HH21 | 1.73                     | 1.01              |
| 3:2:4887:C:N4       | 3:2:4932:U:H3     | 1.58                     | 1.00              |
| 38:g:91:GLU:OE2     | 48:z:259:MET:HE2  | 1.64                     | 0.98              |
| 3:2:417:G:N2        | 7:8:16:G:C2       | 2.32                     | 0.98              |
| 3:2:5016:A:H2       | 3:2:5033:G:N2     | 1.59                     | 0.96              |
| 3:2:417:G:N2        | 7:8:16:G:C4       | 2.33                     | 0.96              |
| 8:A:171:HIS:CD2     | 8:A:174:MET:CG    | 2.48                     | 0.95              |
| 48:z:92:LEU:HD13    | 48:z:290:ARG:HH21 | 1.31                     | 0.95              |
| 48:z:288:LYS:N      | 48:z:288:LYS:HE3  | 1.82                     | 0.94              |
| 3:2:1095:A:H2       | 3:2:1200:G:H1     | 1.03                     | 0.94              |
| 3:2:493:G:N1        | 3:2:660:A:C2      | 2.38                     | 0.92              |
| 38:g:156:ILE:HD12   | 48:z:291:MET:CE   | 2.00                     | 0.91              |
| 4:3:329:ARG:HH12    | 4:3:334:GLY:HA3   | 1.29                     | 0.90              |
| 8:A:171:HIS:HD2     | 8:A:174:MET:CG    | 1.82                     | 0.90              |
| 3:2:493:G:H1        | 3:2:660:A:H2      | 1.08                     | 0.89              |
| 3:2:1094:G:H1       | 3:2:1201:U:H3     | 0.90                     | 0.89              |
| 38:g:156:ILE:CD1    | 48:z:291:MET:HE1  | 2.02                     | 0.88              |
| 3:2:5016:A:H2       | 3:2:5033:G:H21    | 0.96                     | 0.87              |
| 3:2:1095:A:C2       | 3:2:1200:G:N1     | 2.41                     | 0.87              |
| 48:z:147[B]:HIS:HD2 | 48:z:151:GLU:OE2  | 1.56                     | 0.87              |
| 3:2:4254:G:H1       | 3:2:4257:A:H62    | 1.21                     | 0.87              |
| 3:2:452:A:N1        | 46:v:223:ARG:HG2  | 1.93                     | 0.83              |
| 48:z:92:LEU:HD13    | 48:z:290:ARG:NH2  | 1.93                     | 0.83              |
| 4:3:329:ARG:HH11    | 4:3:334:GLY:HA3   | 1.40                     | 0.82              |
| 48:z:243:ARG:HE     | 48:z:290:ARG:HE   | 1.27                     | 0.80              |
| 3:2:3642:A:HO2'     | 19:M:2:THR:N      | 1.79                     | 0.80              |
| 8:A:171:HIS:O       | 8:A:174:MET:HB2   | 1.82                     | 0.79              |
| 48:z:243:ARG:NE     | 48:z:290:ARG:NE   | 2.28                     | 0.79              |
| 4:3:329:ARG:NH2     | 4:3:334:GLY:O     | 2.17                     | 0.78              |
| 3:2:417:G:N2        | 7:8:16:G:C5       | 2.52                     | 0.78              |
| 48:z:283:PHE:HB3    | 48:z:289:ALA:HB2  | 1.65                     | 0.78              |
| 3:2:1095:A:H2       | 3:2:1200:G:N1     | 1.81                     | 0.77              |
| 48:z:288:LYS:HE3    | 48:z:288:LYS:H    | 1.48                     | 0.77              |
| 3:2:417:G:C2        | 7:8:16:G:C6       | 2.73                     | 0.77              |
| 48:z:280:LEU:HD21   | 48:z:293:VAL:HG21 | 1.66                     | 0.77              |
| 48:z:243:ARG:NE     | 48:z:290:ARG:HE   | 1.76                     | 0.77              |
| 8:A:25:ARG:CZ       | 8:A:30:GLU:OE2    | 2.33                     | 0.77              |
| 3:2:684:G:O3'       | 46:v:101:ASN:HB2  | 1.85                     | 0.76              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 48:z:147[B]:HIS:CD2 | 48:z:151:GLU:OE2  | 2.39                     | 0.76              |
| 3:2:417:G:N2        | 7:8:16:G:C6       | 2.54                     | 0.76              |
| 3:2:4993:G:H1       | 3:2:5058:A:H61    | 1.34                     | 0.76              |
| 3:2:4887:C:H42      | 3:2:4932:U:H3     | 0.81                     | 0.76              |
| 3:2:417:G:C2        | 7:8:16:G:N3       | 2.54                     | 0.76              |
| 3:2:493:G:N1        | 3:2:660:A:H2      | 1.76                     | 0.76              |
| 48:z:280:LEU:HD21   | 48:z:293:VAL:CG2  | 2.17                     | 0.75              |
| 48:z:283:PHE:O      | 48:z:286:GLU:CA   | 2.33                     | 0.75              |
| 3:2:417:G:C2        | 7:8:16:G:C4       | 2.75                     | 0.74              |
| 38:g:156:ILE:CG2    | 48:z:291:MET:HE2  | 2.18                     | 0.74              |
| 3:2:4745:G:H1       | 3:2:4955:A:H61    | 1.33                     | 0.74              |
| 4:3:329:ARG:NH1     | 4:3:334:GLY:HA2   | 1.98                     | 0.74              |
| 4:3:329:ARG:NH1     | 4:3:334:GLY:C     | 2.46                     | 0.73              |
| 3:2:417:G:C2        | 7:8:16:G:C2       | 2.77                     | 0.73              |
| 8:A:25:ARG:NH1      | 8:A:30:GLU:OE2    | 2.22                     | 0.72              |
| 6:6:18:LYS:HB3      | 6:6:25:LEU:HB2    | 1.72                     | 0.72              |
| 38:g:156:ILE:HG21   | 48:z:291:MET:HE2  | 1.72                     | 0.72              |
| 3:2:417:G:N2        | 7:8:16:G:N1       | 2.38                     | 0.71              |
| 3:2:1100:U:H3       | 3:2:1194:G:H1     | 1.39                     | 0.71              |
| 8:A:171:HIS:CD2     | 8:A:174:MET:HE3   | 2.26                     | 0.70              |
| 8:A:171:HIS:HD2     | 8:A:174:MET:HG3   | 0.93                     | 0.70              |
| 48:z:92:LEU:HD12    | 48:z:290:ARG:HH21 | 1.57                     | 0.69              |
| 48:z:92:LEU:CD1     | 48:z:290:ARG:NH2  | 2.52                     | 0.69              |
| 3:2:417:G:C2        | 7:8:16:G:C5       | 2.81                     | 0.69              |
| 3:2:1521:C:OP1      | 11:D:100:ARG:NH2  | 2.26                     | 0.69              |
| 3:2:4618:G:H5''     | 36:e:15:ARG:HB2   | 1.74                     | 0.68              |
| 3:2:417:G:C2        | 7:8:16:G:N1       | 2.62                     | 0.67              |
| 3:2:1095:A:N1       | 3:2:1200:G:O6     | 2.27                     | 0.67              |
| 36:e:85:ARG:HE      | 36:e:100:ASP:HA   | 1.59                     | 0.67              |
| 5:5:2:U:H3          | 5:5:117:G:H1      | 1.42                     | 0.67              |
| 46:v:223:ARG:HA     | 46:v:223:ARG:NE   | 2.09                     | 0.67              |
| 9:B:289:GLN:HB3     | 9:B:301:ASN:HB3   | 1.75                     | 0.67              |
| 3:2:684:G:H4'       | 46:v:100:LYS:O    | 1.94                     | 0.67              |
| 3:2:374:G:OP2       | 19:M:56:ARG:NH1   | 2.27                     | 0.67              |
| 25:T:90:ARG:HD3     | 25:T:102:LEU:HD13 | 1.76                     | 0.67              |
| 3:2:2845:A:H61      | 3:2:3843:C:H42    | 1.42                     | 0.66              |
| 24:S:62:LEU:HD21    | 24:S:82:ILE:HD11  | 1.76                     | 0.66              |
| 48:z:280:LEU:CD2    | 48:z:293:VAL:HG21 | 2.25                     | 0.66              |
| 3:2:493:G:O6        | 3:2:660:A:N1      | 2.29                     | 0.66              |
| 3:2:2095:A:N7       | 47:w:32:ARG:NH1   | 2.44                     | 0.66              |
| 3:2:4751:G:N7       | 45:u:52:LYS:NZ    | 2.42                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:329:ARG:NH1   | 4:3:334:GLY:O     | 2.28                     | 0.66              |
| 3:2:1656:U:OP2    | 18:L:26:ARG:NH2   | 2.29                     | 0.66              |
| 46:v:223:ARG:NE   | 46:v:223:ARG:O    | 2.29                     | 0.65              |
| 8:A:25:ARG:NH2    | 8:A:30:GLU:OE2    | 2.28                     | 0.65              |
| 4:3:158:GLN:HB3   | 4:3:160:ARG:HH11  | 1.61                     | 0.65              |
| 44:t:92:ASN:HB3   | 46:v:118:THR:HG21 | 1.78                     | 0.65              |
| 48:z:182:ILE:HD12 | 48:z:229:LEU:HB3  | 1.79                     | 0.65              |
| 46:v:226:ARG:O    | 46:v:226:ARG:HG3  | 1.96                     | 0.65              |
| 8:A:171:HIS:CD2   | 8:A:174:MET:CE    | 2.80                     | 0.64              |
| 24:S:119:ARG:HE   | 27:V:193:THR:HG22 | 1.61                     | 0.64              |
| 8:A:171:HIS:NE2   | 8:A:174:MET:HG3   | 2.10                     | 0.64              |
| 40:i:103:ASP:HB3  | 40:i:106:LEU:HB2  | 1.79                     | 0.64              |
| 38:g:91:GLU:OE2   | 48:z:259:MET:CE   | 2.42                     | 0.64              |
| 36:e:16:ILE:HD11  | 36:e:57:VAL:H     | 1.62                     | 0.64              |
| 3:2:2554:U:O2     | 3:2:2764:A:N7     | 2.30                     | 0.64              |
| 20:N:37:ALA:HB2   | 20:N:70:VAL:HG11  | 1.80                     | 0.64              |
| 8:A:194:LEU:HB3   | 8:A:200:ASN:HD22  | 1.63                     | 0.64              |
| 43:r:232:THR:HG22 | 43:r:234:ASP:H    | 1.62                     | 0.63              |
| 6:6:118:HIS:HB3   | 6:6:121:LEU:HD23  | 1.80                     | 0.63              |
| 43:r:50:ARG:NH2   | 43:r:72:ASP:OD2   | 2.31                     | 0.63              |
| 3:2:1443:A:N1     | 3:2:2104:G:N2     | 2.46                     | 0.63              |
| 33:b:95:ARG:NH1   | 33:b:113:MET:SD   | 2.72                     | 0.63              |
| 3:2:500:G:N3      | 3:2:504:G:N2      | 2.46                     | 0.63              |
| 46:v:190:HIS:HD2  | 46:v:192:LYS:H    | 1.46                     | 0.63              |
| 5:5:60:G:O2'      | 43:r:268:ARG:NH1  | 2.32                     | 0.63              |
| 48:z:243:ARG:HE   | 48:z:290:ARG:NE   | 1.88                     | 0.63              |
| 3:2:1654:G:N2     | 3:2:1678:C:OP1    | 2.32                     | 0.63              |
| 8:A:72:GLN:HE22   | 20:N:34:THR:HB    | 1.63                     | 0.63              |
| 3:2:4077:A:N1     | 3:2:4171:C:N4     | 2.46                     | 0.62              |
| 3:2:417:G:N2      | 3:2:417:G:C2      | 2.67                     | 0.62              |
| 3:2:4941:G:OP2    | 46:v:188:ARG:NH1  | 2.32                     | 0.62              |
| 3:2:2583:C:OP2    | 13:F:76:ARG:NH1   | 2.32                     | 0.62              |
| 3:2:4523:A2M:H5'' | 3:2:4524:G:H5'    | 1.80                     | 0.62              |
| 7:8:51:U:OP2      | 22:P:21:ARG:NH2   | 2.33                     | 0.62              |
| 9:B:92:TYR:HB2    | 9:B:159:VAL:HG13  | 1.82                     | 0.62              |
| 28:W:45:GLN:HE22  | 28:W:52:THR:H     | 1.47                     | 0.62              |
| 3:2:1176:C:H4'    | 43:r:279:ARG:HE   | 1.64                     | 0.61              |
| 4:3:329:ARG:HH12  | 4:3:334:GLY:CA    | 1.93                     | 0.61              |
| 9:B:170:LEU:O     | 9:B:328:ASN:ND2   | 2.33                     | 0.61              |
| 14:G:180:PRO:HA   | 14:G:227:ASN:HD21 | 1.65                     | 0.61              |
| 3:2:1100:U:O2     | 3:2:1194:G:N2     | 2.33                     | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:B:108:GLU:OE2   | 9:B:138:GLN:NE2  | 2.33                     | 0.61              |
| 39:h:112:ASP:O    | 39:h:116:LYS:HB2 | 1.99                     | 0.61              |
| 3:2:2474:G:N2     | 3:2:2502:G:O2'   | 2.33                     | 0.61              |
| 3:2:4646:U:OP2    | 32:a:62:ARG:NH2  | 2.34                     | 0.61              |
| 9:B:10:ARG:NH2    | 9:B:265:SER:O    | 2.33                     | 0.61              |
| 30:Y:125:MET:HB2  | 30:Y:141:SER:HB3 | 1.81                     | 0.61              |
| 3:2:1555:G:N7     | 29:X:4:ARG:NH2   | 2.44                     | 0.61              |
| 3:2:3617:G:OP1    | 37:f:44:ARG:NH2  | 2.34                     | 0.61              |
| 39:h:19:PHE:O     | 39:h:26:ARG:NH2  | 2.34                     | 0.61              |
| 3:2:2573:A:O2'    | 40:i:115:LYS:NZ  | 2.33                     | 0.61              |
| 3:2:1604:G:H2'    | 3:2:1605:7MG:H82 | 1.82                     | 0.61              |
| 3:2:2300:A:N6     | 11:D:178:ASN:OD1 | 2.32                     | 0.61              |
| 15:H:120:ALA:HB2  | 23:Q:48:PRO:HB2  | 1.83                     | 0.61              |
| 5:5:74:A:N3       | 33:b:53:LYS:NZ   | 2.49                     | 0.61              |
| 9:B:230:GLY:O     | 9:B:234:ARG:HB2  | 2.00                     | 0.61              |
| 3:2:4097:G:N7     | 3:2:4099:G:N2    | 2.49                     | 0.60              |
| 4:3:313:LEU:HD21  | 4:3:376:LEU:HD13 | 1.83                     | 0.60              |
| 3:2:88:A:N7       | 31:Z:173:LYS:NZ  | 2.49                     | 0.60              |
| 46:v:222:LEU:HD23 | 46:v:222:LEU:O   | 2.01                     | 0.60              |
| 26:U:68:ARG:NH1   | 26:U:124:ASP:O   | 2.32                     | 0.60              |
| 3:2:4162:C:H5     | 14:G:73:ARG:HH12 | 1.49                     | 0.60              |
| 26:U:138:PHE:HA   | 26:U:143:ARG:HD2 | 1.84                     | 0.60              |
| 48:z:283:PHE:CB   | 48:z:289:ALA:HB2 | 2.32                     | 0.60              |
| 3:2:4985:U:O2     | 9:B:174:ARG:NH1  | 2.35                     | 0.60              |
| 8:A:85:MET:HE3    | 8:A:86:ASP:H     | 1.66                     | 0.60              |
| 12:E:13:SER:N     | 12:E:16:SER:HG   | 2.00                     | 0.60              |
| 16:I:31:ARG:NH1   | 16:I:149:ASN:OD1 | 2.35                     | 0.60              |
| 3:2:691:C:OP1     | 46:v:114:ARG:NH1 | 2.35                     | 0.60              |
| 4:3:329:ARG:CZ    | 4:3:334:GLY:O    | 2.50                     | 0.60              |
| 3:2:308:G:O6      | 26:U:12:ARG:NH1  | 2.35                     | 0.59              |
| 3:2:1952:G:H4'    | 33:b:93:MET:HG3  | 1.83                     | 0.59              |
| 3:2:75:G:O6       | 23:Q:103:ARG:NH1 | 2.35                     | 0.59              |
| 6:6:200:ASN:ND2   | 6:6:203:CYS:SG   | 2.76                     | 0.59              |
| 3:2:417:G:O3'     | 7:8:16:G:N2      | 2.30                     | 0.59              |
| 33:b:95:ARG:NH2   | 33:b:112:ASP:OD2 | 2.34                     | 0.59              |
| 48:z:59:GLU:HA    | 48:z:62:LYS:HE3  | 1.84                     | 0.59              |
| 9:B:222:VAL:O     | 9:B:343:ARG:NH1  | 2.35                     | 0.59              |
| 11:D:204:ARG:NH2  | 11:D:205:ARG:O   | 2.36                     | 0.59              |
| 3:2:4254:G:N2     | 3:2:4257:A:N7    | 2.44                     | 0.59              |
| 8:A:204:LEU:HD13  | 8:A:206:ILE:HG23 | 1.84                     | 0.59              |
| 24:S:81:ASP:OD1   | 24:S:81:ASP:N    | 2.35                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:1176:C:H5''   | 43:r:279:ARG:HH21 | 1.67                     | 0.59              |
| 1:0:450:ARG:NH1   | 30:Y:124:LYS:O    | 2.36                     | 0.59              |
| 3:2:2034:G:O2'    | 33:b:118:ARG:NH2  | 2.36                     | 0.59              |
| 7:8:12:G:N2       | 30:Y:120:ASN:OD1  | 2.31                     | 0.59              |
| 33:b:34:ALA:HB1   | 33:b:39:VAL:HG13  | 1.84                     | 0.59              |
| 3:2:3689:G:O2'    | 3:2:3818:U:OP2    | 2.20                     | 0.58              |
| 30:Y:94:MET:HE2   | 30:Y:148:MET:HE3  | 1.84                     | 0.58              |
| 42:m:14:SER:H     | 42:m:17:ARG:HG3   | 1.67                     | 0.58              |
| 3:2:1380:G:N2     | 3:2:1381:U:O4     | 2.35                     | 0.58              |
| 21:O:12:LEU:HB3   | 21:O:16:ARG:HH21  | 1.68                     | 0.58              |
| 3:2:493:G:C6      | 3:2:660:A:N1      | 2.71                     | 0.58              |
| 9:B:218:ASP:OD2   | 9:B:348:ARG:NH1   | 2.36                     | 0.58              |
| 45:u:33:VAL:HG23  | 45:u:38:GLU:HB3   | 1.84                     | 0.58              |
| 3:2:2517:A:O2'    | 13:F:66:ARG:NH2   | 2.36                     | 0.58              |
| 9:B:220:ILE:HG23  | 9:B:278:THR:HG22  | 1.85                     | 0.58              |
| 6:6:11:CYS:SG     | 6:6:187:ASN:ND2   | 2.75                     | 0.58              |
| 3:2:4373:G:N7     | 28:W:61:LYS:NZ    | 2.51                     | 0.58              |
| 4:3:398:VAL:O     | 8:A:47:LYS:NZ     | 2.36                     | 0.58              |
| 14:G:178:GLY:O    | 14:G:223:ARG:NH2  | 2.37                     | 0.58              |
| 6:6:163:PRO:HA    | 6:6:183:ALA:HB1   | 1.86                     | 0.58              |
| 3:2:1095:A:N1     | 3:2:1200:G:C6     | 2.72                     | 0.58              |
| 3:2:2667:C:OP2    | 32:a:103:ARG:NH1  | 2.37                     | 0.58              |
| 41:l:28:GLU:OE2   | 41:l:31:ASN:ND2   | 2.37                     | 0.58              |
| 43:r:122:GLN:O    | 43:r:248:ARG:NH2  | 2.37                     | 0.58              |
| 11:D:315:LYS:HD2  | 47:w:168:ALA:HB1  | 1.85                     | 0.58              |
| 3:2:24:G:N7       | 19:M:46:LYS:NZ    | 2.52                     | 0.57              |
| 3:2:4993:G:H1     | 3:2:5058:A:N6     | 2.02                     | 0.57              |
| 4:3:329:ARG:HH11  | 4:3:334:GLY:CA    | 2.02                     | 0.57              |
| 9:B:312:LYS:NZ    | 9:B:368:ILE:O     | 2.37                     | 0.57              |
| 3:2:1895:G:OP1    | 47:w:96:ARG:NH2   | 2.37                     | 0.57              |
| 23:Q:171:GLU:O    | 23:Q:175:ASN:ND2  | 2.37                     | 0.57              |
| 45:u:14:TYR:OH    | 45:u:92:LEU:O     | 2.22                     | 0.57              |
| 3:2:280:G:H5''    | 26:U:14:LYS:HE2   | 1.87                     | 0.57              |
| 3:2:1508:A:OP1    | 11:D:110:ARG:NH1  | 2.38                     | 0.57              |
| 6:6:88:LEU:HD12   | 6:6:89:PRO:HD2    | 1.87                     | 0.57              |
| 3:2:137:G:H2'     | 3:2:138:G:H8      | 1.68                     | 0.57              |
| 6:6:85:ARG:NH2    | 6:6:94:ILE:O      | 2.38                     | 0.56              |
| 36:e:71:GLU:O     | 36:e:75:LYS:NZ    | 2.37                     | 0.56              |
| 3:2:3603:G:N2     | 3:2:3604:A:N7     | 2.54                     | 0.56              |
| 36:e:31:ASN:HD21  | 36:e:115:SER:HB3  | 1.70                     | 0.56              |
| 47:w:105:VAL:HG13 | 47:w:136:VAL:HG12 | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:4478:G:O2'    | 3:2:4602:A:N1     | 2.38                     | 0.56              |
| 14:G:211:ASP:OD1  | 14:G:211:ASP:N    | 2.38                     | 0.56              |
| 14:G:229:ARG:NH2  | 14:G:232:GLU:OE1  | 2.39                     | 0.56              |
| 24:S:11:ARG:NH1   | 24:S:58:THR:O     | 2.37                     | 0.56              |
| 42:m:146:THR:O    | 42:m:157:VAL:HA   | 2.06                     | 0.56              |
| 47:w:92:VAL:O     | 47:w:120:GLY:HA2  | 2.06                     | 0.56              |
| 3:2:4199:C:H5''   | 4:3:221:LYS:HD2   | 1.87                     | 0.56              |
| 18:L:38:LEU:O     | 18:L:42:ARG:NH1   | 2.39                     | 0.56              |
| 22:P:42:ARG:HG3   | 22:P:47:THR:HG23  | 1.87                     | 0.56              |
| 31:Z:56:THR:OG1   | 31:Z:146:ARG:NH2  | 2.38                     | 0.56              |
| 43:r:50:ARG:NH1   | 43:r:147:ASP:OD2  | 2.39                     | 0.56              |
| 3:2:2554:U:H3     | 3:2:2764:A:H8     | 1.51                     | 0.56              |
| 3:2:4257:A:H2     | 20:N:27:GLY:HA2   | 1.70                     | 0.56              |
| 3:2:1699:A:O2'    | 11:D:306:ARG:NH1  | 2.39                     | 0.56              |
| 3:2:4217:G:OP1    | 34:c:55:LYS:NZ    | 2.38                     | 0.56              |
| 28:W:11:PHE:O     | 28:W:81:ARG:NH1   | 2.38                     | 0.56              |
| 39:h:4:ASN:HB3    | 39:h:7:VAL:HG12   | 1.88                     | 0.56              |
| 48:z:283:PHE:CB   | 48:z:289:ALA:CB   | 2.84                     | 0.56              |
| 3:2:494:U:O2      | 3:2:659:G:O6      | 2.24                     | 0.55              |
| 3:2:1502:G:OP2    | 31:Z:65:ARG:NH1   | 2.38                     | 0.55              |
| 3:2:1958:A:O2'    | 3:2:2025:A:N1     | 2.36                     | 0.55              |
| 16:I:59:LYS:HE2   | 16:I:66:GLU:HB3   | 1.87                     | 0.55              |
| 16:I:106:GLN:NE2  | 16:I:113:GLU:OE1  | 2.39                     | 0.55              |
| 43:r:62:CYS:HB3   | 43:r:105:LEU:HD22 | 1.88                     | 0.55              |
| 47:w:236:ARG:HB2  | 47:w:239:GLN:HB2  | 1.88                     | 0.55              |
| 48:z:280:LEU:HD11 | 48:z:293:VAL:HG21 | 1.88                     | 0.55              |
| 1:0:311:LYS:HB3   | 1:0:313:LYS:HG2   | 1.88                     | 0.55              |
| 3:2:268:G:H2'     | 3:2:269:G:H8      | 1.70                     | 0.55              |
| 3:2:4097:G:N2     | 3:2:4113:U:O4'    | 2.40                     | 0.55              |
| 4:3:386:ASN:OD1   | 28:W:64:LYS:NZ    | 2.39                     | 0.55              |
| 8:A:46:ASP:N      | 8:A:46:ASP:OD1    | 2.40                     | 0.55              |
| 40:i:36:ARG:NH1   | 40:i:38:TYR:OH    | 2.38                     | 0.55              |
| 3:2:3697:U:H5''   | 3:2:3698:G:H5'    | 1.88                     | 0.55              |
| 3:2:2611:A:H5'    | 3:2:2688:G:H4'    | 1.86                     | 0.55              |
| 3:2:1554:A:H4'    | 29:X:10:ILE:HG13  | 1.89                     | 0.55              |
| 3:2:2525:U:OP2    | 32:a:42:ARG:NH1   | 2.35                     | 0.55              |
| 6:6:78:ASP:OD1    | 6:6:96:ARG:NH1    | 2.40                     | 0.55              |
| 20:N:141:ILE:HG22 | 20:N:144:LYS:HE2  | 1.88                     | 0.55              |
| 3:2:1241:C:O5'    | 46:v:72:LYS:NZ    | 2.38                     | 0.55              |
| 3:2:4741:C:H4'    | 3:2:4742:G:H5'    | 1.89                     | 0.55              |
| 9:B:10:ARG:NH1    | 9:B:11:HIS:O      | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:w:147:LEU:O    | 47:w:151:ASN:HB2  | 2.07                     | 0.55              |
| 3:2:4479:A:OP1    | 16:I:170:LYS:NZ   | 2.39                     | 0.55              |
| 12:E:38:ILE:HD11  | 12:E:46:VAL:HG21  | 1.89                     | 0.55              |
| 23:Q:25:TRP:NE1   | 26:U:199:GLN:OE1  | 2.37                     | 0.55              |
| 3:2:1930:U:OP2    | 27:V:49:ARG:NH2   | 2.39                     | 0.55              |
| 31:Z:158:THR:C    | 31:Z:188:ASN:HD21 | 2.14                     | 0.55              |
| 34:c:100:LYS:HA   | 34:c:103:ASP:HB2  | 1.88                     | 0.55              |
| 3:2:1922:G:OP1    | 33:b:160:ARG:NH1  | 2.40                     | 0.54              |
| 3:2:3642:A:O2'    | 19:M:2:THR:N      | 2.39                     | 0.54              |
| 3:2:5038:A:OP1    | 37:f:61:LYS:NZ    | 2.41                     | 0.54              |
| 25:T:50:ARG:HG3   | 25:T:62:VAL:HG22  | 1.88                     | 0.54              |
| 41:l:56:ASP:OD1   | 41:l:56:ASP:N     | 2.39                     | 0.54              |
| 1:0:394:ARG:NH1   | 35:d:98:ASP:OD1   | 2.40                     | 0.54              |
| 3:2:417:G:N3      | 7:8:16:G:C2       | 2.75                     | 0.54              |
| 3:2:500:G:OP1     | 3:2:503:C:O2'     | 2.25                     | 0.54              |
| 3:2:964:A:H2'     | 3:2:965:G:H4'     | 1.89                     | 0.54              |
| 3:2:1238:A:O2'    | 47:w:52:GLU:OE1   | 2.25                     | 0.54              |
| 4:3:329:ARG:CZ    | 4:3:334:GLY:CA    | 2.83                     | 0.54              |
| 31:Z:155:ALA:HB3  | 31:Z:158:THR:HG23 | 1.88                     | 0.54              |
| 42:m:34:PHE:O     | 42:m:38:HIS:HB2   | 2.07                     | 0.54              |
| 45:u:49:TYR:OH    | 45:u:95:LYS:NZ    | 2.38                     | 0.54              |
| 46:v:46:ARG:HH12  | 46:v:66:LYS:HG2   | 1.72                     | 0.54              |
| 3:2:2651:C:O2'    | 3:2:2653:C:OP1    | 2.24                     | 0.54              |
| 7:8:13:G:O2'      | 30:Y:121:LYS:O    | 2.26                     | 0.54              |
| 32:a:15:LEU:HD22  | 32:a:52:ARG:HB2   | 1.89                     | 0.54              |
| 6:6:145:GLN:NE2   | 36:e:115:SER:OG   | 2.40                     | 0.54              |
| 8:A:111:LEU:HB3   | 8:A:138:LEU:HD11  | 1.88                     | 0.54              |
| 25:T:54:MET:HG2   | 25:T:60:PRO:HA    | 1.88                     | 0.54              |
| 1:0:276:SER:O     | 1:0:276:SER:OG    | 2.24                     | 0.54              |
| 3:2:3688:U:OP2    | 42:m:198:ARG:NH1  | 2.40                     | 0.54              |
| 3:2:3899:BGH:O4'  | 3:2:3899:BGH:C5'  | 2.50                     | 0.54              |
| 3:2:4570:G:H2'    | 3:2:4571:A2M:H8   | 1.88                     | 0.54              |
| 16:I:105:ILE:HD11 | 16:I:134:CYS:HB3  | 1.90                     | 0.54              |
| 3:2:1808:C:OP1    | 34:c:110:LYS:NZ   | 2.41                     | 0.54              |
| 3:2:2544:G:N2     | 7:8:126:C:OP1     | 2.36                     | 0.54              |
| 3:2:2658:G:N2     | 3:2:2676:A:OP2    | 2.40                     | 0.54              |
| 3:2:3699:C:O2'    | 3:2:3775:A:O2'    | 2.23                     | 0.54              |
| 11:D:57:LEU:HB3   | 11:D:61:GLN:HE21  | 1.73                     | 0.54              |
| 46:v:245:GLN:HA   | 46:v:248:ILE:HG12 | 1.89                     | 0.54              |
| 3:2:1596:U:O2'    | 30:Y:135:ARG:NH2  | 2.41                     | 0.54              |
| 3:2:1524:A2M:H62  | 3:2:1651:G:H22    | 1.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:122:ASP:OD1   | 6:6:125:THR:OG1   | 2.26                     | 0.54              |
| 23:Q:43:ALA:O     | 23:Q:149:GLN:NE2  | 2.41                     | 0.54              |
| 1:0:457:LEU:O     | 1:0:461:MET:HB2   | 2.08                     | 0.54              |
| 4:3:354:ASN:HB3   | 8:A:137:LEU:HD23  | 1.90                     | 0.54              |
| 9:B:80:GLU:OE1    | 9:B:323:TYR:OH    | 2.25                     | 0.54              |
| 36:e:99:GLU:HG3   | 37:f:23:ARG:HA    | 1.90                     | 0.54              |
| 1:0:251:ILE:HG21  | 1:0:264:LEU:HD13  | 1.91                     | 0.53              |
| 4:3:387:ASP:HB3   | 4:3:390:VAL:HG22  | 1.89                     | 0.53              |
| 36:e:107:ASN:HD21 | 36:e:111:GLU:HB3  | 1.73                     | 0.53              |
| 38:g:156:ILE:HG23 | 48:z:291:MET:HE2  | 1.88                     | 0.53              |
| 3:2:1368:A:H1'    | 39:h:1:MET:HE2    | 1.90                     | 0.53              |
| 3:2:4895:C:H41    | 24:S:133:ALA:HB2  | 1.74                     | 0.53              |
| 4:3:160:ARG:NH1   | 4:3:196:ASP:OD1   | 2.42                     | 0.53              |
| 33:b:173:ASN:ND2  | 33:b:175:PHE:O    | 2.41                     | 0.53              |
| 3:2:2898:G:H5''   | 32:a:104:ARG:HH21 | 1.73                     | 0.53              |
| 26:U:44:ARG:NH1   | 26:U:120:TRP:O    | 2.40                     | 0.53              |
| 23:Q:80:GLU:OE2   | 23:Q:102:ARG:NH1  | 2.41                     | 0.53              |
| 39:h:31:SER:HA    | 39:h:48:PRO:HA    | 1.89                     | 0.53              |
| 45:u:47:CYS:HA    | 45:u:102:ARG:O    | 2.09                     | 0.53              |
| 3:2:3739:C:O2     | 4:3:263:GLN:NE2   | 2.42                     | 0.53              |
| 10:C:115:GLY:O    | 46:v:72:LYS:NZ    | 2.31                     | 0.53              |
| 20:N:95:ARG:HG2   | 20:N:96:LYS:HG2   | 1.90                     | 0.53              |
| 26:U:17:ASP:HA    | 26:U:20:ARG:HG2   | 1.91                     | 0.53              |
| 3:2:970:G:OP1     | 46:v:123:ARG:NH1  | 2.41                     | 0.53              |
| 3:2:4736:C:H2'    | 3:2:4737:G:H8     | 1.74                     | 0.53              |
| 24:S:123:ILE:HD11 | 27:V:189:ILE:HD13 | 1.90                     | 0.53              |
| 3:2:11:G:N2       | 7:8:146:U:O2      | 2.42                     | 0.53              |
| 19:M:20:ARG:NH2   | 19:M:39:TYR:OH    | 2.42                     | 0.53              |
| 20:N:163:MET:HA   | 20:N:166:PHE:HB3  | 1.91                     | 0.53              |
| 30:Y:5:SER:OG     | 30:Y:118:GLN:NE2  | 2.42                     | 0.53              |
| 12:E:38:ILE:HG21  | 12:E:63:TYR:HB3   | 1.90                     | 0.52              |
| 14:G:160:ASP:OD1  | 14:G:160:ASP:N    | 2.42                     | 0.52              |
| 14:G:188:ALA:O    | 14:G:192:ARG:HB2  | 2.09                     | 0.52              |
| 46:v:254:ASP:HA   | 46:v:257:ILE:HB   | 1.91                     | 0.52              |
| 3:2:1094:G:O6     | 3:2:1201:U:O4     | 2.28                     | 0.52              |
| 6:6:142:VAL:HG22  | 6:6:173:LEU:HD21  | 1.90                     | 0.52              |
| 35:d:64:GLU:HB3   | 35:d:71:THR:HG23  | 1.90                     | 0.52              |
| 36:e:115:SER:O    | 36:e:135:ASN:ND2  | 2.42                     | 0.52              |
| 46:v:155:GLY:O    | 46:v:158:ARG:NH1  | 2.42                     | 0.52              |
| 3:2:1283:G:N1     | 3:2:2076:G:OP1    | 2.38                     | 0.52              |
| 14:G:187:LYS:HG2  | 14:G:198:THR:HB   | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:f:42:SER:OG    | 37:f:44:ARG:NH1   | 2.43                     | 0.52              |
| 3:2:143:C:OP1     | 14:G:111:LYS:NZ   | 2.38                     | 0.52              |
| 3:2:387:G:O2'     | 3:2:412:G:O6      | 2.21                     | 0.52              |
| 26:U:124:ASP:HB3  | 26:U:127:TYR:H    | 1.75                     | 0.52              |
| 39:h:2:LYS:HD3    | 39:h:7:VAL:HG13   | 1.90                     | 0.52              |
| 42:m:30:ARG:NH2   | 42:m:36:GLU:OE2   | 2.42                     | 0.52              |
| 3:2:461:G:H2'     | 3:2:462:G:H8      | 1.73                     | 0.52              |
| 28:W:2:VAL:N      | 28:W:90:HIS:O     | 2.43                     | 0.52              |
| 14:G:165:GLU:OE2  | 26:U:26:ARG:NH1   | 2.35                     | 0.52              |
| 46:v:223:ARG:NE   | 46:v:223:ARG:CA   | 2.73                     | 0.52              |
| 21:O:24:LYS:HG3   | 21:O:67:LYS:HB3   | 1.92                     | 0.52              |
| 35:d:24:ASP:HB2   | 35:d:26:THR:HG23  | 1.92                     | 0.52              |
| 4:3:176:ILE:HG23  | 4:3:181:MET:HB2   | 1.91                     | 0.52              |
| 8:A:69:GLY:HA3    | 8:A:73:HIS:HB3    | 1.92                     | 0.52              |
| 18:L:72:THR:HG22  | 18:L:110:LYS:HB3  | 1.91                     | 0.52              |
| 34:c:135:PRO:HB3  | 47:w:86:GLU:HB2   | 1.92                     | 0.52              |
| 11:D:84:THR:OG1   | 11:D:85:HIS:N     | 2.40                     | 0.52              |
| 14:G:57:TRP:O     | 14:G:62:ARG:NH1   | 2.43                     | 0.52              |
| 3:2:989:U:O2      | 3:2:1064:G:O6     | 2.27                     | 0.51              |
| 3:2:2469:C:H5     | 3:2:2471:G:H1     | 1.58                     | 0.51              |
| 1:0:335:THR:HA    | 1:0:339:ALA:HB3   | 1.90                     | 0.51              |
| 3:2:399:G:OP1     | 30:Y:18:ARG:NH2   | 2.44                     | 0.51              |
| 3:2:1313:C:O2     | 3:2:3881:G:O2'    | 2.26                     | 0.51              |
| 3:2:2434:G:O2'    | 3:2:2527:A:N1     | 2.42                     | 0.51              |
| 34:c:32:ARG:O     | 43:r:41:LYS:NZ    | 2.41                     | 0.51              |
| 39:h:32:SER:OG    | 39:h:101:PRO:O    | 2.27                     | 0.51              |
| 3:2:2288:G:O6     | 18:L:10:LYS:NZ    | 2.43                     | 0.51              |
| 3:2:2380:B8W:N2   | 3:2:2425:U:OP1    | 2.44                     | 0.51              |
| 31:Z:15:ARG:NH1   | 31:Z:52:PHE:O     | 2.41                     | 0.51              |
| 20:N:146:ARG:HH21 | 20:N:147:ARG:HH21 | 1.57                     | 0.51              |
| 1:0:280:PRO:HB3   | 35:d:41:GLN:HE22  | 1.75                     | 0.51              |
| 3:2:1367:C:O2'    | 3:2:1369:C:OP2    | 2.28                     | 0.51              |
| 3:2:1447:C:O2     | 3:2:2099:G:N2     | 2.44                     | 0.51              |
| 3:2:1870:C:H2'    | 3:2:1871:A2M:H8   | 1.92                     | 0.51              |
| 14:G:88:ASP:O     | 14:G:92:ALA:HB2   | 2.10                     | 0.51              |
| 48:z:105:LEU:C    | 48:z:105:LEU:HD23 | 2.35                     | 0.51              |
| 3:2:456:C:H2'     | 3:2:457:G:H8      | 1.75                     | 0.51              |
| 3:2:753:C:H41     | 3:2:910:G:H1      | 1.57                     | 0.51              |
| 8:A:160:LYS:HB3   | 8:A:162:VAL:H     | 1.75                     | 0.51              |
| 3:2:2580:U:OP1    | 40:i:36:ARG:NH2   | 2.43                     | 0.51              |
| 33:b:24:THR:O     | 33:b:24:THR:OG1   | 2.27                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:l:7:TRP:O      | 41:l:11:ARG:HB2   | 2.10                     | 0.51              |
| 45:u:27:LEU:HB3   | 45:u:83:MET:HE1   | 1.92                     | 0.51              |
| 3:2:1502:G:N7     | 18:L:77:LYS:NZ    | 2.44                     | 0.51              |
| 3:2:2630:U:O4     | 35:d:89:LYS:NZ    | 2.41                     | 0.51              |
| 3:2:4637:OMG:OP1  | 25:T:30:HIS:NE2   | 2.40                     | 0.51              |
| 3:2:5030:U:H2'    | 3:2:5031:G:H8     | 1.75                     | 0.51              |
| 4:3:358:GLN:NE2   | 8:A:158:GLN:OE1   | 2.44                     | 0.51              |
| 9:B:317:LEU:HD22  | 9:B:382:MET:HE2   | 1.93                     | 0.51              |
| 38:g:129:ARG:NH1  | 38:g:133:GLU:OE2  | 2.44                     | 0.51              |
| 3:2:355:A:H61     | 3:2:360:A:H2      | 1.56                     | 0.51              |
| 3:2:678:C:H4'     | 41:l:96:MET:HE2   | 1.91                     | 0.51              |
| 21:O:31:ASN:HB3   | 21:O:48:THR:HG22  | 1.93                     | 0.51              |
| 24:S:53:LYS:NZ    | 24:S:54:CYS:SG    | 2.84                     | 0.51              |
| 31:Z:81:VAL:HG22  | 31:Z:101:CYS:HB3  | 1.92                     | 0.51              |
| 32:a:105:LEU:HD23 | 32:a:138:LEU:HD23 | 1.92                     | 0.51              |
| 38:g:122:ALA:N    | 38:g:139:ARG:O    | 2.43                     | 0.51              |
| 48:z:280:LEU:CD1  | 48:z:293:VAL:HG21 | 2.41                     | 0.51              |
| 3:2:185:C:H2'     | 3:2:186:G:H8      | 1.76                     | 0.51              |
| 13:F:46:CYS:SG    | 13:F:47:GLY:N     | 2.84                     | 0.51              |
| 17:K:3:LEU:HB3    | 17:K:4:ARG:HD3    | 1.93                     | 0.51              |
| 1:O:279:ILE:HB    | 1:O:282:ILE:HD11  | 1.93                     | 0.50              |
| 11:D:235:LEU:HG   | 11:D:240:LEU:HD11 | 1.93                     | 0.50              |
| 31:Z:75:ARG:HA    | 31:Z:78:LYS:HD2   | 1.92                     | 0.50              |
| 3:2:3723:A2M:OP2  | 17:K:68:ARG:NH2   | 2.43                     | 0.50              |
| 8:A:32:VAL:HB     | 8:A:169:VAL:HG23  | 1.92                     | 0.50              |
| 43:r:126:THR:HG22 | 43:r:128:ASP:H    | 1.76                     | 0.50              |
| 44:t:86:GLU:OE2   | 44:t:114:ARG:NH2  | 2.44                     | 0.50              |
| 3:2:1870:C:HO2'   | 3:2:4442:PSU:HO2' | 1.58                     | 0.50              |
| 3:2:2870:A:OP2    | 3:2:2879:A:N6     | 2.44                     | 0.50              |
| 5:5:55:A:O2'      | 20:N:151:ILE:O    | 2.29                     | 0.50              |
| 20:N:160:GLU:HA   | 20:N:163:MET:HE2  | 1.94                     | 0.50              |
| 42:m:242:ARG:NH1  | 42:m:243:THR:O    | 2.44                     | 0.50              |
| 43:r:33:ARG:O     | 43:r:37:VAL:HB    | 2.11                     | 0.50              |
| 3:2:137:G:H2'     | 3:2:138:G:C8      | 2.46                     | 0.50              |
| 3:2:138:G:H2'     | 3:2:139:G:H8      | 1.76                     | 0.50              |
| 6:6:14:GLY:O      | 6:6:61:ARG:NH1    | 2.45                     | 0.50              |
| 38:g:104:ALA:O    | 38:g:134:LYS:NZ   | 2.44                     | 0.50              |
| 3:2:405:U:N3      | 3:2:408:A:OP2     | 2.40                     | 0.50              |
| 8:A:114:GLU:HG2   | 8:A:137:LEU:HD11  | 1.93                     | 0.50              |
| 27:V:15:LEU:HB2   | 27:V:18:ARG:HB2   | 1.93                     | 0.50              |
| 44:t:89:LEU:HD13  | 44:t:118:LEU:HD22 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:z:283:PHE:HB2  | 48:z:289:ALA:CB   | 2.41                     | 0.50              |
| 3:2:1187:G:N7     | 43:r:275:GLN:NE2  | 2.59                     | 0.50              |
| 3:2:4589:A:N1     | 3:2:4621:C:O2'    | 2.33                     | 0.50              |
| 8:A:177:ASP:OD1   | 8:A:177:ASP:N     | 2.34                     | 0.50              |
| 14:G:143:VAL:HA   | 14:G:146:LEU:HB2  | 1.93                     | 0.50              |
| 16:I:92:MET:HE3   | 16:I:181:VAL:HG22 | 1.93                     | 0.50              |
| 42:m:101:VAL:HG22 | 42:m:165:VAL:HG22 | 1.92                     | 0.50              |
| 45:u:50:VAL:HG22  | 45:u:69:VAL:HG22  | 1.93                     | 0.50              |
| 3:2:2845:A:H61    | 3:2:3843:C:N4     | 2.07                     | 0.50              |
| 26:U:193:ARG:O    | 26:U:197:THR:OG1  | 2.30                     | 0.50              |
| 42:m:33:ASP:N     | 42:m:33:ASP:OD1   | 2.42                     | 0.50              |
| 43:r:238:GLU:HA   | 43:r:241:LYS:HB2  | 1.94                     | 0.50              |
| 3:2:10:A:N1       | 7:8:147:G:N1      | 2.60                     | 0.50              |
| 3:2:158:A:H5''    | 3:2:159:C:H2'     | 1.94                     | 0.50              |
| 3:2:1562:G:O6     | 3:2:1566:C:N4     | 2.45                     | 0.50              |
| 7:8:61:A:OP1      | 15:H:52:LYS:NZ    | 2.42                     | 0.50              |
| 3:2:2521:G:H4'    | 13:F:26:PRO:HD2   | 1.94                     | 0.49              |
| 3:2:5006:U:H4'    | 3:2:5007:A:H5'    | 1.93                     | 0.49              |
| 10:C:6:ASN:OD1    | 10:C:6:ASN:N      | 2.43                     | 0.49              |
| 20:N:13:ARG:NH1   | 20:N:154:LYS:O    | 2.40                     | 0.49              |
| 1:0:238:GLU:H     | 1:0:239:GLU:HA    | 1.78                     | 0.49              |
| 3:2:2295:C:OP1    | 11:D:199:ARG:NE   | 2.39                     | 0.49              |
| 3:2:2864:A:H5''   | 32:a:84:THR:HG22  | 1.94                     | 0.49              |
| 32:a:134:ASN:N    | 32:a:134:ASN:OD1  | 2.43                     | 0.49              |
| 3:2:4304:A:OP2    | 3:2:4305:G:N2     | 2.43                     | 0.49              |
| 15:H:117:ARG:NH2  | 23:Q:127:PHE:O    | 2.41                     | 0.49              |
| 27:V:152:VAL:HA   | 27:V:155:THR:HG22 | 1.93                     | 0.49              |
| 3:2:124:C:OP1     | 26:U:144:ARG:NH1  | 2.44                     | 0.49              |
| 3:2:702:U:H5'     | 46:v:121:VAL:HG11 | 1.94                     | 0.49              |
| 3:2:1291:G:OP1    | 46:v:219:LYS:NZ   | 2.42                     | 0.49              |
| 43:r:93:THR:O     | 43:r:158:LYS:NZ   | 2.45                     | 0.49              |
| 43:r:271:MET:HE2  | 43:r:275:GLN:HB3  | 1.93                     | 0.49              |
| 48:z:280:LEU:CD2  | 48:z:293:VAL:CG2  | 2.87                     | 0.49              |
| 3:2:1100:U:N3     | 3:2:1194:G:N1     | 2.53                     | 0.49              |
| 3:2:1364:U:OP2    | 23:Q:36:ARG:NH1   | 2.40                     | 0.49              |
| 3:2:2259:G:H2'    | 3:2:2261:G:H21    | 1.76                     | 0.49              |
| 4:3:352:GLU:OE2   | 4:3:357:LYS:NZ    | 2.45                     | 0.49              |
| 15:H:55:ALA:O     | 15:H:59:THR:OG1   | 2.28                     | 0.49              |
| 31:Z:158:THR:HB   | 31:Z:159:PRO:CD   | 2.42                     | 0.49              |
| 34:c:39:ILE:HG13  | 34:c:102:ARG:HD3  | 1.95                     | 0.49              |
| 46:v:179:LEU:HD12 | 46:v:183:ARG:HA   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:2:4084:G:O6     | 42:m:72:ARG:NH2     | 2.46                     | 0.49              |
| 3:2:4369:A:H5''   | 28:W:65:LYS:HD3     | 1.95                     | 0.49              |
| 6:6:100:ARG:HH12  | 6:6:122:ASP:HB3     | 1.78                     | 0.49              |
| 10:C:8:THR:HG22   | 10:C:10:HIS:H       | 1.77                     | 0.49              |
| 43:r:131:ASN:OD1  | 43:r:131:ASN:N      | 2.44                     | 0.49              |
| 47:w:214:SER:OG   | 47:w:215:SER:N      | 2.46                     | 0.49              |
| 3:2:23:C:OP1      | 19:M:44:LYS:NZ      | 2.42                     | 0.48              |
| 3:2:667:A:H5''    | 3:2:668:C:H3'       | 1.95                     | 0.48              |
| 3:2:4163:U:OP2    | 14:G:53:ARG:NH2     | 2.46                     | 0.48              |
| 8:A:52:THR:OG1    | 8:A:155:ILE:O       | 2.26                     | 0.48              |
| 20:N:40:LEU:HD23  | 20:N:43:LEU:HD21    | 1.95                     | 0.48              |
| 37:f:46:PRO:HG2   | 37:f:54:LEU:HD22    | 1.94                     | 0.48              |
| 3:2:1273:G:N7     | 10:C:117:ARG:NE     | 2.61                     | 0.48              |
| 3:2:1378:C:H41    | 23:Q:159:ASN:HB2    | 1.78                     | 0.48              |
| 4:3:295:ASP:OD2   | 4:3:297:SER:OG      | 2.31                     | 0.48              |
| 4:3:329:ARG:HH12  | 4:3:334:GLY:C       | 2.12                     | 0.48              |
| 20:N:144:LYS:O    | 20:N:148:THR:OG1    | 2.23                     | 0.48              |
| 3:2:1509:C:H5''   | 18:L:2:PRO:HD2      | 1.94                     | 0.48              |
| 36:e:65:VAL:HG22  | 36:e:73:ARG:HA      | 1.95                     | 0.48              |
| 3:2:508:G:H21     | 18:L:85:GLN:HE22    | 1.61                     | 0.48              |
| 3:2:2725:A:N6     | 32:a:88:ARG:O       | 2.47                     | 0.48              |
| 43:r:207:TYR:OH   | 43:r:222:GLN:NE2    | 2.46                     | 0.48              |
| 3:2:4196:OMG:HM22 | 3:2:4197:G:H5'      | 1.95                     | 0.48              |
| 6:6:85:ARG:HH21   | 6:6:94:ILE:HG12     | 1.77                     | 0.48              |
| 23:Q:64:VAL:HA    | 23:Q:67:HIS:CD2     | 2.49                     | 0.48              |
| 36:e:30:ASP:OD1   | 36:e:30:ASP:N       | 2.45                     | 0.48              |
| 42:m:56:ALA:HB2   | 42:m:130:SER:HB3    | 1.96                     | 0.48              |
| 1:0:403:ARG:NH2   | 3:2:2706:G:O6       | 2.46                     | 0.48              |
| 3:2:1503:A:H4'    | 3:2:1504:G:H5'      | 1.95                     | 0.48              |
| 3:2:4322:G:N2     | 3:2:4325:A:OP2      | 2.37                     | 0.48              |
| 48:z:227:ASP:CG   | 48:z:320[A]:LYS:HE2 | 2.39                     | 0.48              |
| 1:0:466:THR:HG21  | 11:D:87:SER:HB3     | 1.96                     | 0.48              |
| 3:2:1320:U:O2'    | 3:2:1891:A:N1       | 2.41                     | 0.48              |
| 3:2:1480:C:O2'    | 3:2:1482:G:OP2      | 2.32                     | 0.48              |
| 6:6:42:LEU:HD22   | 6:6:46:ILE:HD11     | 1.96                     | 0.48              |
| 8:A:172:VAL:C     | 8:A:174:MET:N       | 2.71                     | 0.48              |
| 18:L:26:ARG:HB2   | 18:L:29:PRO:HG3     | 1.96                     | 0.48              |
| 45:u:37:ASP:OD1   | 45:u:37:ASP:N       | 2.45                     | 0.48              |
| 3:2:1963:C:H41    | 3:2:2024:G:H21      | 1.61                     | 0.48              |
| 7:8:94:G:H21      | 19:M:82:THR:HB      | 1.78                     | 0.48              |
| 8:A:77:ALA:HB2    | 8:A:144:MET:HE3     | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:109:ARG:HA   | 10:C:112:ILE:HB   | 1.96                     | 0.48              |
| 31:Z:4:ASP:O      | 47:w:115:ARG:NH1  | 2.45                     | 0.48              |
| 3:2:151:G:OP2     | 26:U:4:TYR:OH     | 2.30                     | 0.48              |
| 3:2:982:U:O4      | 3:2:1071:C:N3     | 2.46                     | 0.48              |
| 3:2:1301:C:H2'    | 44:t:17:THR:HG21  | 1.96                     | 0.48              |
| 3:2:4306:OMU:OP2  | 31:Z:159:PRO:HG2  | 2.14                     | 0.48              |
| 24:S:100:ARG:HA   | 24:S:103:LYS:HG2  | 1.95                     | 0.48              |
| 35:d:76:VAL:HG23  | 35:d:78:PHE:HB2   | 1.95                     | 0.48              |
| 43:r:181:PRO:HD2  | 43:r:195:HIS:CD2  | 2.48                     | 0.48              |
| 43:r:195:HIS:O    | 43:r:199:ILE:HB   | 2.14                     | 0.48              |
| 46:v:223:ARG:NH2  | 46:v:238:GLU:OE2  | 2.47                     | 0.48              |
| 3:2:1174:G:H22    | 3:2:1188:C:H42    | 1.62                     | 0.48              |
| 3:2:2041:A:O2'    | 3:2:4464:A:OP1    | 2.32                     | 0.48              |
| 12:E:14:ILE:HD13  | 12:E:17:ARG:HD2   | 1.96                     | 0.48              |
| 20:N:16:ARG:HH12  | 20:N:137:PRO:HD3  | 1.78                     | 0.48              |
| 27:V:37:ARG:HA    | 27:V:107:GLY:H    | 1.79                     | 0.48              |
| 3:2:184:U:O2      | 3:2:253:G:C6      | 2.67                     | 0.47              |
| 3:2:196:C:H4'     | 39:h:126:ARG:HG3  | 1.95                     | 0.47              |
| 3:2:512:U:H3      | 3:2:647:G:H1      | 1.62                     | 0.47              |
| 25:T:36:VAL:HG21  | 25:T:44:ARG:HG2   | 1.95                     | 0.47              |
| 31:Z:66:MET:HE2   | 31:Z:98:LEU:HD13  | 1.97                     | 0.47              |
| 40:i:97:ASN:HB3   | 40:i:99:ASP:H     | 1.79                     | 0.47              |
| 3:2:489:C:H42     | 3:2:664:G:H22     | 1.61                     | 0.47              |
| 3:2:1078:A:H1'    | 3:2:1234:G:C2     | 2.49                     | 0.47              |
| 4:3:167:LYS:HB3   | 4:3:250:CYS:HB3   | 1.95                     | 0.47              |
| 5:5:50:A:OP2      | 43:r:225:GLN:NE2  | 2.47                     | 0.47              |
| 7:8:21:C:OP1      | 11:D:195:LYS:NZ   | 2.37                     | 0.47              |
| 11:D:340:ILE:HG21 | 46:v:50:LEU:HD13  | 1.96                     | 0.47              |
| 13:F:100:GLN:HA   | 13:F:103:VAL:HG22 | 1.96                     | 0.47              |
| 29:X:42:CYS:SG    | 29:X:59:SER:OG    | 2.72                     | 0.47              |
| 3:2:2566:G:H2'    | 3:2:2567:G:H8     | 1.80                     | 0.47              |
| 4:3:329:ARG:CZ    | 4:3:334:GLY:C     | 2.88                     | 0.47              |
| 11:D:13:GLU:HG3   | 11:D:14:LYS:HD2   | 1.96                     | 0.47              |
| 11:D:209:ILE:HB   | 11:D:229:LEU:HD13 | 1.97                     | 0.47              |
| 3:2:453:G:N2      | 3:2:1293:G:N7     | 2.46                     | 0.47              |
| 3:2:2863:G:O2'    | 32:a:82:LYS:O     | 2.33                     | 0.47              |
| 7:8:122:G:O6      | 7:8:126:C:N4      | 2.46                     | 0.47              |
| 26:U:201:HIS:O    | 26:U:204:ARG:NH1  | 2.47                     | 0.47              |
| 27:V:157:GLU:OE2  | 27:V:160:ARG:NE   | 2.40                     | 0.47              |
| 33:b:31:ARG:HH11  | 33:b:129:VAL:HG13 | 1.80                     | 0.47              |
| 3:2:184:U:O2      | 3:2:253:G:O6      | 2.33                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:2:1870:C:O2'   | 3:2:4442:PSU:O2'  | 2.32                     | 0.47              |
| 3:2:3654:G:O2'   | 3:2:3693:U:OP1    | 2.31                     | 0.47              |
| 8:A:31:THR:HG22  | 8:A:61:PRO:HG2    | 1.97                     | 0.47              |
| 9:B:224:LYS:HG3  | 9:B:340:THR:HG22  | 1.97                     | 0.47              |
| 11:D:35:ASP:OD1  | 11:D:35:ASP:N     | 2.47                     | 0.47              |
| 14:G:108:GLN:O   | 14:G:112:GLN:HB2  | 2.15                     | 0.47              |
| 27:V:45:GLY:O    | 27:V:50:ASN:ND2   | 2.47                     | 0.47              |
| 35:d:22:THR:HG22 | 35:d:71:THR:HB    | 1.96                     | 0.47              |
| 4:3:379:ASP:OD2  | 4:3:382:ASN:ND2   | 2.48                     | 0.47              |
| 9:B:302:ASN:ND2  | 9:B:313:SER:OG    | 2.40                     | 0.47              |
| 13:F:23:SER:O    | 13:F:30:ILE:HA    | 2.15                     | 0.47              |
| 33:b:76:LYS:HB3  | 33:b:131:GLU:HG3  | 1.97                     | 0.47              |
| 3:2:1760:G:H2'   | 3:2:1761:G:H8     | 1.79                     | 0.47              |
| 14:G:158:ALA:HB2 | 14:G:190:LEU:HD22 | 1.97                     | 0.47              |
| 34:c:146:LYS:HA  | 34:c:146:LYS:HD3  | 1.78                     | 0.47              |
| 39:h:35:SER:O    | 39:h:39:ARG:HB2   | 2.14                     | 0.47              |
| 3:2:99:A:H5''    | 26:U:184:ILE:HD13 | 1.96                     | 0.47              |
| 3:2:417:G:HO2'   | 7:8:16:G:H1       | 1.61                     | 0.47              |
| 39:h:111:LEU:HA  | 39:h:111:LEU:HD12 | 1.78                     | 0.47              |
| 41:l:49:VAL:HG23 | 41:l:64:ILE:HG22  | 1.96                     | 0.47              |
| 43:r:217:ASP:HA  | 43:r:220:LYS:HG2  | 1.97                     | 0.47              |
| 46:v:93:THR:HG23 | 46:v:104:THR:HG21 | 1.97                     | 0.47              |
| 3:2:1285:U:OP1   | 46:v:127:SER:OG   | 2.33                     | 0.46              |
| 8:A:171:HIS:NE2  | 8:A:174:MET:HE2   | 2.29                     | 0.46              |
| 17:K:23:LYS:HE3  | 17:K:23:LYS:HB2   | 1.77                     | 0.46              |
| 21:O:5:ILE:HD11  | 21:O:11:PHE:HD1   | 1.80                     | 0.46              |
| 26:U:120:TRP:HE1 | 26:U:123:GLU:HG3  | 1.79                     | 0.46              |
| 3:2:2072:C:OP1   | 31:Z:2:GLY:N      | 2.47                     | 0.46              |
| 3:2:2521:G:H2'   | 3:2:2522:7MG:H82  | 1.96                     | 0.46              |
| 13:F:13:TYR:O    | 13:F:18:ASN:ND2   | 2.42                     | 0.46              |
| 15:H:19:LYS:NZ   | 15:H:23:ASP:OD2   | 2.48                     | 0.46              |
| 44:t:114:ARG:HD2 | 44:t:117:GLN:HE21 | 1.81                     | 0.46              |
| 3:2:4911:A:OP2   | 9:B:100:ARG:NH1   | 2.48                     | 0.46              |
| 13:F:3:GLN:HE22  | 13:F:30:ILE:H     | 1.63                     | 0.46              |
| 3:2:1697:G:N2    | 3:2:2084:C:OP1    | 2.48                     | 0.46              |
| 16:I:51:LYS:HA   | 16:I:51:LYS:HD2   | 1.74                     | 0.46              |
| 19:M:33:THR:HA   | 19:M:40:PRO:HD3   | 1.97                     | 0.46              |
| 26:U:75:VAL:HG21 | 26:U:80:THR:HG22  | 1.97                     | 0.46              |
| 28:W:14:LYS:HG2  | 28:W:77:CYS:HB2   | 1.97                     | 0.46              |
| 3:2:1396:G:O2'   | 3:2:1468:C:O2'    | 2.30                     | 0.46              |
| 3:2:2308:A:N3    | 7:8:19:C:O2'      | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:60:ARG:HH11   | 8:A:61:PRO:HD2    | 1.81                     | 0.46              |
| 30:Y:46:LYS:HA    | 30:Y:46:LYS:HD3   | 1.72                     | 0.46              |
| 30:Y:117:ILE:HD12 | 30:Y:148:MET:HE2  | 1.96                     | 0.46              |
| 39:h:54:GLU:HB2   | 39:h:108:ARG:HB3  | 1.96                     | 0.46              |
| 42:m:179:ILE:HG23 | 42:m:184:ARG:HB2  | 1.98                     | 0.46              |
| 44:t:26:ASP:OD1   | 44:t:26:ASP:N     | 2.41                     | 0.46              |
| 47:w:60:GLU:OE2   | 47:w:192:HIS:NE2  | 2.48                     | 0.46              |
| 3:2:907:C:H2'     | 3:2:908:G:H8      | 1.80                     | 0.46              |
| 3:2:931:C:OP1     | 3:2:934:C:N4      | 2.37                     | 0.46              |
| 3:2:4520:G:H8     | 9:B:2:SER:HB2     | 1.81                     | 0.46              |
| 23:Q:16:LYS:O     | 23:Q:21:ARG:NH1   | 2.42                     | 0.46              |
| 30:Y:30:ARG:HD2   | 30:Y:63:TYR:HE2   | 1.81                     | 0.46              |
| 46:v:167:GLN:HE21 | 46:v:171:GLY:HA2  | 1.80                     | 0.46              |
| 46:v:223:ARG:HA   | 46:v:223:ARG:CZ   | 2.45                     | 0.46              |
| 48:z:287:LYS:HB3  | 48:z:288:LYS:CE   | 2.46                     | 0.46              |
| 3:2:4208:U:OP2    | 34:c:4:THR:OG1    | 2.29                     | 0.46              |
| 45:u:110:ILE:O    | 46:v:141:ARG:NH2  | 2.38                     | 0.46              |
| 3:2:1761:G:H5''   | 4:3:167:LYS:HG3   | 1.98                     | 0.46              |
| 3:2:2674:A:N6     | 29:X:41:PHE:O     | 2.49                     | 0.46              |
| 3:2:2695:A:H4'    | 21:O:26:LYS:HE3   | 1.98                     | 0.46              |
| 3:2:4093:G:H2'    | 3:2:4094:G:H8     | 1.81                     | 0.46              |
| 3:2:4620:OMU:H1'  | 3:2:4620:OMU:HM23 | 1.71                     | 0.46              |
| 21:O:54:GLU:HA    | 21:O:57:LYS:HG2   | 1.97                     | 0.46              |
| 31:Z:59:PRO:HG3   | 31:Z:143:ARG:HA   | 1.98                     | 0.46              |
| 43:r:223:PHE:HB3  | 43:r:226:TYR:HB2  | 1.98                     | 0.46              |
| 3:2:942:G:OP1     | 47:w:245:ARG:NH1  | 2.47                     | 0.46              |
| 3:2:977:C:OP2     | 46:v:59:ARG:NH2   | 2.48                     | 0.46              |
| 3:2:1245:C:H2'    | 3:2:1246:G:H8     | 1.80                     | 0.46              |
| 3:2:3886:G:H5''   | 27:V:82:ARG:HH22  | 1.81                     | 0.46              |
| 3:2:4741:C:HO2'   | 3:2:4950:U:H3     | 1.63                     | 0.46              |
| 9:B:300:LYS:O     | 9:B:304:SER:OG    | 2.33                     | 0.46              |
| 17:K:99:LYS:O     | 17:K:103:LYS:NZ   | 2.42                     | 0.46              |
| 43:r:262:LYS:HE2  | 43:r:262:LYS:HB3  | 1.82                     | 0.46              |
| 44:t:91:CYS:HB3   | 44:t:95:TYR:HD2   | 1.80                     | 0.46              |
| 3:2:1458:C:H5''   | 31:Z:69:LYS:HD2   | 1.97                     | 0.46              |
| 4:3:167:LYS:HE2   | 4:3:251:LYS:HB3   | 1.97                     | 0.46              |
| 7:8:102:G:OP2     | 7:8:104:A:O2'     | 2.25                     | 0.46              |
| 14:G:132:ARG:HA   | 14:G:133:PRO:HD3  | 1.84                     | 0.46              |
| 23:Q:170:THR:OG1  | 23:Q:171:GLU:N    | 2.49                     | 0.46              |
| 44:t:64:LYS:HA    | 44:t:67:LYS:HB2   | 1.98                     | 0.46              |
| 1:0:332:LYS:HE2   | 35:d:45:GLU:HA    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:644:G:H3'     | 3:2:645:G:H8      | 1.80                     | 0.45              |
| 3:2:1704:C:OP1    | 47:w:43:ARG:NH1   | 2.49                     | 0.45              |
| 3:2:4139:G:H21    | 3:2:4140:C:H41    | 1.63                     | 0.45              |
| 3:2:4691:A:H4'    | 16:I:71:ARG:HG2   | 1.98                     | 0.45              |
| 3:2:5055:G:H2'    | 3:2:5056:A:H8     | 1.81                     | 0.45              |
| 3:2:382:G:O2'     | 3:2:407:A:N6      | 2.48                     | 0.45              |
| 3:2:1174:G:N2     | 3:2:1188:C:N3     | 2.64                     | 0.45              |
| 5:5:2:U:O4        | 5:5:117:G:O6      | 2.34                     | 0.45              |
| 35:d:106:SER:OG   | 35:d:107:LYS:N    | 2.48                     | 0.45              |
| 48:z:354:LEU:HD12 | 48:z:354:LEU:HA   | 1.87                     | 0.45              |
| 3:2:4363:A:H5''   | 28:W:36:GLN:HG2   | 1.99                     | 0.45              |
| 3:2:4467:A:O2'    | 3:2:4510:A:N3     | 2.41                     | 0.45              |
| 10:C:101:HIS:O    | 10:C:109:ARG:NH1  | 2.46                     | 0.45              |
| 21:O:20:ALA:HA    | 21:O:38:CYS:HA    | 1.99                     | 0.45              |
| 3:2:1326:A2M:OP2  | 3:2:4445:U:O2'    | 2.32                     | 0.45              |
| 3:2:2578:G:OP1    | 40:i:111:ARG:NH2  | 2.49                     | 0.45              |
| 25:T:59:THR:O     | 25:T:59:THR:OG1   | 2.32                     | 0.45              |
| 25:T:64:ILE:HG23  | 25:T:68:LEU:HD23  | 1.99                     | 0.45              |
| 26:U:96:ARG:NH2   | 26:U:104:GLU:OE2  | 2.45                     | 0.45              |
| 3:2:2498:C:H2'    | 3:2:2499:C:H6     | 1.82                     | 0.45              |
| 3:2:4327:C:OP1    | 34:c:70:HIS:NE2   | 2.47                     | 0.45              |
| 4:3:254:VAL:HG13  | 4:3:307:LEU:HB2   | 1.98                     | 0.45              |
| 14:G:55:VAL:HG12  | 38:g:44:PRO:HA    | 1.99                     | 0.45              |
| 14:G:187:LYS:HB3  | 14:G:187:LYS:HE2  | 1.71                     | 0.45              |
| 46:v:74:SER:OG    | 46:v:75:ALA:N     | 2.49                     | 0.45              |
| 3:2:280:G:N2      | 3:2:306:A:OP2     | 2.36                     | 0.45              |
| 3:2:4101:C:H42    | 3:2:4107:G:H22    | 1.65                     | 0.45              |
| 9:B:302:ASN:HB2   | 9:B:313:SER:HA    | 1.99                     | 0.45              |
| 18:L:99:PRO:HG2   | 18:L:122:VAL:HG23 | 1.98                     | 0.45              |
| 26:U:68:ARG:HA    | 26:U:98:LEU:HD21  | 1.99                     | 0.45              |
| 43:r:164:LYS:HD3  | 43:r:195:HIS:HE1  | 1.82                     | 0.45              |
| 8:A:152:LYS:HE2   | 8:A:152:LYS:HB2   | 1.79                     | 0.45              |
| 22:P:16:LYS:HA    | 22:P:16:LYS:HD2   | 1.78                     | 0.45              |
| 31:Z:61:LEU:HB3   | 31:Z:86:ILE:HD13  | 1.97                     | 0.45              |
| 40:i:30:ASP:HA    | 40:i:39:SER:HB2   | 1.99                     | 0.45              |
| 3:2:510:U:OP1     | 23:Q:163:LYS:NZ   | 2.49                     | 0.45              |
| 9:B:136:LYS:HG3   | 9:B:146:LEU:HD11  | 1.99                     | 0.45              |
| 15:H:89:ARG:O     | 15:H:93:ARG:HG2   | 2.17                     | 0.45              |
| 29:X:64:VAL:HG22  | 42:m:83:HIS:HB3   | 1.98                     | 0.45              |
| 36:e:131:ARG:H    | 36:e:131:ARG:HG2  | 1.56                     | 0.45              |
| 48:z:22:LYS:HE3   | 48:z:331:MET:HE1  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:4306:OMU:H1'  | 3:2:4306:OMU:HM23 | 1.71                     | 0.45              |
| 3:2:4992:G:H2'    | 3:2:4993:G:C8     | 2.52                     | 0.45              |
| 6:6:155:SER:OG    | 6:6:158:GLY:O     | 2.34                     | 0.45              |
| 36:e:99:GLU:HB2   | 37:f:24:THR:HG23  | 1.97                     | 0.45              |
| 1:0:236:GLU:HA    | 1:0:237:GLU:HA    | 1.71                     | 0.45              |
| 1:0:436:GLY:O     | 1:0:440:MET:HB2   | 2.17                     | 0.45              |
| 1:0:469:MET:O     | 1:0:470:HIS:ND1   | 2.50                     | 0.45              |
| 3:2:1378:C:N4     | 23:Q:159:ASN:O    | 2.50                     | 0.45              |
| 14:G:123:ALA:HA   | 14:G:124:GLY:HA2  | 1.68                     | 0.45              |
| 27:V:54:TYR:OH    | 27:V:73:PHE:O     | 2.35                     | 0.45              |
| 41:l:26:SER:OG    | 41:l:28:GLU:OE1   | 2.35                     | 0.45              |
| 20:N:40:LEU:O     | 20:N:44:THR:OG1   | 2.36                     | 0.44              |
| 24:S:16:SER:OG    | 24:S:54:CYS:O     | 2.35                     | 0.44              |
| 26:U:135:ILE:HG23 | 26:U:142:ILE:HD13 | 1.99                     | 0.44              |
| 28:W:3:ASN:ND2    | 28:W:96:ASP:O     | 2.50                     | 0.44              |
| 33:b:74:ARG:O     | 33:b:76:LYS:NZ    | 2.43                     | 0.44              |
| 3:2:1963:C:H2'    | 3:2:1964:A:H8     | 1.82                     | 0.44              |
| 3:2:3700:C:O2'    | 3:2:3774:A:N3     | 2.43                     | 0.44              |
| 3:2:4149:C:OP1    | 40:i:59:LYS:N     | 2.49                     | 0.44              |
| 12:E:32:LYS:HB3   | 12:E:32:LYS:HE2   | 1.87                     | 0.44              |
| 18:L:132:ARG:HA   | 18:L:135:GLU:HG2  | 1.98                     | 0.44              |
| 23:Q:50:PRO:HB3   | 23:Q:150:LEU:HB3  | 1.99                     | 0.44              |
| 29:X:46:LYS:HE3   | 29:X:46:LYS:HB3   | 1.81                     | 0.44              |
| 3:2:495:C:H2'     | 3:2:496:G:C5      | 2.52                     | 0.44              |
| 4:3:265:LEU:HD22  | 4:3:292:ALA:HB1   | 1.99                     | 0.44              |
| 8:A:94:ASN:HB3    | 8:A:95:LYS:HD2    | 1.99                     | 0.44              |
| 1:0:473:VAL:HG22  | 1:0:475:VAL:H     | 1.82                     | 0.44              |
| 3:2:1802:A:H5''   | 3:2:1803:G:H5'    | 1.99                     | 0.44              |
| 3:2:2112:G:O2'    | 3:2:2250:C:N4     | 2.50                     | 0.44              |
| 3:2:3799:A:N3     | 3:2:4506:C:O2'    | 2.47                     | 0.44              |
| 3:2:3861:A:H2'    | 3:2:3862:A:C8     | 2.53                     | 0.44              |
| 8:A:36:ILE:HG22   | 8:A:165:LEU:HB2   | 1.99                     | 0.44              |
| 26:U:104:GLU:HA   | 26:U:160:GLU:HG3  | 1.99                     | 0.44              |
| 31:Z:122:THR:H    | 31:Z:125:GLN:HE21 | 1.65                     | 0.44              |
| 3:2:382:G:N1      | 3:2:385:A:OP2     | 2.43                     | 0.44              |
| 3:2:461:G:H2'     | 3:2:462:G:C8      | 2.52                     | 0.44              |
| 3:2:4093:G:H2'    | 3:2:4094:G:C8     | 2.52                     | 0.44              |
| 3:2:4940:C:H5''   | 46:v:219:LYS:HE2  | 1.98                     | 0.44              |
| 8:A:105:LYS:HB3   | 8:A:105:LYS:HE2   | 1.75                     | 0.44              |
| 3:2:97:G:N7       | 23:Q:13:HIS:NE2   | 2.61                     | 0.44              |
| 3:2:2809:G:O2'    | 3:2:4644:G:OP1    | 2.31                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:O:14:THR:HA   | 21:O:17:ARG:HD3   | 1.99                     | 0.44              |
| 38:g:85:SER:HA   | 38:g:88:LYS:HE3   | 2.00                     | 0.44              |
| 41:l:28:GLU:HG2  | 41:l:31:ASN:HB2   | 2.00                     | 0.44              |
| 3:2:180:C:N3     | 3:2:181:C:H1'     | 2.33                     | 0.44              |
| 3:2:2558:C:H2'   | 3:2:2559:G:H8     | 1.82                     | 0.44              |
| 9:B:219:VAL:HG11 | 9:B:337:VAL:HG13  | 1.98                     | 0.44              |
| 13:F:41:ALA:O    | 13:F:52:ARG:NH1   | 2.44                     | 0.44              |
| 24:S:36:ALA:O    | 24:S:49:ALA:HA    | 2.18                     | 0.44              |
| 29:X:80:LYS:HB3  | 29:X:80:LYS:HE2   | 1.66                     | 0.44              |
| 35:d:74:SER:HB3  | 35:d:76:VAL:HG22  | 1.99                     | 0.44              |
| 36:e:82:ILE:HG13 | 36:e:83:ARG:HG3   | 1.99                     | 0.44              |
| 40:i:96:VAL:HG12 | 40:i:110:ALA:HB1  | 2.00                     | 0.44              |
| 48:z:287:LYS:HB3 | 48:z:288:LYS:NZ   | 2.32                     | 0.44              |
| 48:z:295:GLU:O   | 48:z:298:LYS:N    | 2.49                     | 0.44              |
| 1:0:393:HIS:CD2  | 35:d:98:ASP:HB3   | 2.52                     | 0.44              |
| 3:2:1429:C:H4'   | 31:Z:136:THR:HG22 | 2.00                     | 0.44              |
| 3:2:2574:G:N7    | 3:2:2760:G:N2     | 2.66                     | 0.44              |
| 3:2:4686:G:H21   | 16:I:163:GLN:HE22 | 1.66                     | 0.44              |
| 9:B:92:TYR:OH    | 9:B:182:GLU:OE1   | 2.35                     | 0.44              |
| 16:I:104:VAL:HB  | 16:I:113:GLU:HG3  | 2.00                     | 0.44              |
| 28:W:4:VAL:O     | 28:W:94:GLY:N     | 2.49                     | 0.44              |
| 36:e:25:VAL:HA   | 36:e:37:LEU:O     | 2.18                     | 0.44              |
| 36:e:66:LYS:HA   | 36:e:66:LYS:HD3   | 1.73                     | 0.44              |
| 6:6:111:ASN:HD21 | 6:6:114:VAL:HB    | 1.82                     | 0.44              |
| 20:N:120:ASP:HB2 | 20:N:123:ILE:HG12 | 2.00                     | 0.44              |
| 39:h:88:GLU:HA   | 39:h:94:THR:HA    | 2.00                     | 0.44              |
| 3:2:97:G:OP1     | 23:Q:16:LYS:NZ    | 2.46                     | 0.43              |
| 3:2:417:G:N3     | 7:8:16:G:N1       | 2.66                     | 0.43              |
| 3:2:1433:A:N6    | 3:2:1451:G:O2'    | 2.51                     | 0.43              |
| 3:2:2613:C:H4'   | 13:F:2:VAL:HG23   | 1.99                     | 0.43              |
| 4:3:372:GLY:HA3  | 8:A:121:PRO:HB2   | 1.99                     | 0.43              |
| 5:5:11:A:O2'     | 5:5:13:A:OP2      | 2.27                     | 0.43              |
| 29:X:24:LYS:HB3  | 29:X:24:LYS:HE2   | 1.83                     | 0.43              |
| 40:i:94:THR:HG23 | 40:i:95:VAL:HG23  | 2.00                     | 0.43              |
| 3:2:2486:G:H3'   | 3:2:2487:G:C8     | 2.53                     | 0.43              |
| 3:2:4739:C:N4    | 3:2:4740:G:N7     | 2.67                     | 0.43              |
| 6:6:74:ASN:HB3   | 6:6:98:GLU:HA     | 2.00                     | 0.43              |
| 9:B:95:THR:HG22  | 9:B:97:ARG:H      | 1.83                     | 0.43              |
| 10:C:106:LYS:HE2 | 10:C:106:LYS:HB2  | 1.90                     | 0.43              |
| 44:t:124:ASN:OD1 | 44:t:124:ASN:N    | 2.49                     | 0.43              |
| 3:2:667:A:H5''   | 3:2:668:C:H5''    | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:3893:C:O2'    | 3:2:4979:A:N1     | 2.46                     | 0.43              |
| 9:B:49:TYR:OH     | 9:B:168:MET:SD    | 2.74                     | 0.43              |
| 14:G:136:LEU:HD13 | 14:G:202:VAL:HG11 | 1.99                     | 0.43              |
| 15:H:99:GLU:HG2   | 26:U:144:ARG:HG3  | 2.01                     | 0.43              |
| 3:2:320:C:OP1     | 17:K:84:LYS:NZ    | 2.41                     | 0.43              |
| 3:2:3723:A2M:H62  | 3:2:3730:U:H3     | 1.66                     | 0.43              |
| 3:2:4736:C:H2'    | 3:2:4737:G:C8     | 2.52                     | 0.43              |
| 6:6:25:LEU:HD23   | 6:6:49:VAL:HG13   | 1.99                     | 0.43              |
| 6:6:84:ILE:HD12   | 6:6:84:ILE:HA     | 1.85                     | 0.43              |
| 11:D:353:LYS:HD2  | 11:D:353:LYS:HA   | 1.88                     | 0.43              |
| 16:I:129:ARG:HA   | 16:I:129:ARG:HD3  | 1.75                     | 0.43              |
| 23:Q:97:SER:OG    | 23:Q:97:SER:O     | 2.32                     | 0.43              |
| 35:d:38:ASN:OD1   | 35:d:90:TYR:OH    | 2.36                     | 0.43              |
| 46:v:201:ILE:HD13 | 46:v:261:ILE:HG12 | 2.00                     | 0.43              |
| 3:2:469:C:H2'     | 3:2:470:A:H8      | 1.83                     | 0.43              |
| 3:2:2362:U:H2'    | 3:2:2363:A2M:H8   | 2.01                     | 0.43              |
| 3:2:4492:U:O2'    | 3:2:4512:U:O2     | 2.28                     | 0.43              |
| 5:5:6:C:O2'       | 43:r:50:ARG:NH2   | 2.51                     | 0.43              |
| 9:B:48:GLY:HA3    | 9:B:81:THR:HG22   | 2.00                     | 0.43              |
| 11:D:186:SER:O    | 11:D:186:SER:OG   | 2.28                     | 0.43              |
| 16:I:126:VAL:HG11 | 16:I:161:ILE:HG22 | 2.00                     | 0.43              |
| 48:z:63:ILE:O     | 48:z:72:LYS:NZ    | 2.50                     | 0.43              |
| 3:2:2714:G:H2'    | 3:2:2715:G:H8     | 1.83                     | 0.43              |
| 8:A:149:ASP:HA    | 8:A:152:LYS:HB3   | 2.00                     | 0.43              |
| 14:G:37:LYS:HE2   | 14:G:37:LYS:HB3   | 1.85                     | 0.43              |
| 26:U:73:ARG:HA    | 26:U:74:PRO:HD3   | 1.90                     | 0.43              |
| 44:t:91:CYS:O     | 44:t:93:LYS:N     | 2.51                     | 0.43              |
| 6:6:218:VAL:HG23  | 6:6:222:PHE:HD2   | 1.84                     | 0.43              |
| 22:P:21:ARG:HH12  | 22:P:24:PRO:HG3   | 1.83                     | 0.43              |
| 23:Q:80:GLU:OE1   | 23:Q:104:ASN:ND2  | 2.45                     | 0.43              |
| 23:Q:198:ARG:HA   | 23:Q:201:GLU:HG2  | 2.01                     | 0.43              |
| 25:T:59:THR:OG1   | 25:T:104:THR:OG1  | 2.27                     | 0.43              |
| 27:V:12:ARG:HD3   | 27:V:37:ARG:NH2   | 2.34                     | 0.43              |
| 43:r:208:MET:HG3  | 43:r:219:TYR:HE1  | 1.83                     | 0.43              |
| 3:2:975:C:O3'     | 47:w:47:ARG:NH2   | 2.51                     | 0.43              |
| 9:B:36:ASP:OD1    | 9:B:36:ASP:N      | 2.51                     | 0.43              |
| 20:N:46:GLN:HE22  | 20:N:74:VAL:HA    | 1.84                     | 0.43              |
| 36:e:48:ARG:NH1   | 36:e:51:ARG:HH22  | 2.16                     | 0.43              |
| 43:r:60:ILE:HB    | 43:r:80:ALA:HB2   | 2.01                     | 0.43              |
| 43:r:103:LEU:HD11 | 43:r:248:ARG:HE   | 1.84                     | 0.43              |
| 47:w:247:MET:HE3  | 47:w:247:MET:HB2  | 1.85                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:989:U:O2      | 3:2:1064:G:C6     | 2.72                     | 0.43              |
| 3:2:4088:C:H2'    | 3:2:4089:G:C8     | 2.54                     | 0.43              |
| 3:2:4881:U:C4     | 24:S:113:MET:HG3  | 2.53                     | 0.43              |
| 5:5:34:C:N3       | 5:5:46:C:O2'      | 2.49                     | 0.43              |
| 6:6:143:ALA:HB3   | 6:6:162:HIS:CE1   | 2.54                     | 0.43              |
| 11:D:156:ASP:OD2  | 11:D:255:SER:OG   | 2.32                     | 0.43              |
| 21:O:24:LYS:HE2   | 21:O:24:LYS:HB2   | 1.81                     | 0.43              |
| 29:X:42:CYS:N     | 29:X:60:CYS:SG    | 2.91                     | 0.43              |
| 37:f:1:MET:HG3    | 37:f:15:PRO:HG2   | 2.00                     | 0.43              |
| 3:2:352:G:H21     | 3:2:360:A:H62     | 1.67                     | 0.43              |
| 3:2:1355:G:OP1    | 31:Z:108:ARG:NH1  | 2.50                     | 0.43              |
| 3:2:4288:C:O2'    | 3:2:4321:U:OP1    | 2.26                     | 0.43              |
| 15:H:46:LYS:HB2   | 15:H:46:LYS:HE3   | 1.79                     | 0.43              |
| 20:N:109:ILE:O    | 20:N:127:GLY:HA3  | 2.18                     | 0.43              |
| 30:Y:69:ARG:HA    | 30:Y:80:GLN:HA    | 2.01                     | 0.43              |
| 31:Z:97:LYS:HE2   | 31:Z:97:LYS:HB2   | 1.83                     | 0.43              |
| 1:0:328:LYS:HB3   | 1:0:330:HIS:HD2   | 1.84                     | 0.42              |
| 19:M:85:LYS:HA    | 19:M:86:PRO:HD2   | 1.93                     | 0.42              |
| 43:r:218:ALA:HA   | 43:r:221:LYS:HG2  | 2.01                     | 0.42              |
| 44:t:11:LYS:HA    | 44:t:11:LYS:HD2   | 1.77                     | 0.42              |
| 3:2:1397:A:C8     | 18:L:114:LYS:HD2  | 2.54                     | 0.42              |
| 4:3:311:LYS:HG3   | 4:3:312:GLN:HG3   | 2.00                     | 0.42              |
| 23:Q:46:ILE:HB    | 23:Q:49:ARG:HD2   | 2.02                     | 0.42              |
| 31:Z:14:ARG:HE    | 31:Z:14:ARG:HB2   | 1.60                     | 0.42              |
| 32:a:99:MET:HE1   | 32:a:127:VAL:HG12 | 2.01                     | 0.42              |
| 43:r:116:ASP:OD1  | 43:r:117:LYS:NZ   | 2.40                     | 0.42              |
| 46:v:128:HIS:O    | 46:v:128:HIS:ND1  | 2.51                     | 0.42              |
| 3:2:1197:C:H2'    | 3:2:1198:G:C8     | 2.54                     | 0.42              |
| 3:2:1594:C:O2'    | 3:2:1597:G:O2'    | 2.34                     | 0.42              |
| 3:2:1914:C:H4'    | 27:V:89:PRO:HD3   | 2.01                     | 0.42              |
| 3:2:2773:OMG:H5'' | 21:O:39:SER:HB3   | 2.01                     | 0.42              |
| 3:2:4700:A:N1     | 16:I:72:THR:HG21  | 2.34                     | 0.42              |
| 11:D:7:LEU:HG     | 11:D:21:ASN:HB3   | 2.01                     | 0.42              |
| 39:h:2:LYS:HB3    | 39:h:2:LYS:HE3    | 1.79                     | 0.42              |
| 39:h:103:LYS:HA   | 39:h:103:LYS:HD3  | 1.93                     | 0.42              |
| 43:r:51:MET:HA    | 43:r:63:GLN:O     | 2.19                     | 0.42              |
| 3:2:1591:U:N3     | 3:2:4555:U:OP1    | 2.43                     | 0.42              |
| 3:2:2307:A:N3     | 3:2:2333:G:O2'    | 2.49                     | 0.42              |
| 3:2:3716:C:H42    | 3:2:3735:G:H2'    | 1.85                     | 0.42              |
| 30:Y:96:LYS:HA    | 30:Y:99:GLU:HG2   | 2.01                     | 0.42              |
| 36:e:27:ASN:O     | 36:e:102:ALA:HA   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:r:55:VAL:HG13  | 43:r:60:ILE:HG12  | 2.01                     | 0.42              |
| 48:z:274:ASP:HB3  | 48:z:275:ALA:H    | 1.62                     | 0.42              |
| 3:2:110:C:OP1     | 23:Q:89:LYS:NZ    | 2.52                     | 0.42              |
| 4:3:341:THR:HB    | 4:3:367:HIS:HB3   | 2.01                     | 0.42              |
| 11:D:166:GLU:H    | 11:D:166:GLU:HG2  | 1.69                     | 0.42              |
| 16:I:105:ILE:HG13 | 16:I:109:GLY:HA2  | 2.02                     | 0.42              |
| 22:P:26:TRP:CD1   | 22:P:26:TRP:H     | 2.37                     | 0.42              |
| 41:l:20:ARG:O     | 41:l:22:LYS:N     | 2.52                     | 0.42              |
| 3:2:85:G:O2'      | 3:2:97:G:O6       | 2.33                     | 0.42              |
| 3:2:451:C:H3'     | 3:2:1294:A:H2     | 1.85                     | 0.42              |
| 3:2:1578:U:H4'    | 29:X:17:ARG:HH22  | 1.84                     | 0.42              |
| 3:2:4370:OMG:H4'  | 28:W:64:LYS:HE3   | 2.00                     | 0.42              |
| 3:2:4393:G:O4'    | 3:2:4447:5MC:HM52 | 2.20                     | 0.42              |
| 4:3:155:ALA:HA    | 4:3:240:SER:O     | 2.20                     | 0.42              |
| 11:D:320:LYS:HB3  | 11:D:320:LYS:HE3  | 1.86                     | 0.42              |
| 20:N:51:SER:HB3   | 20:N:69:ALA:HB3   | 2.00                     | 0.42              |
| 24:S:114:LYS:HA   | 24:S:114:LYS:HD2  | 1.89                     | 0.42              |
| 3:2:405:U:O2'     | 3:2:407:A:N7      | 2.44                     | 0.42              |
| 3:2:1197:C:H2'    | 3:2:1198:G:H8     | 1.85                     | 0.42              |
| 3:2:2516:G:OP1    | 13:F:60:ARG:NH1   | 2.53                     | 0.42              |
| 3:2:3707:U:O2     | 3:2:3743:G:O6     | 2.37                     | 0.42              |
| 9:B:128:LYS:HB3   | 9:B:128:LYS:HE2   | 1.94                     | 0.42              |
| 11:D:60:HIS:HA    | 11:D:92:PHE:HE1   | 1.84                     | 0.42              |
| 14:G:50:ASP:OD1   | 14:G:52:THR:OG1   | 2.28                     | 0.42              |
| 16:I:28:LYS:HE2   | 16:I:28:LYS:HB2   | 1.75                     | 0.42              |
| 41:l:112:ARG:HB2  | 44:t:90:MET:HE1   | 2.02                     | 0.42              |
| 3:2:1564:A:H2'    | 3:2:1565:A:C5     | 2.55                     | 0.42              |
| 4:3:289:LEU:HD13  | 4:3:342:LEU:HB2   | 2.01                     | 0.42              |
| 6:6:118:HIS:HA    | 6:6:119:PRO:HD3   | 1.87                     | 0.42              |
| 6:6:143:ALA:HB3   | 6:6:162:HIS:HE1   | 1.85                     | 0.42              |
| 19:M:37:CYS:HB2   | 19:M:39:TYR:H     | 1.84                     | 0.42              |
| 24:S:72:TYR:HA    | 24:S:75:GLN:HG2   | 2.02                     | 0.42              |
| 31:Z:158:THR:HB   | 31:Z:159:PRO:HD2  | 2.01                     | 0.42              |
| 46:v:211:HIS:H    | 46:v:211:HIS:CD2  | 2.38                     | 0.42              |
| 1:0:246:LEU:H     | 1:0:301:VAL:HG13  | 1.84                     | 0.42              |
| 3:2:727:C:OP1     | 47:w:73:ARG:NH2   | 2.49                     | 0.42              |
| 3:2:3615:G:H5'    | 37:f:48:GLN:HG2   | 2.02                     | 0.42              |
| 3:2:3717:A:H2'    | 3:2:3718:A2M:C8   | 2.50                     | 0.42              |
| 3:2:3732:A:H2'    | 3:2:3733:A:C8     | 2.55                     | 0.42              |
| 5:5:58:A:H2'      | 5:5:59:G:C8       | 2.55                     | 0.42              |
| 12:E:80:GLU:HA    | 12:E:83:THR:HG22  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:V:58:LEU:HD23  | 27:V:58:LEU:HA    | 1.88                     | 0.42              |
| 31:Z:158:THR:O    | 31:Z:188:ASN:ND2  | 2.39                     | 0.42              |
| 39:h:134:LYS:HD3  | 39:h:134:LYS:HA   | 1.90                     | 0.42              |
| 46:v:157:HIS:HB3  | 46:v:160:LYS:HD2  | 2.01                     | 0.42              |
| 3:2:35:U:O2'      | 3:2:1525:A:N1     | 2.49                     | 0.42              |
| 3:2:66:A:O2'      | 3:2:326:C:O2      | 2.38                     | 0.42              |
| 3:2:3620:G:OP1    | 3:2:3622:C:N4     | 2.53                     | 0.42              |
| 3:2:4577:U:H2'    | 3:2:4578:G:C8     | 2.55                     | 0.42              |
| 3:2:5002:U:H4'    | 9:B:375:GLY:HA3   | 2.02                     | 0.42              |
| 3:2:5055:G:H2'    | 3:2:5056:A:C8     | 2.55                     | 0.42              |
| 10:C:40:LEU:HD12  | 10:C:40:LEU:HA    | 1.83                     | 0.42              |
| 14:G:257:LYS:HA   | 14:G:257:LYS:HD3  | 1.82                     | 0.42              |
| 28:W:66:ILE:HB    | 28:W:85:ILE:HG13  | 2.02                     | 0.42              |
| 33:b:58:SER:O     | 33:b:58:SER:OG    | 2.28                     | 0.42              |
| 41:l:122:LYS:HB2  | 41:l:122:LYS:HE3  | 1.84                     | 0.42              |
| 3:2:3621:A:O2'    | 3:2:4658:G:O2'    | 2.36                     | 0.41              |
| 3:2:3937:C:H1'    | 26:U:125:SER:HB3  | 2.02                     | 0.41              |
| 8:A:58:THR:HG21   | 8:A:182:ASN:HD21  | 1.84                     | 0.41              |
| 24:S:41:PRO:HB2   | 24:S:74:ARG:HB2   | 2.02                     | 0.41              |
| 46:v:177:GLY:HA3  | 46:v:184:VAL:HB   | 2.00                     | 0.41              |
| 47:w:124:LYS:HB3  | 47:w:124:LYS:HE2  | 1.88                     | 0.41              |
| 47:w:161:LYS:HB3  | 47:w:161:LYS:HE2  | 1.84                     | 0.41              |
| 3:2:256:G:H2'     | 3:2:257:C:C6      | 2.55                     | 0.41              |
| 3:2:257:C:H2'     | 3:2:258:G:C8      | 2.55                     | 0.41              |
| 3:2:512:U:O4      | 3:2:647:G:O6      | 2.39                     | 0.41              |
| 3:2:2382:A:N1     | 3:2:2829:U:O2'    | 2.49                     | 0.41              |
| 4:3:344:GLU:HG2   | 4:3:362:ARG:HG2   | 2.02                     | 0.41              |
| 8:A:15:ARG:HH22   | 8:A:216:LEU:HD11  | 1.85                     | 0.41              |
| 11:D:335:MET:O    | 11:D:339:THR:HG23 | 2.20                     | 0.41              |
| 15:H:52:LYS:HA    | 15:H:52:LYS:HD3   | 1.85                     | 0.41              |
| 46:v:72:LYS:HB3   | 46:v:72:LYS:HE2   | 1.84                     | 0.41              |
| 3:2:2422:OMC:HM21 | 3:2:3857:G:H1'    | 2.02                     | 0.41              |
| 3:2:4680:G:H2'    | 3:2:4681:A:C8     | 2.56                     | 0.41              |
| 8:A:100:VAL:HG11  | 8:A:127:GLY:HA3   | 2.02                     | 0.41              |
| 29:X:14:TYR:OH    | 29:X:30:GLU:OE2   | 2.35                     | 0.41              |
| 31:Z:172:ARG:HA   | 31:Z:176:ARG:HG3  | 2.01                     | 0.41              |
| 40:i:121:ARG:HD2  | 40:i:126:LYS:HB3  | 2.01                     | 0.41              |
| 3:2:268:G:H2'     | 3:2:269:G:C8      | 2.54                     | 0.41              |
| 3:2:1084:C:H2'    | 3:2:1085:C:C6     | 2.55                     | 0.41              |
| 3:2:1444:G:N2     | 3:2:2103:G:H1     | 2.18                     | 0.41              |
| 3:2:4939:C:H3'    | 46:v:156:ARG:HH21 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:329:ARG:CZ    | 4:3:334:GLY:HA2   | 2.50                     | 0.41              |
| 9:B:386:LYS:HB2   | 9:B:386:LYS:HE2   | 1.96                     | 0.41              |
| 17:K:52:PRO:HG3   | 17:K:55:ARG:HH21  | 1.85                     | 0.41              |
| 21:O:67:LYS:HA    | 21:O:67:LYS:HD2   | 1.80                     | 0.41              |
| 26:U:116:LEU:HD22 | 26:U:135:ILE:HD11 | 2.02                     | 0.41              |
| 48:z:228:VAL:O    | 48:z:318:GLN:HA   | 2.21                     | 0.41              |
| 3:2:4271:A:OP1    | 3:2:4272:G:N2     | 2.53                     | 0.41              |
| 3:2:4577:U:H2'    | 3:2:4578:G:H8     | 1.86                     | 0.41              |
| 3:2:4882:U:OP1    | 24:S:117:LYS:NZ   | 2.53                     | 0.41              |
| 5:5:28:C:O2'      | 5:5:54:A:N1       | 2.44                     | 0.41              |
| 9:B:28:LYS:HB2    | 9:B:28:LYS:HE3    | 1.81                     | 0.41              |
| 10:C:12:GLN:HB3   | 10:C:16:TRP:CZ3   | 2.56                     | 0.41              |
| 23:Q:200:LYS:HE2  | 23:Q:200:LYS:HB3  | 1.86                     | 0.41              |
| 29:X:11:VAL:HG11  | 29:X:26:VAL:HG23  | 2.03                     | 0.41              |
| 3:2:4238:G:H2'    | 3:2:4239:A:C8     | 2.56                     | 0.41              |
| 3:2:4690:B8K:O4'  | 3:2:4690:B8K:C5'  | 2.55                     | 0.41              |
| 3:2:4940:C:H5'    | 3:2:4941:G:H5''   | 2.01                     | 0.41              |
| 3:2:5030:U:H2'    | 3:2:5031:G:C8     | 2.55                     | 0.41              |
| 6:6:33:ASN:OD1    | 6:6:33:ASN:N      | 2.53                     | 0.41              |
| 9:B:107:ALA:HB2   | 9:B:201:LEU:HD22  | 2.01                     | 0.41              |
| 12:E:48:LEU:HD13  | 12:E:57:LYS:HG3   | 2.02                     | 0.41              |
| 18:L:76:ASP:OD1   | 18:L:76:ASP:N     | 2.53                     | 0.41              |
| 38:g:88:LYS:O     | 38:g:92:ASP:HB2   | 2.21                     | 0.41              |
| 39:h:72:GLN:HB3   | 39:h:81:TYR:HB2   | 2.03                     | 0.41              |
| 3:2:737:C:C4      | 3:2:739:G:H5''    | 2.56                     | 0.41              |
| 3:2:2693:G:H2'    | 3:2:2694:G:N2     | 2.35                     | 0.41              |
| 3:2:4393:G:H22    | 3:2:4397:A:H62    | 1.69                     | 0.41              |
| 3:2:4396:A:H5''   | 3:2:4443:C:C4     | 2.56                     | 0.41              |
| 5:5:58:A:H2'      | 5:5:59:G:H8       | 1.85                     | 0.41              |
| 15:H:104:THR:HG23 | 26:U:146:PRO:HB2  | 2.02                     | 0.41              |
| 16:I:6:SER:HB3    | 16:I:67:LEU:HD22  | 2.02                     | 0.41              |
| 16:I:94:SER:HA    | 16:I:179:ILE:HA   | 2.02                     | 0.41              |
| 16:I:105:ILE:HD12 | 16:I:105:ILE:HA   | 1.93                     | 0.41              |
| 28:W:33:LEU:HA    | 28:W:38:LYS:HG2   | 2.02                     | 0.41              |
| 46:v:149:ILE:O    | 46:v:197:THR:OG1  | 2.27                     | 0.41              |
| 46:v:264:ILE:HA   | 46:v:265:PRO:HD3  | 1.86                     | 0.41              |
| 3:2:416:U:O2      | 7:8:17:A:N6       | 2.53                     | 0.41              |
| 3:2:1259:G:N2     | 3:2:1260:G:O6     | 2.54                     | 0.41              |
| 3:2:1589:C:O2'    | 3:2:2857:A:OP1    | 2.39                     | 0.41              |
| 4:3:384:ASN:N     | 4:3:384:ASN:OD1   | 2.46                     | 0.41              |
| 7:8:37:A:OP2      | 15:H:89:ARG:NH1   | 2.44                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 9:B:57:VAL:HB     | 9:B:367:PHE:HB3     | 2.02                     | 0.41              |
| 33:b:51:LEU:HD12  | 34:c:151:LEU:HD13   | 2.03                     | 0.41              |
| 34:c:27:LEU:HD23  | 43:r:33:ARG:HH21    | 1.85                     | 0.41              |
| 42:m:229:ALA:HB3  | 42:m:234:LYS:HB3    | 2.03                     | 0.41              |
| 46:v:190:HIS:CD2  | 46:v:192:LYS:HB2    | 2.56                     | 0.41              |
| 3:2:120:A:H2'     | 3:2:149:A:N6        | 2.36                     | 0.41              |
| 3:2:138:G:H2'     | 3:2:139:G:C8        | 2.54                     | 0.41              |
| 3:2:459:C:H2'     | 3:2:460:C:H6        | 1.85                     | 0.41              |
| 3:2:1261:G:H2'    | 3:2:1262:G:C8       | 2.56                     | 0.41              |
| 3:2:3641:U:H5     | 3:2:3646:A:N7       | 2.19                     | 0.41              |
| 3:2:4741:C:C4     | 3:2:4950:U:H1'      | 2.56                     | 0.41              |
| 3:2:5016:A:N1     | 3:2:5033:G:N3       | 2.68                     | 0.41              |
| 7:8:8:U:H2'       | 7:8:9:A:C8          | 2.56                     | 0.41              |
| 10:C:32:LEU:HD13  | 10:C:40:LEU:HD11    | 2.02                     | 0.41              |
| 20:N:115:LEU:HA   | 20:N:116:GLY:HA2    | 1.74                     | 0.41              |
| 24:S:71:LYS:HE3   | 24:S:71:LYS:HB2     | 1.91                     | 0.41              |
| 29:X:30:GLU:HA    | 29:X:33:GLN:HG2     | 2.03                     | 0.41              |
| 39:h:54:GLU:OE2   | 39:h:108:ARG:NH1    | 2.54                     | 0.41              |
| 42:m:45:VAL:HB    | 42:m:61:VAL:HG22    | 2.03                     | 0.41              |
| 42:m:147:ARG:HD2  | 42:m:147:ARG:HA     | 1.85                     | 0.41              |
| 44:t:37:LYS:HA    | 44:t:38:PRO:HD3     | 1.93                     | 0.41              |
| 48:z:155:ARG:O    | 48:z:158[B]:LYS:HD2 | 2.20                     | 0.41              |
| 3:2:1302:U:H3'    | 3:2:1303:A:C8       | 2.56                     | 0.41              |
| 3:2:3857:G:H5''   | 30:Y:86:LYS:HB2     | 2.03                     | 0.41              |
| 3:2:4122:G:N7     | 13:F:97:ILE:HD11    | 2.35                     | 0.41              |
| 8:A:36:ILE:HD12   | 8:A:204:LEU:HB3     | 2.02                     | 0.41              |
| 8:A:119:GLN:O     | 8:A:123:ILE:HG12    | 2.21                     | 0.41              |
| 9:B:141:ASP:OD1   | 9:B:144:LYS:NZ      | 2.51                     | 0.41              |
| 11:D:140:LYS:HD3  | 11:D:245:HIS:HB2    | 2.03                     | 0.41              |
| 16:I:53:LYS:HE3   | 16:I:53:LYS:HB3     | 1.95                     | 0.41              |
| 37:f:9:SER:HB3    | 37:f:51:TRP:HZ3     | 1.86                     | 0.41              |
| 37:f:52:THR:O     | 37:f:56:ARG:HG2     | 2.20                     | 0.41              |
| 40:i:92:ASP:HB2   | 40:i:94:THR:HG22    | 2.03                     | 0.41              |
| 3:2:1933:G:H2'    | 3:2:1934:A:C8       | 2.56                     | 0.40              |
| 3:2:2029:A:H2'    | 3:2:2030:A:C8       | 2.56                     | 0.40              |
| 19:M:67:LEU:HD23  | 19:M:67:LEU:HA      | 1.85                     | 0.40              |
| 27:V:202:LEU:HD23 | 27:V:202:LEU:HA     | 1.92                     | 0.40              |
| 28:W:30:LYS:HB3   | 28:W:30:LYS:HE2     | 1.86                     | 0.40              |
| 41:l:96:MET:HE3   | 41:l:96:MET:HB2     | 1.88                     | 0.40              |
| 46:v:207:LYS:O    | 46:v:256:GLN:NE2    | 2.53                     | 0.40              |
| 3:2:92:C:OP2      | 3:2:4341:C:O2'      | 2.33                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:935:A:O2'     | 24:S:44:GLN:O     | 2.33                     | 0.40              |
| 3:2:2870:A:H2'    | 3:2:2871:A:C8     | 2.56                     | 0.40              |
| 3:2:5002:U:H2'    | 3:2:5003:U:C6     | 2.56                     | 0.40              |
| 3:2:185:C:C5      | 23:Q:44:ARG:HD3   | 2.56                     | 0.40              |
| 3:2:2536:A:H5'    | 21:O:42:LEU:HD22  | 2.02                     | 0.40              |
| 8:A:36:ILE:HD12   | 8:A:36:ILE:HA     | 1.99                     | 0.40              |
| 18:L:71:PRO:HG2   | 18:L:108:TYR:HA   | 2.02                     | 0.40              |
| 24:S:107:PHE:HB2  | 46:v:199:THR:HG21 | 2.02                     | 0.40              |
| 38:g:156:ILE:HG23 | 48:z:291:MET:CE   | 2.51                     | 0.40              |
| 1:0:244:PRO:HA    | 1:0:245:PRO:HA    | 1.91                     | 0.40              |
| 3:2:1244:G:H2'    | 3:2:1245:C:C6     | 2.57                     | 0.40              |
| 3:2:2102:G:O2'    | 3:2:2103:G:N7     | 2.51                     | 0.40              |
| 3:2:2739:C:N4     | 42:m:177:LYS:O    | 2.39                     | 0.40              |
| 7:8:78:G:H2'      | 7:8:79:G:O4'      | 2.22                     | 0.40              |
| 9:B:229:LYS:HA    | 9:B:229:LYS:HD2   | 1.84                     | 0.40              |
| 38:g:54:LEU:HD23  | 38:g:54:LEU:HA    | 1.91                     | 0.40              |
| 39:h:10:ASP:HB3   | 39:h:13:LYS:HB2   | 2.03                     | 0.40              |
| 42:m:226:ARG:H    | 42:m:226:ARG:HG2  | 1.66                     | 0.40              |
| 3:2:1548:G:O2'    | 3:2:2812:A:N3     | 2.43                     | 0.40              |
| 3:2:2460:A:O2'    | 26:U:96:ARG:NH1   | 2.53                     | 0.40              |
| 5:5:77:A:H62      | 5:5:99:G:H21      | 1.69                     | 0.40              |
| 9:B:139:ASP:OD2   | 9:B:142:GLY:N     | 2.54                     | 0.40              |
| 12:E:30:GLY:O     | 12:E:34:THR:OG1   | 2.28                     | 0.40              |
| 12:E:49:ALA:O     | 12:E:57:LYS:NZ    | 2.48                     | 0.40              |
| 17:K:87:ARG:O     | 17:K:91:SER:OG    | 2.35                     | 0.40              |
| 20:N:161:GLU:HA   | 20:N:164:ARG:HB2  | 2.02                     | 0.40              |
| 35:d:100:LEU:HD23 | 35:d:112:LEU:HD22 | 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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | 0     | 184/477 (39%) | 158 (86%) | 25 (14%) | 1 (0%)   | 24          | 54  |
| 2   | 1     | 223/658 (34%) | 183 (82%) | 40 (18%) | 0        | 100         | 100 |
| 4   | 3     | 251/534 (47%) | 227 (90%) | 23 (9%)  | 1 (0%)   | 30          | 59  |
| 6   | 6     | 222/245 (91%) | 208 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 8   | A     | 210/217 (97%) | 184 (88%) | 22 (10%) | 4 (2%)   | 6           | 24  |
| 9   | B     | 400/403 (99%) | 372 (93%) | 28 (7%)  | 0        | 100         | 100 |
| 10  | C     | 88/159 (55%)  | 84 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 11  | D     | 355/427 (83%) | 326 (92%) | 28 (8%)  | 1 (0%)   | 36          | 64  |
| 12  | E     | 92/115 (80%)  | 82 (89%)  | 10 (11%) | 0        | 100         | 100 |
| 13  | F     | 107/117 (92%) | 104 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 14  | G     | 229/266 (86%) | 212 (93%) | 17 (7%)  | 0        | 100         | 100 |
| 15  | H     | 120/123 (98%) | 114 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 16  | I     | 188/192 (98%) | 169 (90%) | 19 (10%) | 0        | 100         | 100 |
| 17  | K     | 100/105 (95%) | 92 (92%)  | 7 (7%)   | 1 (1%)   | 12          | 38  |
| 18  | L     | 145/148 (98%) | 131 (90%) | 14 (10%) | 0        | 100         | 100 |
| 19  | M     | 84/97 (87%)   | 79 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 20  | N     | 160/178 (90%) | 146 (91%) | 14 (9%)  | 0        | 100         | 100 |
| 21  | O     | 66/70 (94%)   | 64 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 22  | P     | 48/51 (94%)   | 45 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 23  | Q     | 208/211 (99%) | 188 (90%) | 20 (10%) | 0        | 100         | 100 |
| 24  | S     | 132/215 (61%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 25  | T     | 105/125 (84%) | 96 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 26  | U     | 201/204 (98%) | 190 (94%) | 9 (4%)   | 2 (1%)   | 12          | 38  |
| 27  | V     | 197/203 (97%) | 189 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 28  | W     | 103/106 (97%) | 95 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 29  | X     | 89/92 (97%)   | 85 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 30  | Y     | 151/184 (82%) | 140 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 31  | Z     | 185/188 (98%) | 174 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 32  | a     | 143/196 (73%) | 136 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 33  | b     | 173/176 (98%) | 163 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 34  | c     | 155/160 (97%) | 145 (94%) | 9 (6%)   | 1 (1%)   | 21          | 50  |
| 35  | d     | 97/128 (76%)  | 87 (90%)  | 10 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 36  | e     | 127/140 (91%)   | 119 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 37  | f     | 60/157 (38%)    | 57 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 38  | g     | 115/156 (74%)   | 104 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 39  | h     | 132/145 (91%)   | 123 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 40  | i     | 133/136 (98%)   | 125 (94%)  | 7 (5%)   | 1 (1%)   | 16          | 44  |
| 41  | l     | 123/137 (90%)   | 116 (94%)  | 6 (5%)   | 1 (1%)   | 16          | 44  |
| 42  | m     | 246/257 (96%)   | 221 (90%)  | 24 (10%) | 1 (0%)   | 30          | 59  |
| 43  | r     | 273/297 (92%)   | 252 (92%)  | 21 (8%)  | 0        | 100         | 100 |
| 44  | t     | 126/135 (93%)   | 115 (91%)  | 11 (9%)  | 0        | 100         | 100 |
| 45  | u     | 107/110 (97%)   | 97 (91%)   | 8 (8%)   | 2 (2%)   | 6           | 24  |
| 46  | v     | 231/288 (80%)   | 206 (89%)  | 24 (10%) | 1 (0%)   | 30          | 59  |
| 47  | w     | 224/248 (90%)   | 211 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 48  | z     | 363/394 (92%)   | 354 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| All | All   | 7471/9370 (80%) | 6893 (92%) | 561 (8%) | 17 (0%)  | 44          | 70  |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | v     | 226 | ARG  |
| 4   | 3     | 331 | ALA  |
| 8   | A     | 28  | PHE  |
| 8   | A     | 159 | MET  |
| 8   | A     | 169 | VAL  |
| 8   | A     | 173 | LYS  |
| 17  | K     | 24  | PRO  |
| 41  | l     | 21  | ASN  |
| 34  | c     | 136 | ARG  |
| 40  | i     | 125 | GLY  |
| 45  | u     | 80  | ASN  |
| 11  | D     | 232 | VAL  |
| 45  | u     | 107 | PRO  |
| 26  | U     | 84  | PRO  |
| 26  | U     | 83  | LYS  |
| 42  | m     | 55  | GLY  |
| 1   | 0     | 245 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 165/404 (41%)  | 164 (99%)  | 1 (1%)   | 78          | 80  |
| 4   | 3     | 235/485 (48%)  | 231 (98%)  | 4 (2%)   | 53          | 70  |
| 6   | 6     | 194/213 (91%)  | 194 (100%) | 0        | 100         | 100 |
| 8   | A     | 191/196 (97%)  | 186 (97%)  | 5 (3%)   | 40          | 64  |
| 9   | B     | 348/349 (100%) | 340 (98%)  | 8 (2%)   | 44          | 66  |
| 10  | C     | 77/126 (61%)   | 77 (100%)  | 0        | 100         | 100 |
| 11  | D     | 298/348 (86%)  | 297 (100%) | 1 (0%)   | 86          | 85  |
| 12  | E     | 79/97 (81%)    | 76 (96%)   | 3 (4%)   | 29          | 56  |
| 13  | F     | 94/100 (94%)   | 93 (99%)   | 1 (1%)   | 65          | 75  |
| 14  | G     | 195/223 (87%)  | 193 (99%)  | 2 (1%)   | 68          | 76  |
| 15  | H     | 109/110 (99%)  | 109 (100%) | 0        | 100         | 100 |
| 16  | I     | 169/171 (99%)  | 166 (98%)  | 3 (2%)   | 51          | 69  |
| 17  | K     | 86/89 (97%)    | 85 (99%)   | 1 (1%)   | 63          | 74  |
| 18  | L     | 120/121 (99%)  | 119 (99%)  | 1 (1%)   | 73          | 78  |
| 19  | M     | 73/80 (91%)    | 72 (99%)   | 1 (1%)   | 59          | 72  |
| 20  | N     | 136/149 (91%)  | 132 (97%)  | 4 (3%)   | 37          | 61  |
| 21  | O     | 63/65 (97%)    | 63 (100%)  | 0        | 100         | 100 |
| 22  | P     | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 23  | Q     | 176/177 (99%)  | 176 (100%) | 0        | 100         | 100 |
| 24  | S     | 114/161 (71%)  | 113 (99%)  | 1 (1%)   | 70          | 77  |
| 25  | T     | 98/110 (89%)   | 96 (98%)   | 2 (2%)   | 48          | 68  |
| 26  | U     | 171/172 (99%)  | 171 (100%) | 0        | 100         | 100 |
| 27  | V     | 171/174 (98%)  | 167 (98%)  | 4 (2%)   | 44          | 66  |
| 28  | W     | 93/94 (99%)    | 93 (100%)  | 0        | 100         | 100 |
| 29  | X     | 74/75 (99%)    | 73 (99%)   | 1 (1%)   | 59          | 72  |
| 30  | Y     | 134/163 (82%)  | 133 (99%)  | 1 (1%)   | 76          | 79  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 31  | Z     | 164/165 (99%)   | 161 (98%)  | 3 (2%)   | 51          | 69  |
| 32  | a     | 131/175 (75%)   | 131 (100%) | 0        | 100         | 100 |
| 33  | b     | 156/157 (99%)   | 152 (97%)  | 4 (3%)   | 40          | 64  |
| 34  | c     | 138/140 (99%)   | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 35  | d     | 89/115 (77%)    | 89 (100%)  | 0        | 100         | 100 |
| 36  | e     | 100/107 (94%)   | 98 (98%)   | 2 (2%)   | 48          | 68  |
| 37  | f     | 54/126 (43%)    | 53 (98%)   | 1 (2%)   | 50          | 69  |
| 38  | g     | 105/133 (79%)   | 105 (100%) | 0        | 100         | 100 |
| 39  | h     | 124/135 (92%)   | 124 (100%) | 0        | 100         | 100 |
| 40  | i     | 117/118 (99%)   | 117 (100%) | 0        | 100         | 100 |
| 41  | l     | 109/121 (90%)   | 106 (97%)  | 3 (3%)   | 38          | 62  |
| 42  | m     | 190/199 (96%)   | 185 (97%)  | 5 (3%)   | 40          | 64  |
| 43  | r     | 232/250 (93%)   | 231 (100%) | 1 (0%)   | 84          | 84  |
| 44  | t     | 114/121 (94%)   | 112 (98%)  | 2 (2%)   | 51          | 69  |
| 45  | u     | 88/89 (99%)     | 86 (98%)   | 2 (2%)   | 44          | 66  |
| 46  | v     | 208/252 (82%)   | 205 (99%)  | 3 (1%)   | 59          | 72  |
| 47  | w     | 195/215 (91%)   | 193 (99%)  | 2 (1%)   | 68          | 76  |
| 48  | z     | 316/336 (94%)   | 314 (99%)  | 2 (1%)   | 78          | 80  |
| All | All   | 6340/7454 (85%) | 6265 (99%) | 75 (1%)  | 61          | 74  |

All (75) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 335 | THR  |
| 4   | 3     | 215 | THR  |
| 4   | 3     | 216 | VAL  |
| 4   | 3     | 313 | LEU  |
| 4   | 3     | 404 | ILE  |
| 8   | A     | 30  | GLU  |
| 8   | A     | 55  | LEU  |
| 8   | A     | 175 | THR  |
| 8   | A     | 201 | VAL  |
| 8   | A     | 214 | GLN  |
| 9   | B     | 54  | THR  |
| 9   | B     | 159 | VAL  |
| 9   | B     | 160 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | B     | 184 | GLN  |
| 9   | B     | 205 | VAL  |
| 9   | B     | 251 | VAL  |
| 9   | B     | 351 | LEU  |
| 9   | B     | 370 | THR  |
| 11  | D     | 171 | LEU  |
| 12  | E     | 28  | VAL  |
| 12  | E     | 69  | THR  |
| 12  | E     | 91  | VAL  |
| 13  | F     | 63  | VAL  |
| 14  | G     | 135 | VAL  |
| 14  | G     | 211 | ASP  |
| 16  | I     | 26  | ILE  |
| 16  | I     | 72  | THR  |
| 16  | I     | 136 | VAL  |
| 17  | K     | 18  | THR  |
| 18  | L     | 15  | VAL  |
| 19  | M     | 17  | THR  |
| 20  | N     | 113 | ILE  |
| 20  | N     | 114 | ASP  |
| 20  | N     | 132 | VAL  |
| 20  | N     | 168 | GLN  |
| 24  | S     | 84  | THR  |
| 25  | T     | 62  | VAL  |
| 25  | T     | 100 | ASN  |
| 27  | V     | 34  | VAL  |
| 27  | V     | 49  | ARG  |
| 27  | V     | 64  | THR  |
| 27  | V     | 92  | THR  |
| 29  | X     | 63  | THR  |
| 30  | Y     | 24  | VAL  |
| 31  | Z     | 13  | VAL  |
| 31  | Z     | 72  | LEU  |
| 31  | Z     | 83  | VAL  |
| 33  | b     | 38  | VAL  |
| 33  | b     | 80  | ILE  |
| 33  | b     | 90  | THR  |
| 33  | b     | 129 | VAL  |
| 34  | c     | 72  | VAL  |
| 36  | e     | 65  | VAL  |
| 36  | e     | 81  | VAL  |
| 37  | f     | 5   | LEU  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 41  | l     | 27    | THR  |
| 41  | l     | 63    | VAL  |
| 41  | l     | 78    | VAL  |
| 42  | m     | 4     | VAL  |
| 42  | m     | 45    | VAL  |
| 42  | m     | 143   | THR  |
| 42  | m     | 157   | VAL  |
| 42  | m     | 169   | VAL  |
| 43  | r     | 199   | ILE  |
| 44  | t     | 13    | VAL  |
| 44  | t     | 45    | VAL  |
| 45  | u     | 25    | THR  |
| 45  | u     | 33    | VAL  |
| 46  | v     | 50    | LEU  |
| 46  | v     | 137   | VAL  |
| 46  | v     | 223   | ARG  |
| 47  | w     | 70[A] | ARG  |
| 47  | w     | 70[B] | ARG  |
| 48  | z     | 274   | ASP  |
| 48  | z     | 288   | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 233 | GLN  |
| 1   | 0     | 324 | HIS  |
| 1   | 0     | 393 | HIS  |
| 1   | 0     | 402 | GLN  |
| 4   | 3     | 270 | GLN  |
| 4   | 3     | 290 | GLN  |
| 4   | 3     | 348 | GLN  |
| 4   | 3     | 358 | GLN  |
| 4   | 3     | 364 | HIS  |
| 4   | 3     | 382 | ASN  |
| 4   | 3     | 391 | ASN  |
| 6   | 6     | 9   | ASN  |
| 6   | 6     | 68  | HIS  |
| 6   | 6     | 106 | ASN  |
| 6   | 6     | 145 | GLN  |
| 6   | 6     | 162 | HIS  |
| 8   | A     | 73  | HIS  |
| 8   | A     | 171 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | A     | 197 | ASN  |
| 8   | A     | 200 | ASN  |
| 9   | B     | 167 | GLN  |
| 9   | B     | 204 | GLN  |
| 9   | B     | 209 | GLN  |
| 9   | B     | 236 | HIS  |
| 9   | B     | 258 | HIS  |
| 10  | C     | 19  | ASN  |
| 10  | C     | 27  | GLN  |
| 10  | C     | 49  | HIS  |
| 10  | C     | 60  | ASN  |
| 11  | D     | 50  | GLN  |
| 11  | D     | 60  | HIS  |
| 11  | D     | 61  | GLN  |
| 11  | D     | 212 | ASN  |
| 11  | D     | 231 | ASN  |
| 11  | D     | 310 | HIS  |
| 11  | D     | 346 | ASN  |
| 12  | E     | 50  | ASN  |
| 13  | F     | 3   | GLN  |
| 14  | G     | 159 | HIS  |
| 14  | G     | 195 | HIS  |
| 14  | G     | 208 | ASN  |
| 14  | G     | 227 | ASN  |
| 15  | H     | 101 | ASN  |
| 15  | H     | 108 | GLN  |
| 16  | I     | 42  | ASN  |
| 16  | I     | 102 | ASN  |
| 16  | I     | 163 | GLN  |
| 18  | L     | 44  | ASN  |
| 18  | L     | 60  | HIS  |
| 18  | L     | 93  | ASN  |
| 19  | M     | 13  | ASN  |
| 19  | M     | 48  | ASN  |
| 20  | N     | 46  | GLN  |
| 20  | N     | 65  | ASN  |
| 20  | N     | 104 | ASN  |
| 21  | O     | 28  | ASN  |
| 21  | O     | 58  | GLN  |
| 22  | P     | 25  | GLN  |
| 23  | Q     | 40  | GLN  |
| 24  | S     | 34  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | S     | 48  | GLN  |
| 24  | S     | 66  | HIS  |
| 24  | S     | 75  | GLN  |
| 24  | S     | 125 | ASN  |
| 25  | T     | 28  | ASN  |
| 25  | T     | 93  | ASN  |
| 26  | U     | 15  | GLN  |
| 26  | U     | 32  | GLN  |
| 26  | U     | 149 | GLN  |
| 26  | U     | 156 | HIS  |
| 26  | U     | 158 | HIS  |
| 28  | W     | 18  | HIS  |
| 28  | W     | 45  | GLN  |
| 28  | W     | 51  | GLN  |
| 30  | Y     | 34  | GLN  |
| 30  | Y     | 40  | HIS  |
| 30  | Y     | 80  | GLN  |
| 30  | Y     | 116 | HIS  |
| 30  | Y     | 118 | GLN  |
| 31  | Z     | 7   | HIS  |
| 31  | Z     | 188 | ASN  |
| 33  | b     | 23  | HIS  |
| 33  | b     | 125 | GLN  |
| 33  | b     | 173 | ASN  |
| 34  | c     | 66  | ASN  |
| 35  | d     | 41  | GLN  |
| 35  | d     | 55  | ASN  |
| 35  | d     | 94  | ASN  |
| 36  | e     | 27  | ASN  |
| 36  | e     | 77  | HIS  |
| 37  | f     | 59  | HIS  |
| 38  | g     | 73  | HIS  |
| 38  | g     | 151 | ASN  |
| 39  | h     | 20  | ASN  |
| 40  | i     | 78  | ASN  |
| 41  | l     | 6   | GLN  |
| 41  | l     | 31  | ASN  |
| 42  | m     | 132 | ASN  |
| 42  | m     | 194 | ASN  |
| 43  | r     | 57  | ASN  |
| 43  | r     | 195 | HIS  |
| 43  | r     | 225 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | t     | 23  | HIS  |
| 44  | t     | 63  | ASN  |
| 44  | t     | 92  | ASN  |
| 44  | t     | 107 | ASN  |
| 45  | u     | 20  | ASN  |
| 46  | v     | 190 | HIS  |
| 46  | v     | 211 | HIS  |
| 47  | w     | 24  | ASN  |
| 47  | w     | 63  | GLN  |
| 47  | w     | 235 | ASN  |
| 48  | z     | 8   | GLN  |
| 48  | z     | 162 | GLN  |
| 48  | z     | 193 | HIS  |
| 48  | z     | 242 | GLN  |
| 48  | z     | 299 | HIS  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 3   | 2     | 3464/5070 (68%) | 917 (26%)         | 23 (0%)         |
| 5   | 5     | 119/120 (99%)   | 20 (16%)          | 0               |
| 7   | 8     | 153/156 (98%)   | 35 (22%)          | 0               |
| All | All   | 3736/5346 (69%) | 972 (26%)         | 23 (0%)         |

All (972) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 2   | G    |
| 3   | 2     | 10  | A    |
| 3   | 2     | 18  | C    |
| 3   | 2     | 25  | A    |
| 3   | 2     | 39  | A    |
| 3   | 2     | 42  | A    |
| 3   | 2     | 48  | G    |
| 3   | 2     | 56  | A    |
| 3   | 2     | 59  | A    |
| 3   | 2     | 64  | A    |
| 3   | 2     | 65  | A    |
| 3   | 2     | 67  | C    |
| 3   | 2     | 69  | A    |
| 3   | 2     | 73  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 74  | G    |
| 3   | 2     | 75  | G    |
| 3   | 2     | 91  | G    |
| 3   | 2     | 98  | A    |
| 3   | 2     | 108 | A    |
| 3   | 2     | 109 | G    |
| 3   | 2     | 110 | C    |
| 3   | 2     | 119 | G    |
| 3   | 2     | 120 | A    |
| 3   | 2     | 127 | G    |
| 3   | 2     | 128 | C    |
| 3   | 2     | 131 | C    |
| 3   | 2     | 132 | G    |
| 3   | 2     | 133 | C    |
| 3   | 2     | 134 | G    |
| 3   | 2     | 135 | G    |
| 3   | 2     | 136 | C    |
| 3   | 2     | 141 | C    |
| 3   | 2     | 143 | C    |
| 3   | 2     | 146 | G    |
| 3   | 2     | 151 | G    |
| 3   | 2     | 157 | U    |
| 3   | 2     | 159 | C    |
| 3   | 2     | 165 | A    |
| 3   | 2     | 172 | C    |
| 3   | 2     | 177 | G    |
| 3   | 2     | 180 | C    |
| 3   | 2     | 181 | C    |
| 3   | 2     | 183 | C    |
| 3   | 2     | 184 | U    |
| 3   | 2     | 185 | C    |
| 3   | 2     | 188 | G    |
| 3   | 2     | 189 | G    |
| 3   | 2     | 200 | U    |
| 3   | 2     | 207 | G    |
| 3   | 2     | 209 | U    |
| 3   | 2     | 216 | C    |
| 3   | 2     | 218 | A    |
| 3   | 2     | 219 | G    |
| 3   | 2     | 220 | C    |
| 3   | 2     | 225 | G    |
| 3   | 2     | 233 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 234 | G    |
| 3   | 2     | 236 | G    |
| 3   | 2     | 237 | B9B  |
| 3   | 2     | 250 | C    |
| 3   | 2     | 254 | G    |
| 3   | 2     | 256 | G    |
| 3   | 2     | 257 | C    |
| 3   | 2     | 260 | C    |
| 3   | 2     | 261 | G    |
| 3   | 2     | 262 | G    |
| 3   | 2     | 263 | G    |
| 3   | 2     | 265 | C    |
| 3   | 2     | 278 | G    |
| 3   | 2     | 279 | A    |
| 3   | 2     | 280 | G    |
| 3   | 2     | 297 | U    |
| 3   | 2     | 306 | A    |
| 3   | 2     | 315 | G    |
| 3   | 2     | 316 | U    |
| 3   | 2     | 340 | C    |
| 3   | 2     | 341 | G    |
| 3   | 2     | 347 | A    |
| 3   | 2     | 348 | G    |
| 3   | 2     | 349 | A    |
| 3   | 2     | 350 | C    |
| 3   | 2     | 361 | C    |
| 3   | 2     | 362 | A    |
| 3   | 2     | 363 | A    |
| 3   | 2     | 380 | U    |
| 3   | 2     | 387 | G    |
| 3   | 2     | 388 | A    |
| 3   | 2     | 406 | C    |
| 3   | 2     | 407 | A    |
| 3   | 2     | 408 | A    |
| 3   | 2     | 412 | G    |
| 3   | 2     | 413 | G    |
| 3   | 2     | 433 | A    |
| 3   | 2     | 449 | C    |
| 3   | 2     | 450 | G    |
| 3   | 2     | 452 | A    |
| 3   | 2     | 453 | G    |
| 3   | 2     | 454 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 457 | G    |
| 3   | 2     | 458 | C    |
| 3   | 2     | 467 | U    |
| 3   | 2     | 484 | U    |
| 3   | 2     | 485 | C    |
| 3   | 2     | 486 | C    |
| 3   | 2     | 489 | C    |
| 3   | 2     | 493 | G    |
| 3   | 2     | 494 | U    |
| 3   | 2     | 497 | G    |
| 3   | 2     | 498 | C    |
| 3   | 2     | 499 | G    |
| 3   | 2     | 500 | G    |
| 3   | 2     | 501 | C    |
| 3   | 2     | 502 | C    |
| 3   | 2     | 503 | C    |
| 3   | 2     | 504 | G    |
| 3   | 2     | 505 | G    |
| 3   | 2     | 507 | G    |
| 3   | 2     | 508 | G    |
| 3   | 2     | 509 | A    |
| 3   | 2     | 510 | U    |
| 3   | 2     | 511 | C    |
| 3   | 2     | 512 | U    |
| 3   | 2     | 513 | U    |
| 3   | 2     | 514 | U    |
| 3   | 2     | 515 | C    |
| 3   | 2     | 517 | C    |
| 3   | 2     | 518 | G    |
| 3   | 2     | 519 | C    |
| 3   | 2     | 643 | C    |
| 3   | 2     | 644 | G    |
| 3   | 2     | 645 | G    |
| 3   | 2     | 646 | G    |
| 3   | 2     | 653 | U    |
| 3   | 2     | 656 | C    |
| 3   | 2     | 657 | C    |
| 3   | 2     | 659 | G    |
| 3   | 2     | 660 | A    |
| 3   | 2     | 665 | C    |
| 3   | 2     | 667 | A    |
| 3   | 2     | 668 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 670 | G    |
| 3   | 2     | 673 | C    |
| 3   | 2     | 685 | C    |
| 3   | 2     | 686 | A    |
| 3   | 2     | 687 | U    |
| 3   | 2     | 696 | C    |
| 3   | 2     | 697 | G    |
| 3   | 2     | 703 | G    |
| 3   | 2     | 704 | C    |
| 3   | 2     | 705 | G    |
| 3   | 2     | 708 | G    |
| 3   | 2     | 731 | G    |
| 3   | 2     | 738 | C    |
| 3   | 2     | 739 | G    |
| 3   | 2     | 746 | A    |
| 3   | 2     | 749 | G    |
| 3   | 2     | 753 | C    |
| 3   | 2     | 756 | G    |
| 3   | 2     | 757 | G    |
| 3   | 2     | 760 | G    |
| 3   | 2     | 904 | C    |
| 3   | 2     | 905 | C    |
| 3   | 2     | 906 | C    |
| 3   | 2     | 907 | C    |
| 3   | 2     | 912 | G    |
| 3   | 2     | 913 | U    |
| 3   | 2     | 914 | U    |
| 3   | 2     | 915 | A    |
| 3   | 2     | 916 | C    |
| 3   | 2     | 917 | A    |
| 3   | 2     | 918 | G    |
| 3   | 2     | 923 | C    |
| 3   | 2     | 924 | C    |
| 3   | 2     | 925 | C    |
| 3   | 2     | 932 | A    |
| 3   | 2     | 933 | G    |
| 3   | 2     | 934 | C    |
| 3   | 2     | 935 | A    |
| 3   | 2     | 936 | C    |
| 3   | 2     | 937 | U    |
| 3   | 2     | 941 | C    |
| 3   | 2     | 943 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 944  | A    |
| 3   | 2     | 945  | U    |
| 3   | 2     | 955  | G    |
| 3   | 2     | 956  | A    |
| 3   | 2     | 959  | G    |
| 3   | 2     | 960  | A    |
| 3   | 2     | 961  | G    |
| 3   | 2     | 962  | C    |
| 3   | 2     | 965  | G    |
| 3   | 2     | 966  | A    |
| 3   | 2     | 967  | C    |
| 3   | 2     | 971  | U    |
| 3   | 2     | 977  | C    |
| 3   | 2     | 978  | 2MG  |
| 3   | 2     | 982  | U    |
| 3   | 2     | 985  | C    |
| 3   | 2     | 989  | U    |
| 3   | 2     | 990  | C    |
| 3   | 2     | 991  | C    |
| 3   | 2     | 992  | C    |
| 3   | 2     | 993  | G    |
| 3   | 2     | 995  | C    |
| 3   | 2     | 1048 | G    |
| 3   | 2     | 1049 | C    |
| 3   | 2     | 1051 | G    |
| 3   | 2     | 1065 | G    |
| 3   | 2     | 1068 | G    |
| 3   | 2     | 1070 | G    |
| 3   | 2     | 1071 | C    |
| 3   | 2     | 1072 | C    |
| 3   | 2     | 1075 | G    |
| 3   | 2     | 1078 | A    |
| 3   | 2     | 1080 | C    |
| 3   | 2     | 1083 | U    |
| 3   | 2     | 1084 | C    |
| 3   | 2     | 1095 | A    |
| 3   | 2     | 1098 | G    |
| 3   | 2     | 1171 | G    |
| 3   | 2     | 1172 | C    |
| 3   | 2     | 1173 | G    |
| 3   | 2     | 1174 | G    |
| 3   | 2     | 1176 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 1178 | G    |
| 3   | 2     | 1179 | U    |
| 3   | 2     | 1180 | C    |
| 3   | 2     | 1181 | C    |
| 3   | 2     | 1182 | C    |
| 3   | 2     | 1183 | C    |
| 3   | 2     | 1185 | G    |
| 3   | 2     | 1187 | G    |
| 3   | 2     | 1189 | G    |
| 3   | 2     | 1191 | C    |
| 3   | 2     | 1199 | G    |
| 3   | 2     | 1202 | C    |
| 3   | 2     | 1203 | G    |
| 3   | 2     | 1204 | C    |
| 3   | 2     | 1210 | C    |
| 3   | 2     | 1211 | G    |
| 3   | 2     | 1214 | C    |
| 3   | 2     | 1215 | C    |
| 3   | 2     | 1217 | G    |
| 3   | 2     | 1218 | G    |
| 3   | 2     | 1222 | A    |
| 3   | 2     | 1241 | C    |
| 3   | 2     | 1242 | G    |
| 3   | 2     | 1253 | G    |
| 3   | 2     | 1254 | A    |
| 3   | 2     | 1255 | A    |
| 3   | 2     | 1259 | G    |
| 3   | 2     | 1260 | G    |
| 3   | 2     | 1261 | G    |
| 3   | 2     | 1262 | G    |
| 3   | 2     | 1263 | A    |
| 3   | 2     | 1264 | C    |
| 3   | 2     | 1265 | G    |
| 3   | 2     | 1266 | G    |
| 3   | 2     | 1267 | C    |
| 3   | 2     | 1269 | G    |
| 3   | 2     | 1270 | A    |
| 3   | 2     | 1271 | G    |
| 3   | 2     | 1272 | C    |
| 3   | 2     | 1273 | G    |
| 3   | 2     | 1274 | A    |
| 3   | 2     | 1275 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 1280 | C    |
| 3   | 2     | 1281 | G    |
| 3   | 2     | 1284 | G    |
| 3   | 2     | 1287 | G    |
| 3   | 2     | 1289 | C    |
| 3   | 2     | 1293 | G    |
| 3   | 2     | 1294 | A    |
| 3   | 2     | 1295 | C    |
| 3   | 2     | 1296 | G    |
| 3   | 2     | 1301 | C    |
| 3   | 2     | 1302 | U    |
| 3   | 2     | 1303 | A    |
| 3   | 2     | 1314 | C    |
| 3   | 2     | 1324 | A    |
| 3   | 2     | 1326 | A2M  |
| 3   | 2     | 1337 | A    |
| 3   | 2     | 1354 | A    |
| 3   | 2     | 1358 | G    |
| 3   | 2     | 1359 | G    |
| 3   | 2     | 1365 | C    |
| 3   | 2     | 1366 | G    |
| 3   | 2     | 1367 | C    |
| 3   | 2     | 1370 | G    |
| 3   | 2     | 1377 | G    |
| 3   | 2     | 1378 | C    |
| 3   | 2     | 1379 | C    |
| 3   | 2     | 1387 | A    |
| 3   | 2     | 1394 | G    |
| 3   | 2     | 1397 | A    |
| 3   | 2     | 1399 | G    |
| 3   | 2     | 1403 | G    |
| 3   | 2     | 1404 | G    |
| 3   | 2     | 1405 | C    |
| 3   | 2     | 1407 | C    |
| 3   | 2     | 1408 | G    |
| 3   | 2     | 1409 | C    |
| 3   | 2     | 1410 | U    |
| 3   | 2     | 1411 | C    |
| 3   | 2     | 1412 | G    |
| 3   | 2     | 1420 | A    |
| 3   | 2     | 1425 | G    |
| 3   | 2     | 1435 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 1437 | C    |
| 3   | 2     | 1438 | U    |
| 3   | 2     | 1439 | C    |
| 3   | 2     | 1441 | C    |
| 3   | 2     | 1443 | A    |
| 3   | 2     | 1446 | C    |
| 3   | 2     | 1447 | C    |
| 3   | 2     | 1458 | C    |
| 3   | 2     | 1459 | A    |
| 3   | 2     | 1482 | G    |
| 3   | 2     | 1483 | C    |
| 3   | 2     | 1493 | G    |
| 3   | 2     | 1497 | A    |
| 3   | 2     | 1498 | G    |
| 3   | 2     | 1502 | G    |
| 3   | 2     | 1514 | U    |
| 3   | 2     | 1515 | A    |
| 3   | 2     | 1517 | 2MG  |
| 3   | 2     | 1518 | A    |
| 3   | 2     | 1522 | OMG  |
| 3   | 2     | 1525 | A    |
| 3   | 2     | 1534 | A2M  |
| 3   | 2     | 1547 | A    |
| 3   | 2     | 1566 | C    |
| 3   | 2     | 1574 | B9B  |
| 3   | 2     | 1578 | U    |
| 3   | 2     | 1586 | G    |
| 3   | 2     | 1591 | U    |
| 3   | 2     | 1596 | U    |
| 3   | 2     | 1597 | G    |
| 3   | 2     | 1621 | A    |
| 3   | 2     | 1624 | G    |
| 3   | 2     | 1625 | OMG  |
| 3   | 2     | 1626 | G    |
| 3   | 2     | 1627 | G    |
| 3   | 2     | 1631 | A    |
| 3   | 2     | 1632 | A    |
| 3   | 2     | 1633 | G    |
| 3   | 2     | 1634 | A    |
| 3   | 2     | 1638 | A    |
| 3   | 2     | 1640 | C    |
| 3   | 2     | 1641 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 1642 | A    |
| 3   | 2     | 1651 | G    |
| 3   | 2     | 1654 | G    |
| 3   | 2     | 1655 | C    |
| 3   | 2     | 1661 | C    |
| 3   | 2     | 1676 | C    |
| 3   | 2     | 1677 | PSU  |
| 3   | 2     | 1678 | C    |
| 3   | 2     | 1679 | A    |
| 3   | 2     | 1681 | G    |
| 3   | 2     | 1686 | C    |
| 3   | 2     | 1694 | C    |
| 3   | 2     | 1697 | G    |
| 3   | 2     | 1699 | A    |
| 3   | 2     | 1700 | G    |
| 3   | 2     | 1701 | A    |
| 3   | 2     | 1703 | C    |
| 3   | 2     | 1704 | C    |
| 3   | 2     | 1705 | G    |
| 3   | 2     | 1706 | A    |
| 3   | 2     | 1707 | C    |
| 3   | 2     | 1708 | G    |
| 3   | 2     | 1709 | C    |
| 3   | 2     | 1715 | C    |
| 3   | 2     | 1716 | G    |
| 3   | 2     | 1719 | A    |
| 3   | 2     | 1734 | G    |
| 3   | 2     | 1763 | C    |
| 3   | 2     | 1764 | G    |
| 3   | 2     | 1765 | A    |
| 3   | 2     | 1766 | A    |
| 3   | 2     | 1768 | C    |
| 3   | 2     | 1769 | G    |
| 3   | 2     | 1772 | C    |
| 3   | 2     | 1773 | U    |
| 3   | 2     | 1774 | C    |
| 3   | 2     | 1790 | U    |
| 3   | 2     | 1797 | E7G  |
| 3   | 2     | 1804 | A    |
| 3   | 2     | 1806 | G    |
| 3   | 2     | 1809 | C    |
| 3   | 2     | 1810 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 1815 | G    |
| 3   | 2     | 1820 | C    |
| 3   | 2     | 1821 | G    |
| 3   | 2     | 1822 | U    |
| 3   | 2     | 1829 | G    |
| 3   | 2     | 1836 | G    |
| 3   | 2     | 1837 | A    |
| 3   | 2     | 1842 | G    |
| 3   | 2     | 1855 | G    |
| 3   | 2     | 1862 | U    |
| 3   | 2     | 1863 | U    |
| 3   | 2     | 1866 | UR3  |
| 3   | 2     | 1867 | A    |
| 3   | 2     | 1869 | G    |
| 3   | 2     | 1872 | G    |
| 3   | 2     | 1873 | A    |
| 3   | 2     | 1881 | C    |
| 3   | 2     | 1883 | OMG  |
| 3   | 2     | 1891 | A    |
| 3   | 2     | 1892 | A    |
| 3   | 2     | 1893 | C    |
| 3   | 2     | 1897 | A    |
| 3   | 2     | 1918 | U    |
| 3   | 2     | 1919 | G    |
| 3   | 2     | 1920 | C    |
| 3   | 2     | 1922 | G    |
| 3   | 2     | 1925 | G    |
| 3   | 2     | 1931 | C    |
| 3   | 2     | 1932 | A    |
| 3   | 2     | 1935 | C    |
| 3   | 2     | 1940 | G    |
| 3   | 2     | 1943 | A    |
| 3   | 2     | 1948 | G    |
| 3   | 2     | 1951 | G    |
| 3   | 2     | 1952 | G    |
| 3   | 2     | 1959 | U    |
| 3   | 2     | 1960 | A    |
| 3   | 2     | 1961 | G    |
| 3   | 2     | 1962 | A    |
| 3   | 2     | 1963 | C    |
| 3   | 2     | 2024 | G    |
| 3   | 2     | 2025 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 2026 | A    |
| 3   | 2     | 2033 | A    |
| 3   | 2     | 2034 | G    |
| 3   | 2     | 2046 | G    |
| 3   | 2     | 2048 | U    |
| 3   | 2     | 2055 | G    |
| 3   | 2     | 2056 | G    |
| 3   | 2     | 2069 | A    |
| 3   | 2     | 2070 | U    |
| 3   | 2     | 2071 | A    |
| 3   | 2     | 2084 | C    |
| 3   | 2     | 2085 | G    |
| 3   | 2     | 2089 | G    |
| 3   | 2     | 2090 | U    |
| 3   | 2     | 2091 | C    |
| 3   | 2     | 2092 | G    |
| 3   | 2     | 2093 | A    |
| 3   | 2     | 2094 | G    |
| 3   | 2     | 2095 | A    |
| 3   | 2     | 2096 | G    |
| 3   | 2     | 2097 | U    |
| 3   | 2     | 2098 | G    |
| 3   | 2     | 2100 | A    |
| 3   | 2     | 2101 | C    |
| 3   | 2     | 2103 | G    |
| 3   | 2     | 2104 | G    |
| 3   | 2     | 2106 | G    |
| 3   | 2     | 2108 | G    |
| 3   | 2     | 2111 | G    |
| 3   | 2     | 2112 | G    |
| 3   | 2     | 2251 | G    |
| 3   | 2     | 2252 | G    |
| 3   | 2     | 2253 | A    |
| 3   | 2     | 2256 | C    |
| 3   | 2     | 2259 | G    |
| 3   | 2     | 2262 | G    |
| 3   | 2     | 2263 | A    |
| 3   | 2     | 2280 | G    |
| 3   | 2     | 2289 | C    |
| 3   | 2     | 2297 | E7G  |
| 3   | 2     | 2300 | A    |
| 3   | 2     | 2301 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 2305 | U    |
| 3   | 2     | 2313 | A    |
| 3   | 2     | 2316 | G    |
| 3   | 2     | 2331 | G    |
| 3   | 2     | 2332 | A    |
| 3   | 2     | 2333 | G    |
| 3   | 2     | 2345 | G    |
| 3   | 2     | 2348 | G    |
| 3   | 2     | 2351 | C    |
| 3   | 2     | 2357 | G    |
| 3   | 2     | 2360 | A    |
| 3   | 2     | 2364 | OMG  |
| 3   | 2     | 2380 | B8W  |
| 3   | 2     | 2381 | A    |
| 3   | 2     | 2382 | A    |
| 3   | 2     | 2395 | A    |
| 3   | 2     | 2396 | A    |
| 3   | 2     | 2397 | G    |
| 3   | 2     | 2398 | U    |
| 3   | 2     | 2402 | G    |
| 3   | 2     | 2408 | U    |
| 3   | 2     | 2417 | A    |
| 3   | 2     | 2422 | OMC  |
| 3   | 2     | 2424 | OMG  |
| 3   | 2     | 2425 | U    |
| 3   | 2     | 2437 | C    |
| 3   | 2     | 2441 | C    |
| 3   | 2     | 2447 | U    |
| 3   | 2     | 2450 | G    |
| 3   | 2     | 2453 | A    |
| 3   | 2     | 2460 | A    |
| 3   | 2     | 2465 | C    |
| 3   | 2     | 2467 | U    |
| 3   | 2     | 2471 | G    |
| 3   | 2     | 2474 | G    |
| 3   | 2     | 2475 | G    |
| 3   | 2     | 2478 | C    |
| 3   | 2     | 2480 | G    |
| 3   | 2     | 2481 | G    |
| 3   | 2     | 2483 | G    |
| 3   | 2     | 2484 | A    |
| 3   | 2     | 2485 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 2486 | G    |
| 3   | 2     | 2487 | G    |
| 3   | 2     | 2488 | C    |
| 3   | 2     | 2489 | C    |
| 3   | 2     | 2490 | U    |
| 3   | 2     | 2491 | C    |
| 3   | 2     | 2492 | C    |
| 3   | 2     | 2494 | U    |
| 3   | 2     | 2503 | G    |
| 3   | 2     | 2504 | C    |
| 3   | 2     | 2505 | C    |
| 3   | 2     | 2506 | G    |
| 3   | 2     | 2511 | A    |
| 3   | 2     | 2512 | A    |
| 3   | 2     | 2513 | A    |
| 3   | 2     | 2514 | G    |
| 3   | 2     | 2519 | U    |
| 3   | 2     | 2520 | C    |
| 3   | 2     | 2532 | C    |
| 3   | 2     | 2537 | A    |
| 3   | 2     | 2544 | G    |
| 3   | 2     | 2546 | G    |
| 3   | 2     | 2547 | G    |
| 3   | 2     | 2553 | A    |
| 3   | 2     | 2554 | U    |
| 3   | 2     | 2555 | G    |
| 3   | 2     | 2562 | G    |
| 3   | 2     | 2566 | G    |
| 3   | 2     | 2569 | G    |
| 3   | 2     | 2573 | A    |
| 3   | 2     | 2583 | C    |
| 3   | 2     | 2587 | A    |
| 3   | 2     | 2589 | C    |
| 3   | 2     | 2596 | G    |
| 3   | 2     | 2618 | G    |
| 3   | 2     | 2627 | C    |
| 3   | 2     | 2638 | G    |
| 3   | 2     | 2652 | G    |
| 3   | 2     | 2653 | C    |
| 3   | 2     | 2659 | A    |
| 3   | 2     | 2661 | U    |
| 3   | 2     | 2662 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 2663 | G    |
| 3   | 2     | 2664 | G    |
| 3   | 2     | 2669 | C    |
| 3   | 2     | 2670 | C    |
| 3   | 2     | 2673 | G    |
| 3   | 2     | 2675 | G    |
| 3   | 2     | 2676 | A    |
| 3   | 2     | 2687 | U    |
| 3   | 2     | 2694 | G    |
| 3   | 2     | 2695 | A    |
| 3   | 2     | 2696 | A    |
| 3   | 2     | 2697 | A    |
| 3   | 2     | 2705 | G    |
| 3   | 2     | 2724 | G    |
| 3   | 2     | 2726 | G    |
| 3   | 2     | 2732 | G    |
| 3   | 2     | 2739 | C    |
| 3   | 2     | 2742 | G    |
| 3   | 2     | 2743 | A    |
| 3   | 2     | 2746 | A    |
| 3   | 2     | 2754 | B9B  |
| 3   | 2     | 2756 | G    |
| 3   | 2     | 2761 | U    |
| 3   | 2     | 2763 | U    |
| 3   | 2     | 2764 | A    |
| 3   | 2     | 2769 | U    |
| 3   | 2     | 2770 | C    |
| 3   | 2     | 2773 | OMG  |
| 3   | 2     | 2787 | A    |
| 3   | 2     | 2788 | U    |
| 3   | 2     | 2790 | U    |
| 3   | 2     | 2793 | G    |
| 3   | 2     | 2794 | C    |
| 3   | 2     | 2800 | G    |
| 3   | 2     | 2814 | C    |
| 3   | 2     | 2815 | A    |
| 3   | 2     | 2822 | G    |
| 3   | 2     | 2825 | A    |
| 3   | 2     | 2826 | U    |
| 3   | 2     | 2827 | G    |
| 3   | 2     | 2829 | U    |
| 3   | 2     | 2835 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 2838 | G    |
| 3   | 2     | 2848 | G    |
| 3   | 2     | 2850 | A    |
| 3   | 2     | 2855 | G    |
| 3   | 2     | 2870 | A    |
| 3   | 2     | 2876 | G    |
| 3   | 2     | 2877 | G    |
| 3   | 2     | 2879 | A    |
| 3   | 2     | 2886 | U    |
| 3   | 2     | 2900 | U    |
| 3   | 2     | 3604 | A    |
| 3   | 2     | 3605 | C    |
| 3   | 2     | 3615 | G    |
| 3   | 2     | 3619 | G    |
| 3   | 2     | 3626 | G    |
| 3   | 2     | 3630 | A    |
| 3   | 2     | 3635 | A    |
| 3   | 2     | 3644 | U    |
| 3   | 2     | 3662 | A    |
| 3   | 2     | 3664 | G    |
| 3   | 2     | 3670 | C    |
| 3   | 2     | 3673 | C    |
| 3   | 2     | 3674 | G    |
| 3   | 2     | 3680 | U    |
| 3   | 2     | 3691 | G    |
| 3   | 2     | 3692 | A    |
| 3   | 2     | 3706 | C    |
| 3   | 2     | 3711 | A    |
| 3   | 2     | 3713 | U    |
| 3   | 2     | 3714 | G    |
| 3   | 2     | 3728 | A    |
| 3   | 2     | 3729 | PSU  |
| 3   | 2     | 3735 | G    |
| 3   | 2     | 3736 | A    |
| 3   | 2     | 3748 | A    |
| 3   | 2     | 3750 | G    |
| 3   | 2     | 3776 | G    |
| 3   | 2     | 3777 | G    |
| 3   | 2     | 3784 | A    |
| 3   | 2     | 3785 | A2M  |
| 3   | 2     | 3789 | C    |
| 3   | 2     | 3799 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 3802 | U    |
| 3   | 2     | 3811 | G    |
| 3   | 2     | 3812 | C    |
| 3   | 2     | 3813 | A    |
| 3   | 2     | 3814 | U    |
| 3   | 2     | 3817 | A    |
| 3   | 2     | 3818 | U    |
| 3   | 2     | 3819 | G    |
| 3   | 2     | 3823 | G    |
| 3   | 2     | 3838 | U    |
| 3   | 2     | 3839 | G    |
| 3   | 2     | 3840 | U    |
| 3   | 2     | 3851 | U    |
| 3   | 2     | 3867 | A2M  |
| 3   | 2     | 3876 | A    |
| 3   | 2     | 3877 | A    |
| 3   | 2     | 3878 | C    |
| 3   | 2     | 3879 | G    |
| 3   | 2     | 3880 | P7G  |
| 3   | 2     | 3881 | G    |
| 3   | 2     | 3892 | U    |
| 3   | 2     | 3897 | B8K  |
| 3   | 2     | 3901 | A    |
| 3   | 2     | 3902 | A    |
| 3   | 2     | 3906 | A    |
| 3   | 2     | 3907 | G    |
| 3   | 2     | 3908 | A    |
| 3   | 2     | 3910 | C    |
| 3   | 2     | 3915 | U    |
| 3   | 2     | 3922 | G    |
| 3   | 2     | 3923 | A    |
| 3   | 2     | 3925 | U    |
| 3   | 2     | 3926 | C    |
| 3   | 2     | 3938 | G    |
| 3   | 2     | 3939 | G    |
| 3   | 2     | 3941 | G    |
| 3   | 2     | 3944 | G    |
| 3   | 2     | 3946 | G    |
| 3   | 2     | 4076 | G    |
| 3   | 2     | 4084 | G    |
| 3   | 2     | 4086 | G    |
| 3   | 2     | 4088 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 4097 | G    |
| 3   | 2     | 4098 | A    |
| 3   | 2     | 4099 | G    |
| 3   | 2     | 4101 | C    |
| 3   | 2     | 4102 | C    |
| 3   | 2     | 4103 | C    |
| 3   | 2     | 4104 | G    |
| 3   | 2     | 4105 | A    |
| 3   | 2     | 4106 | G    |
| 3   | 2     | 4107 | G    |
| 3   | 2     | 4108 | G    |
| 3   | 2     | 4111 | U    |
| 3   | 2     | 4112 | C    |
| 3   | 2     | 4113 | U    |
| 3   | 2     | 4114 | C    |
| 3   | 2     | 4115 | G    |
| 3   | 2     | 4116 | C    |
| 3   | 2     | 4117 | U    |
| 3   | 2     | 4118 | U    |
| 3   | 2     | 4119 | C    |
| 3   | 2     | 4127 | A    |
| 3   | 2     | 4133 | C    |
| 3   | 2     | 4138 | C    |
| 3   | 2     | 4139 | G    |
| 3   | 2     | 4140 | C    |
| 3   | 2     | 4141 | G    |
| 3   | 2     | 4142 | C    |
| 3   | 2     | 4143 | G    |
| 3   | 2     | 4145 | C    |
| 3   | 2     | 4146 | G    |
| 3   | 2     | 4148 | C    |
| 3   | 2     | 4157 | A    |
| 3   | 2     | 4162 | C    |
| 3   | 2     | 4163 | U    |
| 3   | 2     | 4170 | A    |
| 3   | 2     | 4177 | C    |
| 3   | 2     | 4183 | G    |
| 3   | 2     | 4184 | G    |
| 3   | 2     | 4191 | G    |
| 3   | 2     | 4195 | G    |
| 3   | 2     | 4196 | OMG  |
| 3   | 2     | 4206 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 4212 | A    |
| 3   | 2     | 4220 | 6MZ  |
| 3   | 2     | 4224 | A    |
| 3   | 2     | 4228 | G    |
| 3   | 2     | 4229 | U    |
| 3   | 2     | 4233 | A    |
| 3   | 2     | 4234 | A    |
| 3   | 2     | 4251 | A    |
| 3   | 2     | 4254 | G    |
| 3   | 2     | 4256 | A    |
| 3   | 2     | 4257 | A    |
| 3   | 2     | 4265 | U    |
| 3   | 2     | 4268 | A    |
| 3   | 2     | 4271 | A    |
| 3   | 2     | 4272 | G    |
| 3   | 2     | 4273 | A    |
| 3   | 2     | 4281 | A    |
| 3   | 2     | 4282 | A    |
| 3   | 2     | 4291 | G    |
| 3   | 2     | 4296 | B8H  |
| 3   | 2     | 4304 | A    |
| 3   | 2     | 4305 | G    |
| 3   | 2     | 4312 | U    |
| 3   | 2     | 4313 | A    |
| 3   | 2     | 4314 | C    |
| 3   | 2     | 4319 | C    |
| 3   | 2     | 4326 | G    |
| 3   | 2     | 4329 | G    |
| 3   | 2     | 4330 | G    |
| 3   | 2     | 4332 | C    |
| 3   | 2     | 4349 | C    |
| 3   | 2     | 4354 | U    |
| 3   | 2     | 4355 | E6G  |
| 3   | 2     | 4364 | G    |
| 3   | 2     | 4371 | MHG  |
| 3   | 2     | 4373 | G    |
| 3   | 2     | 4374 | U    |
| 3   | 2     | 4376 | A    |
| 3   | 2     | 4377 | G    |
| 3   | 2     | 4378 | A    |
| 3   | 2     | 4379 | A    |
| 3   | 2     | 4380 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 4387 | C    |
| 3   | 2     | 4394 | A    |
| 3   | 2     | 4398 | C    |
| 3   | 2     | 4400 | G    |
| 3   | 2     | 4403 | PSU  |
| 3   | 2     | 4443 | C    |
| 3   | 2     | 4444 | C    |
| 3   | 2     | 4448 | G    |
| 3   | 2     | 4450 | PSU  |
| 3   | 2     | 4451 | G    |
| 3   | 2     | 4453 | C    |
| 3   | 2     | 4464 | A    |
| 3   | 2     | 4466 | C    |
| 3   | 2     | 4471 | U    |
| 3   | 2     | 4472 | B8W  |
| 3   | 2     | 4476 | C    |
| 3   | 2     | 4477 | A    |
| 3   | 2     | 4482 | U    |
| 3   | 2     | 4488 | A    |
| 3   | 2     | 4500 | PSU  |
| 3   | 2     | 4510 | A    |
| 3   | 2     | 4512 | U    |
| 3   | 2     | 4513 | A    |
| 3   | 2     | 4518 | A    |
| 3   | 2     | 4519 | C    |
| 3   | 2     | 4523 | A2M  |
| 3   | 2     | 4524 | G    |
| 3   | 2     | 4532 | U    |
| 3   | 2     | 4545 | G    |
| 3   | 2     | 4548 | A    |
| 3   | 2     | 4549 | G    |
| 3   | 2     | 4560 | C    |
| 3   | 2     | 4567 | G    |
| 3   | 2     | 4570 | G    |
| 3   | 2     | 4573 | G    |
| 3   | 2     | 4575 | G    |
| 3   | 2     | 4583 | C    |
| 3   | 2     | 4584 | A    |
| 3   | 2     | 4589 | A    |
| 3   | 2     | 4590 | A    |
| 3   | 2     | 4599 | A    |
| 3   | 2     | 4600 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 4601 | U    |
| 3   | 2     | 4606 | G    |
| 3   | 2     | 4617 | G    |
| 3   | 2     | 4636 | PSU  |
| 3   | 2     | 4637 | OMG  |
| 3   | 2     | 4647 | G    |
| 3   | 2     | 4652 | G    |
| 3   | 2     | 4656 | A    |
| 3   | 2     | 4670 | C    |
| 3   | 2     | 4672 | A    |
| 3   | 2     | 4693 | C    |
| 3   | 2     | 4695 | C    |
| 3   | 2     | 4700 | A    |
| 3   | 2     | 4708 | A    |
| 3   | 2     | 4709 | U    |
| 3   | 2     | 4719 | G    |
| 3   | 2     | 4722 | G    |
| 3   | 2     | 4728 | U    |
| 3   | 2     | 4731 | G    |
| 3   | 2     | 4732 | G    |
| 3   | 2     | 4733 | C    |
| 3   | 2     | 4734 | A    |
| 3   | 2     | 4740 | G    |
| 3   | 2     | 4741 | C    |
| 3   | 2     | 4743 | G    |
| 3   | 2     | 4745 | G    |
| 3   | 2     | 4746 | C    |
| 3   | 2     | 4750 | G    |
| 3   | 2     | 4751 | G    |
| 3   | 2     | 4754 | G    |
| 3   | 2     | 4757 | C    |
| 3   | 2     | 4759 | C    |
| 3   | 2     | 4761 | G    |
| 3   | 2     | 4764 | A    |
| 3   | 2     | 4765 | G    |
| 3   | 2     | 4771 | C    |
| 3   | 2     | 4772 | C    |
| 3   | 2     | 4775 | C    |
| 3   | 2     | 4776 | G    |
| 3   | 2     | 4859 | C    |
| 3   | 2     | 4860 | G    |
| 3   | 2     | 4862 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 4864 | U    |
| 3   | 2     | 4870 | OMG  |
| 3   | 2     | 4871 | C    |
| 3   | 2     | 4872 | 2MG  |
| 3   | 2     | 4874 | A    |
| 3   | 2     | 4875 | G    |
| 3   | 2     | 4877 | G    |
| 3   | 2     | 4882 | U    |
| 3   | 2     | 4883 | C    |
| 3   | 2     | 4887 | C    |
| 3   | 2     | 4889 | G    |
| 3   | 2     | 4895 | C    |
| 3   | 2     | 4896 | G    |
| 3   | 2     | 4900 | C    |
| 3   | 2     | 4901 | G    |
| 3   | 2     | 4904 | G    |
| 3   | 2     | 4910 | G    |
| 3   | 2     | 4912 | G    |
| 3   | 2     | 4914 | C    |
| 3   | 2     | 4915 | G    |
| 3   | 2     | 4925 | U    |
| 3   | 2     | 4926 | C    |
| 3   | 2     | 4927 | G    |
| 3   | 2     | 4928 | C    |
| 3   | 2     | 4935 | C    |
| 3   | 2     | 4936 | G    |
| 3   | 2     | 4937 | C    |
| 3   | 2     | 4938 | A    |
| 3   | 2     | 4941 | G    |
| 3   | 2     | 4943 | A    |
| 3   | 2     | 4945 | G    |
| 3   | 2     | 4949 | G    |
| 3   | 2     | 4950 | U    |
| 3   | 2     | 4951 | G    |
| 3   | 2     | 4955 | A    |
| 3   | 2     | 4960 | G    |
| 3   | 2     | 4966 | A    |
| 3   | 2     | 4975 | G    |
| 3   | 2     | 4976 | U    |
| 3   | 2     | 4985 | U    |
| 3   | 2     | 4988 | U    |
| 3   | 2     | 4989 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 4991 | U    |
| 3   | 2     | 5013 | C    |
| 3   | 2     | 5014 | A    |
| 3   | 2     | 5021 | C    |
| 3   | 2     | 5022 | U    |
| 3   | 2     | 5023 | C    |
| 3   | 2     | 5024 | C    |
| 3   | 2     | 5025 | C    |
| 3   | 2     | 5026 | U    |
| 3   | 2     | 5034 | A    |
| 3   | 2     | 5041 | G    |
| 3   | 2     | 5047 | C    |
| 3   | 2     | 5050 | C    |
| 3   | 2     | 5053 | U    |
| 3   | 2     | 5054 | C    |
| 3   | 2     | 5055 | G    |
| 3   | 2     | 5058 | A    |
| 3   | 2     | 5060 | A    |
| 3   | 2     | 5061 | A    |
| 3   | 2     | 5062 | G    |
| 3   | 2     | 5069 | U    |
| 5   | 5     | 4    | U    |
| 5   | 5     | 5    | A    |
| 5   | 5     | 11   | A    |
| 5   | 5     | 13   | A    |
| 5   | 5     | 22   | A    |
| 5   | 5     | 24   | C    |
| 5   | 5     | 38   | U    |
| 5   | 5     | 42   | A    |
| 5   | 5     | 53   | U    |
| 5   | 5     | 54   | A    |
| 5   | 5     | 61   | G    |
| 5   | 5     | 62   | U    |
| 5   | 5     | 63   | C    |
| 5   | 5     | 64   | G    |
| 5   | 5     | 70   | G    |
| 5   | 5     | 71   | G    |
| 5   | 5     | 74   | A    |
| 5   | 5     | 100  | A    |
| 5   | 5     | 106  | G    |
| 5   | 5     | 110  | G    |
| 7   | 8     | 2    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 8     | 3   | A    |
| 7   | 8     | 23  | C    |
| 7   | 8     | 25  | G    |
| 7   | 8     | 34  | U    |
| 7   | 8     | 35  | C    |
| 7   | 8     | 38  | U    |
| 7   | 8     | 48  | A    |
| 7   | 8     | 59  | A    |
| 7   | 8     | 60  | G    |
| 7   | 8     | 62  | A    |
| 7   | 8     | 63  | U    |
| 7   | 8     | 68  | G    |
| 7   | 8     | 75  | G    |
| 7   | 8     | 80  | A    |
| 7   | 8     | 82  | A    |
| 7   | 8     | 83  | C    |
| 7   | 8     | 84  | A    |
| 7   | 8     | 85  | U    |
| 7   | 8     | 87  | G    |
| 7   | 8     | 103 | A    |
| 7   | 8     | 105 | C    |
| 7   | 8     | 106 | G    |
| 7   | 8     | 110 | U    |
| 7   | 8     | 111 | U    |
| 7   | 8     | 114 | G    |
| 7   | 8     | 123 | U    |
| 7   | 8     | 124 | U    |
| 7   | 8     | 125 | C    |
| 7   | 8     | 126 | C    |
| 7   | 8     | 127 | U    |
| 7   | 8     | 150 | C    |
| 7   | 8     | 151 | G    |
| 7   | 8     | 153 | C    |
| 7   | 8     | 156 | U    |

All (23) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 406 | C    |
| 3   | 2     | 504 | G    |
| 3   | 2     | 914 | U    |
| 3   | 2     | 955 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 2     | 1082 | C    |
| 3   | 2     | 1517 | 2MG  |
| 3   | 2     | 1633 | G    |
| 3   | 2     | 1763 | C    |
| 3   | 2     | 1773 | U    |
| 3   | 2     | 2033 | A    |
| 3   | 2     | 2084 | C    |
| 3   | 2     | 2416 | G    |
| 3   | 2     | 2675 | G    |
| 3   | 2     | 2760 | G    |
| 3   | 2     | 3614 | G    |
| 3   | 2     | 3673 | C    |
| 3   | 2     | 3788 | C    |
| 3   | 2     | 4378 | A    |
| 3   | 2     | 4600 | G    |
| 3   | 2     | 4699 | U    |
| 3   | 2     | 4913 | G    |
| 3   | 2     | 5022 | U    |
| 3   | 2     | 5060 | A    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | B8T  | 2     | 4671 | 3    | 19,22,23     | 3.27 | 8 (42%)     | 26,31,34    | 1.12 | 1 (3%)      |
| 3   | B8K  | 2     | 3897 | 3    | 24,28,29     | 4.32 | 16 (66%)    | 30,42,45    | 2.51 | 12 (40%)    |
| 3   | A2M  | 2     | 2363 | 3,49 | 22,25,26     | 3.60 | 10 (45%)    | 31,36,39    | 2.70 | 11 (35%)    |
| 3   | OMU  | 2     | 4306 | 3    | 19,22,23     | 2.75 | 7 (36%)     | 26,31,34    | 1.74 | 5 (19%)     |
| 3   | A2M  | 2     | 1871 | 3    | 22,25,26     | 3.54 | 10 (45%)    | 31,36,39    | 2.44 | 9 (29%)     |
| 3   | OMG  | 2     | 4196 | 3    | 23,26,27     | 2.37 | 8 (34%)     | 33,38,41    | 1.88 | 8 (24%)     |
| 3   | PSU  | 2     | 1582 | 3    | 18,21,22     | 1.07 | 1 (5%)      | 22,30,33    | 1.76 | 4 (18%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | 2     | 4628 | 3    | 18,21,22     | 0.99 | 1 (5%)   | 22,30,33    | 1.87 | 4 (18%)  |
| 3   | PSU  | 2     | 4500 | 3    | 18,21,22     | 1.09 | 3 (16%)  | 22,30,33    | 1.99 | 5 (22%)  |
| 3   | A2M  | 2     | 4523 | 3    | 22,25,26     | 3.51 | 10 (45%) | 31,36,39    | 2.54 | 12 (38%) |
| 3   | B8W  | 2     | 2380 | 3    | 23,26,27     | 3.66 | 10 (43%) | 33,38,41    | 2.58 | 12 (36%) |
| 3   | OMU  | 2     | 4620 | 3    | 19,22,23     | 2.82 | 8 (42%)  | 26,31,34    | 2.02 | 8 (30%)  |
| 3   | P7G  | 2     | 3880 | 3    | 24,28,29     | 4.22 | 11 (45%) | 27,41,44    | 1.71 | 5 (18%)  |
| 3   | B9B  | 2     | 237  | 3    | 25,28,29     | 3.47 | 12 (48%) | 35,40,43    | 2.51 | 13 (37%) |
| 3   | A2M  | 2     | 398  | 3    | 22,25,26     | 3.44 | 9 (40%)  | 31,36,39    | 2.56 | 8 (25%)  |
| 3   | BGH  | 2     | 3899 | 3    | 25,29,30     | 4.17 | 16 (64%) | 31,43,46    | 2.53 | 12 (38%) |
| 3   | PSU  | 2     | 4450 | 3    | 18,21,22     | 1.07 | 2 (11%)  | 22,30,33    | 2.02 | 5 (22%)  |
| 3   | I4U  | 2     | 4194 | 3    | 21,24,25     | 4.84 | 16 (76%) | 27,34,37    | 1.60 | 6 (22%)  |
| 3   | PSU  | 2     | 1683 | 3    | 18,21,22     | 1.13 | 1 (5%)   | 22,30,33    | 1.84 | 3 (13%)  |
| 3   | OMG  | 2     | 373  | 3    | 23,26,27     | 2.19 | 7 (30%)  | 33,38,41    | 1.83 | 8 (24%)  |
| 3   | E6G  | 2     | 4355 | 3    | 24,27,28     | 3.59 | 11 (45%) | 34,39,42    | 2.59 | 14 (41%) |
| 3   | B8H  | 2     | 4296 | 3    | 19,22,23     | 6.83 | 7 (36%)  | 22,32,35    | 2.40 | 5 (22%)  |
| 3   | 1MA  | 2     | 1322 | 3,49 | 21,25,26     | 2.68 | 6 (28%)  | 31,37,40    | 1.80 | 6 (19%)  |
| 3   | PSU  | 2     | 4636 | 3    | 18,21,22     | 1.17 | 3 (16%)  | 22,30,33    | 1.95 | 4 (18%)  |
| 3   | PSU  | 2     | 3715 | 3    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.49 | 3 (13%)  |
| 3   | B8T  | 2     | 4483 | 3    | 19,22,23     | 3.47 | 8 (42%)  | 26,31,34    | 0.84 | 1 (3%)   |
| 3   | 5MU  | 2     | 4083 | 3    | 19,22,23     | 4.68 | 7 (36%)  | 28,32,35    | 3.85 | 10 (35%) |
| 3   | UR3  | 2     | 4597 | 3    | 19,22,23     | 2.78 | 6 (31%)  | 26,32,35    | 1.24 | 2 (7%)   |
| 3   | 5MC  | 2     | 4335 | 3    | 18,22,23     | 3.29 | 7 (38%)  | 26,32,35    | 1.16 | 2 (7%)   |
| 3   | B9H  | 2     | 2786 | 3    | 20,25,26     | 2.69 | 5 (25%)  | 22,35,38    | 2.62 | 7 (31%)  |
| 3   | OMC  | 2     | 2365 | 3,49 | 19,22,23     | 2.69 | 7 (36%)  | 26,31,34    | 0.72 | 0        |
| 3   | OMC  | 2     | 2804 | 3    | 19,22,23     | 2.64 | 7 (36%)  | 26,31,34    | 0.81 | 0        |
| 3   | OMG  | 2     | 1316 | 3,49 | 23,26,27     | 2.30 | 9 (39%)  | 33,38,41    | 1.99 | 10 (30%) |
| 3   | 2MG  | 2     | 729  | 3    | 23,26,27     | 2.71 | 7 (30%)  | 32,38,41    | 2.23 | 8 (25%)  |
| 3   | P4U  | 2     | 1348 | 3    | 21,24,25     | 3.50 | 8 (38%)  | 27,33,36    | 1.14 | 2 (7%)   |
| 3   | OMG  | 2     | 1522 | 3    | 23,26,27     | 2.29 | 6 (26%)  | 33,38,41    | 1.86 | 10 (30%) |
| 3   | OMG  | 2     | 4370 | 3    | 23,26,27     | 2.23 | 8 (34%)  | 33,38,41    | 1.81 | 8 (24%)  |
| 3   | OMG  | 2     | 1625 | 3,49 | 23,26,27     | 2.22 | 7 (30%)  | 33,38,41    | 1.93 | 8 (24%)  |
| 3   | B9B  | 2     | 1574 | 3    | 25,28,29     | 3.56 | 12 (48%) | 35,40,43    | 2.35 | 14 (40%) |
| 3   | PSU  | 2     | 2508 | 3    | 18,21,22     | 1.03 | 1 (5%)   | 22,30,33    | 1.58 | 3 (13%)  |
| 3   | 5MC  | 2     | 3782 | 3,49 | 18,22,23     | 3.31 | 7 (38%)  | 26,32,35    | 1.15 | 3 (11%)  |
| 3   | OMC  | 2     | 3887 | 3    | 19,22,23     | 2.84 | 7 (36%)  | 26,31,34    | 1.00 | 1 (3%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | 7MG  | 2     | 1605 | 3    | 22,26,27     | 2.99 | 10 (45%) | 29,39,42    | 2.04 | 9 (31%)  |
| 3   | UR3  | 2     | 4530 | 3    | 19,22,23     | 2.75 | 7 (36%)  | 26,32,35    | 1.45 | 5 (19%)  |
| 3   | E7G  | 2     | 1797 | 3    | 24,27,28     | 3.54 | 11 (45%) | 30,40,43    | 2.21 | 9 (30%)  |
| 3   | B8W  | 2     | 4529 | 3    | 23,26,27     | 3.89 | 10 (43%) | 33,38,41    | 3.30 | 16 (48%) |
| 3   | 7MG  | 2     | 4550 | 3    | 22,26,27     | 3.11 | 10 (45%) | 29,39,42    | 2.05 | 10 (34%) |
| 3   | B9B  | 2     | 2754 | 3    | 25,28,29     | 3.46 | 11 (44%) | 35,40,43    | 2.34 | 12 (34%) |
| 3   | PSU  | 2     | 4442 | 3    | 18,21,22     | 1.20 | 1 (5%)   | 22,30,33    | 1.65 | 4 (18%)  |
| 3   | OMG  | 2     | 4623 | 3    | 23,26,27     | 2.25 | 8 (34%)  | 33,38,41    | 1.85 | 9 (27%)  |
| 3   | PSU  | 2     | 4403 | 3    | 18,21,22     | 1.07 | 1 (5%)   | 22,30,33    | 1.57 | 5 (22%)  |
| 3   | B8H  | 2     | 1860 | 3    | 19,22,23     | 6.84 | 7 (36%)  | 22,32,35    | 2.50 | 5 (22%)  |
| 3   | OMG  | 2     | 4494 | 3    | 23,26,27     | 2.22 | 8 (34%)  | 33,38,41    | 1.93 | 8 (24%)  |
| 3   | B8W  | 2     | 4129 | 3    | 23,26,27     | 3.76 | 8 (34%)  | 33,38,41    | 3.06 | 14 (42%) |
| 3   | OMG  | 2     | 2050 | 3    | 23,26,27     | 2.23 | 7 (30%)  | 33,38,41    | 1.90 | 8 (24%)  |
| 3   | OMG  | 2     | 4637 | 3    | 23,26,27     | 2.28 | 6 (26%)  | 33,38,41    | 1.98 | 7 (21%)  |
| 3   | A2M  | 2     | 1524 | 3    | 22,25,26     | 3.51 | 10 (45%) | 31,36,39    | 2.70 | 13 (41%) |
| 3   | B8W  | 2     | 4472 | 3    | 23,26,27     | 3.73 | 9 (39%)  | 33,38,41    | 2.43 | 12 (36%) |
| 3   | 2MG  | 2     | 4872 | 3    | 23,26,27     | 2.55 | 8 (34%)  | 32,38,41    | 2.26 | 12 (37%) |
| 3   | B8K  | 2     | 4690 | 3    | 24,28,29     | 4.33 | 16 (66%) | 30,42,45    | 2.55 | 12 (40%) |
| 3   | PSU  | 2     | 3729 | 3    | 18,21,22     | 1.03 | 2 (11%)  | 22,30,33    | 1.74 | 4 (18%)  |
| 3   | PSU  | 2     | 4531 | 3    | 18,21,22     | 1.04 | 1 (5%)   | 22,30,33    | 1.83 | 4 (18%)  |
| 3   | B8W  | 2     | 4185 | 3    | 23,26,27     | 3.70 | 10 (43%) | 33,38,41    | 2.63 | 13 (39%) |
| 3   | 2MG  | 2     | 978  | 3    | 23,26,27     | 2.68 | 9 (39%)  | 32,38,41    | 2.29 | 10 (31%) |
| 3   | OMG  | 2     | 2773 | 3    | 23,26,27     | 2.34 | 9 (39%)  | 33,38,41    | 1.89 | 9 (27%)  |
| 3   | P7G  | 2     | 1909 | 3    | 24,28,29     | 4.26 | 11 (45%) | 27,41,44    | 1.76 | 3 (11%)  |
| 3   | A2M  | 2     | 1534 | 3,49 | 22,25,26     | 3.59 | 11 (50%) | 31,36,39    | 2.64 | 12 (38%) |
| 3   | 5MC  | 2     | 4447 | 3,49 | 18,22,23     | 3.17 | 7 (38%)  | 26,32,35    | 1.67 | 2 (7%)   |
| 3   | OMG  | 2     | 4870 | 3    | 23,26,27     | 2.39 | 9 (39%)  | 33,38,41    | 2.04 | 11 (33%) |
| 3   | OMC  | 2     | 3869 | 3    | 19,22,23     | 2.74 | 7 (36%)  | 26,31,34    | 0.75 | 0        |
| 3   | OMG  | 2     | 1883 | 3    | 23,26,27     | 2.24 | 6 (26%)  | 33,38,41    | 1.84 | 8 (24%)  |
| 3   | A2M  | 2     | 3723 | 3    | 22,25,26     | 3.55 | 11 (50%) | 31,36,39    | 2.43 | 9 (29%)  |
| 3   | A2M  | 2     | 1326 | 3,49 | 22,25,26     | 3.46 | 9 (40%)  | 31,36,39    | 2.53 | 9 (29%)  |
| 3   | MHG  | 2     | 4371 | 3    | 29,32,33     | 3.68 | 12 (41%) | 34,46,49    | 2.20 | 10 (29%) |
| 3   | E7G  | 2     | 2297 | 3    | 24,27,28     | 3.43 | 11 (45%) | 30,40,43    | 2.17 | 9 (30%)  |
| 3   | OMG  | 2     | 3792 | 3    | 23,26,27     | 2.25 | 7 (30%)  | 33,38,41    | 1.82 | 8 (24%)  |
| 3   | UR3  | 2     | 1866 | 3    | 19,22,23     | 3.01 | 6 (31%)  | 26,32,35    | 1.65 | 4 (15%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMG  | 2     | 2364 | 3    | 23,26,27     | 2.14 | 7 (30%)  | 33,38,41    | 1.94 | 9 (27%)  |
| 3   | A2M  | 2     | 3825 | 3    | 22,25,26     | 3.54 | 10 (45%) | 31,36,39    | 2.55 | 9 (29%)  |
| 3   | PSU  | 2     | 4293 | 3    | 18,21,22     | 1.12 | 2 (11%)  | 22,30,33    | 1.76 | 4 (18%)  |
| 3   | OMG  | 2     | 2424 | 3,49 | 23,26,27     | 2.34 | 8 (34%)  | 33,38,41    | 1.82 | 7 (21%)  |
| 3   | PSU  | 2     | 1677 | 3    | 18,21,22     | 1.31 | 3 (16%)  | 22,30,33    | 2.08 | 5 (22%)  |
| 3   | A2M  | 2     | 2401 | 3    | 22,25,26     | 3.48 | 10 (45%) | 31,36,39    | 2.58 | 9 (29%)  |
| 3   | A2M  | 2     | 3718 | 3    | 22,25,26     | 3.52 | 10 (45%) | 31,36,39    | 2.52 | 10 (32%) |
| 3   | A2M  | 2     | 3867 | 3    | 22,25,26     | 3.50 | 10 (45%) | 31,36,39    | 2.49 | 9 (29%)  |
| 3   | M7A  | 2     | 4564 | 3    | 20,25,26     | 1.90 | 4 (20%)  | 28,37,40    | 3.91 | 7 (25%)  |
| 3   | OMC  | 2     | 2861 | 3    | 19,22,23     | 2.76 | 7 (36%)  | 26,31,34    | 0.66 | 0        |
| 3   | OMC  | 2     | 3701 | 3,49 | 19,22,23     | 2.61 | 8 (42%)  | 26,31,34    | 0.95 | 1 (3%)   |
| 3   | I4U  | 2     | 1659 | 3,49 | 21,24,25     | 4.57 | 15 (71%) | 27,34,37    | 1.31 | 3 (11%)  |
| 3   | B8Q  | 2     | 1456 | 3    | 17,22,23     | 2.85 | 4 (23%)  | 22,32,35    | 2.24 | 6 (27%)  |
| 3   | 2MG  | 2     | 1517 | 3    | 23,26,27     | 2.64 | 8 (34%)  | 32,38,41    | 2.79 | 9 (28%)  |
| 3   | OMC  | 2     | 2422 | 3,49 | 19,22,23     | 2.76 | 7 (36%)  | 26,31,34    | 1.43 | 3 (11%)  |
| 3   | OMC  | 2     | 3909 | 3    | 19,22,23     | 2.96 | 8 (42%)  | 26,31,34    | 1.44 | 4 (15%)  |
| 3   | OMC  | 2     | 4536 | 3    | 19,22,23     | 2.73 | 7 (36%)  | 26,31,34    | 0.75 | 0        |
| 3   | A2M  | 2     | 4571 | 3    | 22,25,26     | 3.63 | 11 (50%) | 31,36,39    | 2.46 | 10 (32%) |
| 3   | A2M  | 2     | 3785 | 3    | 22,25,26     | 3.45 | 10 (45%) | 31,36,39    | 2.76 | 12 (38%) |
| 3   | 6MZ  | 2     | 4220 | 3    | 22,25,26     | 2.52 | 4 (18%)  | 30,36,39    | 3.47 | 11 (36%) |
| 3   | 7MG  | 2     | 2522 | 3    | 22,26,27     | 3.14 | 10 (45%) | 29,39,42    | 2.01 | 7 (24%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | B8T  | 2     | 4671 | 3    | -       | 0/7/27/28  | 0/2/2/2 |
| 3   | B8K  | 2     | 3897 | 3    | -       | 3/11/41/42 | 0/3/3/3 |
| 3   | A2M  | 2     | 2363 | 3,49 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMU  | 2     | 4306 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | A2M  | 2     | 1871 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 2     | 4196 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | 2     | 1582 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | 2     | 4628 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | 2     | 4500 | 3    | -       | 3/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | A2M  | 2     | 4523 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | B8W  | 2     | 2380 | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | OMU  | 2     | 4620 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | P7G  | 2     | 3880 | 3    | -       | 4/10/40/41 | 0/3/3/3 |
| 3   | B9B  | 2     | 237  | 3    | -       | 5/11/29/30 | 0/3/3/3 |
| 3   | A2M  | 2     | 398  | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | BGH  | 2     | 3899 | 3    | -       | 0/13/43/44 | 0/3/3/3 |
| 3   | PSU  | 2     | 4450 | 3    | -       | 5/7/25/26  | 0/2/2/2 |
| 3   | I4U  | 2     | 4194 | 3    | -       | 0/9/29/30  | 0/2/2/2 |
| 3   | PSU  | 2     | 1683 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 2     | 373  | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | E6G  | 2     | 4355 | 3    | -       | 5/10/28/29 | 0/3/3/3 |
| 3   | B8H  | 2     | 4296 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | 1MA  | 2     | 1322 | 3,49 | -       | 1/7/25/26  | 0/3/3/3 |
| 3   | PSU  | 2     | 4636 | 3    | -       | 4/7/25/26  | 0/2/2/2 |
| 3   | PSU  | 2     | 3715 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | B8T  | 2     | 4483 | 3    | -       | 0/7/27/28  | 0/2/2/2 |
| 3   | 5MU  | 2     | 4083 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | UR3  | 2     | 4597 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | 5MC  | 2     | 4335 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | B9H  | 2     | 2786 | 3    | -       | 2/12/47/48 | 0/2/2/2 |
| 3   | OMC  | 2     | 2365 | 3,49 | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMC  | 2     | 2804 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | 2     | 1316 | 3,49 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | 2MG  | 2     | 729  | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | P4U  | 2     | 1348 | 3    | -       | 1/10/29/30 | 0/2/2/2 |
| 3   | OMG  | 2     | 1522 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 2     | 4370 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 2     | 1625 | 3,49 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | B9B  | 2     | 1574 | 3    | -       | 3/11/29/30 | 0/3/3/3 |
| 3   | PSU  | 2     | 2508 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | 5MC  | 2     | 3782 | 3,49 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | 2     | 3887 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | 7MG  | 2     | 1605 | 3    | -       | 0/7/37/38  | 0/3/3/3 |
| 3   | UR3  | 2     | 4530 | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | E7G  | 2     | 1797 | 3    | -       | 2/9/39/40  | 0/3/3/3 |
| 3   | B8W  | 2     | 4529 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | 7MG  | 2     | 4550 | 3    | -       | 2/7/37/38  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | B9B  | 2     | 2754 | 3    | -       | 5/11/29/30 | 0/3/3/3 |
| 3   | PSU  | 2     | 4442 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 2     | 4623 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | 2     | 4403 | 3    | -       | 5/7/25/26  | 0/2/2/2 |
| 3   | B8H  | 2     | 1860 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 2     | 4494 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | B8W  | 2     | 4129 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 2     | 2050 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 2     | 4637 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | 2     | 1524 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | B8W  | 2     | 4472 | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | 2MG  | 2     | 4872 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | B8K  | 2     | 4690 | 3    | -       | 0/11/41/42 | 0/3/3/3 |
| 3   | PSU  | 2     | 3729 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | 2     | 4531 | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | B8W  | 2     | 4185 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | 2MG  | 2     | 978  | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 2     | 2773 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | P7G  | 2     | 1909 | 3    | -       | 3/10/40/41 | 0/3/3/3 |
| 3   | A2M  | 2     | 1534 | 3,49 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | 5MC  | 2     | 4447 | 3,49 | -       | 4/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 2     | 4870 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | OMC  | 2     | 3869 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | 2     | 1883 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | 2     | 3723 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | 2     | 1326 | 3,49 | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | MHG  | 2     | 4371 | 3    | -       | 8/16/46/47 | 0/3/3/3 |
| 3   | E7G  | 2     | 2297 | 3    | -       | 3/9/39/40  | 0/3/3/3 |
| 3   | OMG  | 2     | 3792 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | UR3  | 2     | 1866 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 2     | 2364 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | 2     | 3825 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | PSU  | 2     | 4293 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 2     | 2424 | 3,49 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | 2     | 1677 | 3    | -       | 4/7/25/26  | 0/2/2/2 |
| 3   | A2M  | 2     | 2401 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | 2     | 3718 | 3    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | A2M  | 2     | 3867 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | M7A  | 2     | 4564 | 3    | -       | 0/7/37/38 | 0/3/3/3 |
| 3   | OMC  | 2     | 2861 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | OMC  | 2     | 3701 | 3,49 | -       | 4/9/27/28 | 0/2/2/2 |
| 3   | I4U  | 2     | 1659 | 3,49 | -       | 3/9/29/30 | 0/2/2/2 |
| 3   | B8Q  | 2     | 1456 | 3    | -       | 0/7/42/43 | 0/2/2/2 |
| 3   | 2MG  | 2     | 1517 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMC  | 2     | 2422 | 3,49 | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | OMC  | 2     | 3909 | 3    | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | OMC  | 2     | 4536 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | A2M  | 2     | 4571 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | A2M  | 2     | 3785 | 3    | -       | 3/9/27/28 | 0/3/3/3 |
| 3   | 6MZ  | 2     | 4220 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 3   | 7MG  | 2     | 2522 | 3    | -       | 0/7/37/38 | 0/3/3/3 |

All (762) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 3   | 2     | 1860 | B8H  | C6-C5   | -16.87 | 1.11        | 1.34     |
| 3   | 2     | 4296 | B8H  | C6-C5   | -16.85 | 1.11        | 1.34     |
| 3   | 2     | 4296 | B8H  | C4-N3   | -16.48 | 1.08        | 1.38     |
| 3   | 2     | 1860 | B8H  | C4-N3   | -16.25 | 1.08        | 1.38     |
| 3   | 2     | 1860 | B8H  | C4-C5   | 12.98  | 1.81        | 1.44     |
| 3   | 2     | 4296 | B8H  | C4-C5   | 12.75  | 1.80        | 1.44     |
| 3   | 2     | 3880 | P7G  | C8-N9   | 12.14  | 1.52        | 1.46     |
| 3   | 2     | 1860 | B8H  | C6-N1   | 11.84  | 1.65        | 1.36     |
| 3   | 2     | 4296 | B8H  | C6-N1   | 11.72  | 1.65        | 1.36     |
| 3   | 2     | 1909 | P7G  | C8-N9   | 11.71  | 1.52        | 1.46     |
| 3   | 2     | 1659 | I4U  | C3'-C2' | -10.57 | 1.24        | 1.53     |
| 3   | 2     | 4194 | I4U  | C3'-C2' | -10.57 | 1.24        | 1.53     |
| 3   | 2     | 4083 | 5MU  | C6-N1   | 10.49  | 1.55        | 1.38     |
| 3   | 2     | 4690 | B8K  | C3'-C4' | -10.47 | 1.26        | 1.53     |
| 3   | 2     | 3897 | B8K  | C3'-C4' | -10.10 | 1.27        | 1.53     |
| 3   | 2     | 4220 | 6MZ  | C6-N6   | 10.09  | 1.45        | 1.34     |
| 3   | 2     | 1909 | P7G  | C5-N7   | 10.07  | 1.46        | 1.35     |
| 3   | 2     | 4083 | 5MU  | C2-N1   | 10.05  | 1.54        | 1.38     |
| 3   | 2     | 4472 | B8W  | O4'-C1' | 10.02  | 1.65        | 1.42     |
| 3   | 2     | 4129 | B8W  | O4'-C1' | 9.99   | 1.65        | 1.42     |
| 3   | 2     | 4194 | I4U  | C4-N3   | 9.96   | 1.44        | 1.31     |
| 3   | 2     | 3899 | BGH  | C3'-C4' | -9.92  | 1.27        | 1.53     |
| 3   | 2     | 2380 | B8W  | O4'-C1' | 9.91   | 1.65        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 3897 | B8K  | O4'-C4' | 9.87  | 1.67        | 1.45     |
| 3   | 2     | 4529 | B8W  | O4'-C1' | 9.84  | 1.65        | 1.42     |
| 3   | 2     | 4185 | B8W  | O4'-C1' | 9.82  | 1.65        | 1.42     |
| 3   | 2     | 1348 | P4U  | C4-N3   | 9.66  | 1.43        | 1.31     |
| 3   | 2     | 4690 | B8K  | O4'-C4' | 9.48  | 1.66        | 1.45     |
| 3   | 2     | 4571 | A2M  | C2'-C1' | -9.44 | 1.28        | 1.53     |
| 3   | 2     | 1534 | A2M  | C2'-C1' | -9.29 | 1.29        | 1.53     |
| 3   | 2     | 2363 | A2M  | C2'-C1' | -9.26 | 1.29        | 1.53     |
| 3   | 2     | 3867 | A2M  | C2'-C1' | -9.25 | 1.29        | 1.53     |
| 3   | 2     | 4529 | B8W  | C2-N2   | 9.20  | 1.52        | 1.33     |
| 3   | 2     | 4523 | A2M  | C2'-C1' | -9.17 | 1.29        | 1.53     |
| 3   | 2     | 3899 | BGH  | O4'-C4' | 9.11  | 1.65        | 1.45     |
| 3   | 2     | 3825 | A2M  | C2'-C1' | -9.02 | 1.29        | 1.53     |
| 3   | 2     | 3880 | P7G  | C5-N7   | 9.01  | 1.45        | 1.35     |
| 3   | 2     | 1326 | A2M  | C2'-C1' | -9.01 | 1.29        | 1.53     |
| 3   | 2     | 3718 | A2M  | C2'-C1' | -8.98 | 1.30        | 1.53     |
| 3   | 2     | 3723 | A2M  | C2'-C1' | -8.98 | 1.30        | 1.53     |
| 3   | 2     | 2401 | A2M  | C2'-C1' | -8.93 | 1.30        | 1.53     |
| 3   | 2     | 1659 | I4U  | C4-N3   | 8.92  | 1.42        | 1.31     |
| 3   | 2     | 1524 | A2M  | C2'-C1' | -8.91 | 1.30        | 1.53     |
| 3   | 2     | 4335 | 5MC  | C6-C5   | 8.75  | 1.49        | 1.34     |
| 3   | 2     | 398  | A2M  | C2'-C1' | -8.73 | 1.30        | 1.53     |
| 3   | 2     | 3785 | A2M  | C2'-C1' | -8.71 | 1.30        | 1.53     |
| 3   | 2     | 2297 | E7G  | C5-N7   | 8.70  | 1.45        | 1.35     |
| 3   | 2     | 4083 | 5MU  | C4-C5   | 8.70  | 1.59        | 1.44     |
| 3   | 2     | 4355 | E6G  | O4'-C1' | 8.70  | 1.62        | 1.42     |
| 3   | 2     | 1871 | A2M  | O4'-C1' | 8.64  | 1.62        | 1.42     |
| 3   | 2     | 3782 | 5MC  | C6-C5   | 8.63  | 1.48        | 1.34     |
| 3   | 2     | 1871 | A2M  | C2'-C1' | -8.61 | 1.30        | 1.53     |
| 3   | 2     | 1574 | B9B  | O4'-C1' | 8.55  | 1.62        | 1.42     |
| 3   | 2     | 2754 | B9B  | O4'-C1' | 8.54  | 1.62        | 1.42     |
| 3   | 2     | 4083 | 5MU  | C4-N3   | -8.46 | 1.23        | 1.38     |
| 3   | 2     | 1797 | E7G  | C8-N9   | 8.44  | 1.50        | 1.46     |
| 3   | 2     | 3723 | A2M  | O4'-C1' | 8.43  | 1.62        | 1.42     |
| 3   | 2     | 3718 | A2M  | O4'-C1' | 8.43  | 1.62        | 1.42     |
| 3   | 2     | 4371 | MHG  | C5-N7   | 8.36  | 1.45        | 1.35     |
| 3   | 2     | 4355 | E6G  | O4'-C4' | -8.36 | 1.26        | 1.45     |
| 3   | 2     | 1797 | E7G  | C5-N7   | 8.35  | 1.45        | 1.35     |
| 3   | 2     | 398  | A2M  | O4'-C1' | 8.31  | 1.61        | 1.42     |
| 3   | 2     | 1456 | B8Q  | C6-C5   | 8.30  | 1.52        | 1.33     |
| 3   | 2     | 237  | B9B  | O4'-C4' | -8.29 | 1.26        | 1.45     |
| 3   | 2     | 3825 | A2M  | O4'-C1' | 8.29  | 1.61        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 2786 | B9H  | C2-N3   | 8.28  | 1.47        | 1.37     |
| 3   | 2     | 4447 | 5MC  | C6-C5   | 8.23  | 1.48        | 1.34     |
| 3   | 2     | 4523 | A2M  | O4'-C1' | 8.22  | 1.61        | 1.42     |
| 3   | 2     | 1574 | B9B  | O4'-C4' | -8.21 | 1.26        | 1.45     |
| 3   | 2     | 1534 | A2M  | O4'-C1' | 8.14  | 1.61        | 1.42     |
| 3   | 2     | 1524 | A2M  | O4'-C1' | 8.14  | 1.61        | 1.42     |
| 3   | 2     | 1326 | A2M  | O4'-C1' | 8.13  | 1.61        | 1.42     |
| 3   | 2     | 3867 | A2M  | O4'-C1' | 8.11  | 1.61        | 1.42     |
| 3   | 2     | 4571 | A2M  | O4'-C1' | 8.10  | 1.61        | 1.42     |
| 3   | 2     | 2401 | A2M  | O4'-C1' | 8.09  | 1.61        | 1.42     |
| 3   | 2     | 4371 | MHG  | C8-N9   | 8.07  | 1.50        | 1.46     |
| 3   | 2     | 4129 | B8W  | C2-N2   | 8.07  | 1.50        | 1.33     |
| 3   | 2     | 2297 | E7G  | C8-N9   | 8.05  | 1.50        | 1.46     |
| 3   | 2     | 4472 | B8W  | C2-N2   | 8.03  | 1.50        | 1.33     |
| 3   | 2     | 237  | B9B  | O4'-C1' | 8.00  | 1.60        | 1.42     |
| 3   | 2     | 2363 | A2M  | O4'-C1' | 7.91  | 1.60        | 1.42     |
| 3   | 2     | 237  | B9B  | C2'-C1' | -7.87 | 1.28        | 1.53     |
| 3   | 2     | 1574 | B9B  | C2'-C1' | -7.84 | 1.28        | 1.53     |
| 3   | 2     | 1322 | 1MA  | C2-N3   | 7.83  | 1.45        | 1.30     |
| 3   | 2     | 2754 | B9B  | O4'-C4' | -7.72 | 1.27        | 1.45     |
| 3   | 2     | 1866 | UR3  | C2-N1   | 7.70  | 1.49        | 1.38     |
| 3   | 2     | 1659 | I4U  | O4'-C4' | -7.69 | 1.27        | 1.45     |
| 3   | 2     | 4355 | E6G  | C2'-C1' | -7.68 | 1.28        | 1.53     |
| 3   | 2     | 3785 | A2M  | O4'-C1' | 7.64  | 1.60        | 1.42     |
| 3   | 2     | 4185 | B8W  | C2-N2   | 7.60  | 1.49        | 1.33     |
| 3   | 2     | 729  | 2MG  | C2-N3   | 7.47  | 1.46        | 1.31     |
| 3   | 2     | 4185 | B8W  | C2'-C1' | -7.45 | 1.29        | 1.53     |
| 3   | 2     | 2522 | 7MG  | C5-N7   | 7.42  | 1.44        | 1.35     |
| 3   | 2     | 2754 | B9B  | C2'-C1' | -7.37 | 1.29        | 1.53     |
| 3   | 2     | 4571 | A2M  | O4'-C4' | -7.27 | 1.28        | 1.45     |
| 3   | 2     | 4194 | I4U  | O4'-C4' | -7.27 | 1.28        | 1.45     |
| 3   | 2     | 4550 | 7MG  | C5-N7   | 7.25  | 1.44        | 1.35     |
| 3   | 2     | 4129 | B8W  | C2'-C1' | -7.24 | 1.30        | 1.53     |
| 3   | 2     | 2363 | A2M  | O4'-C4' | -7.23 | 1.28        | 1.45     |
| 3   | 2     | 2380 | B8W  | C2-N2   | 7.23  | 1.48        | 1.33     |
| 3   | 2     | 2380 | B8W  | C2'-C1' | -7.22 | 1.30        | 1.53     |
| 3   | 2     | 1605 | 7MG  | C5-N7   | 7.14  | 1.43        | 1.35     |
| 3   | 2     | 4483 | B8T  | C2-N3   | 7.10  | 1.50        | 1.36     |
| 3   | 2     | 4529 | B8W  | C2'-C1' | -7.04 | 1.31        | 1.53     |
| 3   | 2     | 978  | 2MG  | C2-N3   | 7.00  | 1.45        | 1.31     |
| 3   | 2     | 1524 | A2M  | O4'-C4' | -7.00 | 1.29        | 1.45     |
| 3   | 2     | 4371 | MHG  | C2-N3   | 7.00  | 1.45        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 4483 | B8T  | C4-N3   | 6.92  | 1.44        | 1.32     |
| 3   | 2     | 4472 | B8W  | C2'-C1' | -6.92 | 1.31        | 1.53     |
| 3   | 2     | 4530 | UR3  | C2-N1   | 6.82  | 1.48        | 1.38     |
| 3   | 2     | 1534 | A2M  | O4'-C4' | -6.80 | 1.29        | 1.45     |
| 3   | 2     | 1866 | UR3  | C6-C5   | 6.80  | 1.50        | 1.35     |
| 3   | 2     | 4523 | A2M  | O4'-C4' | -6.79 | 1.29        | 1.45     |
| 3   | 2     | 3723 | A2M  | O4'-C4' | -6.78 | 1.29        | 1.45     |
| 3   | 2     | 3825 | A2M  | O4'-C4' | -6.74 | 1.29        | 1.45     |
| 3   | 2     | 4483 | B8T  | C6-C5   | 6.73  | 1.50        | 1.35     |
| 3   | 2     | 4550 | 7MG  | C8-N9   | 6.72  | 1.49        | 1.46     |
| 3   | 2     | 3718 | A2M  | O4'-C4' | -6.70 | 1.30        | 1.45     |
| 3   | 2     | 3880 | P7G  | C4-N3   | 6.69  | 1.49        | 1.37     |
| 3   | 2     | 1456 | B8Q  | C2-N3   | 6.66  | 1.46        | 1.35     |
| 3   | 2     | 1348 | P4U  | C2-N3   | 6.63  | 1.49        | 1.36     |
| 3   | 2     | 4371 | MHG  | C8-N7   | 6.62  | 1.52        | 1.45     |
| 3   | 2     | 3785 | A2M  | O4'-C4' | -6.60 | 1.30        | 1.45     |
| 3   | 2     | 4671 | B8T  | C6-C5   | 6.59  | 1.50        | 1.35     |
| 3   | 2     | 4872 | 2MG  | C2-N3   | 6.58  | 1.44        | 1.31     |
| 3   | 2     | 4597 | UR3  | C2-N1   | 6.57  | 1.48        | 1.38     |
| 3   | 2     | 398  | A2M  | O4'-C4' | -6.55 | 1.30        | 1.45     |
| 3   | 2     | 1326 | A2M  | O4'-C4' | -6.51 | 1.30        | 1.45     |
| 3   | 2     | 4597 | UR3  | C6-C5   | 6.48  | 1.50        | 1.35     |
| 3   | 2     | 4671 | B8T  | C2-N3   | 6.44  | 1.49        | 1.36     |
| 3   | 2     | 2401 | A2M  | O4'-C4' | -6.44 | 1.30        | 1.45     |
| 3   | 2     | 4194 | I4U  | C6-C5   | 6.40  | 1.49        | 1.35     |
| 3   | 2     | 3867 | A2M  | O4'-C4' | -6.40 | 1.30        | 1.45     |
| 3   | 2     | 1871 | A2M  | O4'-C4' | -6.37 | 1.30        | 1.45     |
| 3   | 2     | 4530 | UR3  | C6-C5   | 6.34  | 1.49        | 1.35     |
| 3   | 2     | 4620 | OMU  | C2-N3   | 6.30  | 1.49        | 1.38     |
| 3   | 2     | 2522 | 7MG  | C8-N9   | 6.28  | 1.49        | 1.46     |
| 3   | 2     | 4196 | OMG  | C4-N3   | 6.16  | 1.48        | 1.34     |
| 3   | 2     | 1909 | P7G  | C4-N3   | 6.16  | 1.48        | 1.37     |
| 3   | 2     | 4306 | OMU  | C2-N3   | 6.16  | 1.48        | 1.38     |
| 3   | 2     | 729  | 2MG  | C4-N3   | 6.15  | 1.48        | 1.34     |
| 3   | 2     | 4620 | OMU  | C2-N1   | 6.13  | 1.48        | 1.38     |
| 3   | 2     | 3909 | OMC  | C2-N3   | 6.11  | 1.48        | 1.36     |
| 3   | 2     | 1866 | UR3  | C2-N3   | 6.08  | 1.50        | 1.39     |
| 3   | 2     | 1517 | 2MG  | C2-N3   | 6.08  | 1.43        | 1.31     |
| 3   | 2     | 4194 | I4U  | C2-N3   | 6.07  | 1.48        | 1.36     |
| 3   | 2     | 4483 | B8T  | C4-N4   | 6.06  | 1.48        | 1.35     |
| 3   | 2     | 3887 | OMC  | C2-N3   | 6.04  | 1.48        | 1.36     |
| 3   | 2     | 3792 | OMG  | C4-N3   | 6.03  | 1.48        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 4870 | OMG  | C4-N3   | 6.03  | 1.48        | 1.34     |
| 3   | 2     | 1322 | 1MA  | C4-N3   | 6.01  | 1.48        | 1.35     |
| 3   | 2     | 3897 | B8K  | O4'-C1' | -6.01 | 1.27        | 1.42     |
| 3   | 2     | 4671 | B8T  | C4-N3   | 6.00  | 1.43        | 1.32     |
| 3   | 2     | 1517 | 2MG  | C4-N3   | 5.99  | 1.48        | 1.34     |
| 3   | 2     | 2861 | OMC  | C2-N3   | 5.99  | 1.48        | 1.36     |
| 3   | 2     | 978  | 2MG  | C4-N3   | 5.96  | 1.48        | 1.34     |
| 3   | 2     | 2773 | OMG  | C4-N3   | 5.95  | 1.48        | 1.34     |
| 3   | 2     | 1348 | P4U  | C6-C5   | 5.94  | 1.48        | 1.35     |
| 3   | 2     | 4371 | MHG  | C2-N1   | 5.88  | 1.46        | 1.36     |
| 3   | 2     | 2050 | OMG  | C4-N3   | 5.86  | 1.48        | 1.34     |
| 3   | 2     | 3887 | OMC  | C6-C5   | 5.85  | 1.48        | 1.35     |
| 3   | 2     | 4370 | OMG  | C4-N3   | 5.83  | 1.48        | 1.34     |
| 3   | 2     | 2786 | B9H  | C6-C5   | 5.82  | 1.46        | 1.33     |
| 3   | 2     | 4494 | OMG  | C4-N3   | 5.80  | 1.48        | 1.34     |
| 3   | 2     | 4536 | OMC  | C2-N3   | 5.79  | 1.48        | 1.36     |
| 3   | 2     | 4371 | MHG  | C2-N2   | 5.79  | 1.46        | 1.33     |
| 3   | 2     | 4671 | B8T  | C4-N4   | 5.77  | 1.47        | 1.35     |
| 3   | 2     | 2422 | OMC  | C6-C5   | 5.76  | 1.48        | 1.35     |
| 3   | 2     | 2365 | OMC  | C2-N3   | 5.76  | 1.48        | 1.36     |
| 3   | 2     | 3782 | 5MC  | C4-N3   | 5.75  | 1.43        | 1.34     |
| 3   | 2     | 1659 | I4U  | C6-C5   | 5.74  | 1.48        | 1.35     |
| 3   | 2     | 4690 | B8K  | O4'-C1' | -5.73 | 1.28        | 1.42     |
| 3   | 2     | 4623 | OMG  | C4-N3   | 5.73  | 1.47        | 1.34     |
| 3   | 2     | 4637 | OMG  | C4-N3   | 5.73  | 1.47        | 1.34     |
| 3   | 2     | 2804 | OMC  | C2-N3   | 5.69  | 1.47        | 1.36     |
| 3   | 2     | 3701 | OMC  | C6-C5   | 5.69  | 1.48        | 1.35     |
| 3   | 2     | 1625 | OMG  | C4-N3   | 5.69  | 1.47        | 1.34     |
| 3   | 2     | 3782 | 5MC  | C2-N3   | 5.68  | 1.47        | 1.36     |
| 3   | 2     | 3869 | OMC  | C2-N3   | 5.67  | 1.47        | 1.36     |
| 3   | 2     | 1522 | OMG  | C4-N3   | 5.66  | 1.47        | 1.34     |
| 3   | 2     | 2861 | OMC  | C6-C5   | 5.66  | 1.48        | 1.35     |
| 3   | 2     | 4690 | B8K  | C2-N3   | 5.65  | 1.46        | 1.33     |
| 3   | 2     | 3909 | OMC  | C6-C5   | 5.65  | 1.48        | 1.35     |
| 3   | 2     | 4529 | B8W  | O4'-C4' | -5.65 | 1.32        | 1.45     |
| 3   | 2     | 4196 | OMG  | C2-N3   | 5.65  | 1.46        | 1.33     |
| 3   | 2     | 4872 | 2MG  | C4-N3   | 5.64  | 1.47        | 1.34     |
| 3   | 2     | 4536 | OMC  | C6-C5   | 5.64  | 1.48        | 1.35     |
| 3   | 2     | 3869 | OMC  | C6-C5   | 5.61  | 1.48        | 1.35     |
| 3   | 2     | 4690 | B8K  | C8-N9   | 5.60  | 1.49        | 1.46     |
| 3   | 2     | 1316 | OMG  | C4-N3   | 5.58  | 1.47        | 1.34     |
| 3   | 2     | 1883 | OMG  | C4-N3   | 5.58  | 1.47        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 2424 | OMG  | C4-N3   | 5.58  | 1.47        | 1.34     |
| 3   | 2     | 1909 | P7G  | C2-N2   | 5.58  | 1.47        | 1.34     |
| 3   | 2     | 373  | OMG  | C4-N3   | 5.58  | 1.47        | 1.34     |
| 3   | 2     | 4335 | 5MC  | C4-N3   | 5.55  | 1.43        | 1.34     |
| 3   | 2     | 2365 | OMC  | C6-C5   | 5.54  | 1.47        | 1.35     |
| 3   | 2     | 4185 | B8W  | O4'-C4' | -5.54 | 1.32        | 1.45     |
| 3   | 2     | 4870 | OMG  | C2-N3   | 5.53  | 1.46        | 1.33     |
| 3   | 2     | 4306 | OMU  | C2-N1   | 5.52  | 1.47        | 1.38     |
| 3   | 2     | 4083 | 5MU  | C6-C5   | 5.51  | 1.43        | 1.34     |
| 3   | 2     | 4129 | B8W  | O4'-C4' | -5.48 | 1.32        | 1.45     |
| 3   | 2     | 1659 | I4U  | C2-N3   | 5.48  | 1.47        | 1.36     |
| 3   | 2     | 1797 | E7G  | C2-N3   | 5.47  | 1.46        | 1.33     |
| 3   | 2     | 3897 | B8K  | C2-N3   | 5.47  | 1.46        | 1.33     |
| 3   | 2     | 2380 | B8W  | O4'-C4' | -5.46 | 1.32        | 1.45     |
| 3   | 2     | 2364 | OMG  | C4-N3   | 5.43  | 1.47        | 1.34     |
| 3   | 2     | 4529 | B8W  | O6-C6   | 5.41  | 1.43        | 1.35     |
| 3   | 2     | 2754 | B9B  | C2-N2   | 5.41  | 1.44        | 1.33     |
| 3   | 2     | 4129 | B8W  | O6-C6   | 5.40  | 1.43        | 1.35     |
| 3   | 2     | 4597 | UR3  | C2-N3   | 5.40  | 1.49        | 1.39     |
| 3   | 2     | 4371 | MHG  | C4-N3   | 5.40  | 1.47        | 1.34     |
| 3   | 2     | 2804 | OMC  | C6-C5   | 5.39  | 1.47        | 1.35     |
| 3   | 2     | 1797 | E7G  | C4-N3   | 5.38  | 1.47        | 1.34     |
| 3   | 2     | 2422 | OMC  | C2-N3   | 5.38  | 1.47        | 1.36     |
| 3   | 2     | 1909 | P7G  | C2-N1   | 5.34  | 1.46        | 1.33     |
| 3   | 2     | 3701 | OMC  | C2-N3   | 5.34  | 1.47        | 1.36     |
| 3   | 2     | 237  | B9B  | C2-N2   | 5.33  | 1.44        | 1.33     |
| 3   | 2     | 4306 | OMU  | C6-C5   | 5.32  | 1.47        | 1.35     |
| 3   | 2     | 4447 | 5MC  | C2-N3   | 5.32  | 1.47        | 1.36     |
| 3   | 2     | 4335 | 5MC  | C2-N3   | 5.28  | 1.47        | 1.36     |
| 3   | 2     | 2424 | OMG  | C2-N3   | 5.28  | 1.45        | 1.33     |
| 3   | 2     | 3880 | P7G  | C2-N2   | 5.28  | 1.46        | 1.34     |
| 3   | 2     | 3899 | BGH  | C4-N3   | 5.27  | 1.46        | 1.34     |
| 3   | 2     | 4472 | B8W  | O4'-C4' | -5.26 | 1.33        | 1.45     |
| 3   | 2     | 2773 | OMG  | C2-N3   | 5.26  | 1.45        | 1.33     |
| 3   | 2     | 2522 | 7MG  | C2-N3   | 5.25  | 1.45        | 1.33     |
| 3   | 2     | 4355 | E6G  | C2-N2   | 5.25  | 1.44        | 1.33     |
| 3   | 2     | 1605 | 7MG  | C2-N3   | 5.24  | 1.45        | 1.33     |
| 3   | 2     | 4447 | 5MC  | C4-N3   | 5.24  | 1.43        | 1.34     |
| 3   | 2     | 4472 | B8W  | O6-C6   | 5.22  | 1.43        | 1.35     |
| 3   | 2     | 1574 | B9B  | C2-N2   | 5.20  | 1.44        | 1.33     |
| 3   | 2     | 4194 | I4U  | C3'-C4' | 5.13  | 1.66        | 1.53     |
| 3   | 2     | 4620 | OMU  | C6-C5   | 5.12  | 1.47        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 4185 | B8W  | O3'-C3' | -5.11 | 1.30        | 1.43     |
| 3   | 2     | 1517 | 2MG  | C2-N2   | 5.11  | 1.44        | 1.33     |
| 3   | 2     | 3792 | OMG  | C2-N3   | 5.09  | 1.45        | 1.33     |
| 3   | 2     | 3909 | OMC  | C2-N1   | 5.08  | 1.51        | 1.40     |
| 3   | 2     | 2297 | E7G  | C2-N3   | 5.06  | 1.45        | 1.33     |
| 3   | 2     | 4637 | OMG  | C2-N3   | 5.06  | 1.45        | 1.33     |
| 3   | 2     | 4530 | UR3  | C2-N3   | 5.05  | 1.48        | 1.39     |
| 3   | 2     | 4494 | OMG  | C2-N3   | 5.05  | 1.45        | 1.33     |
| 3   | 2     | 3899 | BGH  | O4'-C1' | -5.03 | 1.30        | 1.42     |
| 3   | 2     | 4370 | OMG  | C2-N3   | 5.01  | 1.45        | 1.33     |
| 3   | 2     | 1348 | P4U  | O4-C4   | 5.01  | 1.40        | 1.35     |
| 3   | 2     | 2050 | OMG  | C2-N3   | 5.01  | 1.45        | 1.33     |
| 3   | 2     | 3899 | BGH  | C8-N9   | 4.99  | 1.48        | 1.46     |
| 3   | 2     | 3899 | BGH  | C2-N3   | 4.98  | 1.45        | 1.33     |
| 3   | 2     | 1605 | 7MG  | C4-N3   | 4.98  | 1.46        | 1.34     |
| 3   | 2     | 1625 | OMG  | C2-N3   | 4.97  | 1.45        | 1.33     |
| 3   | 2     | 729  | 2MG  | C2-N2   | 4.96  | 1.44        | 1.33     |
| 3   | 2     | 2297 | E7G  | C4-N3   | 4.95  | 1.46        | 1.34     |
| 3   | 2     | 4472 | B8W  | O3'-C3' | -4.94 | 1.31        | 1.43     |
| 3   | 2     | 3897 | B8K  | C8-N9   | 4.93  | 1.48        | 1.46     |
| 3   | 2     | 4550 | 7MG  | C4-N3   | 4.87  | 1.45        | 1.34     |
| 3   | 2     | 4623 | OMG  | C2-N3   | 4.87  | 1.44        | 1.33     |
| 3   | 2     | 4690 | B8K  | C4-N3   | 4.85  | 1.45        | 1.34     |
| 3   | 2     | 4550 | 7MG  | C2-N3   | 4.85  | 1.44        | 1.33     |
| 3   | 2     | 3880 | P7G  | C2-N1   | 4.84  | 1.44        | 1.33     |
| 3   | 2     | 2522 | 7MG  | C4-N3   | 4.84  | 1.45        | 1.34     |
| 3   | 2     | 1316 | OMG  | C2-N3   | 4.83  | 1.44        | 1.33     |
| 3   | 2     | 3909 | OMC  | C4-N4   | 4.82  | 1.45        | 1.33     |
| 3   | 2     | 1348 | P4U  | C5-C4   | 4.80  | 1.49        | 1.43     |
| 3   | 2     | 978  | 2MG  | C2-N2   | 4.79  | 1.44        | 1.33     |
| 3   | 2     | 4564 | M7A  | C6-N6   | 4.76  | 1.46        | 1.34     |
| 3   | 2     | 2364 | OMG  | C2-N3   | 4.76  | 1.44        | 1.33     |
| 3   | 2     | 3897 | B8K  | C4-N3   | 4.74  | 1.45        | 1.34     |
| 3   | 2     | 1522 | OMG  | C2-N3   | 4.74  | 1.44        | 1.33     |
| 3   | 2     | 1797 | E7G  | C2-N2   | 4.74  | 1.45        | 1.34     |
| 3   | 2     | 4194 | I4U  | C1'-N1  | -4.73 | 1.33        | 1.47     |
| 3   | 2     | 4371 | MHG  | C4-N9   | 4.72  | 1.43        | 1.37     |
| 3   | 2     | 3909 | OMC  | C4-N3   | 4.71  | 1.44        | 1.34     |
| 3   | 2     | 4529 | B8W  | O3'-C3' | -4.70 | 1.31        | 1.43     |
| 3   | 2     | 4872 | 2MG  | C2-N2   | 4.69  | 1.43        | 1.33     |
| 3   | 2     | 2422 | OMC  | C4-N4   | 4.65  | 1.44        | 1.33     |
| 3   | 2     | 4129 | B8W  | O3'-C3' | -4.64 | 1.32        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 2422 | OMC  | C2-N1   | 4.64  | 1.50        | 1.40     |
| 3   | 2     | 3897 | B8K  | O2'-C2' | -4.63 | 1.32        | 1.43     |
| 3   | 2     | 1871 | A2M  | C6-N6   | 4.62  | 1.45        | 1.34     |
| 3   | 2     | 3880 | P7G  | C4-N9   | 4.60  | 1.42        | 1.35     |
| 3   | 2     | 3887 | OMC  | C4-N4   | 4.60  | 1.44        | 1.33     |
| 3   | 2     | 1659 | I4U  | C1'-N1  | -4.59 | 1.34        | 1.47     |
| 3   | 2     | 1883 | OMG  | C2-N3   | 4.58  | 1.44        | 1.33     |
| 3   | 2     | 2297 | E7G  | C2-N2   | 4.58  | 1.45        | 1.34     |
| 3   | 2     | 3887 | OMC  | C4-N3   | 4.55  | 1.43        | 1.34     |
| 3   | 2     | 1909 | P7G  | C6-N1   | 4.54  | 1.46        | 1.38     |
| 3   | 2     | 2861 | OMC  | C4-N4   | 4.54  | 1.44        | 1.33     |
| 3   | 2     | 373  | OMG  | C2-N3   | 4.54  | 1.44        | 1.33     |
| 3   | 2     | 4690 | B8K  | O2'-C2' | -4.53 | 1.32        | 1.43     |
| 3   | 2     | 3869 | OMC  | C4-N4   | 4.53  | 1.44        | 1.33     |
| 3   | 2     | 3899 | BGH  | C2-N2   | 4.52  | 1.44        | 1.34     |
| 3   | 2     | 1605 | 7MG  | C8-N9   | 4.50  | 1.48        | 1.46     |
| 3   | 2     | 1605 | 7MG  | C2-N2   | 4.48  | 1.44        | 1.34     |
| 3   | 2     | 2365 | OMC  | C4-N4   | 4.45  | 1.44        | 1.33     |
| 3   | 2     | 3723 | A2M  | C6-N6   | 4.42  | 1.45        | 1.34     |
| 3   | 2     | 2861 | OMC  | C4-N3   | 4.42  | 1.43        | 1.34     |
| 3   | 2     | 2380 | B8W  | O3'-C3' | -4.41 | 1.32        | 1.43     |
| 3   | 2     | 2786 | B9H  | C2-N1   | 4.40  | 1.44        | 1.38     |
| 3   | 2     | 1797 | E7G  | C4-N9   | 4.39  | 1.42        | 1.37     |
| 3   | 2     | 2522 | 7MG  | C2-N2   | 4.38  | 1.44        | 1.34     |
| 3   | 2     | 3869 | OMC  | C4-N3   | 4.38  | 1.43        | 1.34     |
| 3   | 2     | 4442 | PSU  | C6-C5   | 4.38  | 1.40        | 1.35     |
| 3   | 2     | 4550 | 7MG  | C2-N2   | 4.37  | 1.44        | 1.34     |
| 3   | 2     | 4536 | OMC  | C4-N4   | 4.37  | 1.44        | 1.33     |
| 3   | 2     | 1524 | A2M  | C6-N6   | 4.35  | 1.45        | 1.34     |
| 3   | 2     | 3899 | BGH  | C71-N7  | 4.34  | 1.49        | 1.39     |
| 3   | 2     | 2804 | OMC  | C4-N4   | 4.33  | 1.44        | 1.33     |
| 3   | 2     | 3897 | B8K  | C4-N9   | 4.32  | 1.42        | 1.37     |
| 3   | 2     | 978  | 2MG  | C2-N1   | 4.32  | 1.43        | 1.36     |
| 3   | 2     | 3899 | BGH  | O2'-C2' | -4.29 | 1.31        | 1.42     |
| 3   | 2     | 2804 | OMC  | C4-N3   | 4.29  | 1.43        | 1.34     |
| 3   | 2     | 4523 | A2M  | C6-N6   | 4.28  | 1.44        | 1.34     |
| 3   | 2     | 3825 | A2M  | C6-N6   | 4.27  | 1.44        | 1.34     |
| 3   | 2     | 2365 | OMC  | C4-N3   | 4.26  | 1.43        | 1.34     |
| 3   | 2     | 4536 | OMC  | C4-N3   | 4.25  | 1.43        | 1.34     |
| 3   | 2     | 1909 | P7G  | C4-N9   | 4.23  | 1.41        | 1.35     |
| 3   | 2     | 4483 | B8T  | C2-N1   | 4.21  | 1.49        | 1.40     |
| 3   | 2     | 1659 | I4U  | C3'-C4' | 4.21  | 1.63        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 1797 | E7G  | C8-N7   | 4.19  | 1.49        | 1.45     |
| 3   | 2     | 3701 | OMC  | C4-N4   | 4.18  | 1.43        | 1.33     |
| 3   | 2     | 4564 | M7A  | C4-N9   | 4.17  | 1.46        | 1.38     |
| 3   | 2     | 4194 | I4U  | O4'-C1' | 4.17  | 1.51        | 1.42     |
| 3   | 2     | 3718 | A2M  | C6-N6   | 4.15  | 1.44        | 1.34     |
| 3   | 2     | 4690 | B8K  | C5-N7   | 4.13  | 1.46        | 1.39     |
| 3   | 2     | 4690 | B8K  | C4-N9   | 4.13  | 1.42        | 1.37     |
| 3   | 2     | 3880 | P7G  | O6-C6   | -4.11 | 1.17        | 1.23     |
| 3   | 2     | 3880 | P7G  | C8-N7   | 4.11  | 1.49        | 1.45     |
| 3   | 2     | 1517 | 2MG  | C5-N7   | -4.10 | 1.31        | 1.39     |
| 3   | 2     | 4335 | 5MC  | C6-N1   | 4.10  | 1.45        | 1.38     |
| 3   | 2     | 3867 | A2M  | C6-N6   | 4.09  | 1.44        | 1.34     |
| 3   | 2     | 3897 | B8K  | C5-N7   | 4.08  | 1.46        | 1.39     |
| 3   | 2     | 3782 | 5MC  | C4-N4   | 4.07  | 1.44        | 1.34     |
| 3   | 2     | 4447 | 5MC  | C4-N4   | 4.06  | 1.44        | 1.34     |
| 3   | 2     | 4571 | A2M  | C6-N6   | 4.06  | 1.44        | 1.34     |
| 3   | 2     | 3887 | OMC  | C2-N1   | 4.06  | 1.48        | 1.40     |
| 3   | 2     | 1605 | 7MG  | C4-N9   | 4.06  | 1.42        | 1.37     |
| 3   | 2     | 4185 | B8W  | O6-C6   | 4.05  | 1.41        | 1.35     |
| 3   | 2     | 1534 | A2M  | C6-N6   | 4.05  | 1.44        | 1.34     |
| 3   | 2     | 2401 | A2M  | C6-N6   | 4.05  | 1.44        | 1.34     |
| 3   | 2     | 2363 | A2M  | C6-N6   | 4.05  | 1.44        | 1.34     |
| 3   | 2     | 1659 | I4U  | O4'-C1' | 4.03  | 1.51        | 1.42     |
| 3   | 2     | 3701 | OMC  | C4-N3   | 4.01  | 1.42        | 1.34     |
| 3   | 2     | 398  | A2M  | C6-N6   | 3.98  | 1.44        | 1.34     |
| 3   | 2     | 3785 | A2M  | C6-N6   | 3.98  | 1.44        | 1.34     |
| 3   | 2     | 3880 | P7G  | C6-N1   | 3.97  | 1.45        | 1.38     |
| 3   | 2     | 4564 | M7A  | C5-N7   | 3.94  | 1.48        | 1.39     |
| 3   | 2     | 2297 | E7G  | C8-N7   | 3.94  | 1.49        | 1.45     |
| 3   | 2     | 4196 | OMG  | C2-N2   | 3.93  | 1.43        | 1.34     |
| 3   | 2     | 1517 | 2MG  | C2-N1   | 3.93  | 1.43        | 1.36     |
| 3   | 2     | 3899 | BGH  | C5-N7   | 3.92  | 1.46        | 1.39     |
| 3   | 2     | 4335 | 5MC  | C4-N4   | 3.92  | 1.44        | 1.34     |
| 3   | 2     | 4671 | B8T  | C2-N1   | 3.91  | 1.48        | 1.40     |
| 3   | 2     | 2861 | OMC  | C2-N1   | 3.91  | 1.48        | 1.40     |
| 3   | 2     | 2422 | OMC  | C4-N3   | 3.89  | 1.42        | 1.34     |
| 3   | 2     | 1659 | I4U  | C2-N1   | 3.89  | 1.48        | 1.40     |
| 3   | 2     | 1909 | P7G  | C5-C4   | 3.88  | 1.45        | 1.37     |
| 3   | 2     | 2380 | B8W  | O6-C6   | 3.88  | 1.41        | 1.35     |
| 3   | 2     | 1909 | P7G  | O6-C6   | -3.87 | 1.17        | 1.23     |
| 3   | 2     | 4194 | I4U  | C2-N1   | 3.86  | 1.48        | 1.40     |
| 3   | 2     | 729  | 2MG  | C2-N1   | 3.84  | 1.42        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | 2     | 4194 | I4U  | C5-C4 | 3.84  | 1.48        | 1.43     |
| 3   | 2     | 3785 | A2M  | C5-C4 | -3.84 | 1.31        | 1.39     |
| 3   | 2     | 1348 | P4U  | C2-N1 | 3.84  | 1.48        | 1.40     |
| 3   | 2     | 2773 | OMG  | C2-N2 | 3.83  | 1.43        | 1.34     |
| 3   | 2     | 3782 | 5MC  | C6-N1 | 3.82  | 1.44        | 1.38     |
| 3   | 2     | 3897 | B8K  | C2-N2 | 3.80  | 1.43        | 1.34     |
| 3   | 2     | 2424 | OMG  | C2-N2 | 3.79  | 1.43        | 1.34     |
| 3   | 2     | 4296 | B8H  | C2-N3 | 3.79  | 1.44        | 1.38     |
| 3   | 2     | 4447 | 5MC  | C6-N1 | 3.77  | 1.44        | 1.38     |
| 3   | 2     | 1322 | 1MA  | C2-N1 | 3.76  | 1.42        | 1.35     |
| 3   | 2     | 4870 | OMG  | C2-N2 | 3.75  | 1.43        | 1.34     |
| 3   | 2     | 4355 | E6G  | O6-C6 | 3.74  | 1.40        | 1.35     |
| 3   | 2     | 1326 | A2M  | C6-N6 | 3.74  | 1.43        | 1.34     |
| 3   | 2     | 4637 | OMG  | C2-N2 | 3.74  | 1.43        | 1.34     |
| 3   | 2     | 4872 | 2MG  | C2-N1 | 3.74  | 1.42        | 1.36     |
| 3   | 2     | 1860 | B8H  | C2-N3 | 3.73  | 1.44        | 1.38     |
| 3   | 2     | 1522 | OMG  | C2-N2 | 3.73  | 1.43        | 1.34     |
| 3   | 2     | 1574 | B9B  | C5-C4 | -3.73 | 1.32        | 1.39     |
| 3   | 2     | 373  | OMG  | C2-N2 | 3.73  | 1.43        | 1.34     |
| 3   | 2     | 3782 | 5MC  | C2-N1 | 3.72  | 1.48        | 1.40     |
| 3   | 2     | 2804 | OMC  | C2-N1 | 3.72  | 1.48        | 1.40     |
| 3   | 2     | 1883 | OMG  | C5-N7 | -3.71 | 1.31        | 1.39     |
| 3   | 2     | 3899 | BGH  | C2-N1 | 3.70  | 1.46        | 1.37     |
| 3   | 2     | 1883 | OMG  | C2-N2 | 3.69  | 1.43        | 1.34     |
| 3   | 2     | 4403 | PSU  | C6-C5 | 3.69  | 1.39        | 1.35     |
| 3   | 2     | 2754 | B9B  | O6-C6 | 3.68  | 1.40        | 1.35     |
| 3   | 2     | 4550 | 7MG  | C4-N9 | 3.67  | 1.42        | 1.37     |
| 3   | 2     | 1348 | P4U  | C6-N1 | 3.67  | 1.46        | 1.38     |
| 3   | 2     | 4690 | B8K  | C2-N2 | 3.66  | 1.42        | 1.34     |
| 3   | 2     | 4494 | OMG  | C2-N2 | 3.66  | 1.42        | 1.34     |
| 3   | 2     | 4083 | 5MU  | O4-C4 | -3.64 | 1.16        | 1.23     |
| 3   | 2     | 4335 | 5MC  | C2-N1 | 3.63  | 1.47        | 1.40     |
| 3   | 2     | 1625 | OMG  | C2-N2 | 3.63  | 1.42        | 1.34     |
| 3   | 2     | 1322 | 1MA  | C5-N7 | -3.63 | 1.32        | 1.39     |
| 3   | 2     | 2522 | 7MG  | C4-N9 | 3.62  | 1.41        | 1.37     |
| 3   | 2     | 1534 | A2M  | C5-C4 | -3.62 | 1.32        | 1.39     |
| 3   | 2     | 2363 | A2M  | C5-C4 | -3.62 | 1.32        | 1.39     |
| 3   | 2     | 4690 | B8K  | C5-C6 | 3.62  | 1.52        | 1.43     |
| 3   | 2     | 3880 | P7G  | C2-N3 | 3.61  | 1.46        | 1.37     |
| 3   | 2     | 1797 | E7G  | C2-N1 | 3.61  | 1.46        | 1.37     |
| 3   | 2     | 4370 | OMG  | C5-N7 | -3.61 | 1.32        | 1.39     |
| 3   | 2     | 2297 | E7G  | C4-N9 | 3.60  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 3792 | OMG  | C2-N2   | 3.60  | 1.42        | 1.34     |
| 3   | 2     | 729  | 2MG  | C5-N7   | -3.60 | 1.32        | 1.39     |
| 3   | 2     | 4447 | 5MC  | O2-C2   | -3.59 | 1.17        | 1.23     |
| 3   | 2     | 4623 | OMG  | C2-N2   | 3.59  | 1.42        | 1.34     |
| 3   | 2     | 3701 | OMC  | C2-N1   | 3.59  | 1.47        | 1.40     |
| 3   | 2     | 1659 | I4U  | O2-C2   | -3.59 | 1.17        | 1.23     |
| 3   | 2     | 4671 | B8T  | C5-C4   | 3.58  | 1.48        | 1.40     |
| 3   | 2     | 2365 | OMC  | C2-N1   | 3.58  | 1.47        | 1.40     |
| 3   | 2     | 3869 | OMC  | C2-N1   | 3.57  | 1.47        | 1.40     |
| 3   | 2     | 4870 | OMG  | C5-N7   | -3.56 | 1.32        | 1.39     |
| 3   | 2     | 3880 | P7G  | C5-C4   | 3.56  | 1.44        | 1.37     |
| 3   | 2     | 4355 | E6G  | O3'-C3' | -3.55 | 1.34        | 1.43     |
| 3   | 2     | 3899 | BGH  | C6-N1   | 3.55  | 1.45        | 1.38     |
| 3   | 2     | 4620 | OMU  | C4-N3   | 3.54  | 1.44        | 1.38     |
| 3   | 2     | 4306 | OMU  | C4-N3   | 3.53  | 1.44        | 1.38     |
| 3   | 2     | 2424 | OMG  | C5-N7   | -3.52 | 1.32        | 1.39     |
| 3   | 2     | 4371 | MHG  | C5-C6   | 3.52  | 1.52        | 1.43     |
| 3   | 2     | 4690 | B8K  | O6-C6   | -3.51 | 1.16        | 1.23     |
| 3   | 2     | 3899 | BGH  | O6-C6   | -3.50 | 1.16        | 1.23     |
| 3   | 2     | 4306 | OMU  | O4-C4   | -3.50 | 1.17        | 1.24     |
| 3   | 2     | 1316 | OMG  | C2-N2   | 3.49  | 1.42        | 1.34     |
| 3   | 2     | 1909 | P7G  | C2-N3   | 3.49  | 1.46        | 1.37     |
| 3   | 2     | 4483 | B8T  | C5-C4   | 3.48  | 1.48        | 1.40     |
| 3   | 2     | 4536 | OMC  | O2-C2   | -3.47 | 1.17        | 1.23     |
| 3   | 2     | 1316 | OMG  | O6-C6   | -3.46 | 1.17        | 1.23     |
| 3   | 2     | 1522 | OMG  | O6-C6   | -3.46 | 1.17        | 1.23     |
| 3   | 2     | 2364 | OMG  | C2-N2   | 3.46  | 1.42        | 1.34     |
| 3   | 2     | 1574 | B9B  | O2'-C2' | 3.45  | 1.51        | 1.43     |
| 3   | 2     | 2297 | E7G  | C2-N1   | 3.45  | 1.46        | 1.37     |
| 3   | 2     | 1625 | OMG  | C5-N7   | -3.45 | 1.32        | 1.39     |
| 3   | 2     | 4083 | 5MU  | O2-C2   | -3.44 | 1.16        | 1.23     |
| 3   | 2     | 1534 | A2M  | C5-N7   | -3.44 | 1.32        | 1.39     |
| 3   | 2     | 4370 | OMG  | C2-N2   | 3.43  | 1.42        | 1.34     |
| 3   | 2     | 4447 | 5MC  | C2-N1   | 3.43  | 1.47        | 1.40     |
| 3   | 2     | 4571 | A2M  | O3'-C3' | -3.43 | 1.34        | 1.43     |
| 3   | 2     | 1909 | P7G  | C8-N7   | 3.43  | 1.49        | 1.45     |
| 3   | 2     | 3718 | A2M  | C5-C4   | -3.43 | 1.32        | 1.39     |
| 3   | 2     | 237  | B9B  | C5-C4   | -3.42 | 1.32        | 1.39     |
| 3   | 2     | 4597 | UR3  | C6-N1   | 3.41  | 1.46        | 1.38     |
| 3   | 2     | 3825 | A2M  | O3'-C3' | -3.40 | 1.35        | 1.43     |
| 3   | 2     | 3897 | B8K  | C2-N1   | 3.40  | 1.46        | 1.37     |
| 3   | 2     | 1316 | OMG  | C5-N7   | -3.39 | 1.32        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 4194 | I4U  | O2-C2   | -3.38 | 1.17        | 1.23     |
| 3   | 2     | 2754 | B9B  | O2'-C2' | 3.38  | 1.50        | 1.43     |
| 3   | 2     | 2773 | OMG  | C5-N7   | -3.38 | 1.32        | 1.39     |
| 3   | 2     | 3897 | B8K  | C5-C6   | 3.38  | 1.52        | 1.43     |
| 3   | 2     | 4637 | OMG  | C5-N7   | -3.37 | 1.32        | 1.39     |
| 3   | 2     | 2401 | A2M  | C5-C4   | -3.37 | 1.32        | 1.39     |
| 3   | 2     | 1866 | UR3  | C6-N1   | 3.36  | 1.46        | 1.38     |
| 3   | 2     | 2754 | B9B  | C5-C4   | -3.35 | 1.32        | 1.39     |
| 3   | 2     | 4536 | OMC  | C2-N1   | 3.35  | 1.47        | 1.40     |
| 3   | 2     | 1677 | PSU  | C6-C5   | 3.34  | 1.39        | 1.35     |
| 3   | 2     | 1574 | B9B  | O3'-C3' | -3.34 | 1.35        | 1.43     |
| 3   | 2     | 3867 | A2M  | C5-C4   | -3.34 | 1.32        | 1.39     |
| 3   | 2     | 2424 | OMG  | O6-C6   | -3.33 | 1.17        | 1.23     |
| 3   | 2     | 4637 | OMG  | O6-C6   | -3.33 | 1.17        | 1.23     |
| 3   | 2     | 2401 | A2M  | O3'-C3' | -3.33 | 1.35        | 1.43     |
| 3   | 2     | 4371 | MHG  | C6-N1   | 3.32  | 1.45        | 1.38     |
| 3   | 2     | 4571 | A2M  | C5-C4   | -3.32 | 1.32        | 1.39     |
| 3   | 2     | 1871 | A2M  | C5-C4   | -3.32 | 1.32        | 1.39     |
| 3   | 2     | 2050 | OMG  | C2-N2   | 3.32  | 1.42        | 1.34     |
| 3   | 2     | 1574 | B9B  | O6-C6   | 3.32  | 1.40        | 1.35     |
| 3   | 2     | 1326 | A2M  | C5-C4   | -3.31 | 1.32        | 1.39     |
| 3   | 2     | 1522 | OMG  | C5-N7   | -3.31 | 1.32        | 1.39     |
| 3   | 2     | 237  | B9B  | O3'-C3' | -3.30 | 1.35        | 1.43     |
| 3   | 2     | 4620 | OMU  | O4-C4   | -3.29 | 1.18        | 1.24     |
| 3   | 2     | 1871 | A2M  | O3'-C3' | -3.29 | 1.35        | 1.43     |
| 3   | 2     | 2050 | OMG  | O6-C6   | -3.28 | 1.17        | 1.23     |
| 3   | 2     | 2363 | A2M  | C5-N7   | -3.28 | 1.32        | 1.39     |
| 3   | 2     | 4571 | A2M  | C5-N7   | -3.27 | 1.32        | 1.39     |
| 3   | 2     | 4636 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 3   | 2     | 4531 | PSU  | C6-C5   | 3.27  | 1.39        | 1.35     |
| 3   | 2     | 4623 | OMG  | O6-C6   | -3.27 | 1.17        | 1.23     |
| 3   | 2     | 1524 | A2M  | C5-C4   | -3.26 | 1.32        | 1.39     |
| 3   | 2     | 1883 | OMG  | O6-C6   | -3.26 | 1.17        | 1.23     |
| 3   | 2     | 2754 | B9B  | C5-N7   | -3.26 | 1.32        | 1.39     |
| 3   | 2     | 4220 | 6MZ  | C5-C4   | -3.26 | 1.32        | 1.39     |
| 3   | 2     | 978  | 2MG  | C5-N7   | -3.25 | 1.32        | 1.39     |
| 3   | 2     | 398  | A2M  | C5-C4   | -3.25 | 1.32        | 1.39     |
| 3   | 2     | 3869 | OMC  | O2-C2   | -3.24 | 1.17        | 1.23     |
| 3   | 2     | 1524 | A2M  | O3'-C3' | -3.24 | 1.35        | 1.43     |
| 3   | 2     | 2401 | A2M  | C5-N7   | -3.23 | 1.32        | 1.39     |
| 3   | 2     | 4523 | A2M  | C5-C4   | -3.22 | 1.33        | 1.39     |
| 3   | 2     | 398  | A2M  | O3'-C3' | -3.22 | 1.35        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 3897 | B8K  | O6-C6   | -3.22 | 1.17        | 1.23     |
| 3   | 2     | 4671 | B8T  | O2-C2   | -3.21 | 1.17        | 1.23     |
| 3   | 2     | 3825 | A2M  | C5-C4   | -3.21 | 1.33        | 1.39     |
| 3   | 2     | 2422 | OMC  | O2-C2   | -3.21 | 1.17        | 1.23     |
| 3   | 2     | 2050 | OMG  | C5-N7   | -3.21 | 1.32        | 1.39     |
| 3   | 2     | 4530 | UR3  | C6-N1   | 3.21  | 1.45        | 1.38     |
| 3   | 2     | 1326 | A2M  | O3'-C3' | -3.20 | 1.35        | 1.43     |
| 3   | 2     | 3792 | OMG  | C5-N7   | -3.20 | 1.32        | 1.39     |
| 3   | 2     | 2363 | A2M  | O3'-C3' | -3.19 | 1.35        | 1.43     |
| 3   | 2     | 4623 | OMG  | C5-N7   | -3.19 | 1.32        | 1.39     |
| 3   | 2     | 3867 | A2M  | O3'-C3' | -3.19 | 1.35        | 1.43     |
| 3   | 2     | 4306 | OMU  | O2-C2   | -3.18 | 1.17        | 1.23     |
| 3   | 2     | 4196 | OMG  | C5-N7   | -3.18 | 1.32        | 1.39     |
| 3   | 2     | 3899 | BGH  | C4-N9   | 3.18  | 1.41        | 1.37     |
| 3   | 2     | 3909 | OMC  | O2-C2   | -3.18 | 1.17        | 1.23     |
| 3   | 2     | 373  | OMG  | C5-N7   | -3.18 | 1.32        | 1.39     |
| 3   | 2     | 3785 | A2M  | C5-N7   | -3.17 | 1.33        | 1.39     |
| 3   | 2     | 3715 | PSU  | C6-C5   | 3.17  | 1.39        | 1.35     |
| 3   | 2     | 1871 | A2M  | C5-N7   | -3.17 | 1.33        | 1.39     |
| 3   | 2     | 2522 | 7MG  | C5-C6   | 3.16  | 1.51        | 1.43     |
| 3   | 2     | 3723 | A2M  | C5-C4   | -3.16 | 1.33        | 1.39     |
| 3   | 2     | 4872 | 2MG  | C5-N7   | -3.16 | 1.33        | 1.39     |
| 3   | 2     | 3723 | A2M  | C5-N7   | -3.16 | 1.33        | 1.39     |
| 3   | 2     | 4194 | I4U  | O4-C4   | 3.16  | 1.41        | 1.35     |
| 3   | 2     | 4550 | 7MG  | O6-C6   | -3.15 | 1.17        | 1.23     |
| 3   | 2     | 2364 | OMG  | C5-N7   | -3.15 | 1.33        | 1.39     |
| 3   | 2     | 3825 | A2M  | C5-N7   | -3.14 | 1.33        | 1.39     |
| 3   | 2     | 4450 | PSU  | C6-C5   | 3.14  | 1.39        | 1.35     |
| 3   | 2     | 2522 | 7MG  | C2-N1   | 3.14  | 1.45        | 1.37     |
| 3   | 2     | 4355 | E6G  | O2'-C2' | 3.14  | 1.50        | 1.43     |
| 3   | 2     | 4335 | 5MC  | O2-C2   | -3.14 | 1.17        | 1.23     |
| 3   | 2     | 4355 | E6G  | C5-C4   | -3.13 | 1.33        | 1.39     |
| 3   | 2     | 1322 | 1MA  | C5-C6   | 3.13  | 1.52        | 1.43     |
| 3   | 2     | 2364 | OMG  | O6-C6   | -3.12 | 1.17        | 1.23     |
| 3   | 2     | 3909 | OMC  | C6-N1   | 3.11  | 1.45        | 1.38     |
| 3   | 2     | 4523 | A2M  | O3'-C3' | -3.11 | 1.35        | 1.43     |
| 3   | 2     | 4494 | OMG  | C5-N7   | -3.11 | 1.33        | 1.39     |
| 3   | 2     | 3867 | A2M  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 3   | 2     | 1574 | B9B  | C5-N7   | -3.09 | 1.33        | 1.39     |
| 3   | 2     | 3782 | 5MC  | O2-C2   | -3.08 | 1.18        | 1.23     |
| 3   | 2     | 3897 | B8K  | O3'-C3' | 3.07  | 1.50        | 1.43     |
| 3   | 2     | 2363 | A2M  | C8-N9   | -3.07 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 1605 | 7MG  | C2-N1   | 3.07  | 1.45        | 1.37     |
| 3   | 2     | 4194 | I4U  | O2'-C2' | 3.06  | 1.50        | 1.43     |
| 3   | 2     | 237  | B9B  | O2'-C2' | 3.06  | 1.50        | 1.43     |
| 3   | 2     | 4523 | A2M  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 3   | 2     | 3869 | OMC  | C6-N1   | 3.05  | 1.45        | 1.38     |
| 3   | 2     | 398  | A2M  | C5-N7   | -3.04 | 1.33        | 1.39     |
| 3   | 2     | 2365 | OMC  | O2-C2   | -3.04 | 1.18        | 1.23     |
| 3   | 2     | 3723 | A2M  | O3'-C3' | -3.04 | 1.35        | 1.43     |
| 3   | 2     | 1605 | 7MG  | C5-C6   | 3.04  | 1.51        | 1.43     |
| 3   | 2     | 373  | OMG  | O6-C6   | -3.03 | 1.17        | 1.23     |
| 3   | 2     | 4196 | OMG  | O6-C6   | -3.03 | 1.17        | 1.23     |
| 3   | 2     | 1582 | PSU  | C6-C5   | 3.02  | 1.38        | 1.35     |
| 3   | 2     | 4536 | OMC  | C6-N1   | 3.02  | 1.45        | 1.38     |
| 3   | 2     | 3899 | BGH  | C5-C6   | 3.01  | 1.51        | 1.43     |
| 3   | 2     | 237  | B9B  | O6-C6   | 3.01  | 1.39        | 1.35     |
| 3   | 2     | 4370 | OMG  | O6-C6   | -3.01 | 1.17        | 1.23     |
| 3   | 2     | 1517 | 2MG  | O6-C6   | -3.01 | 1.17        | 1.23     |
| 3   | 2     | 4355 | E6G  | C5-N7   | -3.00 | 1.33        | 1.39     |
| 3   | 2     | 4483 | B8T  | C6-N1   | 2.99  | 1.45        | 1.38     |
| 3   | 2     | 4371 | MHG  | C72-C71 | 2.99  | 1.58        | 1.52     |
| 3   | 2     | 1522 | OMG  | C4-N9   | -2.99 | 1.30        | 1.38     |
| 3   | 2     | 1456 | B8Q  | C2-N1   | 2.99  | 1.42        | 1.38     |
| 3   | 2     | 3718 | A2M  | O3'-C3' | -2.98 | 1.35        | 1.43     |
| 3   | 2     | 4620 | OMU  | O2-C2   | -2.98 | 1.17        | 1.23     |
| 3   | 2     | 3887 | OMC  | C6-N1   | 2.96  | 1.45        | 1.38     |
| 3   | 2     | 1659 | I4U  | O4-C4   | 2.96  | 1.41        | 1.35     |
| 3   | 2     | 1534 | A2M  | O3'-C3' | -2.96 | 1.36        | 1.43     |
| 3   | 2     | 4571 | A2M  | C8-N9   | -2.95 | 1.32        | 1.37     |
| 3   | 2     | 2804 | OMC  | O2-C2   | -2.94 | 1.18        | 1.23     |
| 3   | 2     | 1871 | A2M  | O2'-C2' | 2.94  | 1.50        | 1.42     |
| 3   | 2     | 3785 | A2M  | O3'-C3' | -2.93 | 1.36        | 1.43     |
| 3   | 2     | 1797 | E7G  | C5-C6   | 2.92  | 1.51        | 1.43     |
| 3   | 2     | 3792 | OMG  | O6-C6   | -2.92 | 1.18        | 1.23     |
| 3   | 2     | 2754 | B9B  | O3'-C3' | -2.91 | 1.36        | 1.43     |
| 3   | 2     | 4220 | 6MZ  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 3   | 2     | 1326 | A2M  | C5-N7   | -2.90 | 1.33        | 1.39     |
| 3   | 2     | 3785 | A2M  | O2'-C2' | 2.90  | 1.50        | 1.42     |
| 3   | 2     | 2861 | OMC  | C6-N1   | 2.90  | 1.45        | 1.38     |
| 3   | 2     | 4690 | B8K  | C2-N1   | 2.89  | 1.44        | 1.37     |
| 3   | 2     | 3887 | OMC  | O2-C2   | -2.89 | 1.18        | 1.23     |
| 3   | 2     | 2297 | E7G  | O6-C6   | -2.89 | 1.18        | 1.23     |
| 3   | 2     | 4870 | OMG  | O6-C6   | -2.88 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 3897 | B8K  | C6-N1   | 2.88  | 1.44        | 1.38     |
| 3   | 2     | 4494 | OMG  | O6-C6   | -2.87 | 1.18        | 1.23     |
| 3   | 2     | 1524 | A2M  | C5-N7   | -2.87 | 1.33        | 1.39     |
| 3   | 2     | 2522 | 7MG  | O6-C6   | -2.86 | 1.18        | 1.23     |
| 3   | 2     | 2297 | E7G  | C5-C6   | 2.86  | 1.50        | 1.43     |
| 3   | 2     | 4185 | B8W  | C5-C4   | -2.86 | 1.33        | 1.39     |
| 3   | 2     | 2365 | OMC  | C6-N1   | 2.85  | 1.44        | 1.38     |
| 3   | 2     | 1534 | A2M  | C8-N9   | -2.85 | 1.32        | 1.37     |
| 3   | 2     | 2422 | OMC  | C6-N1   | 2.85  | 1.44        | 1.38     |
| 3   | 2     | 1625 | OMG  | O6-C6   | -2.85 | 1.18        | 1.23     |
| 3   | 2     | 3718 | A2M  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 3   | 2     | 1524 | A2M  | C8-N9   | -2.84 | 1.32        | 1.37     |
| 3   | 2     | 1605 | 7MG  | O6-C6   | -2.84 | 1.18        | 1.23     |
| 3   | 2     | 1797 | E7G  | O6-C6   | -2.83 | 1.18        | 1.23     |
| 3   | 2     | 2773 | OMG  | O6-C6   | -2.83 | 1.18        | 1.23     |
| 3   | 2     | 4483 | B8T  | O2-C2   | -2.81 | 1.18        | 1.23     |
| 3   | 2     | 4293 | PSU  | C6-C5   | 2.81  | 1.38        | 1.35     |
| 3   | 2     | 3723 | A2M  | O2'-C2' | 2.80  | 1.49        | 1.42     |
| 3   | 2     | 3701 | OMC  | O2-C2   | -2.79 | 1.18        | 1.23     |
| 3   | 2     | 729  | 2MG  | O6-C6   | -2.78 | 1.18        | 1.23     |
| 3   | 2     | 2380 | B8W  | C5-N7   | -2.78 | 1.33        | 1.39     |
| 3   | 2     | 3701 | OMC  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 3   | 2     | 2861 | OMC  | O2-C2   | -2.76 | 1.18        | 1.23     |
| 3   | 2     | 1316 | OMG  | C4-N9   | -2.73 | 1.31        | 1.38     |
| 3   | 2     | 2786 | B9H  | C6-N1   | 2.73  | 1.44        | 1.38     |
| 3   | 2     | 978  | 2MG  | O6-C6   | -2.72 | 1.18        | 1.23     |
| 3   | 2     | 2380 | B8W  | C5-C4   | -2.72 | 1.33        | 1.39     |
| 3   | 2     | 3785 | A2M  | C8-N9   | -2.72 | 1.32        | 1.37     |
| 3   | 2     | 3718 | A2M  | C8-N9   | -2.72 | 1.32        | 1.37     |
| 3   | 2     | 2522 | 7MG  | C6-N1   | 2.72  | 1.43        | 1.38     |
| 3   | 2     | 4870 | OMG  | C2-N1   | 2.71  | 1.44        | 1.37     |
| 3   | 2     | 237  | B9B  | C5-N7   | -2.70 | 1.33        | 1.39     |
| 3   | 2     | 4872 | 2MG  | O6-C6   | -2.69 | 1.18        | 1.23     |
| 3   | 2     | 1871 | A2M  | C8-N9   | -2.69 | 1.32        | 1.37     |
| 3   | 2     | 1659 | I4U  | C5-C4   | 2.69  | 1.46        | 1.43     |
| 3   | 2     | 4550 | 7MG  | C5-C6   | 2.68  | 1.50        | 1.43     |
| 3   | 2     | 4529 | B8W  | O2'-C2' | 2.67  | 1.49        | 1.43     |
| 3   | 2     | 4550 | 7MG  | C2-N1   | 2.67  | 1.44        | 1.37     |
| 3   | 2     | 3825 | A2M  | O2'-C2' | 2.67  | 1.49        | 1.42     |
| 3   | 2     | 2401 | A2M  | C8-N9   | -2.66 | 1.32        | 1.37     |
| 3   | 2     | 2380 | B8W  | C4-N9   | -2.66 | 1.31        | 1.37     |
| 3   | 2     | 4129 | B8W  | O2'-C2' | 2.65  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 1659 | I4U  | O2'-C2' | 2.65  | 1.49        | 1.43     |
| 3   | 2     | 4870 | OMG  | C6-N1   | 2.65  | 1.43        | 1.38     |
| 3   | 2     | 2754 | B9B  | C5-C6   | -2.65 | 1.36        | 1.41     |
| 3   | 2     | 2297 | E7G  | C6-N1   | 2.64  | 1.43        | 1.38     |
| 3   | 2     | 1797 | E7G  | C6-N1   | 2.64  | 1.43        | 1.38     |
| 3   | 2     | 2380 | B8W  | O2'-C2' | 2.64  | 1.49        | 1.43     |
| 3   | 2     | 3825 | A2M  | C8-N9   | -2.64 | 1.32        | 1.37     |
| 3   | 2     | 237  | B9B  | C8-N9   | -2.63 | 1.32        | 1.37     |
| 3   | 2     | 4690 | B8K  | C71-N7  | 2.62  | 1.45        | 1.39     |
| 3   | 2     | 4671 | B8T  | C6-N1   | 2.62  | 1.44        | 1.38     |
| 3   | 2     | 2786 | B9H  | O2-C2   | -2.62 | 1.17        | 1.22     |
| 3   | 2     | 1326 | A2M  | C8-N9   | -2.61 | 1.32        | 1.37     |
| 3   | 2     | 2773 | OMG  | C6-N1   | 2.60  | 1.43        | 1.38     |
| 3   | 2     | 3718 | A2M  | O2'-C2' | 2.59  | 1.49        | 1.42     |
| 3   | 2     | 2363 | A2M  | O2'-C2' | 2.59  | 1.49        | 1.42     |
| 3   | 2     | 1574 | B9B  | C8-N9   | -2.58 | 1.32        | 1.37     |
| 3   | 2     | 1659 | I4U  | C6-N1   | 2.58  | 1.44        | 1.38     |
| 3   | 2     | 3897 | B8K  | C71-N7  | 2.57  | 1.45        | 1.39     |
| 3   | 2     | 1326 | A2M  | O2'-C2' | 2.56  | 1.49        | 1.42     |
| 3   | 2     | 2804 | OMC  | C6-N1   | 2.56  | 1.44        | 1.38     |
| 3   | 2     | 4529 | B8W  | C5-C4   | -2.56 | 1.34        | 1.39     |
| 3   | 2     | 4196 | OMG  | C2-N1   | 2.55  | 1.44        | 1.37     |
| 3   | 2     | 1883 | OMG  | C4-N9   | -2.54 | 1.31        | 1.38     |
| 3   | 2     | 1456 | B8Q  | C6-N1   | 2.54  | 1.44        | 1.38     |
| 3   | 2     | 2754 | B9B  | C8-N9   | -2.54 | 1.33        | 1.37     |
| 3   | 2     | 4194 | I4U  | C6-N1   | 2.53  | 1.44        | 1.38     |
| 3   | 2     | 1574 | B9B  | C5-C6   | -2.52 | 1.36        | 1.41     |
| 3   | 2     | 4296 | B8H  | O4-C4   | -2.52 | 1.18        | 1.23     |
| 3   | 2     | 398  | A2M  | O2'-C2' | 2.52  | 1.49        | 1.42     |
| 3   | 2     | 4690 | B8K  | C6-N1   | 2.52  | 1.43        | 1.38     |
| 3   | 2     | 4550 | 7MG  | C6-N1   | 2.52  | 1.43        | 1.38     |
| 3   | 2     | 4872 | 2MG  | C5-C6   | 2.51  | 1.53        | 1.44     |
| 3   | 2     | 3867 | A2M  | C8-N9   | -2.50 | 1.33        | 1.37     |
| 3   | 2     | 4371 | MHG  | O6-C6   | -2.50 | 1.18        | 1.23     |
| 3   | 2     | 4623 | OMG  | C4-N9   | -2.50 | 1.31        | 1.38     |
| 3   | 2     | 4196 | OMG  | C6-N1   | 2.49  | 1.43        | 1.38     |
| 3   | 2     | 373  | OMG  | C4-N9   | -2.49 | 1.31        | 1.38     |
| 3   | 2     | 4472 | B8W  | O2'-C2' | 2.48  | 1.48        | 1.43     |
| 3   | 2     | 4690 | B8K  | O3'-C3' | 2.48  | 1.48        | 1.43     |
| 3   | 2     | 3867 | A2M  | O2'-C2' | 2.47  | 1.48        | 1.42     |
| 3   | 2     | 3825 | A2M  | O5'-C5' | -2.46 | 1.38        | 1.44     |
| 3   | 2     | 2424 | OMG  | C4-N9   | -2.45 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 4872 | 2MG  | C4-N9   | -2.45 | 1.31        | 1.38     |
| 3   | 2     | 2508 | PSU  | C6-C5   | 2.45  | 1.38        | 1.35     |
| 3   | 2     | 237  | B9B  | C5-C6   | -2.45 | 1.36        | 1.41     |
| 3   | 2     | 1860 | B8H  | O4-C4   | -2.44 | 1.18        | 1.23     |
| 3   | 2     | 1534 | A2M  | O2'-C2' | 2.43  | 1.48        | 1.42     |
| 3   | 2     | 4571 | A2M  | O2'-C2' | 2.43  | 1.48        | 1.42     |
| 3   | 2     | 1605 | 7MG  | C6-N1   | 2.42  | 1.43        | 1.38     |
| 3   | 2     | 978  | 2MG  | C5-C6   | 2.41  | 1.53        | 1.44     |
| 3   | 2     | 237  | B9B  | O5'-C5' | -2.40 | 1.38        | 1.44     |
| 3   | 2     | 1534 | A2M  | O5'-C5' | -2.40 | 1.38        | 1.44     |
| 3   | 2     | 3785 | A2M  | O5'-C5' | -2.40 | 1.38        | 1.44     |
| 3   | 2     | 4306 | OMU  | C6-N1   | 2.40  | 1.43        | 1.38     |
| 3   | 2     | 4355 | E6G  | O5'-C5' | -2.40 | 1.38        | 1.44     |
| 3   | 2     | 3899 | BGH  | O5'-C5' | -2.39 | 1.38        | 1.44     |
| 3   | 2     | 4637 | OMG  | C4-N9   | -2.39 | 1.31        | 1.38     |
| 3   | 2     | 2773 | OMG  | C2-N1   | 2.38  | 1.43        | 1.37     |
| 3   | 2     | 3723 | A2M  | C8-N9   | -2.38 | 1.33        | 1.37     |
| 3   | 2     | 4529 | B8W  | C6-N1   | 2.37  | 1.35        | 1.32     |
| 3   | 2     | 4185 | B8W  | O2'-C2' | 2.36  | 1.48        | 1.43     |
| 3   | 2     | 2401 | A2M  | O2'-C2' | 2.36  | 1.48        | 1.42     |
| 3   | 2     | 3723 | A2M  | O5'-C5' | -2.34 | 1.39        | 1.44     |
| 3   | 2     | 1322 | 1MA  | C4-N9   | -2.34 | 1.32        | 1.38     |
| 3   | 2     | 2050 | OMG  | C4-N9   | -2.34 | 1.32        | 1.38     |
| 3   | 2     | 1625 | OMG  | C4-N9   | -2.33 | 1.32        | 1.38     |
| 3   | 2     | 2424 | OMG  | C2-N1   | 2.32  | 1.43        | 1.37     |
| 3   | 2     | 4220 | 6MZ  | C8-N9   | -2.31 | 1.33        | 1.37     |
| 3   | 2     | 4194 | I4U  | O5'-C5' | -2.31 | 1.39        | 1.44     |
| 3   | 2     | 2773 | OMG  | C4-N9   | -2.31 | 1.32        | 1.38     |
| 3   | 2     | 1866 | UR3  | C4-N3   | 2.30  | 1.45        | 1.40     |
| 3   | 2     | 978  | 2MG  | C4-N9   | -2.30 | 1.32        | 1.38     |
| 3   | 2     | 4620 | OMU  | C6-N1   | 2.28  | 1.43        | 1.38     |
| 3   | 2     | 1574 | B9B  | C4-N9   | -2.27 | 1.32        | 1.37     |
| 3   | 2     | 4500 | PSU  | C6-C5   | 2.26  | 1.38        | 1.35     |
| 3   | 2     | 4623 | OMG  | C5-C6   | 2.26  | 1.52        | 1.44     |
| 3   | 2     | 2363 | A2M  | O5'-C5' | -2.25 | 1.39        | 1.44     |
| 3   | 2     | 4355 | E6G  | C8-N9   | -2.25 | 1.33        | 1.37     |
| 3   | 2     | 2424 | OMG  | C6-N1   | 2.23  | 1.43        | 1.38     |
| 3   | 2     | 4494 | OMG  | C5-C6   | 2.23  | 1.52        | 1.44     |
| 3   | 2     | 729  | 2MG  | C5-C6   | 2.23  | 1.52        | 1.44     |
| 3   | 2     | 4571 | A2M  | C4-N9   | -2.22 | 1.32        | 1.37     |
| 3   | 2     | 1683 | PSU  | C4-C5   | -2.22 | 1.37        | 1.44     |
| 3   | 2     | 4523 | A2M  | O2'-C2' | 2.22  | 1.48        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 4523 | A2M  | O5'-C5' | -2.21 | 1.39        | 1.44     |
| 3   | 2     | 2364 | OMG  | C4-N9   | -2.21 | 1.32        | 1.38     |
| 3   | 2     | 3729 | PSU  | C6-C5   | 2.21  | 1.37        | 1.35     |
| 3   | 2     | 4571 | A2M  | O5'-C5' | -2.21 | 1.39        | 1.44     |
| 3   | 2     | 398  | A2M  | C8-N9   | -2.20 | 1.33        | 1.37     |
| 3   | 2     | 1677 | PSU  | C4-C5   | -2.20 | 1.37        | 1.44     |
| 3   | 2     | 4529 | B8W  | C4-N9   | -2.20 | 1.32        | 1.37     |
| 3   | 2     | 3729 | PSU  | C4-C5   | -2.20 | 1.37        | 1.44     |
| 3   | 2     | 1860 | B8H  | C2-N1   | -2.19 | 1.34        | 1.38     |
| 3   | 2     | 4523 | A2M  | C4-N9   | -2.19 | 1.32        | 1.37     |
| 3   | 2     | 1348 | P4U  | O2-C2   | -2.19 | 1.19        | 1.23     |
| 3   | 2     | 4472 | B8W  | C5-C4   | -2.19 | 1.34        | 1.39     |
| 3   | 2     | 2401 | A2M  | O5'-C5' | -2.19 | 1.39        | 1.44     |
| 3   | 2     | 4194 | I4U  | O3'-C3' | 2.19  | 1.48        | 1.43     |
| 3   | 2     | 1677 | PSU  | O4'-C1' | -2.18 | 1.40        | 1.43     |
| 3   | 2     | 4597 | UR3  | C5-C4   | 2.17  | 1.49        | 1.43     |
| 3   | 2     | 4500 | PSU  | C4-C5   | -2.17 | 1.38        | 1.44     |
| 3   | 2     | 1517 | 2MG  | C6-N1   | 2.15  | 1.42        | 1.38     |
| 3   | 2     | 4500 | PSU  | O4'-C1' | -2.15 | 1.40        | 1.43     |
| 3   | 2     | 1524 | A2M  | O5'-C5' | -2.15 | 1.39        | 1.44     |
| 3   | 2     | 4636 | PSU  | C4-C5   | -2.14 | 1.38        | 1.44     |
| 3   | 2     | 4530 | UR3  | O2-C2   | -2.14 | 1.18        | 1.22     |
| 3   | 2     | 4494 | OMG  | C4-N9   | -2.14 | 1.32        | 1.38     |
| 3   | 2     | 4370 | OMG  | C4-N9   | -2.13 | 1.32        | 1.38     |
| 3   | 2     | 3792 | OMG  | C5-C6   | 2.13  | 1.52        | 1.44     |
| 3   | 2     | 4370 | OMG  | C5-C6   | 2.13  | 1.52        | 1.44     |
| 3   | 2     | 1659 | I4U  | O5'-C5' | -2.12 | 1.39        | 1.44     |
| 3   | 2     | 4530 | UR3  | C4-N3   | 2.12  | 1.45        | 1.40     |
| 3   | 2     | 4564 | M7A  | C5-C6   | -2.12 | 1.35        | 1.40     |
| 3   | 2     | 2050 | OMG  | C5-C6   | 2.12  | 1.52        | 1.44     |
| 3   | 2     | 4196 | OMG  | C5-C6   | 2.12  | 1.52        | 1.44     |
| 3   | 2     | 4450 | PSU  | C4-C5   | -2.11 | 1.38        | 1.44     |
| 3   | 2     | 4870 | OMG  | C5-C6   | 2.11  | 1.52        | 1.44     |
| 3   | 2     | 2364 | OMG  | C5-C6   | 2.10  | 1.52        | 1.44     |
| 3   | 2     | 373  | OMG  | C5-C6   | 2.09  | 1.52        | 1.44     |
| 3   | 2     | 3792 | OMG  | C4-N9   | -2.09 | 1.32        | 1.38     |
| 3   | 2     | 3723 | A2M  | C4-N9   | -2.08 | 1.33        | 1.37     |
| 3   | 2     | 3718 | A2M  | C4-N9   | -2.08 | 1.33        | 1.37     |
| 3   | 2     | 4129 | B8W  | C4-N9   | -2.08 | 1.33        | 1.37     |
| 3   | 2     | 3701 | OMC  | C5-C4   | 2.08  | 1.47        | 1.42     |
| 3   | 2     | 4628 | PSU  | O4'-C1' | -2.07 | 1.41        | 1.43     |
| 3   | 2     | 4636 | PSU  | O4'-C1' | -2.07 | 1.41        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | 2     | 1316 | OMG  | C5-C6   | 2.07  | 1.52        | 1.44     |
| 3   | 2     | 1316 | OMG  | C2-N1   | 2.07  | 1.42        | 1.37     |
| 3   | 2     | 1866 | UR3  | C5-C4   | 2.06  | 1.49        | 1.43     |
| 3   | 2     | 4472 | B8W  | C5-N7   | -2.06 | 1.35        | 1.39     |
| 3   | 2     | 3909 | OMC  | C5-C4   | 2.06  | 1.47        | 1.42     |
| 3   | 2     | 4530 | UR3  | C5-C4   | 2.05  | 1.49        | 1.43     |
| 3   | 2     | 4597 | UR3  | O2-C2   | -2.05 | 1.18        | 1.22     |
| 3   | 2     | 1625 | OMG  | C5-C6   | 2.04  | 1.52        | 1.44     |
| 3   | 2     | 4870 | OMG  | C4-N9   | -2.04 | 1.32        | 1.38     |
| 3   | 2     | 4370 | OMG  | C2-N1   | 2.04  | 1.42        | 1.37     |
| 3   | 2     | 1517 | 2MG  | C4-N9   | -2.03 | 1.32        | 1.38     |
| 3   | 2     | 978  | 2MG  | C6-N1   | 2.03  | 1.42        | 1.38     |
| 3   | 2     | 1871 | A2M  | C4-N9   | -2.03 | 1.33        | 1.37     |
| 3   | 2     | 4620 | OMU  | O3'-C3' | 2.03  | 1.47        | 1.43     |
| 3   | 2     | 4494 | OMG  | C6-N1   | 2.03  | 1.42        | 1.38     |
| 3   | 2     | 1316 | OMG  | C6-N1   | 2.02  | 1.42        | 1.38     |
| 3   | 2     | 2773 | OMG  | C5-C6   | 2.02  | 1.51        | 1.44     |
| 3   | 2     | 4185 | B8W  | C4-N9   | -2.02 | 1.33        | 1.37     |
| 3   | 2     | 3867 | A2M  | C4-N9   | -2.02 | 1.33        | 1.37     |
| 3   | 2     | 4185 | B8W  | C5-N7   | -2.02 | 1.35        | 1.39     |
| 3   | 2     | 1534 | A2M  | C4-N9   | -2.02 | 1.33        | 1.37     |
| 3   | 2     | 4296 | B8H  | C2-N1   | -2.01 | 1.34        | 1.38     |
| 3   | 2     | 4293 | PSU  | C4-C5   | -2.01 | 1.38        | 1.44     |
| 3   | 2     | 1524 | A2M  | O2'-C2' | 2.01  | 1.47        | 1.42     |
| 3   | 2     | 4623 | OMG  | C2-N1   | 2.00  | 1.42        | 1.37     |

All (702) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 3   | 2     | 4564 | M7A  | C5-C6-N6  | 13.91  | 147.49      | 123.74   |
| 3   | 2     | 4083 | 5MU  | C5-C4-N3  | 12.98  | 126.39      | 115.31   |
| 3   | 2     | 4564 | M7A  | N6-C6-N1  | -11.44 | 93.29       | 118.35   |
| 3   | 2     | 4220 | 6MZ  | C4-N9-C1' | -10.12 | 102.49      | 126.59   |
| 3   | 2     | 4220 | 6MZ  | C1'-N9-C8 | 9.82   | 149.30      | 127.14   |
| 3   | 2     | 4529 | B8W  | C61-O6-C6 | 9.62   | 126.75      | 117.21   |
| 3   | 2     | 4083 | 5MU  | C5-C6-N1  | -9.58  | 113.48      | 123.34   |
| 3   | 2     | 1517 | 2MG  | C2-N3-C4  | 9.31   | 123.58      | 112.04   |
| 3   | 2     | 4129 | B8W  | C61-O6-C6 | 9.13   | 126.26      | 117.21   |
| 3   | 2     | 4185 | B8W  | C5-C4-N3  | -7.70  | 118.53      | 127.19   |
| 3   | 2     | 2786 | B9H  | C31-N3-C2 | 7.69   | 126.82      | 117.21   |
| 3   | 2     | 4472 | B8W  | C5-C4-N3  | -7.19  | 119.11      | 127.19   |
| 3   | 2     | 1517 | 2MG  | C5-C4-N3  | -7.08  | 116.97      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 1860 | B8H  | C4-N3-C2   | -6.99 | 118.30      | 127.35   |
| 3   | 2     | 4296 | B8H  | C4-N3-C2   | -6.89 | 118.43      | 127.35   |
| 3   | 2     | 2363 | A2M  | N6-C6-N1   | -6.88 | 103.29      | 118.35   |
| 3   | 2     | 4355 | E6G  | C5-C4-N3   | -6.83 | 119.50      | 127.19   |
| 3   | 2     | 4355 | E6G  | N2-C2-N3   | 6.80  | 127.82      | 117.25   |
| 3   | 2     | 2754 | B9B  | C5-C4-N3   | -6.78 | 119.56      | 127.19   |
| 3   | 2     | 237  | B9B  | C5-C4-N3   | -6.77 | 119.58      | 127.19   |
| 3   | 2     | 3880 | P7G  | C4-C5-N7   | 6.72  | 110.22      | 106.67   |
| 3   | 2     | 2380 | B8W  | C5-C4-N3   | -6.70 | 119.66      | 127.19   |
| 3   | 2     | 4872 | 2MG  | C2-N3-C4   | 6.67  | 120.31      | 112.04   |
| 3   | 2     | 4529 | B8W  | C5-C4-N3   | -6.64 | 119.72      | 127.19   |
| 3   | 2     | 1871 | A2M  | N3-C2-N1   | -6.46 | 118.49      | 128.60   |
| 3   | 2     | 1860 | B8H  | N3-C2-N1   | 6.44  | 122.10      | 115.14   |
| 3   | 2     | 3718 | A2M  | N6-C6-N1   | -6.43 | 104.26      | 118.35   |
| 3   | 2     | 4564 | M7A  | N3-C2-N1   | -6.37 | 118.63      | 128.60   |
| 3   | 2     | 4129 | B8W  | C5-C4-N3   | -6.36 | 120.04      | 127.19   |
| 3   | 2     | 729  | 2MG  | C2-N3-C4   | 6.36  | 119.92      | 112.04   |
| 3   | 2     | 978  | 2MG  | C2-N3-C4   | 6.32  | 119.87      | 112.04   |
| 3   | 2     | 3867 | A2M  | C5-C4-N3   | -6.29 | 118.54      | 126.75   |
| 3   | 2     | 398  | A2M  | N6-C6-N1   | -6.28 | 104.60      | 118.35   |
| 3   | 2     | 4447 | 5MC  | C5-C6-N1   | -6.25 | 116.91      | 123.34   |
| 3   | 2     | 4129 | B8W  | N2-C2-N3   | 6.24  | 126.96      | 117.25   |
| 3   | 2     | 3825 | A2M  | N6-C6-N1   | -6.23 | 104.72      | 118.35   |
| 3   | 2     | 237  | B9B  | O6-C6-C5   | 6.20  | 124.41      | 116.57   |
| 3   | 2     | 3785 | A2M  | N6-C6-N1   | -6.19 | 104.79      | 118.35   |
| 3   | 2     | 1524 | A2M  | N6-C6-N1   | -6.18 | 104.82      | 118.35   |
| 3   | 2     | 4523 | A2M  | N6-C6-N1   | -6.11 | 104.98      | 118.35   |
| 3   | 2     | 2401 | A2M  | N3-C2-N1   | -6.06 | 119.12      | 128.60   |
| 3   | 2     | 4220 | 6MZ  | N1-C2-N3   | -6.05 | 119.13      | 128.60   |
| 3   | 2     | 729  | 2MG  | C5-C4-N3   | -6.04 | 118.66      | 128.46   |
| 3   | 2     | 4690 | B8K  | C5-C6-N1   | 6.03  | 121.62      | 110.99   |
| 3   | 2     | 398  | A2M  | N3-C2-N1   | -6.03 | 119.17      | 128.60   |
| 3   | 2     | 4371 | MHG  | C2-N3-C4   | 6.03  | 119.51      | 112.04   |
| 3   | 2     | 3723 | A2M  | N3-C2-N1   | -6.02 | 119.18      | 128.60   |
| 3   | 2     | 1456 | B8Q  | C31-N3-C4  | 6.01  | 123.31      | 114.25   |
| 3   | 2     | 2363 | A2M  | N3-C2-N1   | -5.99 | 119.23      | 128.60   |
| 3   | 2     | 3897 | B8K  | C72-C71-N7 | 5.99  | 127.87      | 118.86   |
| 3   | 2     | 1326 | A2M  | N6-C6-N1   | -5.94 | 105.34      | 118.35   |
| 3   | 2     | 1326 | A2M  | N3-C2-N1   | -5.94 | 119.31      | 128.60   |
| 3   | 2     | 4571 | A2M  | N3-C2-N1   | -5.87 | 119.42      | 128.60   |
| 3   | 2     | 2401 | A2M  | N6-C6-N1   | -5.83 | 105.57      | 118.35   |
| 3   | 2     | 1574 | B9B  | C5-C4-N3   | -5.83 | 120.63      | 127.19   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 2363 | A2M  | C5-C6-N6   | 5.78  | 136.01      | 123.43   |
| 3   | 2     | 1517 | 2MG  | C2-N1-C6   | -5.77 | 117.84      | 124.48   |
| 3   | 2     | 4220 | 6MZ  | C5-C4-N3   | -5.75 | 119.25      | 126.75   |
| 3   | 2     | 3825 | A2M  | N3-C2-N1   | -5.75 | 119.61      | 128.60   |
| 3   | 2     | 4564 | M7A  | N3-C4-N9   | 5.74  | 134.12      | 126.87   |
| 3   | 2     | 2401 | A2M  | C5-C4-N3   | -5.73 | 119.27      | 126.75   |
| 3   | 2     | 3867 | A2M  | N6-C6-N1   | -5.72 | 105.83      | 118.35   |
| 3   | 2     | 3785 | A2M  | N3-C2-N1   | -5.71 | 119.66      | 128.60   |
| 3   | 2     | 4690 | B8K  | C72-C71-N7 | 5.71  | 127.44      | 118.86   |
| 3   | 2     | 4083 | 5MU  | O4-C4-C5   | -5.68 | 118.31      | 124.90   |
| 3   | 2     | 4296 | B8H  | N3-C2-N1   | 5.68  | 121.28      | 115.14   |
| 3   | 2     | 4571 | A2M  | N6-C6-N1   | -5.58 | 106.13      | 118.35   |
| 3   | 2     | 1322 | 1MA  | N1-C2-N3   | -5.57 | 119.38      | 126.00   |
| 3   | 2     | 1524 | A2M  | N3-C2-N1   | -5.56 | 119.90      | 128.60   |
| 3   | 2     | 4870 | OMG  | C5-C4-N3   | -5.55 | 119.46      | 128.46   |
| 3   | 2     | 2786 | B9H  | C6-N1-C2   | -5.55 | 116.82      | 121.79   |
| 3   | 2     | 1326 | A2M  | C5-C4-N3   | -5.53 | 119.53      | 126.75   |
| 3   | 2     | 3899 | BGH  | C5-C6-N1   | 5.50  | 120.69      | 110.99   |
| 3   | 2     | 1797 | E7G  | C4-C5-N7   | 5.49  | 109.80      | 104.91   |
| 3   | 2     | 1534 | A2M  | N3-C2-N1   | -5.49 | 120.02      | 128.60   |
| 3   | 2     | 4083 | 5MU  | C4-N3-C2   | -5.48 | 120.25      | 127.35   |
| 3   | 2     | 1574 | B9B  | O6-C6-C5   | 5.48  | 123.50      | 116.57   |
| 3   | 2     | 3718 | A2M  | C5-C6-N6   | 5.47  | 135.34      | 123.43   |
| 3   | 2     | 4529 | B8W  | C5-N7-C8   | 5.47  | 111.28      | 103.51   |
| 3   | 2     | 1524 | A2M  | C5-C4-N3   | -5.47 | 119.62      | 126.75   |
| 3   | 2     | 3723 | A2M  | N6-C6-N1   | -5.46 | 106.39      | 118.35   |
| 3   | 2     | 1534 | A2M  | N6-C6-N1   | -5.45 | 106.42      | 118.35   |
| 3   | 2     | 1625 | OMG  | C5-C4-N3   | -5.43 | 119.65      | 128.46   |
| 3   | 2     | 4083 | 5MU  | N3-C2-N1   | 5.43  | 122.10      | 114.89   |
| 3   | 2     | 4529 | B8W  | N9-C8-N7   | -5.41 | 106.51      | 113.91   |
| 3   | 2     | 1534 | A2M  | C5-C4-N3   | -5.41 | 119.69      | 126.75   |
| 3   | 2     | 2297 | E7G  | C5-C6-N1   | 5.41  | 120.53      | 110.99   |
| 3   | 2     | 4620 | OMU  | C4-N3-C2   | -5.41 | 119.44      | 126.58   |
| 3   | 2     | 2297 | E7G  | C4-C5-N7   | 5.39  | 109.70      | 104.91   |
| 3   | 2     | 1456 | B8Q  | N3-C2-N1   | 5.38  | 123.46      | 117.13   |
| 3   | 2     | 3825 | A2M  | C5-C4-N3   | -5.38 | 119.73      | 126.75   |
| 3   | 2     | 4529 | B8W  | C4-C5-N7   | -5.37 | 104.08      | 110.62   |
| 3   | 2     | 4523 | A2M  | N3-C2-N1   | -5.35 | 120.23      | 128.60   |
| 3   | 2     | 2050 | OMG  | C5-C4-N3   | -5.34 | 119.81      | 128.46   |
| 3   | 2     | 1677 | PSU  | N1-C2-N3   | 5.33  | 121.17      | 115.13   |
| 3   | 2     | 4494 | OMG  | C5-C4-N3   | -5.32 | 119.83      | 128.46   |
| 3   | 2     | 4872 | 2MG  | C5-C4-N3   | -5.31 | 119.85      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | 2     | 3899 | BGH  | C4-C5-N7  | 5.30  | 109.63      | 104.91   |
| 3   | 2     | 4306 | OMU  | C4-N3-C2  | -5.29 | 119.60      | 126.58   |
| 3   | 2     | 4523 | A2M  | C5-C6-N6  | 5.29  | 134.94      | 123.43   |
| 3   | 2     | 398  | A2M  | C5-C6-N6  | 5.28  | 134.92      | 123.43   |
| 3   | 2     | 3718 | A2M  | N3-C2-N1  | -5.28 | 120.35      | 128.60   |
| 3   | 2     | 4450 | PSU  | N1-C2-N3  | 5.27  | 121.10      | 115.13   |
| 3   | 2     | 978  | 2MG  | C5-C4-N3  | -5.27 | 119.92      | 128.46   |
| 3   | 2     | 4637 | OMG  | C5-C4-N3  | -5.26 | 119.93      | 128.46   |
| 3   | 2     | 3785 | A2M  | C5-C4-N3  | -5.26 | 119.89      | 126.75   |
| 3   | 2     | 398  | A2M  | C5-C4-N3  | -5.26 | 119.89      | 126.75   |
| 3   | 2     | 3718 | A2M  | C5-C4-N3  | -5.25 | 119.90      | 126.75   |
| 3   | 2     | 2522 | 7MG  | C5-C6-N1  | 5.25  | 120.24      | 110.99   |
| 3   | 2     | 1524 | A2M  | C5-C6-N6  | 5.25  | 134.85      | 123.43   |
| 3   | 2     | 1871 | A2M  | N6-C6-N1  | -5.23 | 106.89      | 118.35   |
| 3   | 2     | 2754 | B9B  | O6-C6-C5  | 5.22  | 123.18      | 116.57   |
| 3   | 2     | 4636 | PSU  | C4-N3-C2  | -5.21 | 118.84      | 126.34   |
| 3   | 2     | 4370 | OMG  | C5-C4-N3  | -5.19 | 120.03      | 128.46   |
| 3   | 2     | 2363 | A2M  | C5-C4-N3  | -5.18 | 119.99      | 126.75   |
| 3   | 2     | 4196 | OMG  | C5-C4-N3  | -5.18 | 120.06      | 128.46   |
| 3   | 2     | 1909 | P7G  | C4-C5-N7  | 5.16  | 109.39      | 106.67   |
| 3   | 2     | 4690 | B8K  | C4-C5-N7  | 5.16  | 109.50      | 104.91   |
| 3   | 2     | 4550 | 7MG  | C5-C6-N1  | 5.16  | 120.09      | 110.99   |
| 3   | 2     | 4529 | B8W  | N1-C2-N3  | -5.15 | 117.33      | 125.42   |
| 3   | 2     | 3867 | A2M  | N3-C2-N1  | -5.14 | 120.55      | 128.60   |
| 3   | 2     | 4870 | OMG  | C2-N3-C4  | 5.13  | 121.44      | 112.30   |
| 3   | 2     | 3897 | B8K  | C5-C6-N1  | 5.13  | 120.03      | 110.99   |
| 3   | 2     | 978  | 2MG  | C2-N1-C6  | -5.13 | 118.58      | 124.48   |
| 3   | 2     | 1677 | PSU  | C4-N3-C2  | -5.11 | 118.97      | 126.34   |
| 3   | 2     | 2364 | OMG  | C5-C4-N3  | -5.11 | 120.17      | 128.46   |
| 3   | 2     | 3825 | A2M  | C5-C6-N6  | 5.10  | 134.53      | 123.43   |
| 3   | 2     | 1797 | E7G  | C5-C6-N1  | 5.10  | 119.97      | 110.99   |
| 3   | 2     | 2380 | B8W  | C61-O6-C6 | -5.09 | 112.17      | 117.21   |
| 3   | 2     | 2401 | A2M  | C5-C6-N6  | 5.05  | 134.42      | 123.43   |
| 3   | 2     | 4531 | PSU  | N1-C2-N3  | 5.04  | 120.84      | 115.13   |
| 3   | 2     | 4500 | PSU  | N1-C2-N3  | 5.03  | 120.83      | 115.13   |
| 3   | 2     | 4872 | 2MG  | C2-N1-C6  | -5.02 | 118.70      | 124.48   |
| 3   | 2     | 1883 | OMG  | C5-C4-N3  | -5.00 | 120.35      | 128.46   |
| 3   | 2     | 4628 | PSU  | N1-C2-N3  | 4.98  | 120.78      | 115.13   |
| 3   | 2     | 3792 | OMG  | C5-C4-N3  | -4.98 | 120.39      | 128.46   |
| 3   | 2     | 4185 | B8W  | N2-C2-N3  | 4.96  | 124.97      | 117.25   |
| 3   | 2     | 4500 | PSU  | C4-N3-C2  | -4.96 | 119.20      | 126.34   |
| 3   | 2     | 3785 | A2M  | C5-C6-N6  | 4.94  | 134.18      | 123.43   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 4450 | PSU  | C4-N3-C2   | -4.93 | 119.24      | 126.34   |
| 3   | 2     | 1605 | 7MG  | C5-C6-N1   | 4.93  | 119.67      | 110.99   |
| 3   | 2     | 4371 | MHG  | C5-C6-N1   | 4.91  | 119.65      | 110.99   |
| 3   | 2     | 1871 | A2M  | C5-C4-N3   | -4.91 | 120.34      | 126.75   |
| 3   | 2     | 4371 | MHG  | C4-C5-N7   | 4.90  | 109.27      | 104.91   |
| 3   | 2     | 1582 | PSU  | N1-C2-N3   | 4.88  | 120.66      | 115.13   |
| 3   | 2     | 3899 | BGH  | C72-C71-N7 | 4.88  | 126.19      | 118.86   |
| 3   | 2     | 4523 | A2M  | C5-C4-N3   | -4.87 | 120.40      | 126.75   |
| 3   | 2     | 4636 | PSU  | N1-C2-N3   | 4.83  | 120.61      | 115.13   |
| 3   | 2     | 1316 | OMG  | C5-C4-N3   | -4.83 | 120.63      | 128.46   |
| 3   | 2     | 3897 | B8K  | C4-C5-N7   | 4.82  | 109.20      | 104.91   |
| 3   | 2     | 3723 | A2M  | C5-C4-N3   | -4.79 | 120.50      | 126.75   |
| 3   | 2     | 4494 | OMG  | C2-N3-C4   | 4.78  | 120.83      | 112.30   |
| 3   | 2     | 1326 | A2M  | C5-C6-N6   | 4.78  | 133.84      | 123.43   |
| 3   | 2     | 4571 | A2M  | C5-C6-N6   | 4.77  | 133.82      | 123.43   |
| 3   | 2     | 729  | 2MG  | C2-N1-C6   | -4.77 | 118.99      | 124.48   |
| 3   | 2     | 4637 | OMG  | C2-N3-C4   | 4.77  | 120.80      | 112.30   |
| 3   | 2     | 4623 | OMG  | C5-C4-N3   | -4.77 | 120.73      | 128.46   |
| 3   | 2     | 1683 | PSU  | C4-N3-C2   | -4.77 | 119.47      | 126.34   |
| 3   | 2     | 3723 | A2M  | C5-C6-N6   | 4.76  | 133.79      | 123.43   |
| 3   | 2     | 1517 | 2MG  | N9-C4-N3   | 4.75  | 135.47      | 125.94   |
| 3   | 2     | 4129 | B8W  | O6-C6-C5   | 4.75  | 122.92      | 116.97   |
| 3   | 2     | 4571 | A2M  | C5-C4-N3   | -4.73 | 120.58      | 126.75   |
| 3   | 2     | 1866 | UR3  | C1'-N1-C2  | 4.67  | 124.88      | 116.99   |
| 3   | 2     | 4550 | 7MG  | C2-N3-C4   | 4.66  | 120.60      | 112.30   |
| 3   | 2     | 1322 | 1MA  | C5-C4-N3   | -4.66 | 120.31      | 127.26   |
| 3   | 2     | 2773 | OMG  | C5-C4-N3   | -4.66 | 120.90      | 128.46   |
| 3   | 2     | 1625 | OMG  | C2-N3-C4   | 4.65  | 120.58      | 112.30   |
| 3   | 2     | 3785 | A2M  | N9-C8-N7   | -4.63 | 107.58      | 113.91   |
| 3   | 2     | 4628 | PSU  | C4-N3-C2   | -4.62 | 119.69      | 126.34   |
| 3   | 2     | 1522 | OMG  | C2-N3-C4   | 4.61  | 120.51      | 112.30   |
| 3   | 2     | 1683 | PSU  | N1-C2-N3   | 4.59  | 120.33      | 115.13   |
| 3   | 2     | 4293 | PSU  | N1-C2-N3   | 4.59  | 120.33      | 115.13   |
| 3   | 2     | 373  | OMG  | C5-C4-N3   | -4.58 | 121.02      | 128.46   |
| 3   | 2     | 4442 | PSU  | N1-C2-N3   | 4.58  | 120.31      | 115.13   |
| 3   | 2     | 237  | B9B  | N9-C8-N7   | -4.57 | 107.67      | 113.91   |
| 3   | 2     | 2424 | OMG  | C5-C4-N3   | -4.56 | 121.06      | 128.46   |
| 3   | 2     | 2422 | OMC  | O2-C2-N3   | -4.53 | 114.97      | 122.33   |
| 3   | 2     | 1316 | OMG  | C2-N3-C4   | 4.53  | 120.36      | 112.30   |
| 3   | 2     | 4530 | UR3  | C4-N3-C2   | -4.50 | 120.32      | 124.56   |
| 3   | 2     | 2364 | OMG  | C2-N3-C4   | 4.50  | 120.32      | 112.30   |
| 3   | 2     | 1909 | P7G  | N9-C8-N7   | 4.49  | 109.79      | 103.38   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 4597 | UR3  | C4-N3-C2   | -4.48 | 120.34      | 124.56   |
| 3   | 2     | 2380 | B8W  | N9-C8-N7   | -4.48 | 107.79      | 113.91   |
| 3   | 2     | 1871 | A2M  | C5-C6-N6   | 4.47  | 133.15      | 123.43   |
| 3   | 2     | 4472 | B8W  | N2-C2-N3   | 4.46  | 124.19      | 117.25   |
| 3   | 2     | 4690 | B8K  | C2-N3-C4   | 4.46  | 120.25      | 112.30   |
| 3   | 2     | 4531 | PSU  | C4-N3-C2   | -4.46 | 119.91      | 126.34   |
| 3   | 2     | 3729 | PSU  | N1-C2-N3   | 4.45  | 120.17      | 115.13   |
| 3   | 2     | 1522 | OMG  | C5-C4-N3   | -4.45 | 121.24      | 128.46   |
| 3   | 2     | 2522 | 7MG  | C2-N3-C4   | 4.44  | 120.21      | 112.30   |
| 3   | 2     | 2297 | E7G  | C2-N3-C4   | 4.43  | 120.20      | 112.30   |
| 3   | 2     | 1534 | A2M  | C5-C6-N6   | 4.43  | 133.06      | 123.43   |
| 3   | 2     | 3899 | BGH  | C2-N3-C4   | 4.41  | 120.15      | 112.30   |
| 3   | 2     | 1582 | PSU  | C4-N3-C2   | -4.40 | 119.99      | 126.34   |
| 3   | 2     | 1524 | A2M  | N9-C8-N7   | -4.40 | 107.90      | 113.91   |
| 3   | 2     | 4620 | OMU  | N3-C2-N1   | 4.40  | 120.73      | 114.89   |
| 3   | 2     | 1797 | E7G  | C2-N3-C4   | 4.39  | 120.13      | 112.30   |
| 3   | 2     | 2050 | OMG  | C2-N3-C4   | 4.39  | 120.12      | 112.30   |
| 3   | 2     | 3897 | B8K  | C2-N3-C4   | 4.37  | 120.08      | 112.30   |
| 3   | 2     | 1534 | A2M  | N9-C8-N7   | -4.37 | 107.94      | 113.91   |
| 3   | 2     | 2773 | OMG  | C2-N3-C4   | 4.36  | 120.07      | 112.30   |
| 3   | 2     | 1883 | OMG  | C2-N3-C4   | 4.36  | 120.06      | 112.30   |
| 3   | 2     | 2380 | B8W  | N2-C2-N3   | 4.35  | 124.02      | 117.25   |
| 3   | 2     | 4185 | B8W  | N3-C4-N9   | 4.35  | 133.03      | 126.99   |
| 3   | 2     | 3867 | A2M  | C5-C6-N6   | 4.35  | 132.89      | 123.43   |
| 3   | 2     | 373  | OMG  | C2-N3-C4   | 4.34  | 120.04      | 112.30   |
| 3   | 2     | 237  | B9B  | O6-C6-N1   | -4.34 | 113.95      | 120.00   |
| 3   | 2     | 4370 | OMG  | C2-N3-C4   | 4.31  | 119.97      | 112.30   |
| 3   | 2     | 4529 | B8W  | O6-C6-C5   | 4.30  | 122.36      | 116.97   |
| 3   | 2     | 4623 | OMG  | C2-N3-C4   | 4.30  | 119.96      | 112.30   |
| 3   | 2     | 1456 | B8Q  | O2-C2-N3   | -4.30 | 116.64      | 122.95   |
| 3   | 2     | 3899 | BGH  | N9-C8-N7   | 4.28  | 109.08      | 103.33   |
| 3   | 2     | 4293 | PSU  | C4-N3-C2   | -4.27 | 120.19      | 126.34   |
| 3   | 2     | 1909 | P7G  | C71-N7-C5  | 4.26  | 134.62      | 124.52   |
| 3   | 2     | 237  | B9B  | N3-C4-N9   | 4.26  | 132.90      | 126.99   |
| 3   | 2     | 4194 | I4U  | C5-C4-N3   | -4.24 | 118.45      | 124.91   |
| 3   | 2     | 4185 | B8W  | N9-C8-N7   | -4.21 | 108.16      | 113.91   |
| 3   | 2     | 4472 | B8W  | N3-C4-N9   | 4.21  | 132.82      | 126.99   |
| 3   | 2     | 1534 | A2M  | O4'-C1'-N9 | -4.20 | 99.79       | 108.06   |
| 3   | 2     | 4220 | 6MZ  | N9-C8-N7   | -4.17 | 108.21      | 113.91   |
| 3   | 2     | 2380 | B8W  | O6-C6-N1   | 4.13  | 124.71      | 119.01   |
| 3   | 2     | 3792 | OMG  | C2-N3-C4   | 4.12  | 119.64      | 112.30   |
| 3   | 2     | 2754 | B9B  | N3-C4-N9   | 4.11  | 132.70      | 126.99   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 4306 | OMU  | N3-C2-N1   | 4.11  | 120.34      | 114.89   |
| 3   | 2     | 1574 | B9B  | N9-C8-N7   | -4.11 | 108.30      | 113.91   |
| 3   | 2     | 4335 | 5MC  | C5-C6-N1   | -4.10 | 119.12      | 123.34   |
| 3   | 2     | 1605 | 7MG  | C2-N3-C4   | 4.09  | 119.58      | 112.30   |
| 3   | 2     | 3729 | PSU  | C4-N3-C2   | -4.08 | 120.46      | 126.34   |
| 3   | 2     | 4196 | OMG  | C2-N3-C4   | 4.07  | 119.56      | 112.30   |
| 3   | 2     | 398  | A2M  | N9-C8-N7   | -4.06 | 108.37      | 113.91   |
| 3   | 2     | 3785 | A2M  | O4'-C1'-N9 | 4.05  | 116.05      | 108.06   |
| 3   | 2     | 2363 | A2M  | N9-C8-N7   | -4.05 | 108.37      | 113.91   |
| 3   | 2     | 2424 | OMG  | C2-N3-C4   | 4.05  | 119.51      | 112.30   |
| 3   | 2     | 4355 | E6G  | N3-C4-N9   | 4.05  | 132.61      | 126.99   |
| 3   | 2     | 4220 | 6MZ  | N3-C4-N9   | 4.03  | 133.73      | 127.08   |
| 3   | 2     | 4083 | 5MU  | C5M-C5-C4  | 4.03  | 123.21      | 118.77   |
| 3   | 2     | 4442 | PSU  | C4-N3-C2   | -4.03 | 120.54      | 126.34   |
| 3   | 2     | 1797 | E7G  | C5-C4-N3   | -4.03 | 120.46      | 128.13   |
| 3   | 2     | 1866 | UR3  | C6-N1-C2   | -4.03 | 118.18      | 121.79   |
| 3   | 2     | 2508 | PSU  | C4-N3-C2   | -4.02 | 120.55      | 126.34   |
| 3   | 2     | 4571 | A2M  | N9-C8-N7   | -4.00 | 108.44      | 113.91   |
| 3   | 2     | 3909 | OMC  | O2-C2-N3   | -3.99 | 115.83      | 122.33   |
| 3   | 2     | 2401 | A2M  | N9-C8-N7   | -3.98 | 108.47      | 113.91   |
| 3   | 2     | 4355 | E6G  | N9-C8-N7   | -3.97 | 108.48      | 113.91   |
| 3   | 2     | 4523 | A2M  | N9-C8-N7   | -3.97 | 108.49      | 113.91   |
| 3   | 2     | 1871 | A2M  | N9-C8-N7   | -3.96 | 108.50      | 113.91   |
| 3   | 2     | 4220 | 6MZ  | C2-N3-C4   | 3.95  | 121.07      | 111.75   |
| 3   | 2     | 1326 | A2M  | N9-C8-N7   | -3.94 | 108.52      | 113.91   |
| 3   | 2     | 729  | 2MG  | N9-C4-N3   | 3.94  | 133.85      | 125.94   |
| 3   | 2     | 4472 | B8W  | O6-C6-N1   | 3.93  | 124.44      | 119.01   |
| 3   | 2     | 2508 | PSU  | N1-C2-N3   | 3.93  | 119.59      | 115.13   |
| 3   | 2     | 4472 | B8W  | N9-C8-N7   | -3.91 | 108.56      | 113.91   |
| 3   | 2     | 4083 | 5MU  | C5M-C5-C6  | -3.90 | 117.64      | 122.85   |
| 3   | 2     | 1574 | B9B  | O4'-C1'-N9 | 3.90  | 115.74      | 108.06   |
| 3   | 2     | 4129 | B8W  | C2-N1-C6   | 3.89  | 122.11      | 115.93   |
| 3   | 2     | 4403 | PSU  | N1-C2-N3   | 3.88  | 119.53      | 115.13   |
| 3   | 2     | 1322 | 1MA  | C2-N3-C4   | 3.88  | 120.03      | 112.41   |
| 3   | 2     | 3723 | A2M  | N9-C8-N7   | -3.87 | 108.62      | 113.91   |
| 3   | 2     | 3718 | A2M  | N9-C8-N7   | -3.83 | 108.67      | 113.91   |
| 3   | 2     | 3867 | A2M  | N3-C4-N9   | 3.83  | 133.39      | 127.08   |
| 3   | 2     | 3715 | PSU  | N1-C2-N3   | 3.83  | 119.46      | 115.13   |
| 3   | 2     | 2754 | B9B  | N9-C8-N7   | -3.82 | 108.69      | 113.91   |
| 3   | 2     | 4870 | OMG  | N9-C4-N3   | 3.80  | 133.56      | 125.94   |
| 3   | 2     | 2401 | A2M  | C2-N3-C4   | 3.79  | 120.72      | 111.75   |
| 3   | 2     | 1866 | UR3  | C4-N3-C2   | -3.79 | 121.00      | 124.56   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 3867 | A2M  | C2-N3-C4    | 3.78  | 120.69      | 111.75   |
| 3   | 2     | 3825 | A2M  | C2-N3-C4    | 3.78  | 120.68      | 111.75   |
| 3   | 2     | 1326 | A2M  | C2-N3-C4    | 3.78  | 120.67      | 111.75   |
| 3   | 2     | 1534 | A2M  | N3-C4-N9    | 3.77  | 133.30      | 127.08   |
| 3   | 2     | 1871 | A2M  | C2-N3-C4    | 3.76  | 120.64      | 111.75   |
| 3   | 2     | 4129 | B8W  | C5-C6-N1    | -3.76 | 118.23      | 123.46   |
| 3   | 2     | 4220 | 6MZ  | C4-C5-C6    | 3.76  | 119.72      | 116.81   |
| 3   | 2     | 3897 | B8K  | N9-C8-N7    | 3.75  | 108.36      | 103.33   |
| 3   | 2     | 2363 | A2M  | C2-N3-C4    | 3.75  | 120.60      | 111.75   |
| 3   | 2     | 1605 | 7MG  | C5-C4-N3    | -3.73 | 121.02      | 128.13   |
| 3   | 2     | 1524 | A2M  | C2-N3-C4    | 3.72  | 120.54      | 111.75   |
| 3   | 2     | 2401 | A2M  | N3-C4-N9    | 3.72  | 133.21      | 127.08   |
| 3   | 2     | 4129 | B8W  | N9-C8-N7    | -3.70 | 108.85      | 113.91   |
| 3   | 2     | 4129 | B8W  | C5-N7-C8    | 3.70  | 108.76      | 103.51   |
| 3   | 2     | 1860 | B8H  | C5-C4-N3    | 3.68  | 124.91      | 116.58   |
| 3   | 2     | 398  | A2M  | C2-N3-C4    | 3.67  | 120.43      | 111.75   |
| 3   | 2     | 4185 | B8W  | O6-C6-N1    | 3.66  | 124.07      | 119.01   |
| 3   | 2     | 2522 | 7MG  | C5-C4-N9    | 3.66  | 111.10      | 106.35   |
| 3   | 2     | 1348 | P4U  | C5-C4-N3    | -3.66 | 119.34      | 124.91   |
| 3   | 2     | 237  | B9B  | N3-C2-N1    | -3.66 | 119.68      | 125.42   |
| 3   | 2     | 1659 | I4U  | C5-C4-N3    | -3.66 | 119.35      | 124.91   |
| 3   | 2     | 4296 | B8H  | C5-C4-N3    | 3.65  | 124.84      | 116.58   |
| 3   | 2     | 3785 | A2M  | C2-N3-C4    | 3.64  | 120.36      | 111.75   |
| 3   | 2     | 2522 | 7MG  | C5-C4-N3    | -3.64 | 121.19      | 128.13   |
| 3   | 2     | 2380 | B8W  | C5-N7-C8    | 3.64  | 108.68      | 103.51   |
| 3   | 2     | 1326 | A2M  | N3-C4-N9    | 3.63  | 133.07      | 127.08   |
| 3   | 2     | 4690 | B8K  | C5-C4-N9    | 3.63  | 111.05      | 106.35   |
| 3   | 2     | 2380 | B8W  | N3-C4-N9    | 3.62  | 132.01      | 126.99   |
| 3   | 2     | 4371 | MHG  | C2-N1-C6    | -3.62 | 120.32      | 124.48   |
| 3   | 2     | 1605 | 7MG  | N9-C8-N7    | 3.61  | 108.55      | 103.38   |
| 3   | 2     | 2786 | B9H  | O3'-C3'-C2' | 3.60  | 121.38      | 111.17   |
| 3   | 2     | 3718 | A2M  | C2-N3-C4    | 3.59  | 120.23      | 111.75   |
| 3   | 2     | 4371 | MHG  | C5-C4-N9    | 3.59  | 111.01      | 106.35   |
| 3   | 2     | 2786 | B9H  | C32-C31-N3  | 3.57  | 119.93      | 112.47   |
| 3   | 2     | 3825 | A2M  | N9-C8-N7    | -3.57 | 109.03      | 113.91   |
| 3   | 2     | 2786 | B9H  | O2-C2-N1    | -3.57 | 114.37      | 122.72   |
| 3   | 2     | 3715 | PSU  | C4-N3-C2    | -3.56 | 121.20      | 126.34   |
| 3   | 2     | 4403 | PSU  | C4-N3-C2    | -3.56 | 121.21      | 126.34   |
| 3   | 2     | 4129 | B8W  | N1-C2-N3    | -3.56 | 119.83      | 125.42   |
| 3   | 2     | 978  | 2MG  | CM2-N2-C2   | -3.56 | 116.00      | 123.86   |
| 3   | 2     | 1534 | A2M  | C2-N3-C4    | 3.54  | 120.12      | 111.75   |
| 3   | 2     | 3723 | A2M  | C2-N3-C4    | 3.54  | 120.12      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 4472 | B8W  | C5-N7-C8   | 3.53  | 108.52      | 103.51   |
| 3   | 2     | 2297 | E7G  | C5-C4-N3   | -3.52 | 121.42      | 128.13   |
| 3   | 2     | 4529 | B8W  | C2-N3-C4   | 3.52  | 123.62      | 113.89   |
| 3   | 2     | 1316 | OMG  | N9-C8-N7   | -3.52 | 106.77      | 113.39   |
| 3   | 2     | 4529 | B8W  | C5-C4-N9   | 3.51  | 109.87      | 105.78   |
| 3   | 2     | 3909 | OMC  | C1'-N1-C2  | 3.51  | 126.25      | 118.42   |
| 3   | 2     | 4447 | 5MC  | CM5-C5-C6  | -3.50 | 118.17      | 122.85   |
| 3   | 2     | 4550 | 7MG  | C5-C4-N3   | -3.50 | 121.46      | 128.13   |
| 3   | 2     | 4129 | B8W  | C4-C5-N7   | -3.46 | 106.40      | 110.62   |
| 3   | 2     | 3897 | B8K  | C5-C4-N9   | 3.46  | 110.83      | 106.35   |
| 3   | 2     | 4196 | OMG  | N9-C4-N3   | 3.45  | 132.87      | 125.94   |
| 3   | 2     | 373  | OMG  | N9-C8-N7   | -3.45 | 106.89      | 113.39   |
| 3   | 2     | 4185 | B8W  | C5-N7-C8   | 3.45  | 108.41      | 103.51   |
| 3   | 2     | 4690 | B8K  | N9-C8-N7   | 3.43  | 107.93      | 103.33   |
| 3   | 2     | 2364 | OMG  | N9-C8-N7   | -3.43 | 106.94      | 113.39   |
| 3   | 2     | 1517 | 2MG  | O6-C6-C5   | -3.41 | 117.55      | 126.60   |
| 3   | 2     | 1860 | B8H  | O2-C2-N1   | -3.41 | 119.03      | 122.87   |
| 3   | 2     | 3867 | A2M  | N9-C8-N7   | -3.41 | 109.25      | 113.91   |
| 3   | 2     | 4355 | E6G  | N2-C2-N1   | -3.41 | 111.95      | 117.25   |
| 3   | 2     | 4571 | A2M  | C2-N3-C4   | 3.40  | 119.79      | 111.75   |
| 3   | 2     | 4523 | A2M  | C2-N3-C4   | 3.40  | 119.79      | 111.75   |
| 3   | 2     | 1524 | A2M  | N3-C4-N9   | 3.40  | 132.68      | 127.08   |
| 3   | 2     | 2754 | B9B  | N3-C2-N1   | -3.40 | 120.09      | 125.42   |
| 3   | 2     | 4637 | OMG  | N9-C4-N3   | 3.39  | 132.75      | 125.94   |
| 3   | 2     | 237  | B9B  | C5-N7-C8   | 3.39  | 108.32      | 103.51   |
| 3   | 2     | 4355 | E6G  | C5-N7-C8   | 3.38  | 108.32      | 103.51   |
| 3   | 2     | 4529 | B8W  | C2-N1-C6   | 3.38  | 121.30      | 115.93   |
| 3   | 2     | 4637 | OMG  | C2-N1-C6   | -3.38 | 118.94      | 125.10   |
| 3   | 2     | 1316 | OMG  | C2-N1-C6   | -3.37 | 118.96      | 125.10   |
| 3   | 2     | 4296 | B8H  | O2-C2-N1   | -3.36 | 119.08      | 122.87   |
| 3   | 2     | 1522 | OMG  | N9-C8-N7   | -3.36 | 107.06      | 113.39   |
| 3   | 2     | 1574 | B9B  | C2'-C1'-N9 | -3.34 | 104.84      | 113.30   |
| 3   | 2     | 4623 | OMG  | N9-C8-N7   | -3.33 | 107.12      | 113.39   |
| 3   | 2     | 4185 | B8W  | O4'-C1'-N9 | 3.33  | 114.61      | 108.06   |
| 3   | 2     | 3792 | OMG  | N9-C4-N3   | 3.32  | 132.61      | 125.94   |
| 3   | 2     | 4306 | OMU  | C5-C4-N3   | 3.32  | 119.81      | 114.84   |
| 3   | 2     | 1574 | B9B  | N3-C2-N1   | -3.32 | 120.21      | 125.42   |
| 3   | 2     | 4185 | B8W  | N1-C2-N3   | -3.32 | 120.21      | 125.42   |
| 3   | 2     | 2364 | OMG  | C2-N1-C6   | -3.32 | 119.05      | 125.10   |
| 3   | 2     | 4355 | E6G  | N3-C2-N1   | -3.32 | 120.22      | 125.42   |
| 3   | 2     | 2424 | OMG  | C2-N1-C6   | -3.32 | 119.05      | 125.10   |
| 3   | 2     | 4571 | A2M  | N3-C4-N9   | 3.31  | 132.54      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 1517 | 2MG  | C5-C6-N1    | 3.31  | 121.59      | 113.19   |
| 3   | 2     | 4355 | E6G  | O6-C6-N1    | 3.30  | 124.60      | 120.00   |
| 3   | 2     | 1574 | B9B  | O6-C6-N1    | -3.30 | 115.40      | 120.00   |
| 3   | 2     | 2773 | OMG  | N9-C8-N7    | -3.29 | 107.19      | 113.39   |
| 3   | 2     | 2380 | B8W  | C3'-C2'-C1' | 3.29  | 107.69      | 101.43   |
| 3   | 2     | 1625 | OMG  | N9-C4-N3    | 3.29  | 132.55      | 125.94   |
| 3   | 2     | 4690 | B8K  | C6-C5-C4    | -3.28 | 115.85      | 122.62   |
| 3   | 2     | 3899 | BGH  | C6-C5-C4    | -3.27 | 115.88      | 122.62   |
| 3   | 2     | 4620 | OMU  | C5-C4-N3    | 3.26  | 119.72      | 114.84   |
| 3   | 2     | 4371 | MHG  | C72-C71-N7  | 3.26  | 115.61      | 112.41   |
| 3   | 2     | 2050 | OMG  | N9-C4-N3    | 3.25  | 132.47      | 125.94   |
| 3   | 2     | 1625 | OMG  | C2-N1-C6    | -3.24 | 119.19      | 125.10   |
| 3   | 2     | 2050 | OMG  | C2-N1-C6    | -3.24 | 119.19      | 125.10   |
| 3   | 2     | 3785 | A2M  | C5-N7-C8    | 3.23  | 108.10      | 103.51   |
| 3   | 2     | 4450 | PSU  | C6-C5-C4    | 3.22  | 120.45      | 118.20   |
| 3   | 2     | 2363 | A2M  | C5-N7-C8    | 3.22  | 108.08      | 103.51   |
| 3   | 2     | 1871 | A2M  | N3-C4-N9    | 3.22  | 132.39      | 127.08   |
| 3   | 2     | 4637 | OMG  | N9-C8-N7    | -3.18 | 107.39      | 113.39   |
| 3   | 2     | 4472 | B8W  | N1-C2-N3    | -3.18 | 120.43      | 125.42   |
| 3   | 2     | 4494 | OMG  | N9-C4-N3    | 3.18  | 132.32      | 125.94   |
| 3   | 2     | 3785 | A2M  | N3-C4-N9    | 3.18  | 132.31      | 127.08   |
| 3   | 2     | 4371 | MHG  | C5-C4-N3    | -3.17 | 122.09      | 128.13   |
| 3   | 2     | 1605 | 7MG  | C4-C5-N7    | 3.17  | 109.93      | 105.53   |
| 3   | 2     | 2364 | OMG  | N9-C4-N3    | 3.16  | 132.28      | 125.94   |
| 3   | 2     | 4196 | OMG  | C2-N1-C6    | -3.14 | 119.37      | 125.10   |
| 3   | 2     | 1524 | A2M  | C5-N7-C8    | 3.14  | 107.97      | 103.51   |
| 3   | 2     | 3729 | PSU  | C6-N1-C2    | -3.13 | 119.48      | 122.68   |
| 3   | 2     | 2424 | OMG  | N9-C8-N7    | -3.13 | 107.49      | 113.39   |
| 3   | 2     | 4531 | PSU  | C6-N1-C2    | -3.13 | 119.48      | 122.68   |
| 3   | 2     | 1605 | 7MG  | C5-C4-N9    | 3.13  | 110.41      | 106.35   |
| 3   | 2     | 4637 | OMG  | C5-C6-N1    | 3.13  | 121.13      | 113.19   |
| 3   | 2     | 2050 | OMG  | N9-C8-N7    | -3.12 | 107.51      | 113.39   |
| 3   | 2     | 4620 | OMU  | O4-C4-C5    | -3.11 | 119.69      | 125.16   |
| 3   | 2     | 4494 | OMG  | C2-N1-C6    | -3.10 | 119.44      | 125.10   |
| 3   | 2     | 2773 | OMG  | C2-N1-C6    | -3.10 | 119.45      | 125.10   |
| 3   | 2     | 4620 | OMU  | O3'-C3'-C4' | 3.09  | 119.99      | 111.05   |
| 3   | 2     | 1883 | OMG  | C2-N1-C6    | -3.09 | 119.47      | 125.10   |
| 3   | 2     | 4623 | OMG  | C2-N1-C6    | -3.09 | 119.47      | 125.10   |
| 3   | 2     | 4564 | M7A  | C2-N3-C4    | 3.08  | 119.04      | 111.75   |
| 3   | 2     | 3899 | BGH  | C5-C4-N9    | 3.07  | 110.33      | 106.35   |
| 3   | 2     | 4550 | 7MG  | C4-C5-N7    | 3.07  | 109.79      | 105.53   |
| 3   | 2     | 4083 | 5MU  | O2-C2-N1    | -3.06 | 118.71      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 2754 | B9B  | O6-C6-N1    | -3.06 | 115.73      | 120.00   |
| 3   | 2     | 398  | A2M  | N3-C4-N9    | 3.06  | 132.13      | 127.08   |
| 3   | 2     | 2773 | OMG  | N9-C4-N3    | 3.06  | 132.08      | 125.94   |
| 3   | 2     | 4355 | E6G  | C5-C6-N1    | -3.05 | 119.21      | 123.46   |
| 3   | 2     | 2754 | B9B  | O4'-C1'-N9  | 3.05  | 114.07      | 108.06   |
| 3   | 2     | 4550 | 7MG  | C5-C4-N9    | 3.05  | 110.31      | 106.35   |
| 3   | 2     | 4370 | OMG  | C2-N1-C6    | -3.04 | 119.55      | 125.10   |
| 3   | 2     | 4500 | PSU  | C6-C5-C4    | 3.04  | 120.32      | 118.20   |
| 3   | 2     | 3729 | PSU  | O2-C2-N1    | -3.04 | 119.45      | 122.79   |
| 3   | 2     | 4529 | B8W  | C5-C6-N1    | -3.03 | 119.24      | 123.46   |
| 3   | 2     | 1524 | A2M  | C4'-O4'-C1' | -3.03 | 102.79      | 109.47   |
| 3   | 2     | 2773 | OMG  | O6-C6-C5    | -3.02 | 118.58      | 126.60   |
| 3   | 2     | 1517 | 2MG  | N1-C2-N3    | -3.02 | 119.28      | 123.95   |
| 3   | 2     | 2424 | OMG  | O6-C6-C5    | -3.02 | 118.59      | 126.60   |
| 3   | 2     | 3825 | A2M  | N3-C4-N9    | 3.01  | 132.05      | 127.08   |
| 3   | 2     | 4628 | PSU  | O2-C2-N1    | -3.01 | 119.48      | 122.79   |
| 3   | 2     | 4870 | OMG  | C1'-N9-C8   | -3.01 | 118.14      | 126.70   |
| 3   | 2     | 1522 | OMG  | C5-C6-N1    | 2.99  | 120.79      | 113.19   |
| 3   | 2     | 398  | A2M  | C5-N7-C8    | 2.99  | 107.76      | 103.51   |
| 3   | 2     | 4531 | PSU  | O2-C2-N1    | -2.99 | 119.50      | 122.79   |
| 3   | 2     | 1797 | E7G  | C5-C4-N9    | 2.96  | 110.19      | 106.35   |
| 3   | 2     | 4671 | B8T  | C6-C5-C4    | 2.95  | 120.57      | 116.96   |
| 3   | 2     | 2297 | E7G  | C5-C4-N9    | 2.95  | 110.18      | 106.35   |
| 3   | 2     | 4494 | OMG  | N9-C8-N7    | -2.95 | 107.83      | 113.39   |
| 3   | 2     | 2424 | OMG  | N9-C4-N3    | 2.95  | 131.86      | 125.94   |
| 3   | 2     | 1883 | OMG  | N9-C4-N3    | 2.95  | 131.85      | 125.94   |
| 3   | 2     | 4293 | PSU  | O2-C2-N1    | -2.94 | 119.55      | 122.79   |
| 3   | 2     | 4472 | B8W  | C61-O6-C6   | 2.94  | 120.12      | 117.21   |
| 3   | 2     | 1316 | OMG  | C5-C6-N1    | 2.93  | 120.63      | 113.19   |
| 3   | 2     | 2050 | OMG  | C5-C6-N1    | 2.93  | 120.63      | 113.19   |
| 3   | 2     | 3792 | OMG  | N9-C8-N7    | -2.93 | 107.87      | 113.39   |
| 3   | 2     | 4370 | OMG  | N9-C4-N3    | 2.93  | 131.82      | 125.94   |
| 3   | 2     | 3785 | A2M  | C2'-C1'-N9  | -2.92 | 108.61      | 113.53   |
| 3   | 2     | 4355 | E6G  | O4'-C4'-C3' | -2.92 | 99.34       | 105.11   |
| 3   | 2     | 2364 | OMG  | C5-C6-N1    | 2.92  | 120.60      | 113.19   |
| 3   | 2     | 1574 | B9B  | N3-C4-N9    | 2.92  | 131.04      | 126.99   |
| 3   | 2     | 4220 | 6MZ  | C5-N7-C8    | 2.91  | 107.64      | 103.51   |
| 3   | 2     | 2522 | 7MG  | C2-N1-C6    | -2.90 | 119.80      | 125.10   |
| 3   | 2     | 373  | OMG  | C2-N1-C6    | -2.90 | 119.82      | 125.10   |
| 3   | 2     | 4523 | A2M  | C5-N7-C8    | 2.89  | 107.62      | 103.51   |
| 3   | 2     | 1683 | PSU  | O2-C2-N1    | -2.89 | 119.61      | 122.79   |
| 3   | 2     | 1677 | PSU  | O2-C2-N1    | -2.89 | 119.61      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 4129 | B8W  | N3-C4-N9    | 2.88  | 130.99      | 126.99   |
| 3   | 2     | 4194 | I4U  | C3'-C2'-C1' | 2.88  | 106.91      | 101.43   |
| 3   | 2     | 3723 | A2M  | N3-C4-N9    | 2.88  | 131.83      | 127.08   |
| 3   | 2     | 1574 | B9B  | C5-N7-C8    | 2.87  | 107.59      | 103.51   |
| 3   | 2     | 4870 | OMG  | N1-C2-N3    | -2.87 | 117.97      | 123.32   |
| 3   | 2     | 1625 | OMG  | N9-C8-N7    | -2.86 | 108.00      | 113.39   |
| 3   | 2     | 4637 | OMG  | O6-C6-C5    | -2.86 | 119.02      | 126.60   |
| 3   | 2     | 4494 | OMG  | C5-C6-N1    | 2.86  | 120.45      | 113.19   |
| 3   | 2     | 2424 | OMG  | C5-C6-N1    | 2.86  | 120.44      | 113.19   |
| 3   | 2     | 4530 | UR3  | C1'-N1-C2   | 2.85  | 121.81      | 116.99   |
| 3   | 2     | 1316 | OMG  | O6-C6-C5    | -2.85 | 119.03      | 126.60   |
| 3   | 2     | 4355 | E6G  | C2-N1-C6    | 2.85  | 120.46      | 115.93   |
| 3   | 2     | 1860 | B8H  | O4-C4-N3    | -2.85 | 114.65      | 120.12   |
| 3   | 2     | 2401 | A2M  | C5-N7-C8    | 2.85  | 107.56      | 103.51   |
| 3   | 2     | 2297 | E7G  | C2-N1-C6    | -2.85 | 119.91      | 125.10   |
| 3   | 2     | 4690 | B8K  | C5-C4-N3    | -2.84 | 122.72      | 128.13   |
| 3   | 2     | 3897 | B8K  | C6-C5-C4    | -2.84 | 116.77      | 122.62   |
| 3   | 2     | 1522 | OMG  | C2-N1-C6    | -2.83 | 119.94      | 125.10   |
| 3   | 2     | 2773 | OMG  | C5-C6-N1    | 2.83  | 120.36      | 113.19   |
| 3   | 2     | 1625 | OMG  | C5-C6-N1    | 2.82  | 120.34      | 113.19   |
| 3   | 2     | 1883 | OMG  | N9-C8-N7    | -2.82 | 108.09      | 113.39   |
| 3   | 2     | 3718 | A2M  | C5-N7-C8    | 2.81  | 107.50      | 103.51   |
| 3   | 2     | 4220 | 6MZ  | C5-C6-N1    | 2.80  | 121.19      | 118.20   |
| 3   | 2     | 1534 | A2M  | C5-N7-C8    | 2.79  | 107.48      | 103.51   |
| 3   | 2     | 978  | 2MG  | N9-C4-N3    | 2.79  | 131.54      | 125.94   |
| 3   | 2     | 4529 | B8W  | N2-C2-N3    | 2.79  | 121.59      | 117.25   |
| 3   | 2     | 4472 | B8W  | C5-C6-N1    | -2.79 | 119.58      | 123.46   |
| 3   | 2     | 1883 | OMG  | O6-C6-C5    | -2.79 | 119.21      | 126.60   |
| 3   | 2     | 2754 | B9B  | C5-N7-C8    | 2.79  | 107.47      | 103.51   |
| 3   | 2     | 4196 | OMG  | N9-C8-N7    | -2.78 | 108.15      | 113.39   |
| 3   | 2     | 978  | 2MG  | C5-C6-N1    | 2.78  | 120.25      | 113.19   |
| 3   | 2     | 4623 | OMG  | C5-C6-N1    | 2.78  | 120.25      | 113.19   |
| 3   | 2     | 4196 | OMG  | O6-C6-C5    | -2.78 | 119.23      | 126.60   |
| 3   | 2     | 2297 | E7G  | O6-C6-C5    | -2.77 | 120.73      | 127.54   |
| 3   | 2     | 1582 | PSU  | C6-N1-C2    | -2.77 | 119.85      | 122.68   |
| 3   | 2     | 4870 | OMG  | N9-C8-N7    | -2.77 | 108.17      | 113.39   |
| 3   | 2     | 4293 | PSU  | C6-N1-C2    | -2.77 | 119.85      | 122.68   |
| 3   | 2     | 4628 | PSU  | C6-N1-C2    | -2.77 | 119.85      | 122.68   |
| 3   | 2     | 4872 | 2MG  | C5-C6-N1    | 2.75  | 120.17      | 113.19   |
| 3   | 2     | 1677 | PSU  | C6-N1-C2    | -2.74 | 119.88      | 122.68   |
| 3   | 2     | 2786 | B9H  | O3'-C3'-C4' | 2.74  | 118.96      | 111.05   |
| 3   | 2     | 4129 | B8W  | C5-C4-N9    | 2.73  | 108.96      | 105.78   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | 2     | 978  | 2MG  | N9-C8-N7   | -2.73 | 108.25      | 113.39   |
| 3   | 2     | 4872 | 2MG  | N9-C8-N7   | -2.72 | 108.27      | 113.39   |
| 3   | 2     | 3825 | A2M  | C5-N7-C8   | 2.72  | 107.37      | 103.51   |
| 3   | 2     | 729  | 2MG  | C5-C6-N1   | 2.72  | 120.09      | 113.19   |
| 3   | 2     | 3897 | B8K  | C5-C4-N3   | -2.71 | 122.96      | 128.13   |
| 3   | 2     | 4370 | OMG  | N9-C8-N7   | -2.71 | 108.29      | 113.39   |
| 3   | 2     | 1797 | E7G  | N9-C8-N7   | 2.69  | 107.23      | 103.38   |
| 3   | 2     | 3792 | OMG  | C1'-N9-C8  | -2.69 | 119.03      | 126.70   |
| 3   | 2     | 373  | OMG  | N9-C4-N3   | 2.68  | 131.33      | 125.94   |
| 3   | 2     | 3792 | OMG  | C2-N1-C6   | -2.68 | 120.21      | 125.10   |
| 3   | 2     | 3899 | BGH  | N1-C2-N3   | -2.68 | 118.32      | 123.32   |
| 3   | 2     | 1456 | B8Q  | C31-N3-C2  | 2.68  | 121.68      | 117.79   |
| 3   | 2     | 1883 | OMG  | C5-C6-N1   | 2.68  | 119.99      | 113.19   |
| 3   | 2     | 1326 | A2M  | C5-N7-C8   | 2.68  | 107.31      | 103.51   |
| 3   | 2     | 1456 | B8Q  | C1'-N1-C2  | 2.67  | 121.50      | 116.99   |
| 3   | 2     | 2754 | B9B  | C2'-C1'-N9 | -2.67 | 106.53      | 113.30   |
| 3   | 2     | 1677 | PSU  | C6-C5-C4   | 2.67  | 120.06      | 118.20   |
| 3   | 2     | 1456 | B8Q  | C6-N1-C2   | -2.67 | 119.40      | 121.79   |
| 3   | 2     | 373  | OMG  | C5-C6-N1   | 2.66  | 119.95      | 113.19   |
| 3   | 2     | 4306 | OMU  | O2-C2-N1   | -2.66 | 119.26      | 122.79   |
| 3   | 2     | 4529 | B8W  | C6-C5-N7   | 2.65  | 137.15      | 133.63   |
| 3   | 2     | 4185 | B8W  | C4-C5-N7   | -2.64 | 107.40      | 110.62   |
| 3   | 2     | 4185 | B8W  | C2-N3-C4   | 2.64  | 121.19      | 113.89   |
| 3   | 2     | 4083 | 5MU  | C6-N1-C2   | -2.64 | 118.62      | 121.30   |
| 3   | 2     | 4530 | UR3  | O2-C2-N3   | -2.63 | 117.63      | 121.34   |
| 3   | 2     | 4370 | OMG  | C5-C6-N1   | 2.63  | 119.88      | 113.19   |
| 3   | 2     | 2380 | B8W  | C4-C5-N7   | -2.63 | 107.41      | 110.62   |
| 3   | 2     | 3899 | BGH  | O6-C6-C5   | -2.62 | 121.11      | 127.54   |
| 3   | 2     | 1322 | 1MA  | N9-C8-N7   | -2.61 | 108.47      | 113.39   |
| 3   | 2     | 1797 | E7G  | C2-N1-C6   | -2.61 | 120.33      | 125.10   |
| 3   | 2     | 4196 | OMG  | C5-C6-N1   | 2.61  | 119.83      | 113.19   |
| 3   | 2     | 1605 | 7MG  | C2-N1-C6   | -2.61 | 120.33      | 125.10   |
| 3   | 2     | 1625 | OMG  | O6-C6-C5   | -2.61 | 119.67      | 126.60   |
| 3   | 2     | 4129 | B8W  | N2-C2-N1   | -2.60 | 113.21      | 117.25   |
| 3   | 2     | 1866 | UR3  | O2-C2-N3   | -2.60 | 117.68      | 121.34   |
| 3   | 2     | 1797 | E7G  | N9-C4-N3   | 2.60  | 129.35      | 125.47   |
| 3   | 2     | 2522 | 7MG  | C4-C5-N7   | 2.59  | 109.13      | 105.53   |
| 3   | 2     | 1316 | OMG  | N9-C4-N3   | 2.59  | 131.14      | 125.94   |
| 3   | 2     | 4571 | A2M  | C4-N9-C8   | 2.58  | 108.53      | 105.73   |
| 3   | 2     | 2363 | A2M  | C4-C5-N7   | -2.58 | 107.47      | 110.62   |
| 3   | 2     | 4450 | PSU  | C6-N1-C2   | -2.58 | 120.05      | 122.68   |
| 3   | 2     | 2422 | OMC  | O2-C2-N1   | 2.58  | 124.21      | 118.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 3718 | A2M  | N3-C4-N9    | 2.58  | 131.33      | 127.08   |
| 3   | 2     | 4872 | 2MG  | N9-C4-N3    | 2.57  | 131.11      | 125.94   |
| 3   | 2     | 3899 | BGH  | N2-C2-N1    | 2.57  | 122.19      | 116.71   |
| 3   | 2     | 3718 | A2M  | C5-C4-N9    | 2.57  | 108.78      | 105.78   |
| 3   | 2     | 4442 | PSU  | C6-N1-C2    | -2.57 | 120.05      | 122.68   |
| 3   | 2     | 4403 | PSU  | C6-N1-C2    | -2.57 | 120.06      | 122.68   |
| 3   | 2     | 1871 | A2M  | C5-N7-C8    | 2.57  | 107.16      | 103.51   |
| 3   | 2     | 1534 | A2M  | C4-N9-C8    | 2.57  | 108.51      | 105.73   |
| 3   | 2     | 3897 | B8K  | N1-C2-N3    | -2.56 | 118.54      | 123.32   |
| 3   | 2     | 4571 | A2M  | C5-N7-C8    | 2.56  | 107.14      | 103.51   |
| 3   | 2     | 2363 | A2M  | N3-C4-N9    | 2.55  | 131.29      | 127.08   |
| 3   | 2     | 4296 | B8H  | O4-C4-N3    | -2.54 | 115.24      | 120.12   |
| 3   | 2     | 4690 | B8K  | C2-N1-C6    | -2.53 | 120.49      | 125.10   |
| 3   | 2     | 4196 | OMG  | C1'-N9-C8   | -2.53 | 119.50      | 126.70   |
| 3   | 2     | 237  | B9B  | C4-N9-C8    | 2.53  | 108.47      | 105.73   |
| 3   | 2     | 1524 | A2M  | C4-N9-C8    | 2.53  | 108.47      | 105.73   |
| 3   | 2     | 237  | B9B  | C2-N3-C4    | 2.53  | 120.87      | 113.89   |
| 3   | 2     | 1797 | E7G  | O6-C6-C5    | -2.53 | 121.35      | 127.54   |
| 3   | 2     | 1524 | A2M  | O4'-C4'-C3' | -2.52 | 100.12      | 105.11   |
| 3   | 2     | 4450 | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 3   | 2     | 3887 | OMC  | O2-C2-N3    | -2.52 | 118.23      | 122.33   |
| 3   | 2     | 4083 | 5MU  | O4-C4-N3    | -2.52 | 115.29      | 120.12   |
| 3   | 2     | 4472 | B8W  | C2-N1-C6    | 2.52  | 119.93      | 115.93   |
| 3   | 2     | 2363 | A2M  | C5-C4-N9    | 2.51  | 108.71      | 105.78   |
| 3   | 2     | 3723 | A2M  | C5-N7-C8    | 2.51  | 107.07      | 103.51   |
| 3   | 2     | 3792 | OMG  | C5-C6-N1    | 2.50  | 119.54      | 113.19   |
| 3   | 2     | 2754 | B9B  | N2-C2-N3    | 2.50  | 121.13      | 117.25   |
| 3   | 2     | 4472 | B8W  | C4-C5-N7    | -2.49 | 107.59      | 110.62   |
| 3   | 2     | 4550 | 7MG  | O6-C6-C5    | -2.49 | 121.44      | 127.54   |
| 3   | 2     | 3897 | B8K  | O6-C6-C5    | -2.49 | 121.44      | 127.54   |
| 3   | 2     | 2422 | OMC  | C1'-N1-C2   | 2.48  | 123.95      | 118.42   |
| 3   | 2     | 4306 | OMU  | O4-C4-C5    | -2.47 | 120.81      | 125.16   |
| 3   | 2     | 3867 | A2M  | C5-N7-C8    | 2.47  | 107.02      | 103.51   |
| 3   | 2     | 978  | 2MG  | C1'-N9-C4   | -2.46 | 119.19      | 126.50   |
| 3   | 2     | 4529 | B8W  | N3-C4-N9    | 2.46  | 130.40      | 126.99   |
| 3   | 2     | 4494 | OMG  | O6-C6-C5    | -2.46 | 120.08      | 126.60   |
| 3   | 2     | 2786 | B9H  | C1'-N1-C6   | 2.46  | 126.20      | 120.84   |
| 3   | 2     | 4529 | B8W  | N2-C2-N1    | 2.45  | 121.07      | 117.25   |
| 3   | 2     | 3897 | B8K  | N2-C2-N1    | 2.45  | 121.93      | 116.71   |
| 3   | 2     | 4620 | OMU  | O2-C2-N1    | -2.45 | 119.53      | 122.79   |
| 3   | 2     | 978  | 2MG  | O6-C6-C5    | -2.44 | 120.13      | 126.60   |
| 3   | 2     | 3899 | BGH  | C5-C4-N3    | -2.44 | 123.49      | 128.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 1316 | OMG  | C8-N7-C5    | 2.43  | 108.64      | 104.24   |
| 3   | 2     | 2364 | OMG  | C1'-N9-C8   | -2.43 | 119.78      | 126.70   |
| 3   | 2     | 729  | 2MG  | N9-C8-N7    | -2.43 | 108.82      | 113.39   |
| 3   | 2     | 2754 | B9B  | C2-N3-C4    | 2.42  | 120.58      | 113.89   |
| 3   | 2     | 4523 | A2M  | C5-C4-N9    | 2.41  | 108.59      | 105.78   |
| 3   | 2     | 3867 | A2M  | C6-C5-C4    | 2.41  | 120.42      | 117.18   |
| 3   | 2     | 4371 | MHG  | O6-C6-C5    | -2.41 | 121.63      | 127.54   |
| 3   | 2     | 373  | OMG  | O6-C6-C5    | -2.41 | 120.22      | 126.60   |
| 3   | 2     | 3792 | OMG  | O6-C6-C5    | -2.40 | 120.22      | 126.60   |
| 3   | 2     | 1534 | A2M  | C6-C5-C4    | 2.40  | 120.41      | 117.18   |
| 3   | 2     | 4185 | B8W  | C5-C6-N1    | -2.40 | 120.12      | 123.46   |
| 3   | 2     | 4550 | 7MG  | N1-C2-N3    | -2.40 | 118.84      | 123.32   |
| 3   | 2     | 1517 | 2MG  | CM2-N2-C2   | -2.40 | 118.57      | 123.86   |
| 3   | 2     | 237  | B9B  | C3'-C2'-C1' | 2.40  | 105.98      | 101.43   |
| 3   | 2     | 3718 | A2M  | C4-C5-N7    | -2.40 | 107.70      | 110.62   |
| 3   | 2     | 2380 | B8W  | N1-C2-N3    | -2.40 | 121.66      | 125.42   |
| 3   | 2     | 2380 | B8W  | C5-C6-N1    | -2.39 | 120.13      | 123.46   |
| 3   | 2     | 2522 | 7MG  | O6-C6-C5    | -2.39 | 121.67      | 127.54   |
| 3   | 2     | 4194 | I4U  | C5'-C4'-C3' | -2.39 | 106.22      | 115.18   |
| 3   | 2     | 4403 | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 3   | 2     | 4523 | A2M  | N3-C4-N9    | 2.38  | 131.01      | 127.08   |
| 3   | 2     | 3880 | P7G  | N2-C2-N3    | 2.38  | 121.78      | 116.71   |
| 3   | 2     | 3715 | PSU  | C6-N1-C2    | -2.38 | 120.25      | 122.68   |
| 3   | 2     | 3880 | P7G  | N9-C8-N7    | 2.38  | 106.78      | 103.38   |
| 3   | 2     | 4355 | E6G  | C2-N3-C4    | 2.37  | 120.45      | 113.89   |
| 3   | 2     | 4636 | PSU  | C6-C5-C4    | 2.37  | 119.86      | 118.20   |
| 3   | 2     | 4623 | OMG  | C8-N7-C5    | 2.37  | 108.53      | 104.24   |
| 3   | 2     | 4370 | OMG  | O6-C6-C5    | -2.37 | 120.32      | 126.60   |
| 3   | 2     | 4371 | MHG  | N1-C2-N3    | -2.36 | 120.30      | 123.95   |
| 3   | 2     | 3785 | A2M  | C4-N9-C8    | 2.36  | 108.29      | 105.73   |
| 3   | 2     | 4530 | UR3  | C6-N1-C2    | -2.36 | 119.67      | 121.79   |
| 3   | 2     | 3897 | B8K  | O4'-C1'-C2' | -2.36 | 101.50      | 106.64   |
| 3   | 2     | 1625 | OMG  | C1'-N9-C8   | -2.36 | 119.99      | 126.70   |
| 3   | 2     | 4623 | OMG  | N9-C4-N3    | 2.35  | 130.66      | 125.94   |
| 3   | 2     | 4872 | 2MG  | C1'-N9-C4   | -2.35 | 119.53      | 126.50   |
| 3   | 2     | 4597 | UR3  | C6-N1-C2    | -2.35 | 119.69      | 121.79   |
| 3   | 2     | 2754 | B9B  | C3'-C2'-C1' | 2.35  | 105.88      | 101.43   |
| 3   | 2     | 237  | B9B  | N2-C2-N3    | 2.34  | 120.89      | 117.25   |
| 3   | 2     | 4870 | OMG  | O6-C6-C5    | -2.34 | 120.40      | 126.60   |
| 3   | 2     | 3909 | OMC  | O2-C2-N1    | 2.33  | 123.71      | 118.89   |
| 3   | 2     | 1605 | 7MG  | O6-C6-C5    | -2.33 | 121.82      | 127.54   |
| 3   | 2     | 2401 | A2M  | C6-C5-C4    | 2.33  | 120.32      | 117.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 4529 | B8W  | C4-N9-C8    | 2.33  | 108.25      | 105.73   |
| 3   | 2     | 4472 | B8W  | C2-N3-C4    | 2.32  | 120.32      | 113.89   |
| 3   | 2     | 1522 | OMG  | N1-C2-N3    | -2.32 | 119.00      | 123.32   |
| 3   | 2     | 3880 | P7G  | C71-N7-C5   | 2.32  | 130.01      | 124.52   |
| 3   | 2     | 4185 | B8W  | C2-N1-C6    | 2.31  | 119.59      | 115.93   |
| 3   | 2     | 4530 | UR3  | C3U-N3-C4   | 2.31  | 121.18      | 117.89   |
| 3   | 2     | 1522 | OMG  | O6-C6-C5    | -2.30 | 120.49      | 126.60   |
| 3   | 2     | 4550 | 7MG  | C6-C5-C4    | -2.30 | 117.88      | 122.62   |
| 3   | 2     | 1316 | OMG  | N2-C2-N1    | 2.30  | 121.61      | 116.71   |
| 3   | 2     | 4870 | OMG  | C1'-N9-C4   | 2.30  | 133.32      | 126.50   |
| 3   | 2     | 2364 | OMG  | O6-C6-C5    | -2.29 | 120.52      | 126.60   |
| 3   | 2     | 4870 | OMG  | C2-N1-C6    | -2.29 | 120.93      | 125.10   |
| 3   | 2     | 4185 | B8W  | C5-C4-N9    | 2.28  | 108.44      | 105.78   |
| 3   | 2     | 4690 | B8K  | N1-C2-N3    | -2.28 | 119.06      | 123.32   |
| 3   | 2     | 4500 | PSU  | O2-C2-N1    | -2.28 | 120.28      | 122.79   |
| 3   | 2     | 4220 | 6MZ  | C4-N9-C8    | 2.28  | 108.20      | 105.73   |
| 3   | 2     | 237  | B9B  | C2-N1-C6    | 2.28  | 119.55      | 115.93   |
| 3   | 2     | 2364 | OMG  | C8-N7-C5    | 2.28  | 108.36      | 104.24   |
| 3   | 2     | 3782 | 5MC  | C5-C4-N3    | -2.27 | 119.22      | 121.67   |
| 3   | 2     | 4870 | OMG  | C5-C6-N1    | 2.26  | 118.94      | 113.19   |
| 3   | 2     | 1574 | B9B  | C4-N9-C1'   | -2.26 | 121.21      | 126.59   |
| 3   | 2     | 1322 | 1MA  | N9-C4-N3    | 2.26  | 132.20      | 126.94   |
| 3   | 2     | 4500 | PSU  | C6-N1-C2    | -2.26 | 120.38      | 122.68   |
| 3   | 2     | 1348 | P4U  | O2-C2-N3    | -2.25 | 118.67      | 122.33   |
| 3   | 2     | 4194 | I4U  | C2'-C3'-C4' | 2.25  | 107.01      | 102.64   |
| 3   | 2     | 729  | 2MG  | O6-C6-C5    | -2.25 | 120.63      | 126.60   |
| 3   | 2     | 3899 | BGH  | O4'-C4'-C3' | -2.25 | 100.67      | 105.11   |
| 3   | 2     | 1322 | 1MA  | C1'-N9-C4   | -2.24 | 119.84      | 126.50   |
| 3   | 2     | 1871 | A2M  | C4-N9-C8    | 2.24  | 108.15      | 105.73   |
| 3   | 2     | 1574 | B9B  | C2-N3-C4    | 2.23  | 120.07      | 113.89   |
| 3   | 2     | 4194 | I4U  | O4-C41-C43  | 2.23  | 113.08      | 107.14   |
| 3   | 2     | 978  | 2MG  | C1'-N9-C8   | 2.23  | 133.05      | 126.70   |
| 3   | 2     | 4623 | OMG  | C4-C5-N7    | -2.23 | 107.19      | 110.72   |
| 3   | 2     | 3782 | 5MC  | O2-C2-N3    | -2.23 | 118.71      | 122.33   |
| 3   | 2     | 3785 | A2M  | C4'-O4'-C1' | -2.22 | 104.58      | 109.47   |
| 3   | 2     | 4355 | E6G  | C4-C5-N7    | -2.22 | 107.92      | 110.62   |
| 3   | 2     | 373  | OMG  | C8-N7-C5    | 2.22  | 108.25      | 104.24   |
| 3   | 2     | 3782 | 5MC  | C5-C6-N1    | -2.21 | 121.06      | 123.34   |
| 3   | 2     | 4872 | 2MG  | C4-C5-N7    | -2.21 | 107.23      | 110.72   |
| 3   | 2     | 4872 | 2MG  | CM2-N2-C2   | -2.20 | 119.00      | 123.86   |
| 3   | 2     | 1582 | PSU  | O2-C2-N1    | -2.20 | 120.37      | 122.79   |
| 3   | 2     | 1517 | 2MG  | N9-C8-N7    | -2.19 | 109.26      | 113.39   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 2380 | B8W  | C5-C4-N9    | 2.19  | 108.33      | 105.78   |
| 3   | 2     | 1574 | B9B  | C5-C4-N9    | 2.19  | 108.33      | 105.78   |
| 3   | 2     | 3909 | OMC  | C1'-N1-C6   | -2.18 | 116.08      | 120.84   |
| 3   | 2     | 4129 | B8W  | C2-N3-C4    | 2.18  | 119.92      | 113.89   |
| 3   | 2     | 4550 | 7MG  | C2-N1-C6    | -2.18 | 121.13      | 125.10   |
| 3   | 2     | 1534 | A2M  | O3'-C3'-C4' | -2.18 | 104.76      | 111.05   |
| 3   | 2     | 4371 | MHG  | C6-C5-C4    | -2.18 | 118.14      | 122.62   |
| 3   | 2     | 1524 | A2M  | C4-C5-N7    | -2.17 | 107.97      | 110.62   |
| 3   | 2     | 4523 | A2M  | O4'-C1'-N9  | 2.17  | 112.34      | 108.06   |
| 3   | 2     | 4872 | 2MG  | C1'-N9-C8   | 2.16  | 132.86      | 126.70   |
| 3   | 2     | 4872 | 2MG  | O6-C6-C5    | -2.16 | 120.87      | 126.60   |
| 3   | 2     | 4355 | E6G  | C2'-C3'-C4' | -2.15 | 98.46       | 102.64   |
| 3   | 2     | 4523 | A2M  | O4'-C4'-C3' | -2.15 | 100.85      | 105.11   |
| 3   | 2     | 1522 | OMG  | N9-C4-N3    | 2.15  | 130.26      | 125.94   |
| 3   | 2     | 1524 | A2M  | C2'-C1'-N9  | -2.15 | 109.91      | 113.53   |
| 3   | 2     | 1326 | A2M  | C4-N9-C8    | 2.15  | 108.06      | 105.73   |
| 3   | 2     | 4690 | B8K  | O6-C6-C5    | -2.15 | 122.27      | 127.54   |
| 3   | 2     | 4403 | PSU  | O4-C4-N3    | -2.15 | 116.00      | 120.12   |
| 3   | 2     | 4335 | 5MC  | O2-C2-N3    | -2.14 | 118.85      | 122.33   |
| 3   | 2     | 1316 | OMG  | C4-C5-N7    | -2.14 | 107.33      | 110.72   |
| 3   | 2     | 1659 | I4U  | O2-C2-N3    | -2.14 | 118.86      | 122.33   |
| 3   | 2     | 4194 | I4U  | O4'-C4'-C3' | 2.14  | 109.34      | 105.11   |
| 3   | 2     | 2050 | OMG  | C8-N7-C5    | 2.13  | 108.10      | 104.24   |
| 3   | 2     | 237  | B9B  | C4-C5-N7    | -2.13 | 108.02      | 110.62   |
| 3   | 2     | 2297 | E7G  | C6-C5-C4    | -2.13 | 118.24      | 122.62   |
| 3   | 2     | 2297 | E7G  | N9-C8-N7    | 2.11  | 106.40      | 103.38   |
| 3   | 2     | 4564 | M7A  | C2-N1-C6    | 2.11  | 122.39      | 118.77   |
| 3   | 2     | 4620 | OMU  | O3'-C3'-C2' | 2.11  | 117.16      | 111.17   |
| 3   | 2     | 2050 | OMG  | O6-C6-C5    | -2.11 | 121.01      | 126.60   |
| 3   | 2     | 2773 | OMG  | C8-N7-C5    | 2.10  | 108.04      | 104.24   |
| 3   | 2     | 3825 | A2M  | C5-C4-N9    | 2.10  | 108.22      | 105.78   |
| 3   | 2     | 1522 | OMG  | C8-N7-C5    | 2.10  | 108.03      | 104.24   |
| 3   | 2     | 4623 | OMG  | O6-C6-C5    | -2.10 | 121.04      | 126.60   |
| 3   | 2     | 4690 | B8K  | O6-C6-N1    | -2.09 | 116.11      | 120.12   |
| 3   | 2     | 4620 | OMU  | C6-N1-C2    | -2.09 | 118.32      | 120.99   |
| 3   | 2     | 4523 | A2M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 3   | 2     | 1883 | OMG  | N2-C2-N1    | 2.08  | 121.14      | 116.71   |
| 3   | 2     | 4564 | M7A  | C5-C4-N3    | -2.08 | 121.74      | 126.62   |
| 3   | 2     | 4442 | PSU  | O2-C2-N1    | -2.08 | 120.50      | 122.79   |
| 3   | 2     | 1605 | 7MG  | N9-C4-N3    | 2.08  | 128.57      | 125.47   |
| 3   | 2     | 4550 | 7MG  | N9-C8-N7    | 2.07  | 106.34      | 103.38   |
| 3   | 2     | 1574 | B9B  | C2-N1-C6    | 2.07  | 119.21      | 115.93   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | 2     | 4370 | OMG  | C8-N7-C5    | 2.07  | 107.98      | 104.24   |
| 3   | 2     | 4872 | 2MG  | C8-N7-C5    | 2.06  | 107.97      | 104.24   |
| 3   | 2     | 4870 | OMG  | N2-C2-N1    | 2.05  | 121.08      | 116.71   |
| 3   | 2     | 1574 | B9B  | C4-C5-N7    | -2.04 | 108.13      | 110.62   |
| 3   | 2     | 4571 | A2M  | C5'-C4'-C3' | -2.04 | 107.53      | 115.18   |
| 3   | 2     | 3701 | OMC  | C5-C6-N1    | -2.04 | 118.39      | 121.81   |
| 3   | 2     | 1659 | I4U  | O4'-C4'-C3' | -2.04 | 101.08      | 105.11   |
| 3   | 2     | 2363 | A2M  | C2'-C1'-N9  | 2.04  | 116.96      | 113.53   |
| 3   | 2     | 4483 | B8T  | C6-C5-C4    | 2.03  | 119.45      | 116.96   |
| 3   | 2     | 2773 | OMG  | N2-C2-N1    | 2.03  | 121.04      | 116.71   |
| 3   | 2     | 2508 | PSU  | O2-C2-N1    | -2.02 | 120.56      | 122.79   |
| 3   | 2     | 3723 | A2M  | O4'-C4'-C3' | -2.02 | 101.12      | 105.11   |
| 3   | 2     | 3880 | P7G  | N3-C2-N1    | -2.02 | 119.56      | 123.32   |
| 3   | 2     | 4636 | PSU  | O4'-C1'-C2' | 2.02  | 107.99      | 105.14   |
| 3   | 2     | 1522 | OMG  | C2'-C1'-N9  | -2.01 | 110.32      | 114.22   |
| 3   | 2     | 4494 | OMG  | C8-N7-C5    | 2.01  | 107.88      | 104.24   |
| 3   | 2     | 729  | 2MG  | CM2-N2-C2   | -2.01 | 119.43      | 123.86   |

There are no chirality outliers.

All (159) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | 2     | 237  | B9B  | C5-C6-O6-C61    |
| 3   | 2     | 237  | B9B  | N1-C6-O6-C61    |
| 3   | 2     | 237  | B9B  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1348 | P4U  | N3-C4-O4-C41    |
| 3   | 2     | 1574 | B9B  | C5-C6-O6-C61    |
| 3   | 2     | 1574 | B9B  | N1-C6-O6-C61    |
| 3   | 2     | 1625 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 1677 | PSU  | C3'-C4'-C5'-O5' |
| 3   | 2     | 1797 | E7G  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1883 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1883 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 1909 | P7G  | C72-C71-N7-C5   |
| 3   | 2     | 2297 | E7G  | C3'-C4'-C5'-O5' |
| 3   | 2     | 2297 | E7G  | O4'-C4'-C5'-O5' |
| 3   | 2     | 2364 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 2380 | B8W  | C5-C6-O6-C61    |
| 3   | 2     | 2424 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 2754 | B9B  | C5-C6-O6-C61    |
| 3   | 2     | 2754 | B9B  | N1-C6-O6-C61    |
| 3   | 2     | 2786 | B9H  | C32-C31-N3-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | 2     | 2786 | B9H  | C32-C31-N3-C4   |
| 3   | 2     | 3701 | OMC  | C2'-C1'-N1-C2   |
| 3   | 2     | 3701 | OMC  | C2'-C1'-N1-C6   |
| 3   | 2     | 3867 | A2M  | O4'-C4'-C5'-O5' |
| 3   | 2     | 3867 | A2M  | C3'-C4'-C5'-O5' |
| 3   | 2     | 3880 | P7G  | O4'-C4'-C5'-O5' |
| 3   | 2     | 3897 | B8K  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4129 | B8W  | C5-C6-O6-C61    |
| 3   | 2     | 4129 | B8W  | N1-C6-O6-C61    |
| 3   | 2     | 4185 | B8W  | C5-C6-O6-C61    |
| 3   | 2     | 4185 | B8W  | N1-C6-O6-C61    |
| 3   | 2     | 4196 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4196 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4306 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | 2     | 4355 | E6G  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4355 | E6G  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4355 | E6G  | C5-C6-O6-C61    |
| 3   | 2     | 4355 | E6G  | N1-C6-O6-C61    |
| 3   | 2     | 4371 | MHG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4371 | MHG  | C71-C72-C73-C75 |
| 3   | 2     | 4403 | PSU  | C2'-C1'-C5-C4   |
| 3   | 2     | 4403 | PSU  | O4'-C1'-C5-C4   |
| 3   | 2     | 4403 | PSU  | O4'-C1'-C5-C6   |
| 3   | 2     | 4403 | PSU  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4403 | PSU  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4450 | PSU  | C2'-C1'-C5-C4   |
| 3   | 2     | 4472 | B8W  | C5-C6-O6-C61    |
| 3   | 2     | 4472 | B8W  | N1-C6-O6-C61    |
| 3   | 2     | 4472 | B8W  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4472 | B8W  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4500 | PSU  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4523 | A2M  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4529 | B8W  | C5-C6-O6-C61    |
| 3   | 2     | 4529 | B8W  | N1-C6-O6-C61    |
| 3   | 2     | 4620 | OMU  | C1'-C2'-O2'-CM2 |
| 3   | 2     | 4636 | PSU  | C2'-C1'-C5-C6   |
| 3   | 2     | 4636 | PSU  | O4'-C1'-C5-C6   |
| 3   | 2     | 4636 | PSU  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4636 | PSU  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4637 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4870 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 237  | B9B  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | 2     | 398  | A2M  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1677 | PSU  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1797 | E7G  | C3'-C4'-C5'-O5' |
| 3   | 2     | 1866 | UR3  | O4'-C4'-C5'-O5' |
| 3   | 2     | 2364 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 2424 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 2773 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 3729 | PSU  | O4'-C4'-C5'-O5' |
| 3   | 2     | 3785 | A2M  | O4'-C4'-C5'-O5' |
| 3   | 2     | 3785 | A2M  | C3'-C4'-C5'-O5' |
| 3   | 2     | 3897 | B8K  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4450 | PSU  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4500 | PSU  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4523 | A2M  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4637 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4870 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4872 | 2MG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 978  | 2MG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 1860 | B8H  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1866 | UR3  | C3'-C4'-C5'-O5' |
| 3   | 2     | 2773 | OMG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 3880 | P7G  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4450 | PSU  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4872 | 2MG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 3880 | P7G  | N7-C71-C72-C73  |
| 3   | 2     | 1909 | P7G  | C72-C71-N7-C8   |
| 3   | 2     | 4355 | E6G  | C62-C61-O6-C6   |
| 3   | 2     | 3729 | PSU  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4371 | MHG  | C71-C72-C73-C74 |
| 3   | 2     | 237  | B9B  | O6-C61-C62-C63  |
| 3   | 2     | 729  | 2MG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4220 | 6MZ  | C3'-C4'-C5'-O5' |
| 3   | 2     | 398  | A2M  | C3'-C4'-C5'-O5' |
| 3   | 2     | 978  | 2MG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1625 | OMG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1659 | I4U  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1871 | A2M  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4220 | 6MZ  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4296 | B8H  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1909 | P7G  | N7-C71-C72-C73  |
| 3   | 2     | 4371 | MHG  | C75-C73-C74-C76 |
| 3   | 2     | 729  | 2MG  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | 2     | 4296 | B8H  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4371 | MHG  | C2'-C1'-N9-C8   |
| 3   | 2     | 1574 | B9B  | O6-C61-C62-C63  |
| 3   | 2     | 1860 | B8H  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4447 | 5MC  | C2'-C1'-N1-C6   |
| 3   | 2     | 2754 | B9B  | O4'-C4'-C5'-O5' |
| 3   | 2     | 2297 | E7G  | C72-C71-N7-C8   |
| 3   | 2     | 2401 | A2M  | C3'-C2'-O2'-CM' |
| 3   | 2     | 3897 | B8K  | C4'-C5'-O5'-P   |
| 3   | 2     | 2754 | B9B  | C3'-C4'-C5'-O5' |
| 3   | 2     | 2754 | B9B  | O6-C61-C62-C63  |
| 3   | 2     | 4447 | 5MC  | O4'-C1'-N1-C6   |
| 3   | 2     | 4371 | MHG  | C72-C71-N7-C5   |
| 3   | 2     | 373  | OMG  | C4'-C5'-O5'-P   |
| 3   | 2     | 2380 | B8W  | N1-C6-O6-C61    |
| 3   | 2     | 2380 | B8W  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4530 | UR3  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4550 | 7MG  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4447 | 5MC  | C2'-C1'-N1-C2   |
| 3   | 2     | 1517 | 2MG  | C4'-C5'-O5'-P   |
| 3   | 2     | 4500 | PSU  | C4'-C5'-O5'-P   |
| 3   | 2     | 4870 | OMG  | C4'-C5'-O5'-P   |
| 3   | 2     | 3701 | OMC  | O4'-C1'-N1-C6   |
| 3   | 2     | 1524 | A2M  | C3'-C2'-O2'-CM' |
| 3   | 2     | 3825 | A2M  | C3'-C2'-O2'-CM' |
| 3   | 2     | 3701 | OMC  | O4'-C1'-N1-C2   |
| 3   | 2     | 4447 | 5MC  | O4'-C1'-N1-C2   |
| 3   | 2     | 1534 | A2M  | C4'-C5'-O5'-P   |
| 3   | 2     | 2422 | OMC  | O4'-C4'-C5'-O5' |
| 3   | 2     | 3880 | P7G  | C72-C71-N7-C8   |
| 3   | 2     | 4371 | MHG  | C72-C71-N7-C8   |
| 3   | 2     | 1677 | PSU  | O4'-C1'-C5-C4   |
| 3   | 2     | 4450 | PSU  | O4'-C1'-C5-C4   |
| 3   | 2     | 4531 | PSU  | O4'-C1'-C5-C4   |
| 3   | 2     | 4370 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | 2     | 4494 | OMG  | C3'-C2'-O2'-CM2 |
| 3   | 2     | 1326 | A2M  | C4'-C5'-O5'-P   |
| 3   | 2     | 3887 | OMC  | C4'-C5'-O5'-P   |
| 3   | 2     | 1534 | A2M  | O4'-C4'-C5'-O5' |
| 3   | 2     | 4371 | MHG  | O4'-C1'-N9-C8   |
| 3   | 2     | 1524 | A2M  | O4'-C1'-N9-C8   |
| 3   | 2     | 3909 | OMC  | C2'-C1'-N1-C6   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | 2     | 1871 | A2M  | C3'-C4'-C5'-O5' |
| 3   | 2     | 1524 | A2M  | C1'-C2'-O2'-CM' |
| 3   | 2     | 2401 | A2M  | C1'-C2'-O2'-CM' |
| 3   | 2     | 1322 | 1MA  | O4'-C4'-C5'-O5' |
| 3   | 2     | 1677 | PSU  | O4'-C1'-C5-C6   |
| 3   | 2     | 4450 | PSU  | O4'-C1'-C5-C6   |
| 3   | 2     | 3909 | OMC  | C2'-C1'-N1-C2   |
| 3   | 2     | 1659 | I4U  | C42-C41-O4-C4   |
| 3   | 2     | 1659 | I4U  | C43-C41-O4-C4   |
| 3   | 2     | 3785 | A2M  | C3'-C2'-O2'-CM' |
| 3   | 2     | 2380 | B8W  | C3'-C4'-C5'-O5' |
| 3   | 2     | 4550 | 7MG  | C3'-C4'-C5'-O5' |
| 3   | 2     | 2422 | OMC  | C2'-C1'-N1-C2   |

There are no ring outliers.

29 monomers are involved in 35 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | 2     | 3897 | B8K  | 1       | 0            |
| 3   | 2     | 2363 | A2M  | 1       | 0            |
| 3   | 2     | 4306 | OMU  | 2       | 0            |
| 3   | 2     | 1871 | A2M  | 1       | 0            |
| 3   | 2     | 4196 | OMG  | 1       | 0            |
| 3   | 2     | 4523 | A2M  | 1       | 0            |
| 3   | 2     | 2380 | B8W  | 2       | 0            |
| 3   | 2     | 4620 | OMU  | 1       | 0            |
| 3   | 2     | 3899 | BGH  | 2       | 0            |
| 3   | 2     | 4296 | B8H  | 1       | 0            |
| 3   | 2     | 4370 | OMG  | 1       | 0            |
| 3   | 2     | 1605 | 7MG  | 1       | 0            |
| 3   | 2     | 4529 | B8W  | 1       | 0            |
| 3   | 2     | 4442 | PSU  | 2       | 0            |
| 3   | 2     | 1860 | B8H  | 1       | 0            |
| 3   | 2     | 4129 | B8W  | 1       | 0            |
| 3   | 2     | 4637 | OMG  | 1       | 0            |
| 3   | 2     | 1524 | A2M  | 1       | 0            |
| 3   | 2     | 4472 | B8W  | 1       | 0            |
| 3   | 2     | 4690 | B8K  | 2       | 0            |
| 3   | 2     | 4185 | B8W  | 1       | 0            |
| 3   | 2     | 2773 | OMG  | 1       | 0            |
| 3   | 2     | 4447 | 5MC  | 1       | 0            |
| 3   | 2     | 3723 | A2M  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | 2     | 1326 | A2M  | 1       | 0            |
| 3   | 2     | 3718 | A2M  | 1       | 0            |
| 3   | 2     | 2422 | OMC  | 1       | 0            |
| 3   | 2     | 4571 | A2M  | 1       | 0            |
| 3   | 2     | 2522 | 7MG  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 246 ligands modelled in this entry, 246 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

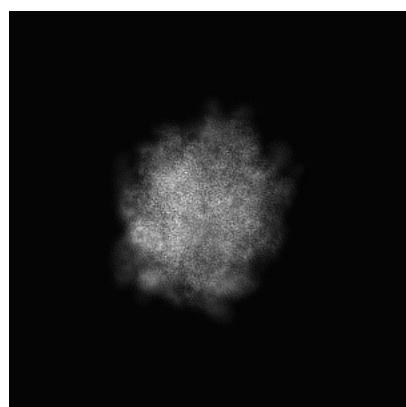
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0963. These allow visual inspection of the internal detail of the map and identification of artifacts.

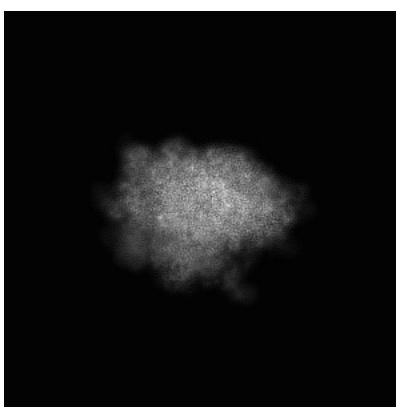
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

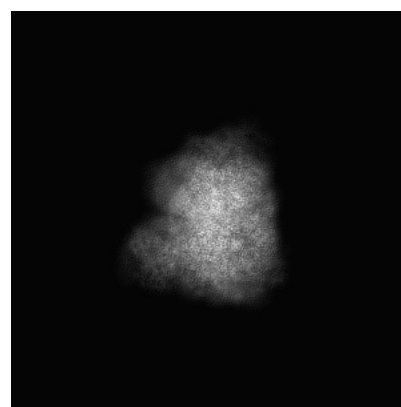
#### 6.1.1 Primary map



X



Y

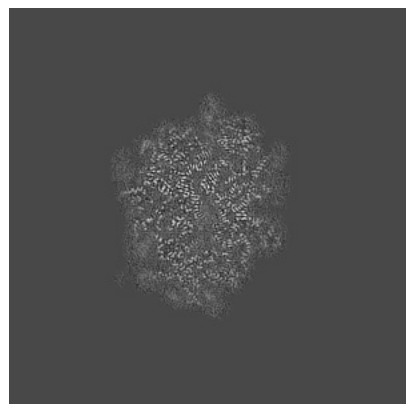


Z

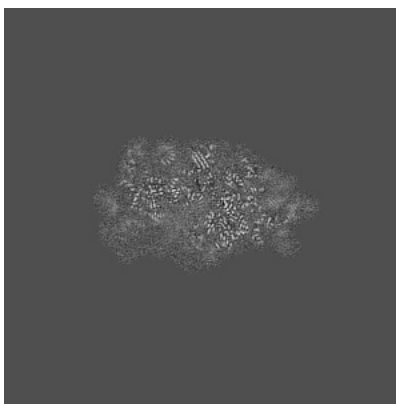
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

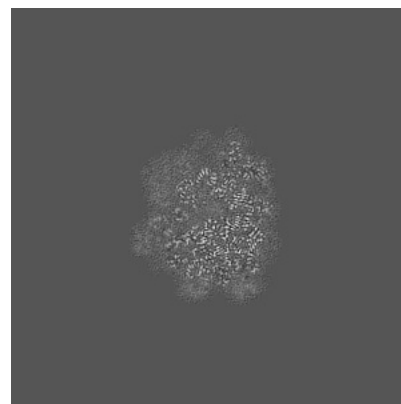
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

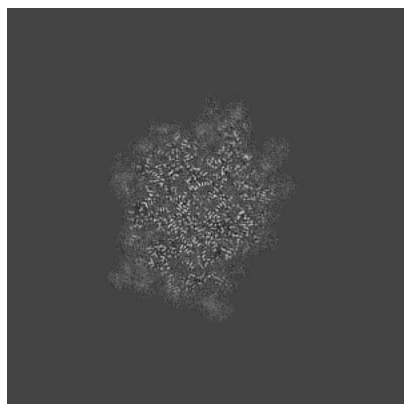


Z Index: 240

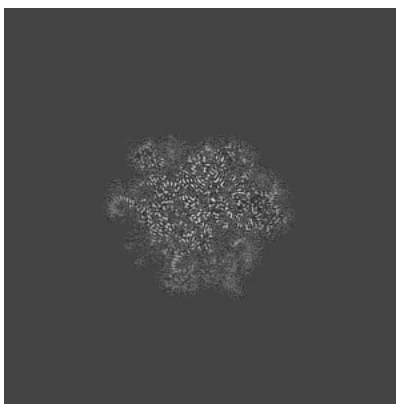
The images above show central slices of the map in three orthogonal directions.

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

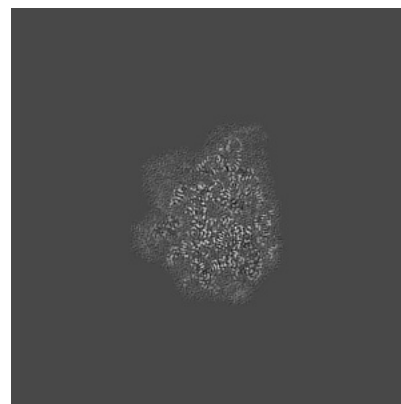
### 6.3.1 Primary map



X Index: 253



Y Index: 201

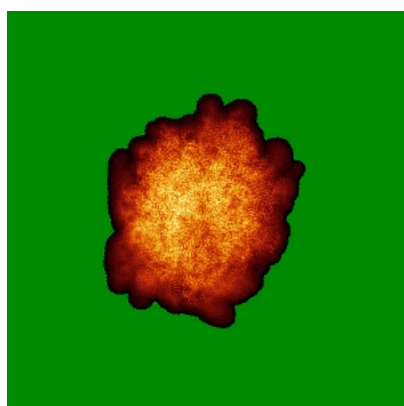


Z Index: 251

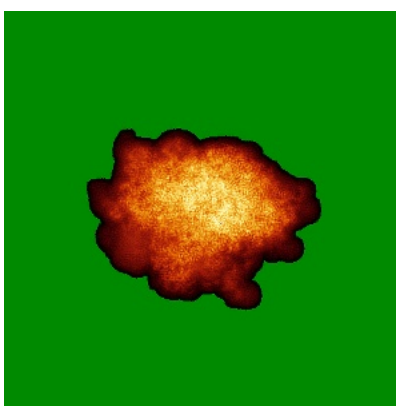
The images above show the largest variance slices of the map in three orthogonal directions.

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

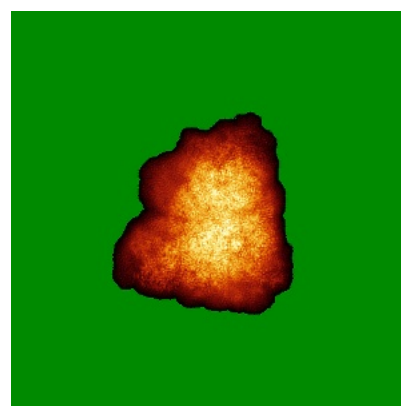
### 6.4.1 Primary map



X



Y

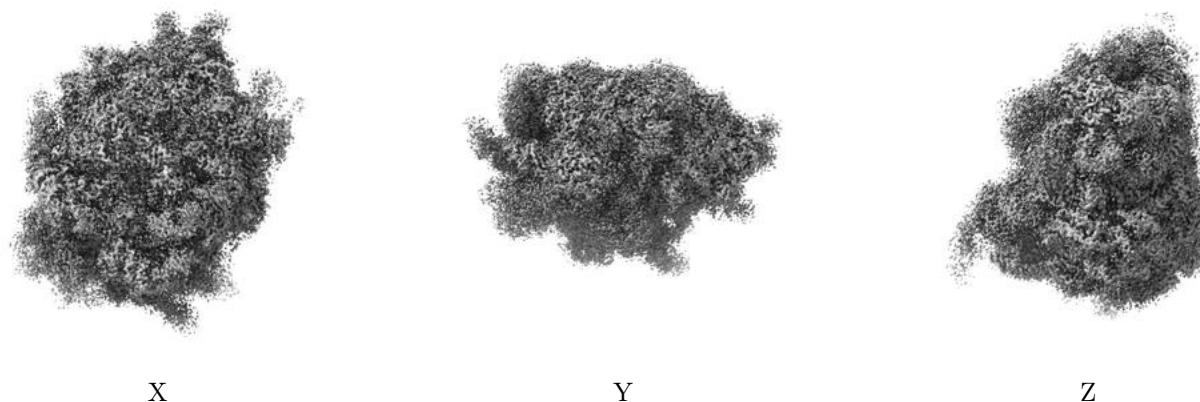


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

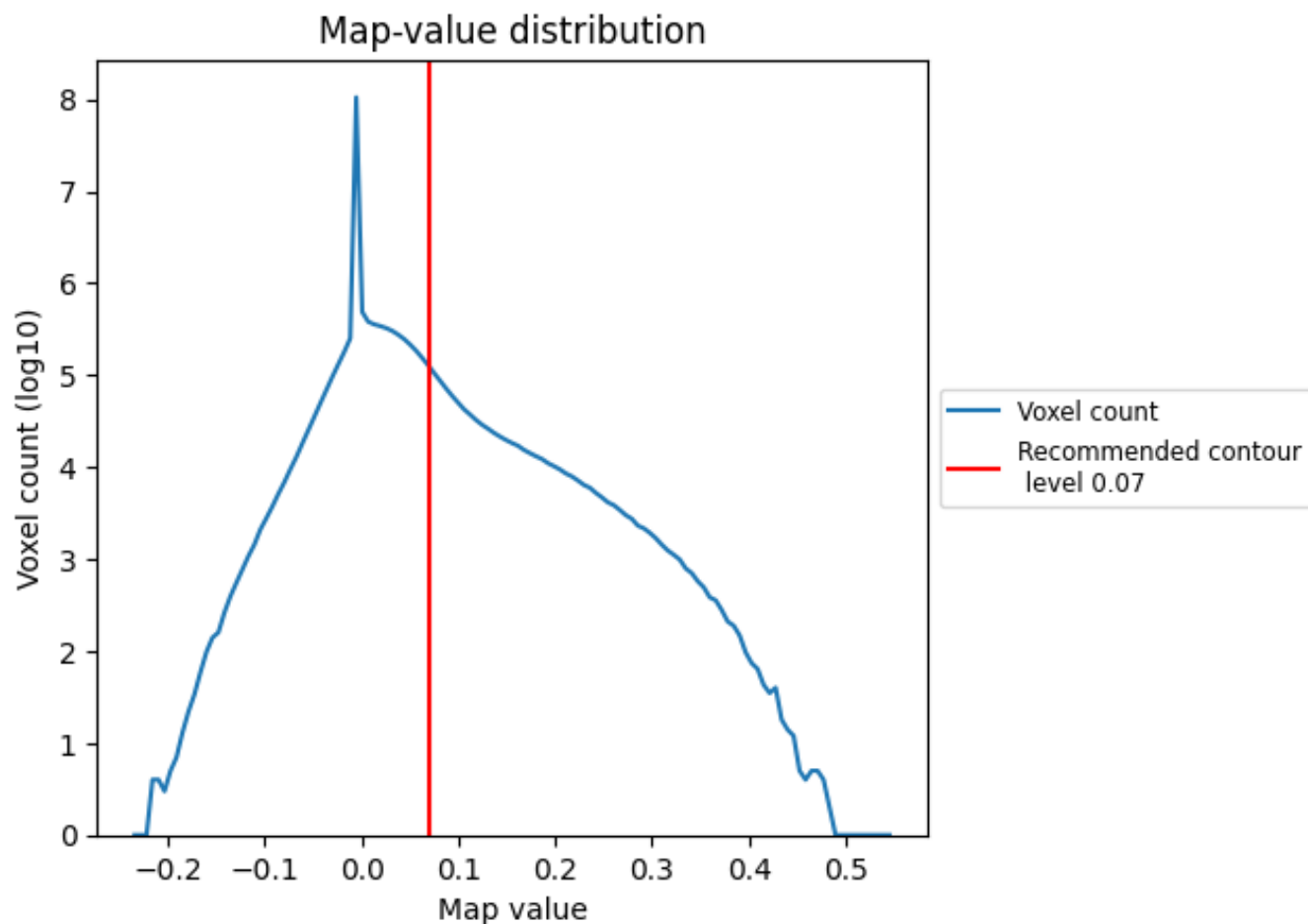
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

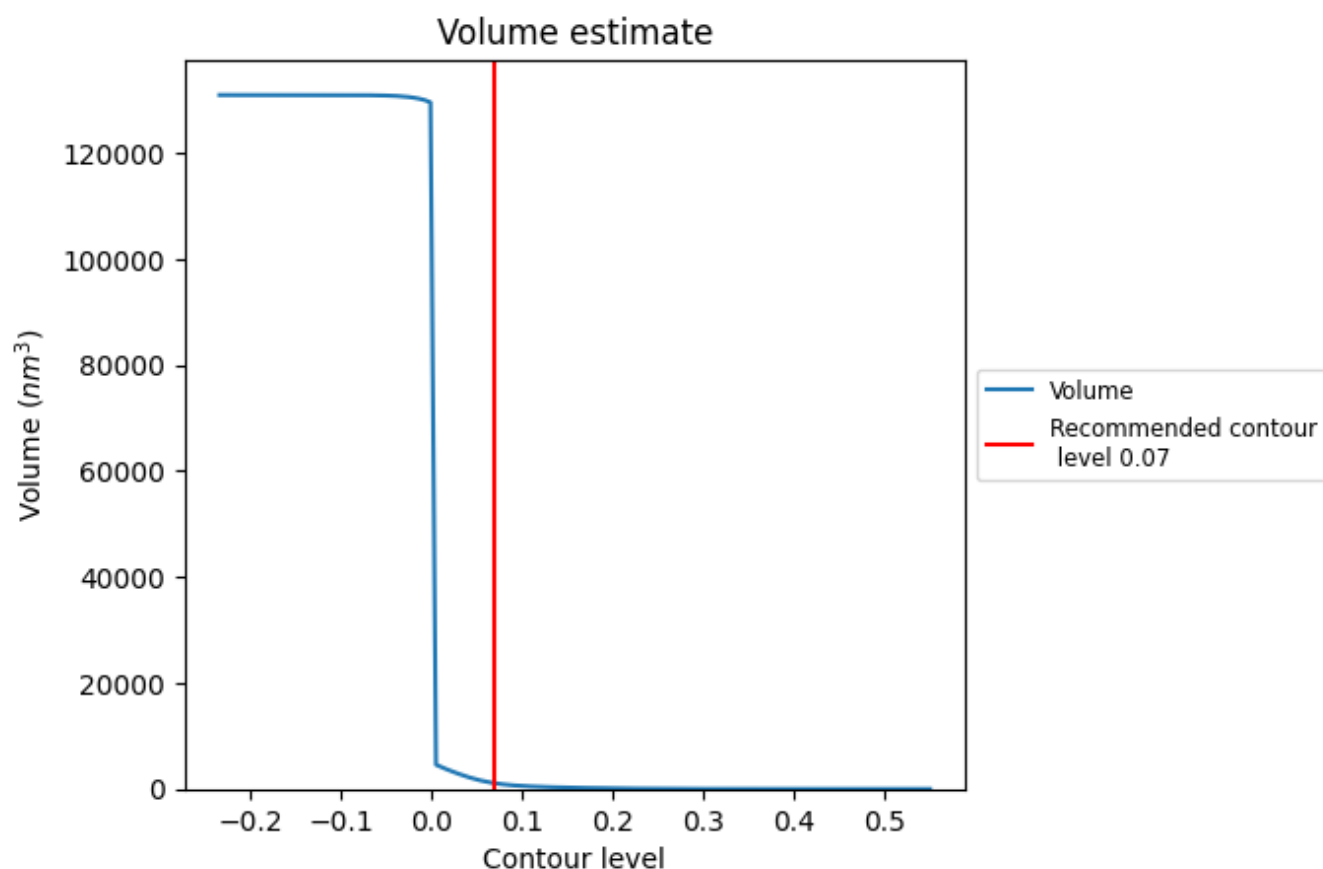
This section contains the results of statistical analysis of the map.

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



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

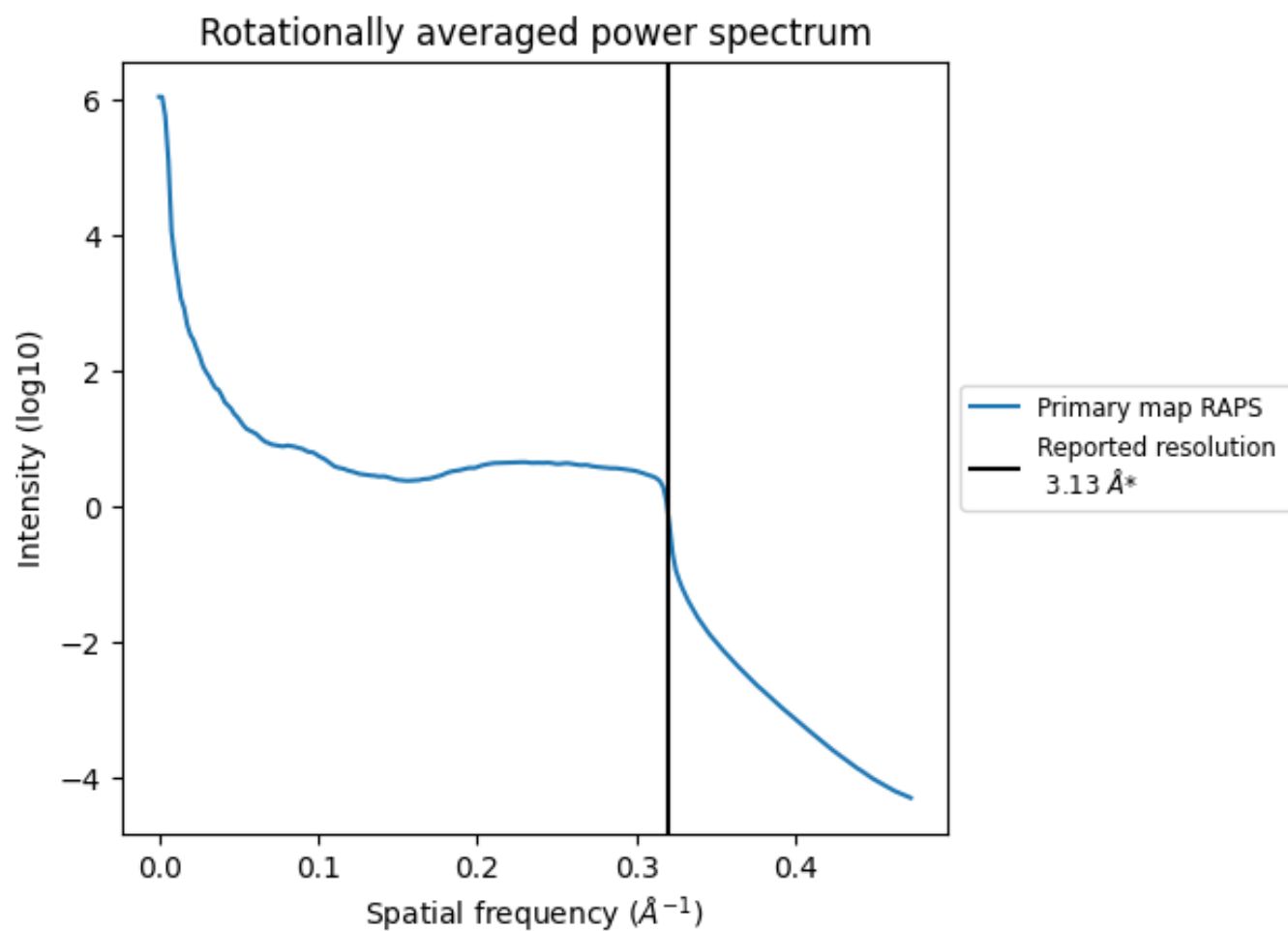
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1084  $\text{nm}^3$ ; this corresponds to an approximate mass of 979 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 0.319 Å<sup>-1</sup>

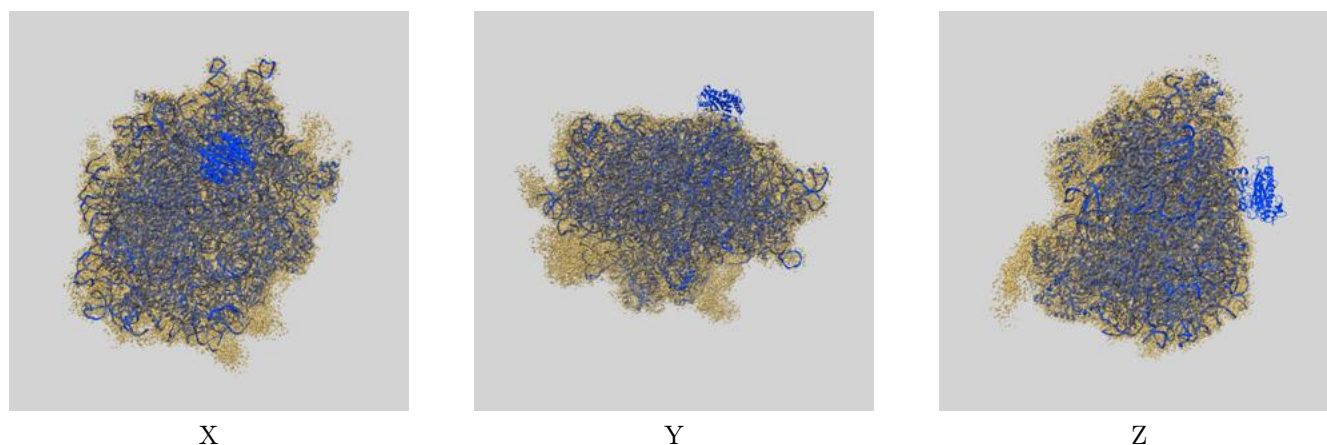
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

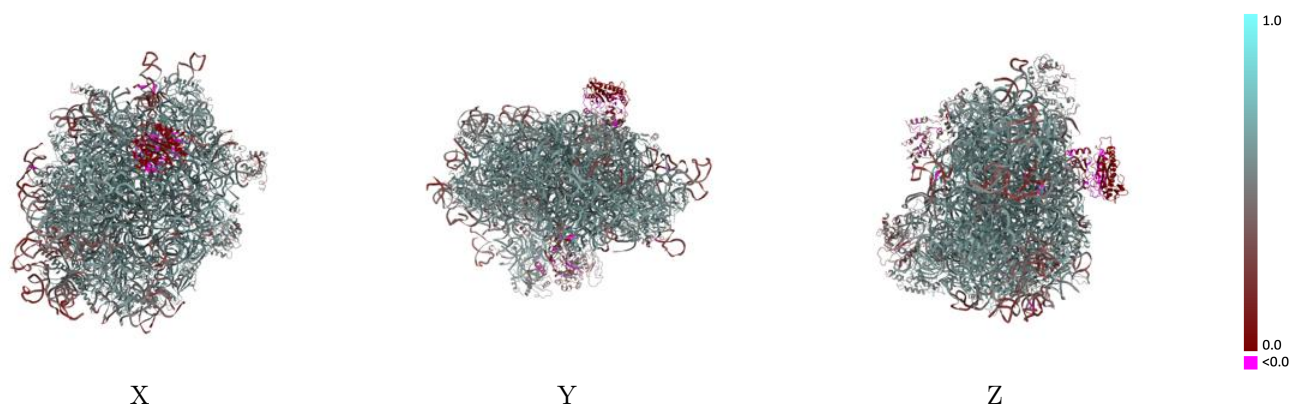
This section contains information regarding the fit between EMDB map EMD-0963 and PDB model 6LSR. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



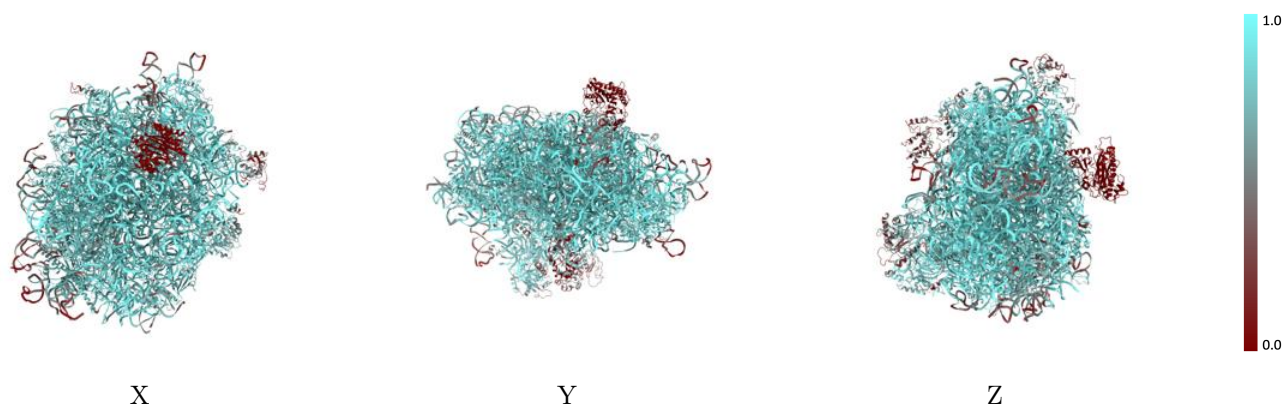
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



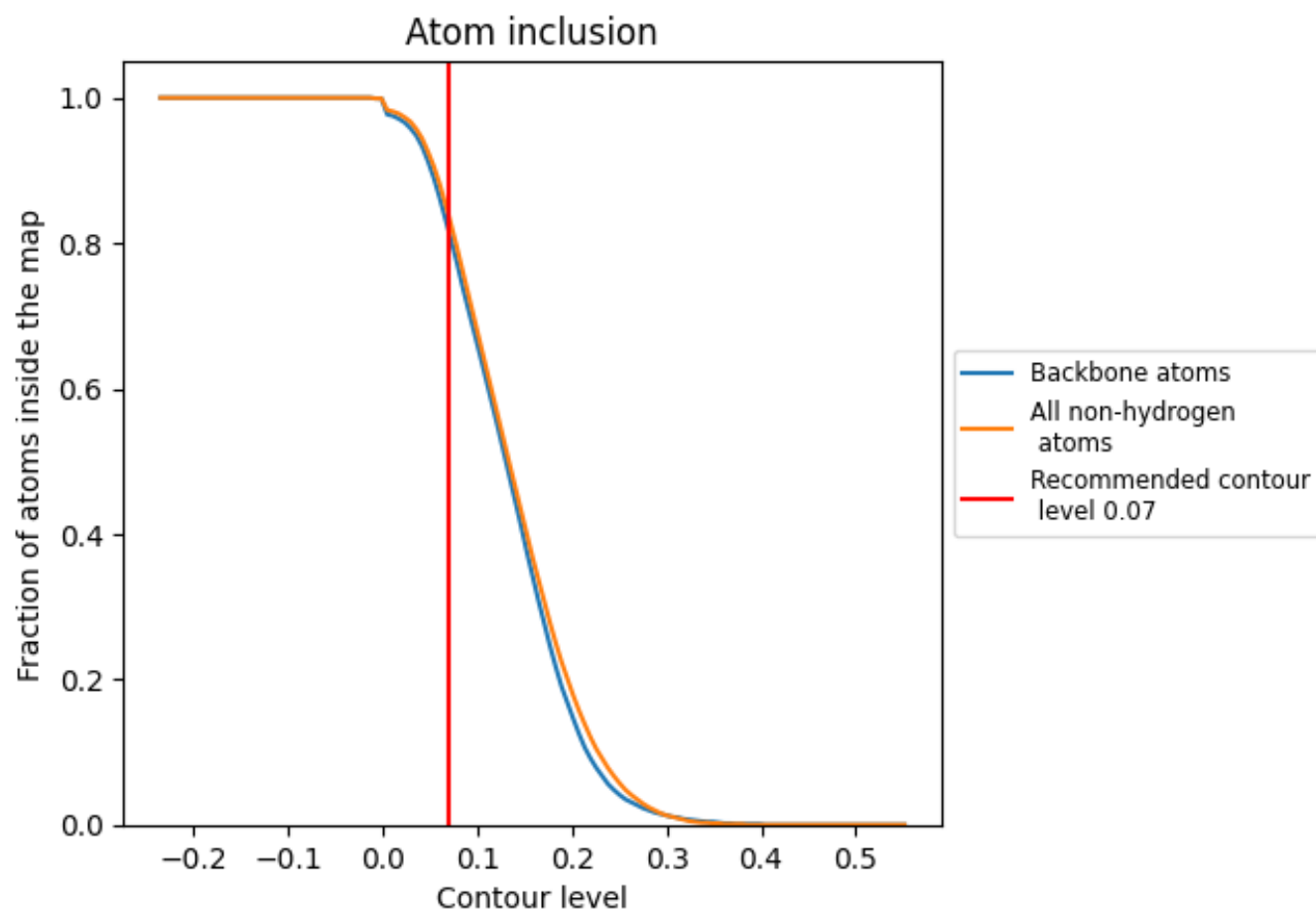
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8380   |  0.5320   |
| 0     |  0.5020   |  0.4460   |
| 1     |  0.3130   |  0.2480   |
| 2     |  0.8730   |  0.5340   |
| 3     |  0.8300   |  0.5350   |
| 5     |  0.9430   |  0.5660   |
| 6     |  0.6740   |  0.4860   |
| 8     |  0.9210   |  0.5590   |
| A     |  0.3870   |  0.3470   |
| B     |  0.8710   |  0.5770   |
| C     |  0.8140   |  0.5190   |
| D     |  0.9140   |  0.5890   |
| E     |  0.8010   |  0.5350   |
| F     |  0.8950   |  0.5820   |
| G     |  0.8060  |  0.5430  |
| H     |  0.8470 |  0.5710 |
| I     |  0.8080 |  0.5500 |
| K     |  0.8300 |  0.5470 |
| L     |  0.9340 |  0.6080 |
| M     |  0.9520 |  0.6010 |
| N     |  0.6780 |  0.4610 |
| O     |  0.7510 |  0.5350 |
| P     |  0.9290 |  0.5950 |
| Q     |  0.8430 |  0.5670 |
| S     |  0.8770 |  0.5680 |
| T     |  0.8440 |  0.5730 |
| U     |  0.9590 |  0.6120 |
| V     |  0.9130 |  0.5880 |
| W     |  0.8450 |  0.5550 |
| X     |  0.8470 |  0.5610 |
| Y     |  0.9100 |  0.5940 |
| Z     |  0.9320 |  0.5970 |
| a     |  0.8980 |  0.5770 |
| b     |  0.9210 |  0.5870 |
| c     |  0.8710 |  0.5710 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| d     |  0.7220 |  0.4980 |
| e     |  0.8810 |  0.5780 |
| f     |  0.8120 |  0.5590 |
| g     |  0.8690 |  0.5640 |
| h     |  0.8770 |  0.5760 |
| i     |  0.8160 |  0.5560 |
| l     |  0.8990 |  0.5810 |
| m     |  0.9320 |  0.5970 |
| r     |  0.7870 |  0.5330 |
| t     |  0.9350 |  0.5980 |
| u     |  0.9530 |  0.6020 |
| v     |  0.7760 |  0.5240 |
| w     |  0.9040 |  0.5830 |
| z     |  0.0120 |  0.0190 |