



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:05 PM UTC

PDB ID : 7N8B / pdb\_00007n8b  
EMDB ID : EMD-24235  
Title : Cycloheximide bound vacant 80S structure isolated from cbf5-D95A  
Authors : Rai, J.; Zhao, Y.; Li, H.  
Deposited on : 2021-06-14  
Resolution : 3.05 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| EMDB validation analysis       | : | 0.0.1.dev132                                                     |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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                                                             |

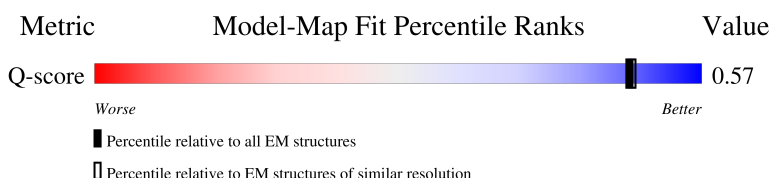
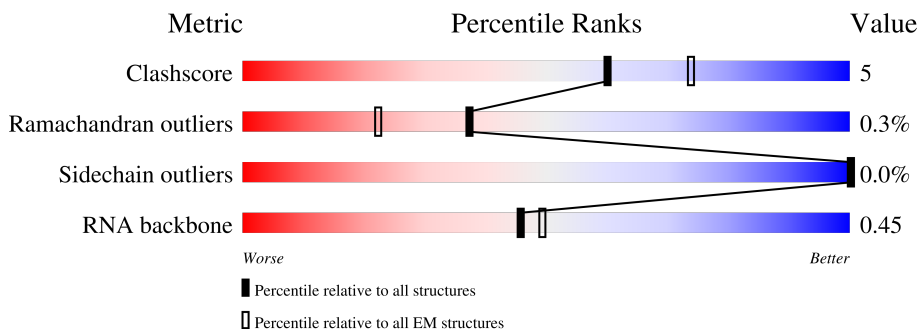
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.05 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.



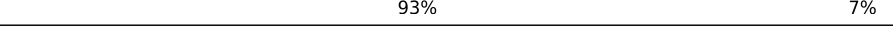
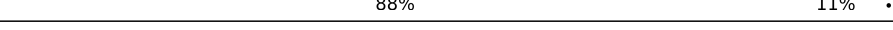
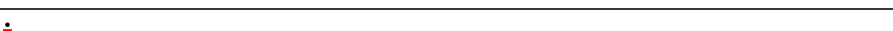
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13971 ( 2.55 - 3.55 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A1    | 3156   |                  |
| 2   | A3    | 121    |                  |
| 3   | A4    | 158    |                  |

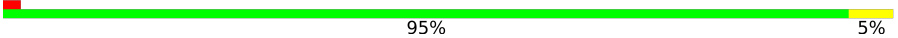
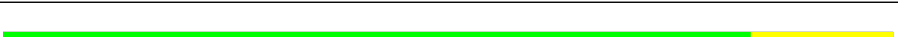
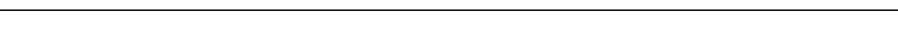
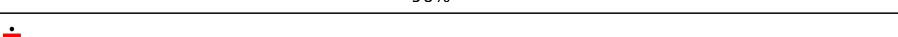
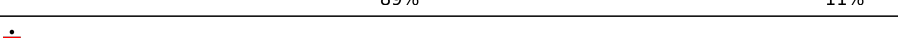
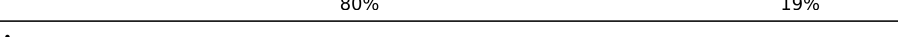
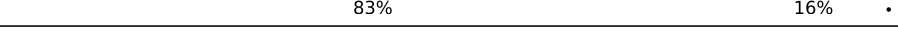
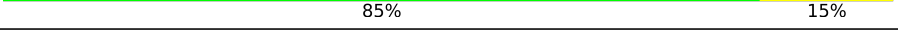
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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 4   | AA    | 247    |  78%22%     |
| 5   | AB    | 386    |  81%19%     |
| 6   | AC    | 361    |  86%14%     |
| 7   | AD    | 292    |  88%12%     |
| 8   | AE    | 156    |  90%10%     |
| 9   | AF    | 222    |  82%17%     |
| 10  | AG    | 230    |  88%11%     |
| 11  | AH    | 190    |  87%13%     |
| 12  | AI    | 205    |  80%20%     |
| 13  | AJ    | 169    |  5%83%17%   |
| 14  | AL    | 193    |  84%14%     |
| 15  | AM    | 136    |  93%7%     |
| 16  | AN    | 203    |  81%18%   |
| 17  | AO    | 197    |  88%11%   |
| 18  | AP    | 175    |  89%11%   |
| 19  | AQ    | 185    |  91%9%    |
| 20  | AR    | 188    |  7%89%11% |
| 21  | AS    | 172    |  87%12%   |
| 22  | AT    | 159    |  79%20%   |
| 23  | AU    | 100    |  92%7%    |
| 24  | AV    | 136    |  88%12%   |
| 25  | AW    | 63     |  90%10%   |
| 26  | AX    | 121    |  90%10%   |
| 27  | AY    | 126    |  80%20%   |
| 28  | AZ    | 135    |  82%18%   |

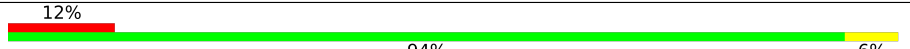
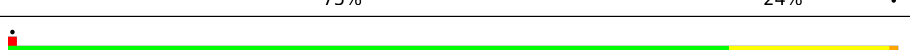
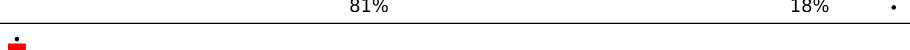
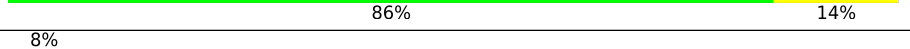
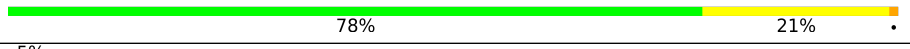
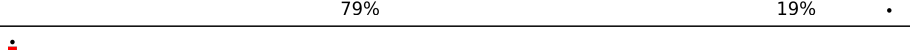
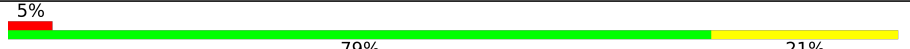
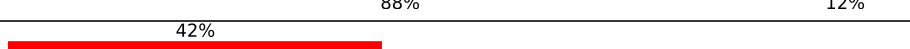
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | Aa    | 148    |    |
| 30  | Ab    | 58     |    |
| 31  | Ac    | 97     |    |
| 32  | Ad    | 109    |    |
| 33  | Ae    | 127    |    |
| 34  | Af    | 106    |    |
| 35  | Ag    | 112    |    |
| 36  | Ah    | 119    |    |
| 37  | Ai    | 99     |    |
| 38  | Aj    | 87     |    |
| 39  | Ak    | 77     |    |
| 40  | Al    | 50     |    |
| 41  | Am    | 52     |  |
| 42  | An    | 25     |  |
| 43  | Ao    | 105    |  |
| 44  | Ap    | 91     |  |
| 45  | BA    | 206    |  |
| 46  | BB    | 214    |  |
| 47  | BC    | 217    |  |
| 48  | BD    | 223    |  |
| 49  | BE    | 260    |  |
| 50  | BF    | 206    |  |
| 51  | BG    | 226    |  |
| 52  | BH    | 184    |  |
| 53  | BI    | 188    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | BJ    | 185    |    |
| 55  | BK    | 96     |    |
| 56  | BL    | 155    |    |
| 57  | BM    | 121    |    |
| 58  | BN    | 150    |    |
| 59  | BO    | 127    |    |
| 60  | BP    | 124    |    |
| 61  | BQ    | 141    |    |
| 62  | BR    | 121    |    |
| 63  | BS    | 145    |    |
| 64  | BT    | 141    |    |
| 65  | BU    | 107    |    |
| 66  | BV    | 87     |   |
| 67  | BW    | 129    |  |
| 68  | BX    | 144    |  |
| 69  | BY    | 134    |  |
| 70  | BZ    | 69     |  |
| 71  | Ba    | 97     |  |
| 72  | Bb    | 81     |  |
| 73  | Bc    | 63     |  |
| 74  | Bd    | 53     |  |
| 75  | Be    | 60     |  |
| 76  | Bf    | 57     |  |
| 77  | Bg    | 312    |  |
| 78  | Bh    | 89     |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 79  | B5    | 1783   |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 79  | 3AU  | B5    | 1191 | X         | -        | -       | -                |
| 79  | G7M  | B5    | 1575 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 199900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | A1    | 3156     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 67535 | 30189 | 12152 | 22038 | 3156 |         |       |

- Molecule 2 is a RNA chain called 5S.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2   | A3    | 121      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |       |

- Molecule 3 is a RNA chain called 5.8S.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | A4    | 158      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | AA    | 247      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1878  | 1170 | 381 | 326 | 1 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | AB    | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3079  | 1954 | 584 | 533 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | AC    | 361      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | AD    | 292      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2341  | 1478 | 408 | 453 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | AE    | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1239  | 800 | 222 | 216 | 1 |         |       |

There are 19 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AE    | ?       | -        | LYS    | deletion | UNP Q02326 |
| AE    | ?       | -        | LEU    | deletion | UNP Q02326 |
| AE    | ?       | -        | THR    | deletion | UNP Q02326 |
| AE    | ?       | -        | LYS    | deletion | UNP Q02326 |
| AE    | ?       | -        | LYS    | deletion | UNP Q02326 |
| AE    | ?       | -        | GLU    | deletion | UNP Q02326 |
| AE    | ?       | -        | LYS    | deletion | UNP Q02326 |
| AE    | ?       | -        | LYS    | deletion | UNP Q02326 |
| AE    | ?       | -        | GLU    | deletion | UNP Q02326 |
| AE    | ?       | -        | ALA    | deletion | UNP Q02326 |
| AE    | ?       | -        | ASN    | deletion | UNP Q02326 |
| AE    | ?       | -        | LEU    | deletion | UNP Q02326 |
| AE    | ?       | -        | PHE    | deletion | UNP Q02326 |
| AE    | ?       | -        | PRO    | deletion | UNP Q02326 |
| AE    | ?       | -        | GLU    | deletion | UNP Q02326 |
| AE    | ?       | -        | GLN    | deletion | UNP Q02326 |
| AE    | ?       | -        | GLN    | deletion | UNP Q02326 |
| AE    | ?       | -        | ASN    | deletion | UNP Q02326 |
| AE    | ?       | -        | LYS    | deletion | UNP Q02326 |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | AF    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L8-A.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | AG    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1798  | 1149 | 323 | 323 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | AH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1510  | 957 | 273 | 276 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | AI    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1672  | 1063 | 316 | 288 | 5 |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AI    | ?       | -        | MET    | deletion | UNP P41805 |
| AI    | ?       | -        | LEU    | deletion | UNP P41805 |
| AI    | ?       | -        | SER    | deletion | UNP P41805 |
| AI    | ?       | -        | CYS    | deletion | UNP P41805 |
| AI    | ?       | -        | ALA    | deletion | UNP P41805 |
| AI    | ?       | -        | GLY    | deletion | UNP P41805 |
| AI    | ?       | -        | ALA    | deletion | UNP P41805 |
| AI    | ?       | -        | ASP    | deletion | UNP P41805 |
| AI    | ?       | -        | ARG    | deletion | UNP P41805 |
| AI    | ?       | -        | LEU    | deletion | UNP P41805 |
| AI    | ?       | -        | GLN    | deletion | UNP P41805 |
| AI    | ?       | -        | GLN    | deletion | UNP P41805 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | AJ    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14  | AL    | 193      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | AN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | AO    | 197      | Total | C    | N   | O   | S | 197     | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 18  | AP    | 175      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1388  | 862 | 277 | 249 |  |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AP    | ?       | -        | ALA    | deletion | UNP P05740 |
| AP    | ?       | -        | VAL    | deletion | UNP P05740 |
| AP    | ?       | -        | ALA    | deletion | UNP P05740 |
| AP    | ?       | -        | LYS    | deletion | UNP P05740 |
| AP    | ?       | -        | ALA    | deletion | UNP P05740 |
| AP    | ?       | -        | ALA    | deletion | UNP P05740 |
| AP    | ?       | -        | GLU    | deletion | UNP P05740 |
| AP    | ?       | -        | LYS    | deletion | UNP P05740 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AQ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20  | AR    | 188      | Total | C   | N   | O   |         |       |
|     |       |          | 1521  | 935 | 326 | 260 | 0       | 0     |

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | AS    | 172      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1445  | 930 | 267 | 244 | 4 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | AT    | 159      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1276  | 805 | 246 | 221 | 4 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 23  | AU    | 100      | Total | C   | N   | O   |         |       |
|     |       |          | 796   | 516 | 131 | 149 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | AV    | 136      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1003  | 628 | 189 | 179 | 7 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 25  | AW    | 63       | Total | C   | N   | O  | S |         |       |
|     |       |          | 521   | 336 | 102 | 82 | 1 | 0       | 0     |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | AX    | 121      | Total | C   | N   | O   | S |         |       |
|     |       |          | 968   | 623 | 170 | 173 | 2 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 27  | AY    | 126      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28  | AZ    | 135      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | Aa    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 30  | Ab    | 58       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Ac    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 743   | 479 | 124 | 139 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Ad    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 890   | 565 | 168 | 156 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Ae    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Af    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Ag    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Ah    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Ai    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Aj    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39  | Ak    | 77       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | Al    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | Am    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | An    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Ao    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Ap    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |       |

- Molecule 45 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45  | BA    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1612  | 1034 | 285 | 291 | 2 |         |       |

- Molecule 46 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | BB    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1709  | 1084 | 310 | 311 | 4 |         |       |

- Molecule 47 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | BC    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |       |

- Molecule 48 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | BD    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |       |

- Molecule 49 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | BE    | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | BF    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | BG    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1820  | 1142 | 350 | 325 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 52  | BH    | 184      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | BI    | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BI    | ?       | -        | LYS    | deletion | UNP P0CX39 |
| BI    | ?       | -        | LYS    | deletion | UNP P0CX39 |
| BI    | ?       | -        | ASN    | deletion | UNP P0CX39 |
| BI    | ?       | -        | VAL    | deletion | UNP P0CX39 |
| BI    | ?       | -        | LYS    | deletion | UNP P0CX39 |
| BI    | ?       | -        | GLU    | deletion | UNP P0CX39 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BI    | ?       | -        | GLU    | deletion | UNP P0CX39 |
| BI    | ?       | -        | GLU    | deletion | UNP P0CX39 |
| BI    | ?       | -        | THR    | deletion | UNP P0CX39 |
| BI    | ?       | -        | VAL    | deletion | UNP P0CX39 |
| BI    | ?       | -        | ALA    | deletion | UNP P0CX39 |

- Molecule 54 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | BJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | BK    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 529 | 133 | 153 | 2 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | BL    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1244  | 798 | 235 | 208 | 3 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | BM    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 913   | 574 | 162 | 175 | 2 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | BN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | BO    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 941   | 578 | 186 | 174 | 3 |         |       |



- Molecule 60 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | BP    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 991   | 631 | 187 | 166 | 7 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 708 | 203 | 194 |   |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | BR    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 975   | 611 | 183 | 179 | 2 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BR    | ?       | -        | SER    | deletion | UNP P02407 |
| BR    | ?       | -        | ASN    | deletion | UNP P02407 |
| BR    | ?       | -        | GLY    | deletion | UNP P02407 |
| BR    | ?       | -        | VAL    | deletion | UNP P02407 |

- Molecule 63 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | BS    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | BT    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1095  | 685 | 206 | 202 | 2 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | BU    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 855   | 539 | 156 | 159 | 1 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | BV    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | BW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | BX    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | BY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |   |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 70  | BZ    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 558   | 357 | 103 | 98 |   |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | Ba    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | Bb    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 73  | Bc    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 74  | Bd    | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 75  | Be    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 475   | 299 | 98 | 77 | 1 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 76  | Bf    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 454   | 288 | 86 | 77 | 3 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Bf    | 97      | ALA      | LYS    | conflict | UNP P05759 |
| Bf    | ?       | -        | CYS    | deletion | UNP P05759 |
| Bf    | ?       | -        | GLY    | deletion | UNP P05759 |
| Bf    | ?       | -        | ALA    | deletion | UNP P05759 |

- Molecule 77 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 77  | Bg    | 312      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2401  | 1522 | 410 | 461 | 8 |         |       |

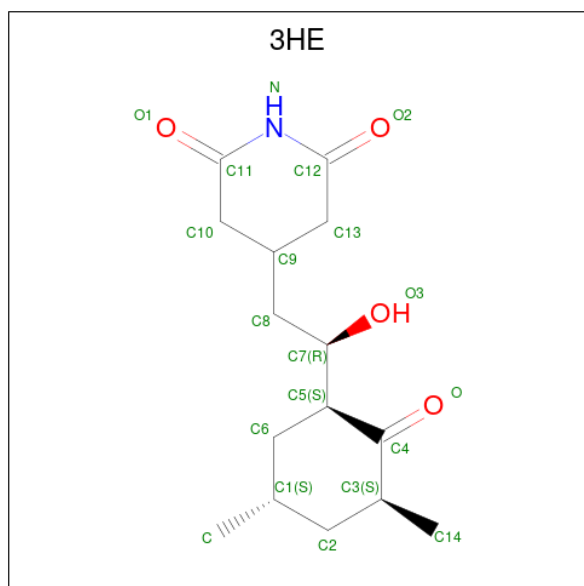
- Molecule 78 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 78  | Bh    | 89       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 675   | 391 | 137 | 147 |         |       |

- Molecule 79 is a RNA chain called 18S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 79  | B5    | 1783     | Total | C     | N    | O     | P    | 1       | 0     |
|     |       |          | 37891 | 16950 | 6664 | 12494 | 1783 |         |       |

- Molecule 80 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 80  | A1    | 1        | Total | C  | N | O | 0       |
|     |       |          | 20    | 15 | 1 | 4 |         |

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 81  | A1    | 247      | Total | Mg  | 0       |
|     |       |          | 247   | 247 |         |
| 81  | A3    | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 81  | A4    | 9        | Total | Mg  | 0       |
|     |       |          | 9     | 9   |         |
| 81  | AB    | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 81  | AC    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 81  | AG    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 81  | AL    | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 81  | AN    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | AO    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | AP    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | AR    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | AV    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | Aa    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | Ae    | 2        | Total<br>2  | Mg<br>2  | 0       |
| 81  | Af    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | Aj    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | BE    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | BG    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | BJ    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | Ba    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 81  | B5    | 90       | Total<br>90 | Mg<br>90 | 0       |

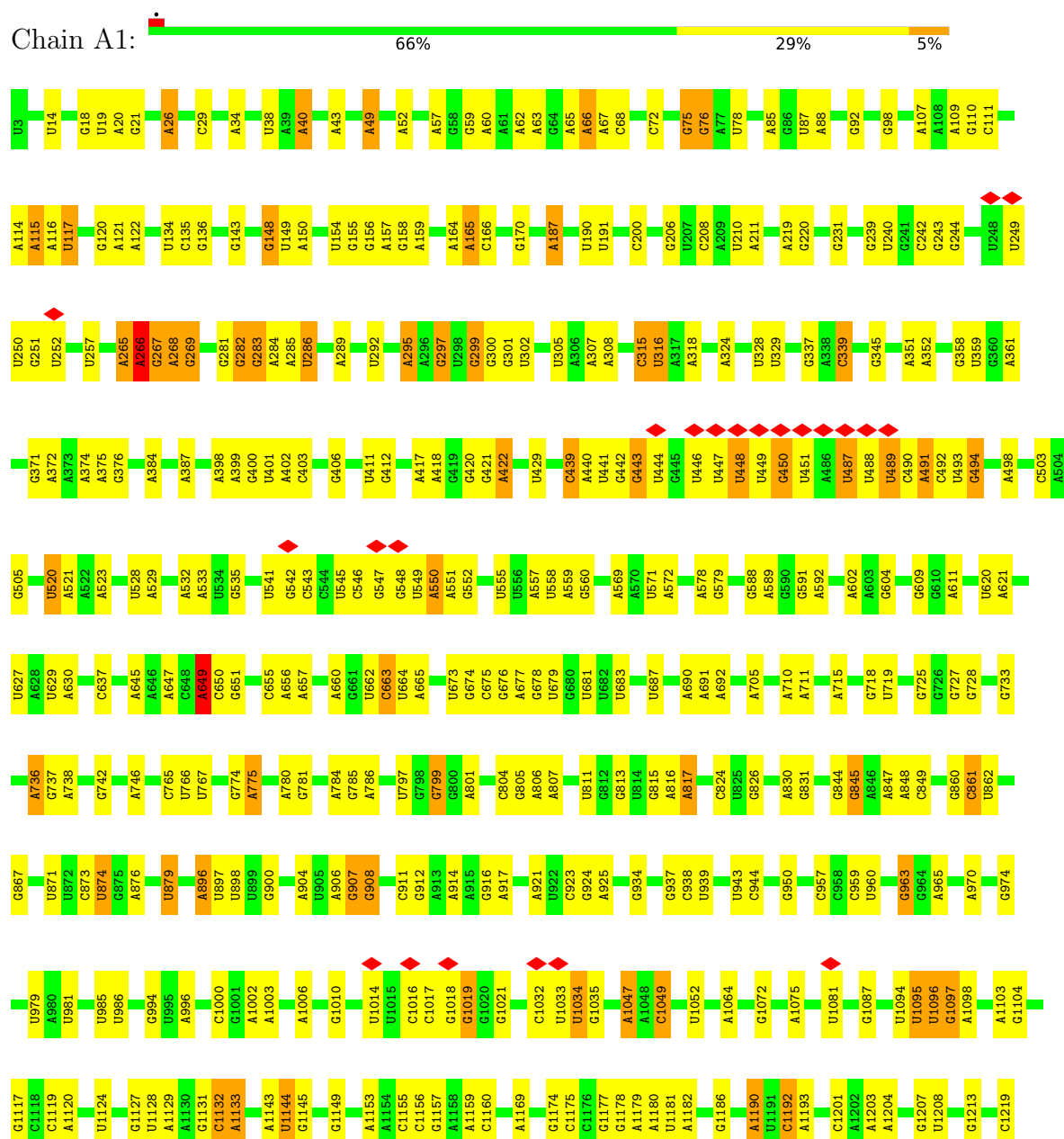
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 82  | Ao    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 82  | Bb    | 1        | Total<br>1 | Zn<br>1 | 0       |

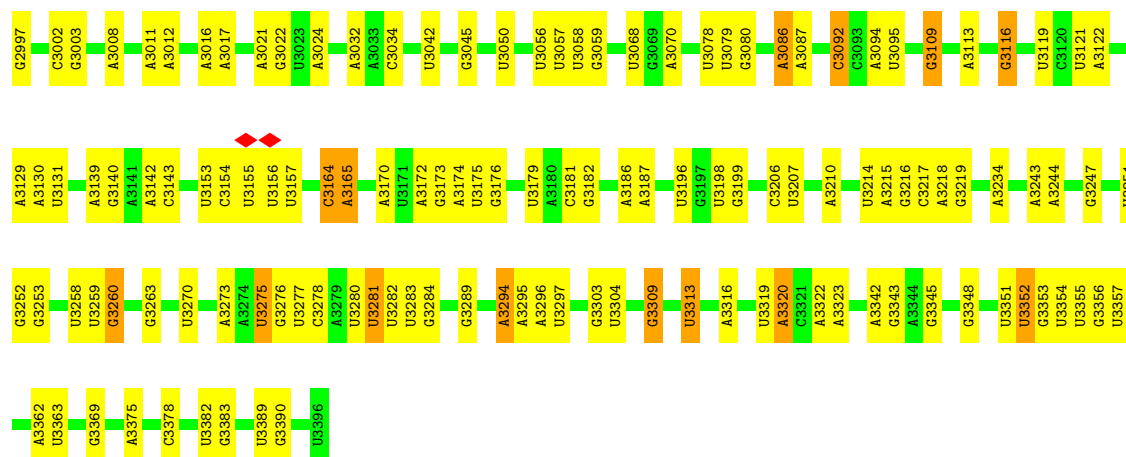
### 3 Residue-property plots [i](#)

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

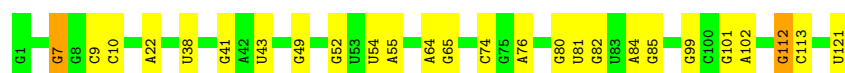
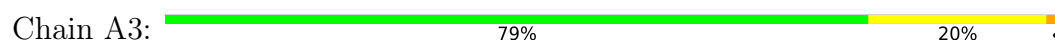
#### • Molecule 1: 25S



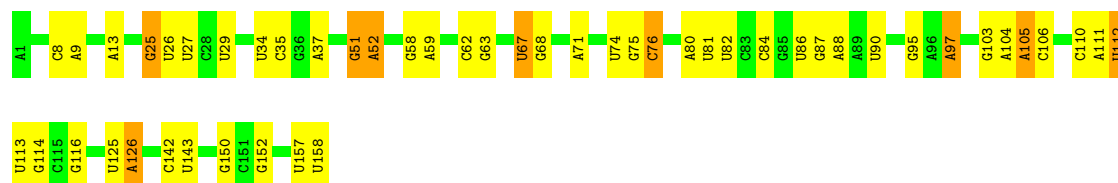




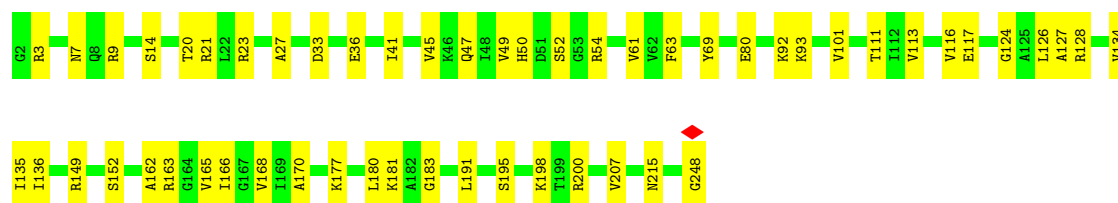
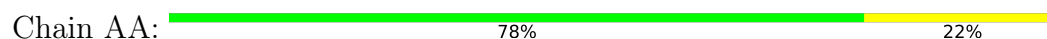
• Molecule 2: 5S



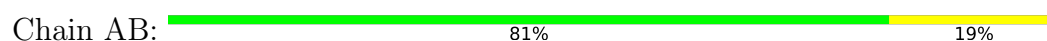
• Molecule 3: 5.8S



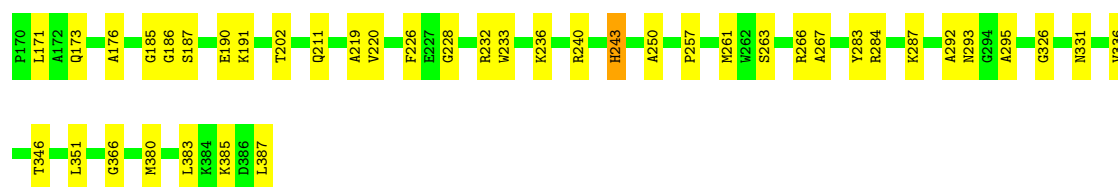
• Molecule 4: 60S ribosomal protein L2-A



• Molecule 5: 60S ribosomal protein L3

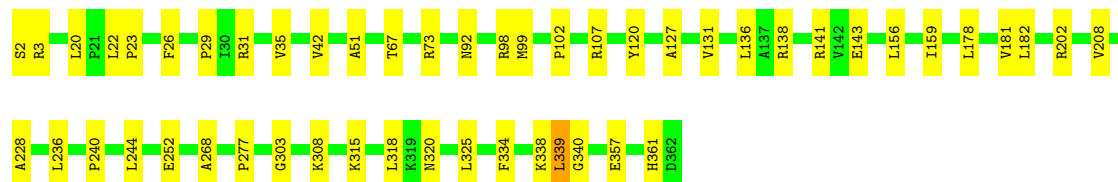






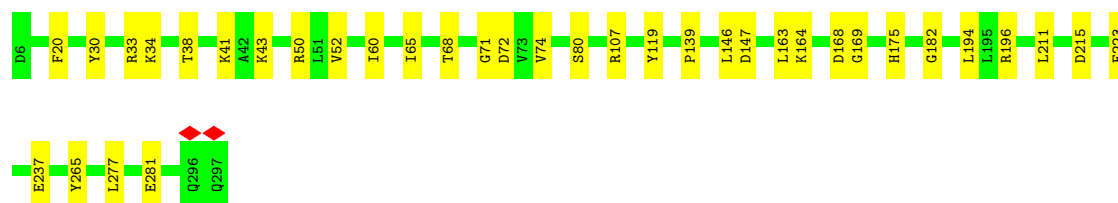
- Molecule 6: 60S ribosomal protein L4-A

Chain AC: 86% 14%



- Molecule 7: 60S ribosomal protein L5

Chain AD: 88% 12%



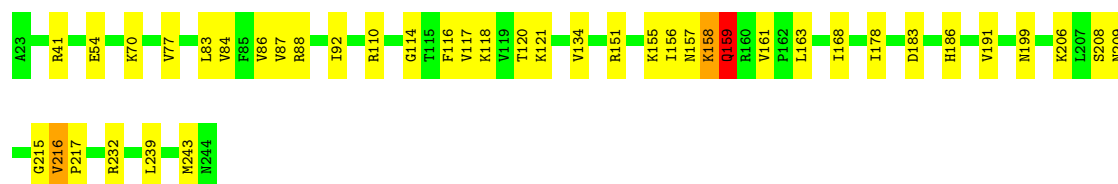
- Molecule 8: 60S ribosomal protein L6-A

Chain AE: 90% 10%



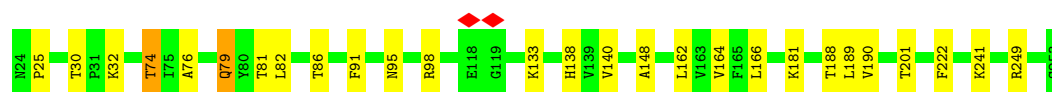
- Molecule 9: 60S ribosomal protein L7-A

Chain AF: 82% 17%

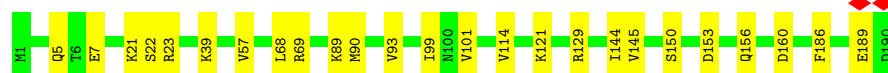
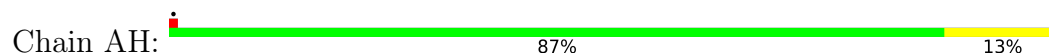


- Molecule 10: 60S ribosomal protein L8-A

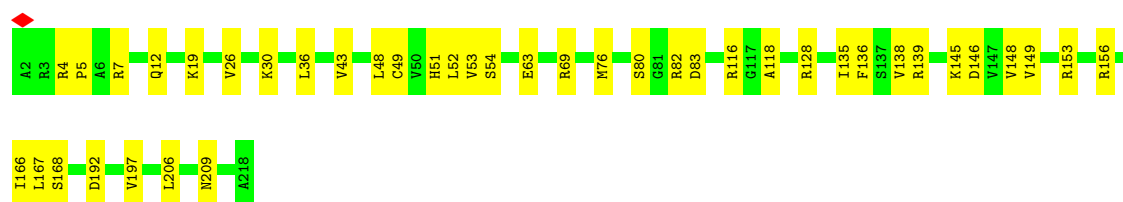
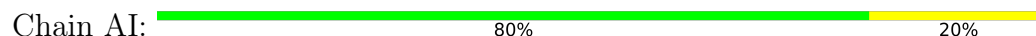
Chain AG: 88% 11%



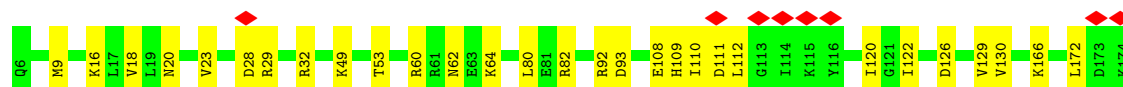
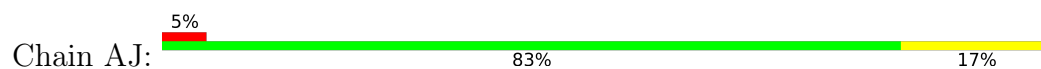
- Molecule 11: 60S ribosomal protein L9-A



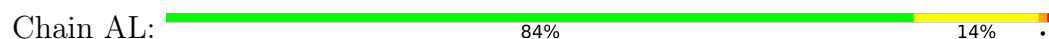
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-A



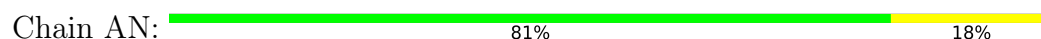
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A



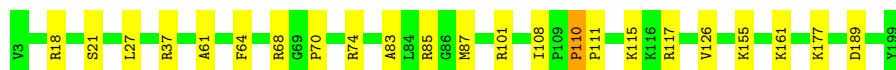
- Molecule 16: 60S ribosomal protein L15-A





- Molecule 17: 60S ribosomal protein L16-A

Chain AO: 88% 11%



- Molecule 18: 60S ribosomal protein L17-A

Chain AP: 89% 11%



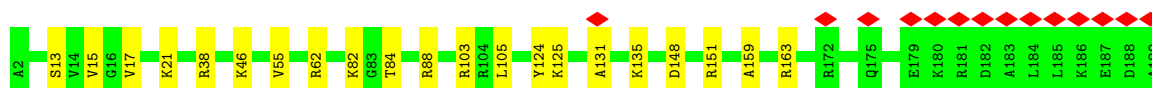
- Molecule 19: 60S ribosomal protein L18-A

Chain AQ: 91% 9%



- Molecule 20: 60S ribosomal protein L19-A

Chain AR: 7% 89% 11%



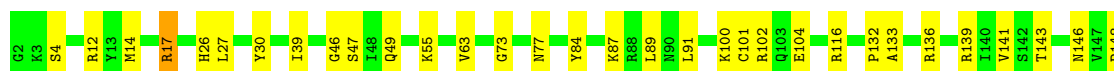
- Molecule 21: 60S ribosomal protein L20-A

Chain AS: 87% 12%

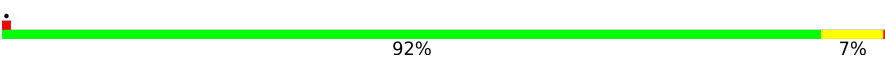
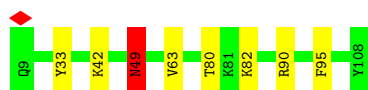


- Molecule 22: 60S ribosomal protein L21-A

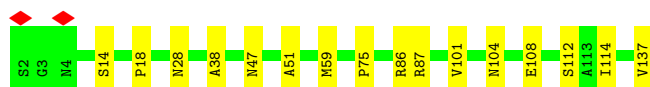
Chain AT: 79% 20%



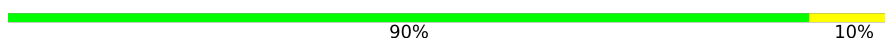
## • Molecule 23: 60S ribosomal protein L22-A

Chain AU:  92% 7%

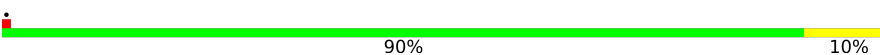
## • Molecule 24: 60S ribosomal protein L23-A

Chain AV:  88% 12%

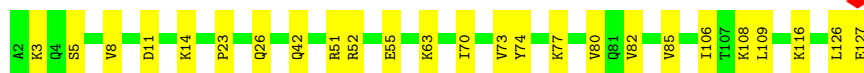
## • Molecule 25: 60S ribosomal protein L24-A

Chain AW:  90% 10%

## • Molecule 26: 60S ribosomal protein L25

Chain AX:  90% 10%

## • Molecule 27: 60S ribosomal protein L26-A

Chain AY:  80% 20%

## • Molecule 28: 60S ribosomal protein L27-A

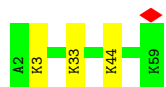
Chain AZ:  82% 18%

## • Molecule 29: 60S ribosomal protein L28

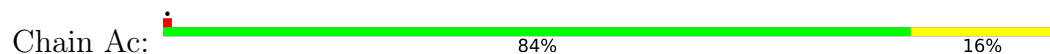
Chain Aa:  78% 21%



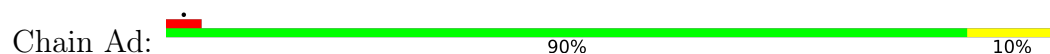
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30



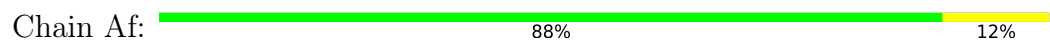
- Molecule 32: 60S ribosomal protein L31-A



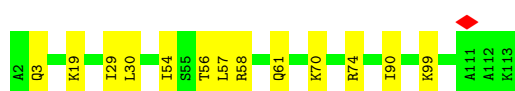
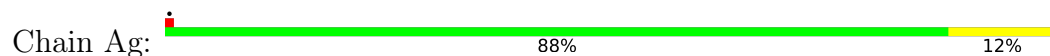
- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-A



- Molecule 36: 60S ribosomal protein L35-A

Chain Ah:  88% 11%



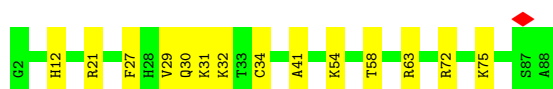
- Molecule 37: 60S ribosomal protein L36-A

Chain Ai:  91% 9%



- Molecule 38: 60S ribosomal protein L37-A

Chain Aj:  84% 16%

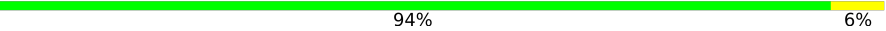


- Molecule 39: 60S ribosomal protein L38

Chain Ak:  84% 16%



- Molecule 40: 60S ribosomal protein L39

Chain Al:  94% 6%

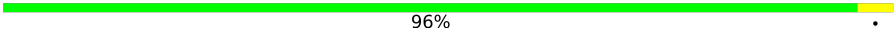


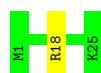
- Molecule 41: 60S ribosomal protein L40-A

Chain Am:  69% 31%



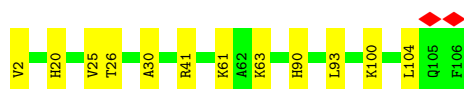
- Molecule 42: 60S ribosomal protein L41-A

Chain An:  96%



- Molecule 43: 60S ribosomal protein L42-A

Chain Ao:  89% 11%



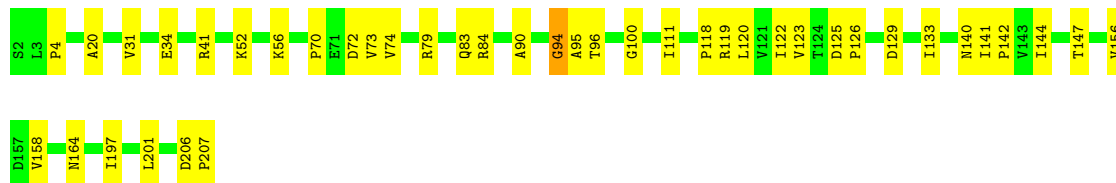
- Molecule 44: 60S ribosomal protein L43-A

Chain Ap:  80% 20%



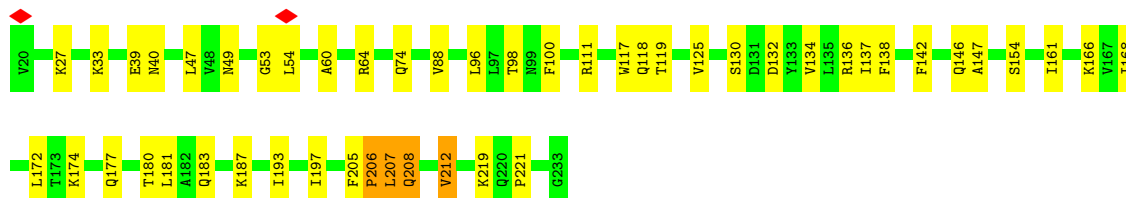
- Molecule 45: 40S ribosomal protein S0-A

Chain BA:  80% 19%



- Molecule 46: 40S ribosomal protein S1-A

Chain BB:  77% 21%



- Molecule 47: 40S ribosomal protein S2

Chain BC:  83% 16%



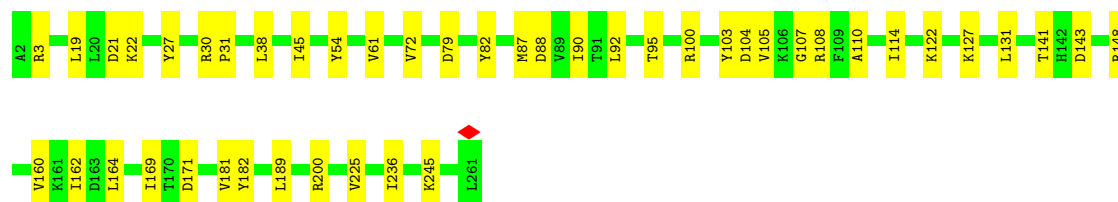
- Molecule 48: 40S ribosomal protein S3

Chain BD:  85% 15%



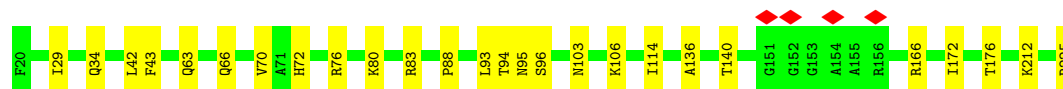
- Molecule 49: 40S ribosomal protein S4-A

Chain BE: 83% 17%



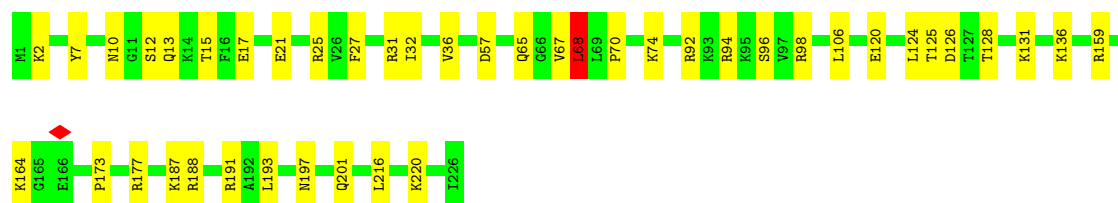
- Molecule 50: 40S ribosomal protein S5

Chain BF: 87% 13%



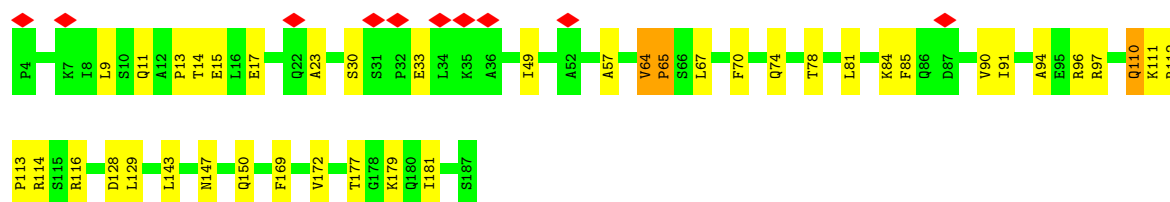
- Molecule 51: 40S ribosomal protein S6-A

Chain BG: 81% 19%



- Molecule 52: 40S ribosomal protein S7-A

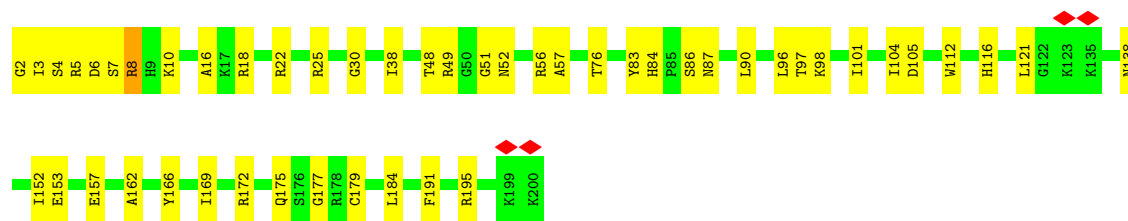
Chain BH: 5% 78% 21%



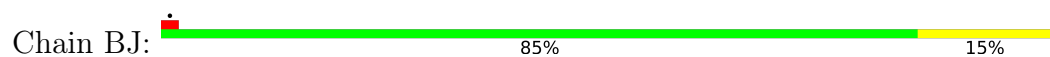
- Molecule 53: 40S ribosomal protein S8-A

Chain BI: 74% 26%

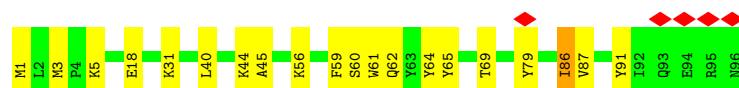
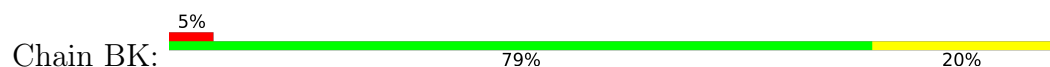




- Molecule 54: 40S ribosomal protein S9-A



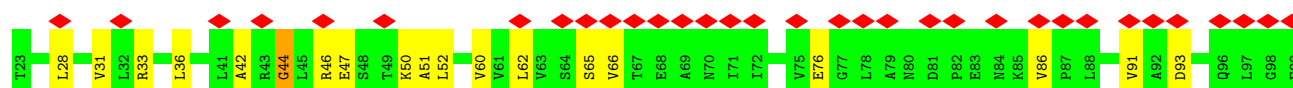
- Molecule 55: 40S ribosomal protein S10-A



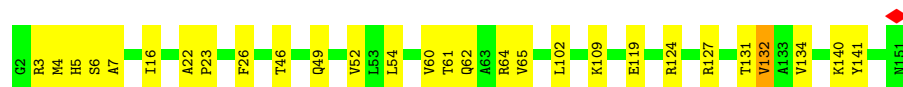
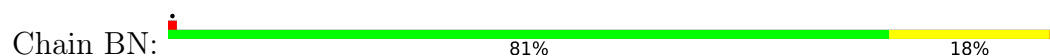
- Molecule 56: 40S ribosomal protein S11-A



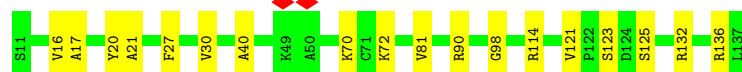
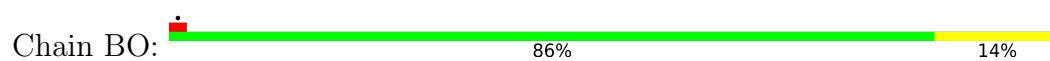
- Molecule 57: 40S ribosomal protein S12



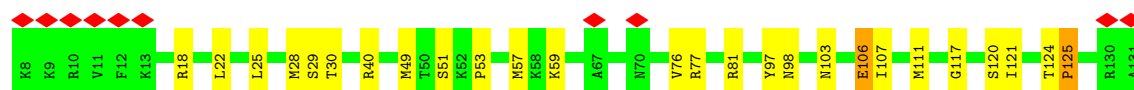
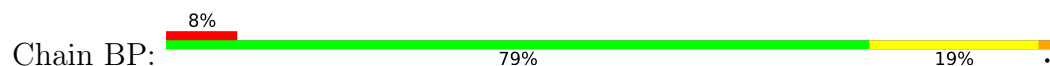
- Molecule 58: 40S ribosomal protein S13



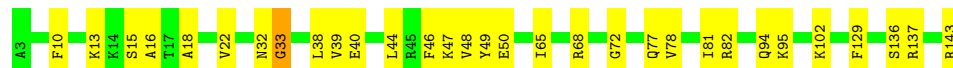
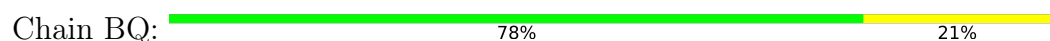
- Molecule 59: 40S ribosomal protein S14-A



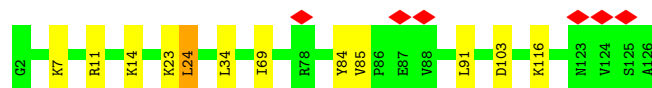
- Molecule 60: 40S ribosomal protein S15



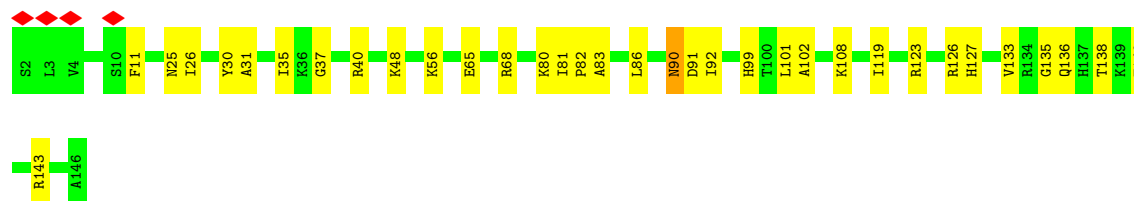
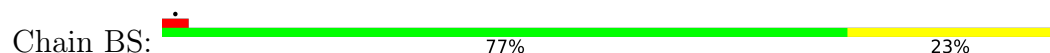
- Molecule 61: 40S ribosomal protein S16-A



- Molecule 62: 40S ribosomal protein S17-A



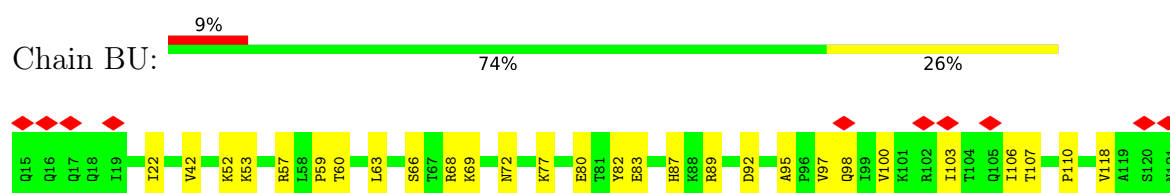
- Molecule 63: 40S ribosomal protein S18-A



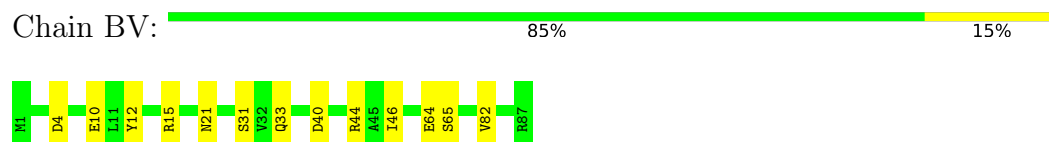
- Molecule 64: 40S ribosomal protein S19-A



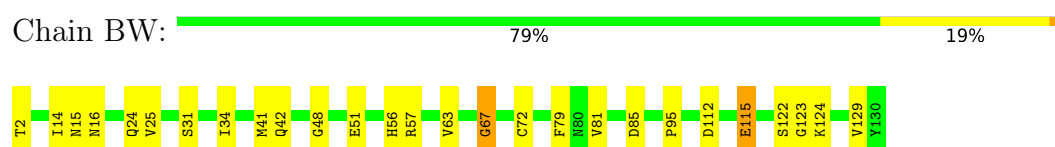
- Molecule 65: 40S ribosomal protein S20



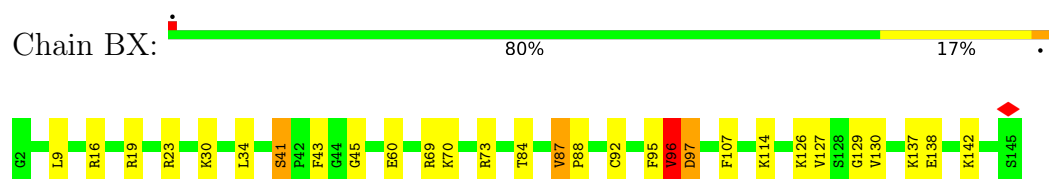
- Molecule 66: 40S ribosomal protein S21-A



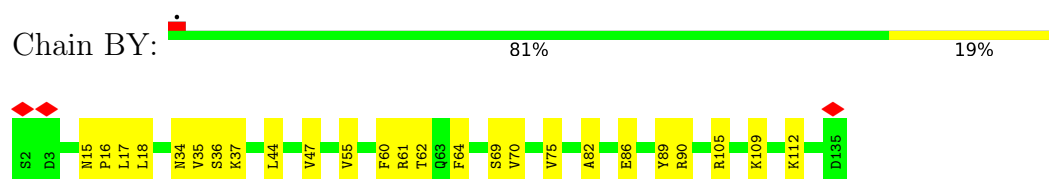
- Molecule 67: 40S ribosomal protein S22-A



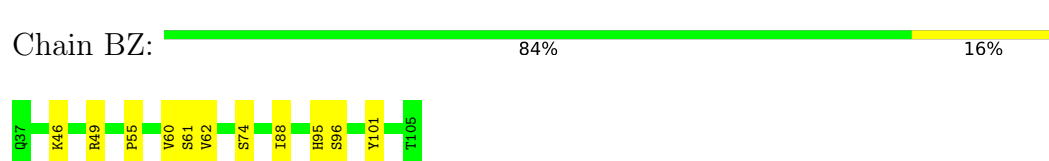
- Molecule 68: 40S ribosomal protein S23-A



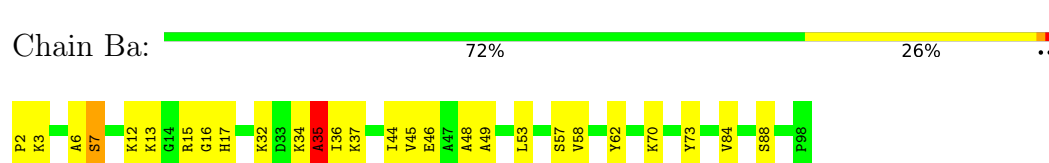
- Molecule 69: 40S ribosomal protein S24-A



- Molecule 70: 40S ribosomal protein S25-A



- Molecule 71: 40S ribosomal protein S26-B



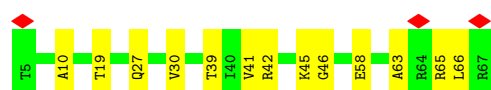
- Molecule 72: 40S ribosomal protein S27-A

Chain Bb:  80% 19%



- Molecule 73: 40S ribosomal protein S28-A

Chain Bc:  5% 79% 21%



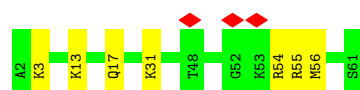
- Molecule 74: 40S ribosomal protein S29-A

Chain Bd:  68% 32%



- Molecule 75: 40S ribosomal protein S30-A

Chain Be:  5% 88% 12%



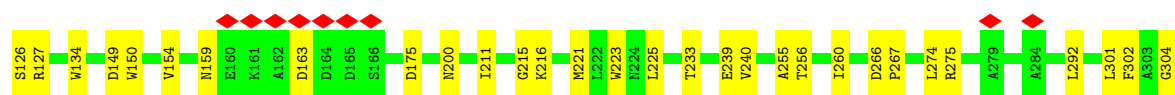
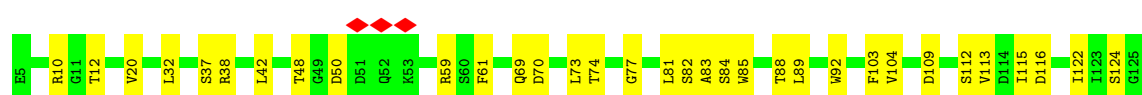
- Molecule 76: 40S ribosomal protein S31

Chain Bf:  42% 86% 14%

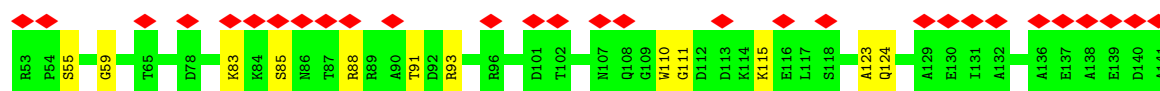
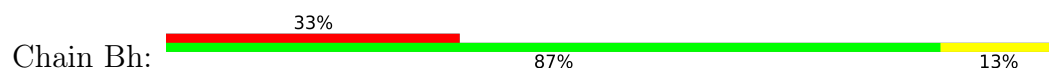


- Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein

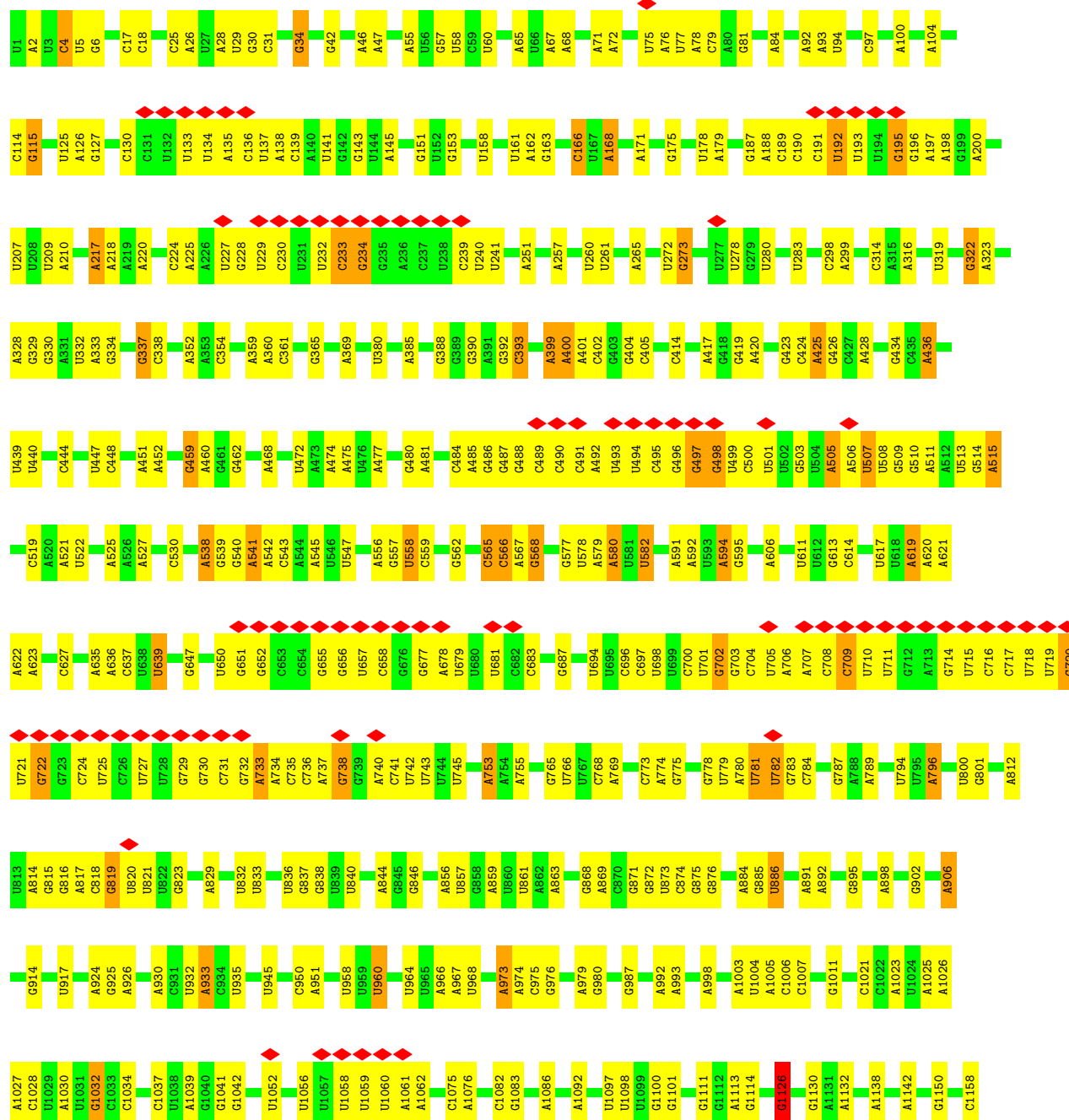
Chain Bg:  79% 21%

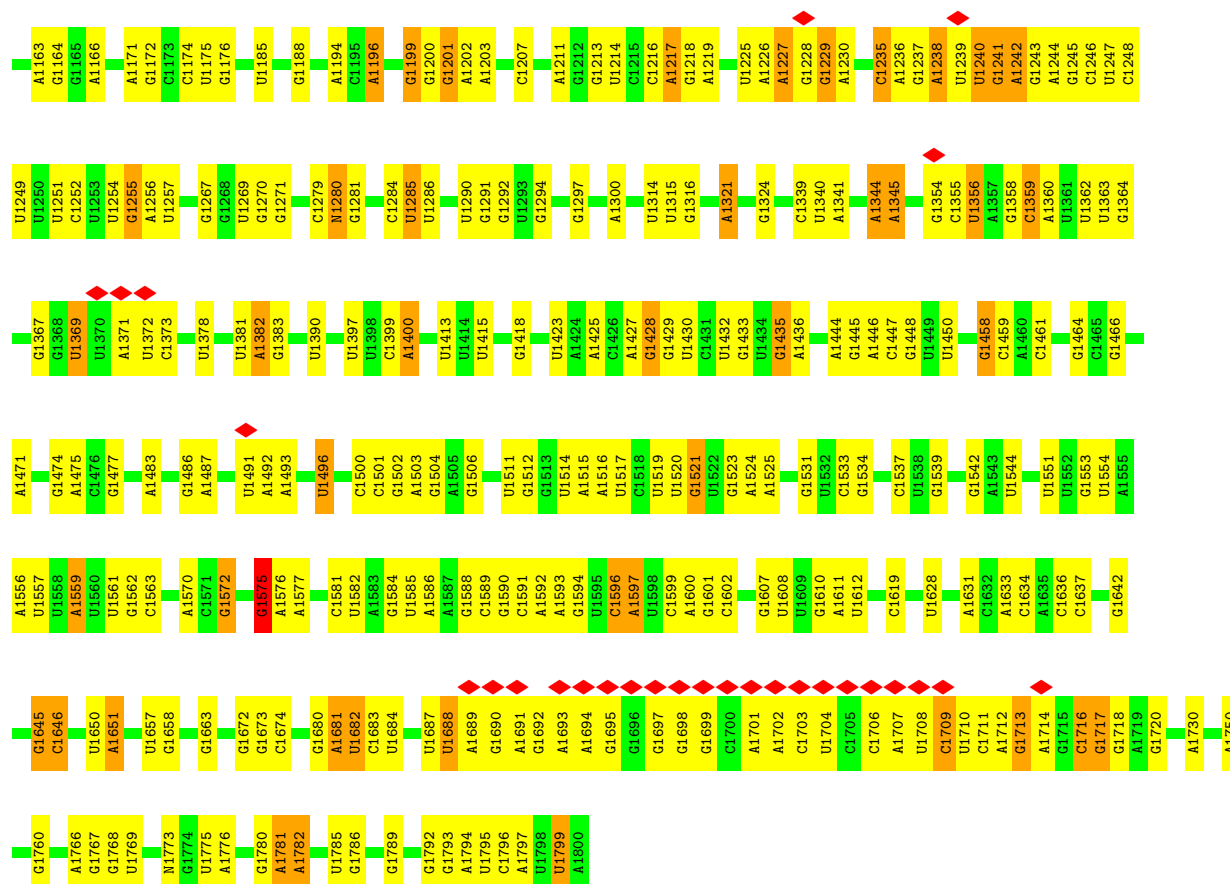


- Molecule 78: Suppressor protein STM1



• Molecule 79: 18S RIBOSOMAL RNA





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 178990                                  | Depositor |
| Resolution determination method      | OTHER                                   | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 61                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.233                                   | Depositor |
| Minimum map value                    | -0.020                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.008                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size (Å)                         | 455.75998, 455.75998, 455.75998         | wwPDB     |
| Map dimensions                       | 432, 432, 432                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.055, 1.055, 1.055                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3HE, 3AU, 1MA, OMC, MG, ZN, G7M, A2M, MA6, UR3, 5MC, 4AC, OMU, OMG, HIC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 1   | A1    | 0.51         | 0/74562     | 0.46        | 10/116239 (0.0%) |
| 2   | A3    | 0.43         | 0/2883      | 0.38        | 0/4491           |
| 3   | A4    | 0.54         | 0/3745      | 0.49        | 1/5828 (0.0%)    |
| 4   | AA    | 0.49         | 0/1912      | 0.59        | 0/2569           |
| 5   | AB    | 0.54         | 0/3137      | 0.66        | 4/4215 (0.1%)    |
| 6   | AC    | 0.49         | 0/2800      | 0.69        | 1/3790 (0.0%)    |
| 7   | AD    | 0.37         | 0/2390      | 0.62        | 0/3225           |
| 8   | AE    | 0.45         | 0/1260      | 0.58        | 0/1694           |
| 9   | AF    | 0.49         | 0/1821      | 0.70        | 3/2451 (0.1%)    |
| 10  | AG    | 0.44         | 0/1830      | 0.66        | 1/2469 (0.0%)    |
| 11  | AH    | 0.45         | 0/1531      | 0.61        | 0/2062           |
| 12  | AI    | 0.35         | 0/1708      | 0.55        | 0/2290           |
| 13  | AJ    | 0.33         | 0/1374      | 0.70        | 0/1842           |
| 14  | AL    | 0.49         | 0/1568      | 0.73        | 1/2106 (0.0%)    |
| 15  | AM    | 0.49         | 0/1068      | 0.60        | 0/1438           |
| 16  | AN    | 0.56         | 0/1757      | 0.71        | 0/2354           |
| 17  | AO    | 0.50         | 0/1585      | 0.59        | 0/2128           |
| 18  | AP    | 0.49         | 0/1410      | 0.58        | 0/1893           |
| 19  | AQ    | 0.47         | 0/1465      | 0.61        | 1/1965 (0.1%)    |
| 20  | AR    | 0.42         | 0/1538      | 0.61        | 0/2050           |
| 21  | AS    | 0.54         | 0/1481      | 0.67        | 0/1990           |
| 22  | AT    | 0.46         | 0/1300      | 0.66        | 0/1743           |
| 23  | AU    | 0.39         | 0/812       | 0.69        | 2/1099 (0.2%)    |
| 24  | AV    | 0.48         | 0/1018      | 0.58        | 0/1369           |
| 25  | AW    | 0.46         | 0/533       | 0.62        | 0/707            |
| 26  | AX    | 0.49         | 0/983       | 0.59        | 0/1325           |
| 27  | AY    | 0.49         | 0/1004      | 0.63        | 0/1341           |
| 28  | AZ    | 0.44         | 0/1118      | 0.71        | 2/1497 (0.1%)    |
| 29  | Aa    | 0.51         | 0/1204      | 0.79        | 3/1612 (0.2%)    |
| 30  | Ab    | 0.36         | 0/473       | 0.64        | 0/629            |
| 31  | Ac    | 0.40         | 0/751       | 0.57        | 0/1008           |
| 32  | Ad    | 0.49         | 0/904       | 0.56        | 0/1213           |



| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 33  | Ae    | 0.49         | 0/1041  | 0.55        | 0/1394        |
| 34  | Af    | 0.54         | 0/868   | 0.51        | 0/1168        |
| 35  | Ag    | 0.53         | 0/890   | 0.68        | 0/1189        |
| 36  | Ah    | 0.44         | 0/978   | 0.61        | 0/1301        |
| 37  | Ai    | 0.44         | 0/778   | 0.72        | 0/1034        |
| 38  | Aj    | 0.55         | 0/696   | 0.62        | 0/923         |
| 39  | Ak    | 0.48         | 0/618   | 0.60        | 0/826         |
| 40  | Al    | 0.55         | 0/443   | 0.71        | 0/588         |
| 41  | Am    | 0.46         | 0/423   | 0.55        | 0/562         |
| 42  | An    | 0.30         | 0/234   | 0.62        | 0/300         |
| 43  | Ao    | 0.39         | 0/860   | 0.61        | 0/1136        |
| 44  | Ap    | 0.44         | 0/701   | 0.71        | 0/934         |
| 45  | BA    | 0.37         | 0/1653  | 0.58        | 0/2261        |
| 46  | BB    | 0.40         | 0/1735  | 0.80        | 4/2335 (0.2%) |
| 47  | BC    | 0.42         | 0/1665  | 0.69        | 3/2263 (0.1%) |
| 48  | BD    | 0.36         | 0/1759  | 0.62        | 0/2368        |
| 49  | BE    | 0.42         | 0/2109  | 0.64        | 0/2839        |
| 50  | BF    | 0.37         | 0/1629  | 0.67        | 0/2202        |
| 51  | BG    | 0.36         | 0/1844  | 0.67        | 3/2464 (0.1%) |
| 52  | BH    | 0.36         | 0/1506  | 0.70        | 0/2028        |
| 53  | BI    | 0.41         | 0/1514  | 0.69        | 0/2021        |
| 54  | BJ    | 0.40         | 0/1519  | 0.69        | 0/2035        |
| 55  | BK    | 0.40         | 0/837   | 0.82        | 1/1131 (0.1%) |
| 56  | BL    | 0.38         | 0/1272  | 0.53        | 0/1712        |
| 57  | BM    | 0.26         | 0/921   | 0.75        | 1/1245 (0.1%) |
| 58  | BN    | 0.41         | 0/1215  | 0.72        | 1/1638 (0.1%) |
| 59  | BO    | 0.39         | 0/952   | 0.77        | 0/1279        |
| 60  | BP    | 0.41         | 0/1012  | 0.78        | 4/1356 (0.3%) |
| 61  | BQ    | 0.40         | 0/1125  | 0.65        | 1/1510 (0.1%) |
| 62  | BR    | 0.31         | 0/984   | 0.68        | 0/1318        |
| 63  | BS    | 0.41         | 0/1211  | 0.71        | 0/1628        |
| 64  | BT    | 0.44         | 0/1113  | 0.78        | 3/1494 (0.2%) |
| 65  | BU    | 0.37         | 0/865   | 0.63        | 0/1169        |
| 66  | BV    | 0.40         | 0/692   | 0.58        | 0/932         |
| 67  | BW    | 0.48         | 0/1038  | 0.68        | 1/1395 (0.1%) |
| 68  | BX    | 0.44         | 0/1139  | 0.79        | 2/1518 (0.1%) |
| 69  | BY    | 0.39         | 0/1087  | 0.71        | 0/1449        |
| 70  | BZ    | 0.35         | 0/566   | 0.70        | 0/761         |
| 71  | Ba    | 0.44         | 0/782   | 0.86        | 2/1047 (0.2%) |
| 72  | Bb    | 0.36         | 0/620   | 0.62        | 0/838         |
| 73  | Bc    | 0.35         | 0/499   | 0.65        | 0/670         |
| 74  | Bd    | 0.42         | 0/452   | 0.66        | 0/600         |
| 75  | Be    | 0.34         | 0/483   | 0.55        | 0/643         |

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 76  | Bf    | 0.30         | 0/462       | 0.70        | 0/617            |
| 77  | Bg    | 0.36         | 0/2454      | 0.63        | 0/3340           |
| 78  | Bh    | 0.26         | 0/678       | 0.65        | 0/905            |
| 79  | B5    | 0.41         | 0/41746     | 0.44        | 1/65032 (0.0%)   |
| All | All   | 0.46         | 0/212593    | 0.54        | 56/312030 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | AC    | 0                   | 2                   |
| 7   | AD    | 0                   | 1                   |
| 8   | AE    | 0                   | 1                   |
| 9   | AF    | 0                   | 3                   |
| 10  | AG    | 0                   | 4                   |
| 13  | AJ    | 0                   | 2                   |
| 14  | AL    | 0                   | 2                   |
| 16  | AN    | 0                   | 1                   |
| 17  | AO    | 0                   | 1                   |
| 20  | AR    | 0                   | 1                   |
| 21  | AS    | 0                   | 1                   |
| 22  | AT    | 0                   | 1                   |
| 28  | AZ    | 0                   | 1                   |
| 36  | Ah    | 0                   | 1                   |
| 37  | Ai    | 0                   | 1                   |
| 45  | BA    | 0                   | 1                   |
| 46  | BB    | 0                   | 4                   |
| 47  | BC    | 0                   | 1                   |
| 50  | BF    | 0                   | 2                   |
| 51  | BG    | 0                   | 1                   |
| 52  | BH    | 0                   | 3                   |
| 53  | BI    | 0                   | 2                   |
| 54  | BJ    | 0                   | 2                   |
| 59  | BO    | 0                   | 1                   |
| 60  | BP    | 0                   | 4                   |
| 61  | BQ    | 0                   | 3                   |
| 63  | BS    | 0                   | 3                   |
| 67  | BW    | 0                   | 1                   |
| 68  | BX    | 0                   | 5                   |
| 71  | Ba    | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 76  | Bf    | 0                   | 1                   |
| 78  | Bh    | 0                   | 1                   |
| 79  | B5    | 4                   | 0                   |
| All | All   | 4                   | 61                  |

There are no bond length outliers.

All (56) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | A1    | 266  | A    | OP1-P-OP2 | -14.25 | 76.86       | 119.60   |
| 1   | A1    | 266  | A    | O5'-P-OP1 | -10.95 | 75.14       | 108.00   |
| 1   | A1    | 265  | A    | OP2-P-O3' | -10.59 | 76.24       | 108.00   |
| 1   | A1    | 1947 | G    | OP2-P-O3' | -9.65  | 79.06       | 108.00   |
| 1   | A1    | 265  | A    | OP1-P-O3' | 8.62   | 133.87      | 108.00   |
| 1   | A1    | 266  | A    | O5'-P-OP2 | 8.27   | 132.82      | 108.00   |
| 57  | BM    | 44   | GLY  | N-CA-C    | 7.85   | 122.61      | 111.00   |
| 51  | BG    | 67   | VAL  | CA-C-N    | 7.69   | 136.24      | 121.54   |
| 51  | BG    | 67   | VAL  | C-N-CA    | 7.69   | 136.24      | 121.54   |
| 9   | AF    | 157  | ASN  | CA-C-N    | 7.65   | 136.15      | 121.54   |
| 9   | AF    | 157  | ASN  | C-N-CA    | 7.65   | 136.15      | 121.54   |
| 29  | Aa    | 47   | LYS  | CA-C-N    | 7.46   | 135.78      | 121.54   |
| 29  | Aa    | 47   | LYS  | C-N-CA    | 7.46   | 135.78      | 121.54   |
| 71  | Ba    | 35   | ALA  | CA-C-N    | 7.32   | 135.15      | 121.97   |
| 71  | Ba    | 35   | ALA  | C-N-CA    | 7.32   | 135.15      | 121.97   |
| 46  | BB    | 147  | ALA  | CA-C-N    | 6.97   | 134.86      | 121.54   |
| 46  | BB    | 147  | ALA  | C-N-CA    | 6.97   | 134.86      | 121.54   |
| 1   | A1    | 1947 | G    | OP1-P-O3' | -6.70  | 87.90       | 108.00   |
| 1   | A1    | 1948 | G    | OP1-P-OP2 | 6.70   | 139.70      | 119.60   |
| 55  | BK    | 86   | ILE  | N-CA-C    | -6.70  | 107.35      | 113.71   |
| 46  | BB    | 212  | VAL  | CA-C-N    | 6.56   | 134.08      | 121.54   |
| 46  | BB    | 212  | VAL  | C-N-CA    | 6.56   | 134.08      | 121.54   |
| 47  | BC    | 146  | THR  | N-CA-C    | -6.52  | 97.70       | 108.07   |
| 58  | BN    | 132  | VAL  | N-CA-C    | -6.50  | 106.18      | 112.29   |
| 23  | AU    | 49   | ASN  | CA-CB-CG  | 6.22   | 118.82      | 112.60   |
| 64  | BT    | 7    | ARG  | N-CA-C    | -6.21  | 106.93      | 114.75   |
| 29  | Aa    | 56   | VAL  | N-CA-C    | -6.15  | 96.55       | 109.34   |
| 28  | AZ    | 102  | GLU  | CA-C-N    | -5.99  | 112.71      | 122.65   |
| 28  | AZ    | 102  | GLU  | C-N-CA    | -5.99  | 112.71      | 122.65   |
| 68  | BX    | 96   | VAL  | CA-C-N    | 5.87   | 132.76      | 121.54   |
| 68  | BX    | 96   | VAL  | C-N-CA    | 5.87   | 132.76      | 121.54   |
| 14  | AL    | 48   | PRO  | N-CA-C    | 5.86   | 124.54      | 112.47   |
| 9   | AF    | 159  | GLN  | N-CA-C    | 5.86   | 123.27      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 67  | BW    | 115  | GLU  | CA-CB-CG    | 5.83  | 125.77      | 114.10   |
| 1   | A1    | 1385 | C    | C2'-C3'-O3' | 5.79  | 122.39      | 113.70   |
| 10  | AG    | 79   | GLN  | CA-CB-CG    | 5.63  | 125.36      | 114.10   |
| 19  | AQ    | 180  | ARG  | CA-CB-CG    | 5.57  | 125.24      | 114.10   |
| 5   | AB    | 138  | ALA  | CA-C-N      | 5.55  | 132.14      | 121.54   |
| 5   | AB    | 138  | ALA  | C-N-CA      | 5.55  | 132.14      | 121.54   |
| 60  | BP    | 106  | GLU  | CA-CB-CG    | 5.48  | 125.06      | 114.10   |
| 5   | AB    | 4    | ARG  | CA-C-N      | 5.48  | 132.00      | 121.54   |
| 5   | AB    | 4    | ARG  | C-N-CA      | 5.48  | 132.00      | 121.54   |
| 60  | BP    | 28   | MET  | CA-C-N      | 5.45  | 131.94      | 121.54   |
| 60  | BP    | 28   | MET  | C-N-CA      | 5.45  | 131.94      | 121.54   |
| 64  | BT    | 52   | GLY  | CA-C-N      | 5.38  | 131.82      | 121.54   |
| 64  | BT    | 52   | GLY  | C-N-CA      | 5.38  | 131.82      | 121.54   |
| 3   | A4    | 67   | U    | C2'-C3'-O3' | 5.28  | 121.61      | 113.70   |
| 79  | B5    | 1285 | U    | P-O3'-C3'   | 5.27  | 128.10      | 120.20   |
| 60  | BP    | 30   | THR  | N-CA-C      | 5.23  | 119.13      | 112.34   |
| 47  | BC    | 145  | GLY  | CA-C-N      | 5.22  | 134.21      | 122.19   |
| 47  | BC    | 145  | GLY  | C-N-CA      | 5.22  | 134.21      | 122.19   |
| 23  | AU    | 49   | ASN  | CB-CA-C     | 5.07  | 118.91      | 111.06   |
| 61  | BQ    | 38   | LEU  | CA-CB-CG    | 5.03  | 133.91      | 116.30   |
| 51  | BG    | 68   | LEU  | N-CA-C      | -5.03 | 100.09      | 110.80   |
| 6   | AC    | 182  | LEU  | CA-CB-CG    | 5.02  | 133.87      | 116.30   |
| 1   | A1    | 406  | G    | O4'-C1'-N9  | 5.01  | 115.71      | 108.20   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom        |
|-----|-------|------|------|-------------|
| 79  | B5    | 1191 | 3AU  | C12         |
| 79  | B5    | 1575 | G7M  | C2',C4',C3' |

All (61) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 6   | AC    | 131 | VAL  | Peptide |
| 6   | AC    | 318 | LEU  | Peptide |
| 7   | AD    | 43  | LYS  | Peptide |
| 8   | AE    | 67  | GLY  | Peptide |
| 9   | AF    | 158 | LYS  | Peptide |
| 9   | AF    | 215 | GLY  | Peptide |
| 9   | AF    | 232 | ARG  | Peptide |
| 10  | AG    | 30  | THR  | Peptide |
| 10  | AG    | 74  | THR  | Peptide |

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| Mol | Chain | Res    | Type | Group   |
|-----|-------|--------|------|---------|
| 10  | AG    | 76     | ALA  | Peptide |
| 10  | AG    | 79     | GLN  | Peptide |
| 13  | AJ    | 109    | HIS  | Peptide |
| 13  | AJ    | 166    | LYS  | Peptide |
| 14  | AL    | 47     | ALA  | Peptide |
| 14  | AL    | 75     | PHE  | Peptide |
| 16  | AN    | 80     | THR  | Peptide |
| 17  | AO    | 110[A] | PRO  | Peptide |
| 20  | AR    | 131    | ALA  | Peptide |
| 21  | AS    | 22     | PRO  | Peptide |
| 22  | AT    | 17     | ARG  | Peptide |
| 28  | AZ    | 123    | GLN  | Peptide |
| 36  | Ah    | 90     | ARG  | Peptide |
| 37  | Ai    | 27     | SER  | Peptide |
| 45  | BA    | 94     | GLY  | Peptide |
| 46  | BB    | 177    | GLN  | Peptide |
| 46  | BB    | 205    | PHE  | Peptide |
| 46  | BB    | 206    | PRO  | Peptide |
| 46  | BB    | 208    | GLN  | Peptide |
| 47  | BC    | 148    | LEU  | Peptide |
| 50  | BF    | 42     | LEU  | Peptide |
| 50  | BF    | 43     | PHE  | Peptide |
| 51  | BG    | 68     | LEU  | Peptide |
| 52  | BH    | 110    | GLN  | Peptide |
| 52  | BH    | 64     | VAL  | Peptide |
| 52  | BH    | 65     | PRO  | Peptide |
| 53  | BI    | 51     | GLY  | Peptide |
| 53  | BI    | 8      | ARG  | Peptide |
| 54  | BJ    | 117    | GLY  | Peptide |
| 54  | BJ    | 133    | HIS  | Peptide |
| 59  | BO    | 123    | SER  | Peptide |
| 60  | BP    | 106    | GLU  | Peptide |
| 60  | BP    | 124    | THR  | Peptide |
| 60  | BP    | 125    | PRO  | Peptide |
| 60  | BP    | 29     | SER  | Peptide |
| 61  | BQ    | 32     | ASN  | Peptide |
| 61  | BQ    | 33     | GLY  | Peptide |
| 61  | BQ    | 40     | GLU  | Peptide |
| 63  | BS    | 56     | LYS  | Peptide |
| 63  | BS    | 81     | ILE  | Peptide |
| 63  | BS    | 90     | ASN  | Peptide |
| 67  | BW    | 115    | GLU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 68  | BX    | 137 | LYS  | Peptide |
| 68  | BX    | 138 | GLU  | Peptide |
| 68  | BX    | 41  | SER  | Peptide |
| 68  | BX    | 87  | VAL  | Peptide |
| 68  | BX    | 97  | ASP  | Peptide |
| 71  | Ba    | 34  | LYS  | Peptide |
| 71  | Ba    | 35  | ALA  | Peptide |
| 71  | Ba    | 7   | SER  | Peptide |
| 76  | Bf    | 105 | TYR  | Peptide |
| 78  | Bh    | 85  | SER  | 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   | A1    | 67535 | 0        | 33991    | 368     | 0            |
| 2   | A3    | 2579  | 0        | 1303     | 11      | 0            |
| 3   | A4    | 3353  | 0        | 1695     | 19      | 0            |
| 4   | AA    | 1878  | 0        | 1946     | 40      | 0            |
| 5   | AB    | 3079  | 0        | 3154     | 51      | 0            |
| 6   | AC    | 2748  | 0        | 2859     | 34      | 0            |
| 7   | AD    | 2341  | 0        | 2290     | 23      | 0            |
| 8   | AE    | 1239  | 0        | 1326     | 10      | 0            |
| 9   | AF    | 1784  | 0        | 1862     | 25      | 0            |
| 10  | AG    | 1798  | 0        | 1894     | 16      | 0            |
| 11  | AH    | 1510  | 0        | 1576     | 17      | 0            |
| 12  | AI    | 1672  | 0        | 1711     | 27      | 0            |
| 13  | AJ    | 1353  | 0        | 1383     | 18      | 0            |
| 14  | AL    | 1543  | 0        | 1608     | 23      | 0            |
| 15  | AM    | 1053  | 0        | 1149     | 6       | 0            |
| 16  | AN    | 1720  | 0        | 1779     | 35      | 0            |
| 17  | AO    | 1555  | 0        | 1659     | 19      | 0            |
| 18  | AP    | 1388  | 0        | 1423     | 13      | 0            |
| 19  | AQ    | 1441  | 0        | 1543     | 12      | 0            |
| 20  | AR    | 1521  | 0        | 1617     | 16      | 0            |
| 21  | AS    | 1445  | 0        | 1487     | 17      | 0            |
| 22  | AT    | 1276  | 0        | 1323     | 26      | 0            |
| 23  | AU    | 796   | 0        | 812      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | AV    | 1003  | 0        | 1048     | 10      | 0            |
| 25  | AW    | 521   | 0        | 551      | 4       | 0            |
| 26  | AX    | 968   | 0        | 1036     | 7       | 0            |
| 27  | AY    | 993   | 0        | 1081     | 14      | 0            |
| 28  | AZ    | 1092  | 0        | 1155     | 14      | 0            |
| 29  | Aa    | 1173  | 0        | 1215     | 26      | 0            |
| 30  | Ab    | 462   | 0        | 491      | 3       | 0            |
| 31  | Ac    | 743   | 0        | 797      | 12      | 0            |
| 32  | Ad    | 890   | 0        | 938      | 7       | 0            |
| 33  | Ae    | 1020  | 0        | 1090     | 6       | 0            |
| 34  | Af    | 850   | 0        | 880      | 9       | 0            |
| 35  | Ag    | 880   | 0        | 945      | 11      | 0            |
| 36  | Ah    | 969   | 0        | 1078     | 9       | 0            |
| 37  | Ai    | 771   | 0        | 849      | 5       | 0            |
| 38  | Aj    | 681   | 0        | 687      | 9       | 0            |
| 39  | Ak    | 612   | 0        | 682      | 10      | 0            |
| 40  | Al    | 436   | 0        | 475      | 3       | 0            |
| 41  | Am    | 417   | 0        | 459      | 12      | 0            |
| 42  | An    | 233   | 0        | 284      | 1       | 0            |
| 43  | Ao    | 847   | 0        | 914      | 9       | 0            |
| 44  | Ap    | 694   | 0        | 738      | 14      | 0            |
| 45  | BA    | 1612  | 0        | 1623     | 27      | 0            |
| 46  | BB    | 1709  | 0        | 1784     | 29      | 0            |
| 47  | BC    | 1635  | 0        | 1723     | 21      | 0            |
| 48  | BD    | 1734  | 0        | 1817     | 25      | 0            |
| 49  | BE    | 2068  | 0        | 2154     | 30      | 0            |
| 50  | BF    | 1609  | 0        | 1675     | 18      | 0            |
| 51  | BG    | 1820  | 0        | 1918     | 31      | 0            |
| 52  | BH    | 1481  | 0        | 1572     | 24      | 0            |
| 53  | BI    | 1489  | 0        | 1525     | 33      | 0            |
| 54  | BJ    | 1494  | 0        | 1573     | 19      | 0            |
| 55  | BK    | 817   | 0        | 804      | 15      | 0            |
| 56  | BL    | 1244  | 0        | 1314     | 8       | 0            |
| 57  | BM    | 913   | 0        | 955      | 22      | 0            |
| 58  | BN    | 1192  | 0        | 1255     | 19      | 0            |
| 59  | BO    | 941   | 0        | 979      | 13      | 0            |
| 60  | BP    | 991   | 0        | 1035     | 13      | 0            |
| 61  | BQ    | 1105  | 0        | 1166     | 20      | 0            |
| 62  | BR    | 975   | 0        | 1039     | 11      | 0            |
| 63  | BS    | 1192  | 0        | 1222     | 22      | 0            |
| 64  | BT    | 1095  | 0        | 1114     | 28      | 0            |
| 65  | BU    | 855   | 0        | 917      | 19      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 66  | BV    | 684    | 0        | 671      | 10      | 0            |
| 67  | BW    | 1021   | 0        | 1060     | 19      | 0            |
| 68  | BX    | 1121   | 0        | 1196     | 18      | 0            |
| 69  | BY    | 1073   | 0        | 1132     | 19      | 0            |
| 70  | BZ    | 558    | 0        | 598      | 6       | 0            |
| 71  | Ba    | 769    | 0        | 818      | 18      | 0            |
| 72  | Bb    | 610    | 0        | 630      | 10      | 0            |
| 73  | Bc    | 497    | 0        | 535      | 9       | 0            |
| 74  | Bd    | 442    | 0        | 432      | 13      | 0            |
| 75  | Be    | 475    | 0        | 525      | 5       | 0            |
| 76  | Bf    | 454    | 0        | 468      | 5       | 0            |
| 77  | Bg    | 2401   | 0        | 2356     | 41      | 0            |
| 78  | Bh    | 675    | 0        | 654      | 10      | 0            |
| 79  | B5    | 37891  | 0        | 19102    | 265     | 0            |
| 80  | A1    | 20     | 0        | 23       | 0       | 0            |
| 81  | A1    | 247    | 0        | 0        | 0       | 0            |
| 81  | A3    | 5      | 0        | 0        | 0       | 0            |
| 81  | A4    | 9      | 0        | 0        | 0       | 0            |
| 81  | AB    | 4      | 0        | 0        | 0       | 0            |
| 81  | AC    | 1      | 0        | 0        | 0       | 0            |
| 81  | AG    | 1      | 0        | 0        | 0       | 0            |
| 81  | AL    | 3      | 0        | 0        | 0       | 0            |
| 81  | AN    | 1      | 0        | 0        | 0       | 0            |
| 81  | AO    | 1      | 0        | 0        | 0       | 0            |
| 81  | AP    | 1      | 0        | 0        | 0       | 0            |
| 81  | AR    | 1      | 0        | 0        | 0       | 0            |
| 81  | AV    | 1      | 0        | 0        | 0       | 0            |
| 81  | Aa    | 1      | 0        | 0        | 0       | 0            |
| 81  | Ae    | 2      | 0        | 0        | 0       | 0            |
| 81  | Af    | 1      | 0        | 0        | 0       | 0            |
| 81  | Aj    | 1      | 0        | 0        | 0       | 0            |
| 81  | B5    | 90     | 0        | 0        | 0       | 0            |
| 81  | BE    | 1      | 0        | 0        | 0       | 0            |
| 81  | BG    | 1      | 0        | 0        | 0       | 0            |
| 81  | BJ    | 1      | 0        | 0        | 0       | 0            |
| 81  | Ba    | 1      | 0        | 0        | 0       | 0            |
| 82  | Ao    | 1      | 0        | 0        | 0       | 0            |
| 82  | Bb    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 199900 | 0        | 148147   | 1521    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.



All (1521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:A1:3348:G:H1     | 1:A1:3357:U:H3       | 1.04                     | 0.99              |
| 79:B5:1356:U:H3    | 79:B5:1367:G:H1      | 0.96                     | 0.95              |
| 79:B5:868:G:H1     | 79:B5:960:U:H3       | 1.15                     | 0.88              |
| 79:B5:1588:G:H1    | 79:B5:1608:U:H3      | 1.24                     | 0.86              |
| 79:B5:976:G:H1     | 79:B5:1023:A:HO2'    | 1.24                     | 0.85              |
| 16:AN:16:SER:O     | 16:AN:20:ARG:HB2     | 1.79                     | 0.81              |
| 2:A3:52:G:H21      | 13:AJ:9:MET:HE3      | 1.50                     | 0.76              |
| 28:AZ:88:ASP:HB3   | 28:AZ:121:ARG:HH12   | 1.54                     | 0.73              |
| 79:B5:1213:G:H1    | 79:B5:1450:U:H3      | 1.37                     | 0.72              |
| 63:BS:48:LYS:HD3   | 64:BT:35:ASP:HB3     | 1.72                     | 0.70              |
| 79:B5:895:G:H1     | 79:B5:917:U:H3       | 1.38                     | 0.70              |
| 72:Bb:56:CYS:HB2   | 72:Bb:59:CYS:H       | 1.56                     | 0.68              |
| 1:A1:2392:C:O2'    | 5:AB:266:ARG:NH2     | 2.27                     | 0.68              |
| 49:BE:87:MET:HE1   | 49:BE:236:ILE:HD13   | 1.76                     | 0.68              |
| 62:BR:24:LEU:HB3   | 62:BR:34:LEU:HD11    | 1.76                     | 0.67              |
| 70:BZ:95:HIS:ND1   | 70:BZ:96:SER:O       | 2.26                     | 0.67              |
| 1:A1:2987:A:H5''   | 17:AO:68[A]:ARG:HH12 | 1.60                     | 0.67              |
| 32:Ad:51:LEU:HB3   | 32:Ad:55:LEU:HD23    | 1.77                     | 0.66              |
| 1:A1:1213:G:H4'    | 21:AS:90:MET:HG2     | 1.77                     | 0.66              |
| 24:AV:104:ASN:HD21 | 24:AV:108:GLU:HB2    | 1.60                     | 0.66              |
| 39:Ak:5:ILE:HG22   | 39:Ak:7:ASP:H        | 1.58                     | 0.66              |
| 1:A1:1766:G:N7     | 20:AR:46:LYS:NZ      | 2.43                     | 0.66              |
| 1:A1:2721:A:H5''   | 30:Ab:33:LYS:HE2     | 1.76                     | 0.66              |
| 50:BF:166:ARG:HH12 | 73:Bc:45:LYS:HE3     | 1.59                     | 0.65              |
| 59:BO:16:VAL:O     | 59:BO:30:VAL:HA      | 1.97                     | 0.65              |
| 4:AA:27:ALA:O      | 4:AA:128:ARG:NH2     | 2.29                     | 0.65              |
| 1:A1:687:U:OP2     | 14:AL:36:ARG:NH2     | 2.30                     | 0.65              |
| 79:B5:737:A:C2     | 79:B5:738:G:O6       | 2.50                     | 0.65              |
| 5:AB:10:ARG:NH1    | 5:AB:11:HIS:O        | 2.30                     | 0.64              |
| 52:BH:70:PHE:O     | 52:BH:74:GLN:HB2     | 1.97                     | 0.64              |
| 79:B5:513:U:H3     | 79:B5:538:A:H2       | 1.44                     | 0.64              |
| 1:A1:860:G:OP1     | 44:Ap:17:ARG:NH1     | 2.29                     | 0.64              |
| 47:BC:38:VAL:HG13  | 47:BC:39:THR:HG23    | 1.80                     | 0.64              |
| 65:BU:82:TYR:HB3   | 74:Bd:52:PHE:HB3     | 1.79                     | 0.64              |
| 7:AD:50:ARG:NH2    | 7:AD:72:ASP:OD2      | 2.31                     | 0.64              |
| 1:A1:1682:U:O4     | 23:AU:90:ARG:NH1     | 2.31                     | 0.64              |
| 50:BF:63:GLN:HE22  | 50:BF:66:GLN:HG2     | 1.63                     | 0.64              |
| 1:A1:1097:G:N7     | 22:AT:116:ARG:NH2    | 2.45                     | 0.63              |
| 57:BM:47:GLU:HB2   | 79:B5:1229:G:H1      | 1.62                     | 0.63              |
| 67:BW:15:ASN:ND2   | 67:BW:72:CYS:O       | 2.32                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A1:912:G:OP2     | 4:AA:9:ARG:NH1      | 2.32                     | 0.63              |
| 9:AF:87:VAL:HG11   | 9:AF:243:MET:HE1    | 1.80                     | 0.63              |
| 77:Bg:216:LYS:HA   | 77:Bg:239:GLU:HG3   | 1.79                     | 0.63              |
| 1:A1:1575:A:O2'    | 1:A1:1576:G:N3      | 2.32                     | 0.63              |
| 46:BB:132:ASP:HB3  | 46:BB:221:PRO:HB3   | 1.80                     | 0.63              |
| 67:BW:31:SER:H     | 67:BW:34:ILE:HD12   | 1.64                     | 0.62              |
| 68:BX:96:VAL:O     | 68:BX:142:LYS:NZ    | 2.30                     | 0.62              |
| 71:Ba:46:GLU:HB3   | 71:Ba:49:ALA:H      | 1.64                     | 0.62              |
| 63:BS:135:GLY:HA3  | 79:B5:1559:A:H5''   | 1.81                     | 0.62              |
| 16:AN:183:THR:HG22 | 16:AN:187:ARG:HB3   | 1.80                     | 0.62              |
| 44:Ap:46:THR:OG1   | 44:Ap:57:CYS:SG     | 2.57                     | 0.62              |
| 1:A1:3045:G:OP1    | 5:AB:19:ARG:NH2     | 2.33                     | 0.62              |
| 72:Bb:48:SER:HG    | 72:Bb:49:HIS:HD1    | 1.48                     | 0.62              |
| 5:AB:10:ARG:NH2    | 5:AB:263:SER:O      | 2.33                     | 0.62              |
| 16:AN:155:VAL:O    | 16:AN:162:ARG:NH2   | 2.32                     | 0.62              |
| 1:A1:299:G:HO2'    | 1:A1:300:G:H8       | 1.48                     | 0.62              |
| 1:A1:1639:C:OP2    | 35:Ag:74:ARG:NH2    | 2.31                     | 0.62              |
| 9:AF:163:LEU:HA    | 9:AF:168:ILE:HD11   | 1.81                     | 0.61              |
| 64:BT:38:LYS:O     | 64:BT:43:ASN:ND2    | 2.33                     | 0.61              |
| 21:AS:112:ALA:O    | 21:AS:115:ARG:NH1   | 2.33                     | 0.61              |
| 36:Ah:85:THR:HB    | 36:Ah:88:LEU:HB2    | 1.82                     | 0.61              |
| 61:BQ:39:VAL:HG21  | 61:BQ:48:VAL:HG21   | 1.82                     | 0.61              |
| 67:BW:2:THR:N      | 79:B5:1034:C:HO2'   | 1.98                     | 0.61              |
| 4:AA:101:VAL:HG22  | 4:AA:165:VAL:HG22   | 1.82                     | 0.61              |
| 26:AX:103:TYR:O    | 26:AX:138:ARG:NH1   | 2.34                     | 0.61              |
| 41:Am:104:PRO:HG2  | 41:Am:107:ALA:HB2   | 1.83                     | 0.61              |
| 50:BF:225:ARG:NH1  | 73:Bc:58:GLU:OE2    | 2.34                     | 0.61              |
| 66:BV:40:ASP:HB3   | 66:BV:46:ILE:HD11   | 1.81                     | 0.61              |
| 1:A1:1317:A:O2'    | 17:AO:18[A]:ARG:NH2 | 2.34                     | 0.61              |
| 4:AA:117:GLU:HG2   | 4:AA:124:GLY:H      | 1.66                     | 0.61              |
| 6:AC:136:LEU:HD11  | 6:AC:143:GLU:HG3    | 1.83                     | 0.61              |
| 50:BF:72:HIS:NE2   | 79:B5:1610:G:OP1    | 2.28                     | 0.60              |
| 53:BI:98:LYS:HB3   | 79:B5:329:G:H5''    | 1.83                     | 0.60              |
| 77:Bg:81:LEU:HD11  | 77:Bg:122:ILE:HD12  | 1.83                     | 0.60              |
| 1:A1:676:G:HO2'    | 1:A1:678:G:HO2'     | 1.46                     | 0.60              |
| 1:A1:1348:U:OP1    | 19:AQ:39:ARG:NH1    | 2.35                     | 0.60              |
| 5:AB:37:ARG:HD3    | 5:AB:186:GLY:HA2    | 1.83                     | 0.60              |
| 31:Ac:13:LYS:HB3   | 31:Ac:100:ILE:HG22  | 1.84                     | 0.60              |
| 57:BM:62:LEU:HD22  | 57:BM:76:GLU:HG2    | 1.83                     | 0.60              |
| 79:B5:1354:G:O6    | 79:B5:1369:U:O4     | 2.19                     | 0.60              |
| 12:AI:36:LEU:HD11  | 12:AI:69:ARG:HH11   | 1.66                     | 0.60              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:BI:172:ARG:HE   | 53:BI:175:GLN:HG3   | 1.65                     | 0.60              |
| 74:Bd:14:TYR:HH    | 79:B5:1553:G:HO2'   | 1.49                     | 0.60              |
| 1:A1:3034:C:H5     | 11:AH:121:LYS:H     | 1.49                     | 0.60              |
| 12:AI:76:MET:HE1   | 12:AI:138:VAL:HG21  | 1.83                     | 0.60              |
| 31:Ac:17:VAL:HG11  | 31:Ac:92:ILE:HD12   | 1.82                     | 0.60              |
| 20:AR:148:ASP:OD1  | 20:AR:151:ARG:NH1   | 2.34                     | 0.60              |
| 68:BX:70:LYS:NZ    | 79:B5:567:A:OP1     | 2.34                     | 0.60              |
| 1:A1:2878:G:H5''   | 5:AB:5:LYS:HE2      | 1.84                     | 0.60              |
| 68:BX:69:ARG:NH2   | 79:B5:568:G:N7      | 2.50                     | 0.60              |
| 69:BY:61:ARG:NH1   | 79:B5:530:C:O2      | 2.35                     | 0.60              |
| 3:A4:52:A:H62      | 40:Al:27:ILE:HD13   | 1.67                     | 0.60              |
| 23:AU:49:ASN:O     | 23:AU:49:ASN:ND2    | 2.35                     | 0.60              |
| 54:BJ:119:ALA:O    | 54:BJ:124:HIS:ND1   | 2.32                     | 0.60              |
| 61:BQ:129:PHE:O    | 61:BQ:137:ARG:NH2   | 2.35                     | 0.60              |
| 3:A4:71:A:O2'      | 27:AY:52:ARG:NH2    | 2.35                     | 0.60              |
| 5:AB:284:ARG:NH1   | 5:AB:293:ASN:O      | 2.35                     | 0.60              |
| 65:BU:72:ASN:ND2   | 79:B5:1429:G:N3     | 2.50                     | 0.60              |
| 78:Bh:93:ARG:HH22  | 79:B5:1636:C:H5''   | 1.65                     | 0.60              |
| 3:A4:150:G:OP1     | 26:AX:27:ARG:NH2    | 2.35                     | 0.59              |
| 1:A1:1385:C:OP1    | 6:AC:141:ARG:NH1    | 2.34                     | 0.59              |
| 51:BG:13:GLN:NE2   | 79:B5:151:G:N3      | 2.50                     | 0.59              |
| 6:AC:20:LEU:HD11   | 6:AC:252:GLU:HG3    | 1.85                     | 0.59              |
| 18:AP:118:GLN:NE2  | 18:AP:120:ASN:OD1   | 2.35                     | 0.59              |
| 66:BV:10:GLU:O     | 66:BV:12:TYR:N      | 2.35                     | 0.59              |
| 65:BU:95:ALA:HB1   | 65:BU:100:VAL:HG21  | 1.82                     | 0.59              |
| 1:A1:1390:A:N6     | 1:A1:1418:A:O2'     | 2.34                     | 0.59              |
| 16:AN:80:THR:HG22  | 16:AN:82:GLY:H      | 1.68                     | 0.59              |
| 74:Bd:43:PHE:O     | 74:Bd:47:ALA:HB2    | 2.02                     | 0.59              |
| 1:A1:2901:G:O2'    | 1:A1:3024:A:N1      | 2.33                     | 0.59              |
| 60:BP:18:ARG:NH1   | 63:BS:90:ASN:O      | 2.35                     | 0.59              |
| 6:AC:99:MET:HE3    | 6:AC:102:PRO:HA     | 1.83                     | 0.59              |
| 79:B5:1023:A:OP1   | 79:B5:1126:OMG:N2   | 2.35                     | 0.59              |
| 1:A1:2779:A:O2'    | 14:AL:180:ARG:NH2   | 2.36                     | 0.58              |
| 1:A1:2842:U:OP1    | 1:A1:2844:C:N4      | 2.33                     | 0.58              |
| 3:A4:51:G:OP2      | 40:Al:21:ARG:NH1    | 2.34                     | 0.58              |
| 54:BJ:139:GLN:NE2  | 69:BY:64:PHE:O      | 2.35                     | 0.58              |
| 71:Ba:84:VAL:O     | 79:B5:1797:A:N6     | 2.36                     | 0.58              |
| 17:AO:61[A]:ALA:HA | 17:AO:70[A]:PRO:HD2 | 1.84                     | 0.58              |
| 1:A1:1361:U:O2     | 9:AF:159:GLN:NE2    | 2.35                     | 0.58              |
| 1:A1:439:C:H1'     | 1:A1:494:G:H21      | 1.68                     | 0.58              |
| 29:Aa:104:THR:HG21 | 29:Aa:112:ILE:HD11  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:BG:57:ASP:HA   | 51:BG:106:LEU:HA  | 1.86                     | 0.58              |
| 79:B5:233:C:O2'   | 79:B5:234:G:N2    | 2.35                     | 0.58              |
| 79:B5:1354:G:O6   | 79:B5:1369:U:C4   | 2.56                     | 0.58              |
| 1:A1:2406:C:O2'   | 1:A1:2619:OMG:N2  | 2.36                     | 0.58              |
| 55:BK:40:LEU:O    | 55:BK:44:LYS:HB2  | 2.04                     | 0.58              |
| 45:BA:72:ASP:HB2  | 45:BA:118:PRO:HA  | 1.84                     | 0.58              |
| 1:A1:2848:G:OP1   | 41:Am:100:TYR:OH  | 2.22                     | 0.58              |
| 57:BM:44:GLY:HA2  | 79:B5:1227:A:H2   | 1.69                     | 0.58              |
| 1:A1:831:G:O2'    | 1:A1:1864:A:N3    | 2.32                     | 0.58              |
| 79:B5:979:A:N3    | 79:B5:1775:U:O2'  | 2.36                     | 0.58              |
| 79:B5:1291:G:H1   | 79:B5:1324:G:H22  | 1.50                     | 0.58              |
| 47:BC:199:GLN:NE2 | 79:B5:2:A:N3      | 2.52                     | 0.58              |
| 64:BT:102:ARG:NH2 | 79:B5:1502:G:N7   | 2.51                     | 0.58              |
| 79:B5:730:G:N2    | 79:B5:733:A:OP1   | 2.36                     | 0.58              |
| 1:A1:3297:U:O4    | 5:AB:124:LYS:NZ   | 2.36                     | 0.58              |
| 10:AG:81:THR:HG21 | 10:AG:181:LYS:HB2 | 1.84                     | 0.58              |
| 54:BJ:109:LEU:HB2 | 54:BJ:146:PHE:HB3 | 1.86                     | 0.58              |
| 79:B5:709:C:N4    | 79:B5:730:G:O2'   | 2.37                     | 0.58              |
| 1:A1:1669:C:H5'   | 35:Ag:30:LEU:HD11 | 1.86                     | 0.57              |
| 1:A1:1722:U:OP2   | 20:AR:103:ARG:NH1 | 2.37                     | 0.57              |
| 6:AC:338:LYS:O    | 6:AC:340:GLY:N    | 2.37                     | 0.57              |
| 57:BM:47:GLU:OE1  | 79:B5:1229:G:N2   | 2.36                     | 0.57              |
| 1:A1:443:G:N2     | 1:A1:492:C:O2'    | 2.38                     | 0.57              |
| 1:A1:799:G:O2'    | 14:AL:18:TRP:NE1  | 2.35                     | 0.57              |
| 22:AT:73:GLY:HA2  | 22:AT:89:LEU:O    | 2.04                     | 0.57              |
| 50:BF:76:ARG:O    | 50:BF:83:ARG:NH1  | 2.37                     | 0.57              |
| 1:A1:38:U:H4'     | 29:Aa:32:ARG:HD2  | 1.86                     | 0.57              |
| 5:AB:185:GLY:O    | 5:AB:191:LYS:NZ   | 2.36                     | 0.57              |
| 46:BB:39:GLU:HB3  | 46:BB:74:GLN:HA   | 1.85                     | 0.57              |
| 77:Bg:149:ASP:H   | 77:Bg:175:ASP:HB3 | 1.69                     | 0.57              |
| 1:A1:1592:G:OP1   | 35:Ag:58:ARG:NH2  | 2.37                     | 0.57              |
| 11:AH:57:VAL:HG23 | 11:AH:68:LEU:HD13 | 1.87                     | 0.57              |
| 16:AN:35:VAL:O    | 16:AN:64:VAL:HA   | 2.04                     | 0.57              |
| 54:BJ:3:ARG:NH2   | 79:B5:462:G:OP1   | 2.37                     | 0.57              |
| 58:BN:23:PRO:HD2  | 58:BN:26:PHE:HB2  | 1.86                     | 0.57              |
| 74:Bd:30:LEU:HA   | 74:Bd:39:CYS:HA   | 1.85                     | 0.57              |
| 1:A1:1124:U:O2'   | 1:A1:2635:A:OP1   | 2.22                     | 0.57              |
| 5:AB:113:GLU:HB3  | 5:AB:176:ALA:HB2  | 1.87                     | 0.57              |
| 6:AC:357:GLU:O    | 6:AC:361:HIS:HB2  | 2.04                     | 0.57              |
| 1:A1:2890:A:O2'   | 1:A1:2933:A:N3    | 2.34                     | 0.57              |
| 22:AT:89:LEU:HB3  | 22:AT:91:LEU:HD13 | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:BE:19:LEU:HD11  | 49:BE:108:ARG:HD2  | 1.85                     | 0.57              |
| 65:BU:42:VAL:HG13  | 65:BU:52:LYS:HE2   | 1.87                     | 0.57              |
| 57:BM:135:MET:SD   | 57:BM:139:HIS:NE2  | 2.78                     | 0.57              |
| 79:B5:220:A:H5''   | 79:B5:832:U:H1'    | 1.85                     | 0.57              |
| 79:B5:1238:A:H61   | 79:B5:1246:C:H42   | 1.51                     | 0.57              |
| 1:A1:2631:U:OP2    | 22:AT:4:SER:OG     | 2.23                     | 0.57              |
| 50:BF:70:VAL:HG12  | 61:BQ:47:LYS:HE3   | 1.87                     | 0.57              |
| 1:A1:284:A:OP2     | 43:Ao:41:ARG:NH1   | 2.34                     | 0.56              |
| 1:A1:692:A:OP1     | 16:AN:201:ARG:NH2  | 2.33                     | 0.56              |
| 1:A1:938:C:OP2     | 29:Aa:26:ARG:NH1   | 2.39                     | 0.56              |
| 69:BY:105:ARG:NH2  | 79:B5:459:G:OP2    | 2.38                     | 0.56              |
| 1:A1:541:U:H3      | 1:A1:550:A:H61     | 1.51                     | 0.56              |
| 4:AA:36:GLU:OE1    | 4:AA:163:ARG:NH1   | 2.38                     | 0.56              |
| 5:AB:17:LEU:HD11   | 5:AB:233:TRP:HH2   | 1.69                     | 0.56              |
| 45:BA:144:ILE:HG12 | 45:BA:158:VAL:HB   | 1.86                     | 0.56              |
| 51:BG:31:ARG:NH1   | 79:B5:1681:A:O2'   | 2.38                     | 0.56              |
| 79:B5:1339:C:O2'   | 79:B5:1341:A:N7    | 2.33                     | 0.56              |
| 49:BE:103:TYR:O    | 49:BE:182:TYR:OH   | 2.23                     | 0.56              |
| 53:BI:172:ARG:NH1  | 79:B5:330:G:OP2    | 2.38                     | 0.56              |
| 1:A1:939:U:O2'     | 1:A1:2402:A:N1     | 2.38                     | 0.56              |
| 1:A1:2622:C:H42    | 12:AI:116:ARG:HH12 | 1.54                     | 0.56              |
| 11:AH:89:LYS:HG2   | 11:AH:145:VAL:HG22 | 1.88                     | 0.56              |
| 42:An:18:ARG:NH2   | 79:B5:1126:OMG:OP2 | 2.38                     | 0.56              |
| 56:BL:129:ARG:HD3  | 79:B5:115:G:H5'    | 1.87                     | 0.56              |
| 62:BR:7:LYS:HD2    | 62:BR:11:ARG:HH22  | 1.71                     | 0.56              |
| 78:Bh:111:GLY:HA3  | 78:Bh:115:LYS:HE2  | 1.88                     | 0.56              |
| 1:A1:1322:U:O2     | 21:AS:108:GLN:NE2  | 2.39                     | 0.56              |
| 1:A1:3343:G:H21    | 1:A1:3362:A:H2     | 1.54                     | 0.56              |
| 6:AC:35:VAL:HG21   | 6:AC:244:LEU:HD21  | 1.88                     | 0.56              |
| 7:AD:50:ARG:NH1    | 7:AD:147:ASP:OD2   | 2.38                     | 0.56              |
| 8:AE:40:LEU:HB3    | 8:AE:84:VAL:HG13   | 1.88                     | 0.56              |
| 37:Ai:70:ARG:HD3   | 37:Ai:84:LYS:HG2   | 1.88                     | 0.56              |
| 53:BI:87:ASN:HB3   | 53:BI:90:LEU:HG    | 1.88                     | 0.56              |
| 77:Bg:127:ARG:HA   | 77:Bg:150:TRP:HB2  | 1.88                     | 0.56              |
| 6:AC:29:PRO:HD2    | 6:AC:277:PRO:HB2   | 1.87                     | 0.56              |
| 9:AF:121:LYS:HB2   | 22:AT:133:ALA:HB3  | 1.87                     | 0.56              |
| 47:BC:181:SER:HB3  | 79:B5:4:C:H4'      | 1.87                     | 0.56              |
| 57:BM:66:VAL:HG11  | 57:BM:93:ASP:HB2   | 1.88                     | 0.56              |
| 57:BM:103:LEU:HD11 | 57:BM:121:VAL:HG21 | 1.87                     | 0.56              |
| 1:A1:63:A:N3       | 1:A1:78:U:O2'      | 2.36                     | 0.56              |
| 1:A1:1047:A:N3     | 1:A1:2633:U:O2'    | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:2552:C:H2'    | 31:Ac:50:VAL:HG11  | 1.86                     | 0.56              |
| 26:AX:77:GLU:HB3   | 26:AX:133:LEU:HD13 | 1.88                     | 0.56              |
| 63:BS:11:PHE:HZ    | 63:BS:25:ASN:H     | 1.53                     | 0.56              |
| 14:AL:48:PRO:HA    | 14:AL:137:GLN:HB2  | 1.88                     | 0.55              |
| 46:BB:111:ARG:NH2  | 79:B5:930:A:N3     | 2.50                     | 0.55              |
| 51:BG:201:GLN:NE2  | 79:B5:125:U:OP1    | 2.39                     | 0.55              |
| 50:BF:94:THR:HG22  | 50:BF:114:ILE:HG13 | 1.89                     | 0.55              |
| 51:BG:10:ASN:HB3   | 51:BG:128:THR:HA   | 1.89                     | 0.55              |
| 1:A1:1448:U:H2'    | 1:A1:1449:A2M:H8   | 1.87                     | 0.55              |
| 28:AZ:90:GLU:HA    | 28:AZ:93:LYS:HG2   | 1.88                     | 0.55              |
| 63:BS:136:GLN:NE2  | 79:B5:1544:U:OP1   | 2.37                     | 0.55              |
| 64:BT:102:ARG:NH1  | 79:B5:1501:C:OP2   | 2.39                     | 0.55              |
| 1:A1:1940:G:H21    | 1:A1:3362:A:H8     | 1.54                     | 0.55              |
| 1:A1:549:U:H3'     | 1:A1:550:A:H8      | 1.72                     | 0.55              |
| 1:A1:816:A:H5'     | 1:A1:906:A:H61     | 1.72                     | 0.55              |
| 13:AJ:53:THR:HG23  | 13:AJ:60:ARG:HA    | 1.88                     | 0.55              |
| 21:AS:22:PRO:O     | 22:AT:146:ASN:ND2  | 2.33                     | 0.55              |
| 1:A1:1128:U:OP1    | 12:AI:4:ARG:NH2    | 2.36                     | 0.55              |
| 1:A1:1334:U:H5''   | 9:AF:206:LYS:HB3   | 1.89                     | 0.55              |
| 1:A1:2433:U:H1'    | 16:AN:125:SER:HB3  | 1.88                     | 0.55              |
| 22:AT:39:ILE:HG12  | 22:AT:63:VAL:HG22  | 1.87                     | 0.55              |
| 54:BJ:52:ILE:HG23  | 54:BJ:76:LEU:HD11  | 1.89                     | 0.55              |
| 77:Bg:32:LEU:HD22  | 77:Bg:73:LEU:HD21  | 1.89                     | 0.55              |
| 41:Am:109:ASN:ND2  | 41:Am:117:HIS:O    | 2.38                     | 0.55              |
| 47:BC:170:ILE:HB   | 47:BC:197:TYR:HB2  | 1.88                     | 0.55              |
| 52:BH:143:LEU:HD12 | 52:BH:147:ASN:HB3  | 1.89                     | 0.55              |
| 1:A1:1192:C:N4     | 1:A1:1301:A:O2'    | 2.32                     | 0.55              |
| 4:AA:135:ILE:HD12  | 4:AA:149:ARG:HE    | 1.71                     | 0.55              |
| 16:AN:143:ARG:NH2  | 36:Ah:90:ARG:O     | 2.40                     | 0.55              |
| 1:A1:68:C:OP2      | 1:A1:301:G:N2      | 2.39                     | 0.54              |
| 1:A1:117:U:OP2     | 16:AN:2:GLY:N      | 2.39                     | 0.54              |
| 1:A1:2219:A:H2'    | 1:A1:2220:A2M:H8   | 1.90                     | 0.54              |
| 5:AB:10:ARG:HH21   | 5:AB:14:LEU:HD21   | 1.72                     | 0.54              |
| 35:Ag:54:ILE:HG23  | 35:Ag:70:LYS:HA    | 1.90                     | 0.54              |
| 1:A1:845:G:H21     | 1:A1:848:A:H2      | 1.53                     | 0.54              |
| 47:BC:40:LYS:HE3   | 47:BC:248:SER:HB3  | 1.88                     | 0.54              |
| 55:BK:3:MET:HE1    | 55:BK:45:ALA:HB2   | 1.89                     | 0.54              |
| 1:A1:149:U:OP2     | 16:AN:49:ARG:NH2   | 2.40                     | 0.54              |
| 1:A1:1618:G:O2'    | 3:A4:126:A:N1      | 2.39                     | 0.54              |
| 45:BA:41:ARG:NH2   | 62:BR:103:ASP:OD2  | 2.40                     | 0.54              |
| 1:A1:1178:G:N3     | 1:A1:1328:C:O2'    | 2.39                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:1243:G:H21    | 1:A1:1244:A:H62    | 1.56                     | 0.54              |
| 52:BH:110:GLN:NE2  | 79:B5:816:G:N3     | 2.51                     | 0.54              |
| 79:B5:1585:U:H3    | 79:B5:1611:A:H2    | 1.54                     | 0.54              |
| 1:A1:98:G:N7       | 14:AL:13:HIS:NE2   | 2.56                     | 0.54              |
| 5:AB:169:THR:HG22  | 5:AB:171:LEU:HD13  | 1.89                     | 0.54              |
| 7:AD:196:ARG:NH2   | 7:AD:237:GLU:OE2   | 2.40                     | 0.54              |
| 13:AJ:82:ARG:NH2   | 13:AJ:112:LEU:O    | 2.41                     | 0.54              |
| 1:A1:1779:C:N4     | 1:A1:2102:U:OP1    | 2.39                     | 0.54              |
| 5:AB:57:VAL:HG22   | 5:AB:73:VAL:HG22   | 1.89                     | 0.54              |
| 16:AN:137:PRO:O    | 16:AN:143:ARG:NH1  | 2.41                     | 0.54              |
| 47:BC:148:LEU:O    | 47:BC:174:ARG:NH2  | 2.41                     | 0.54              |
| 53:BI:2:GLY:N      | 79:B5:393:C:OP2    | 2.41                     | 0.54              |
| 53:BI:152:ILE:HG13 | 53:BI:153:GLU:H    | 1.73                     | 0.54              |
| 57:BM:46:ARG:HH21  | 79:B5:1229:G:H2'   | 1.73                     | 0.54              |
| 64:BT:49:ASP:HB3   | 64:BT:53:TRP:HB3   | 1.90                     | 0.54              |
| 79:B5:1594:G:OP2   | 79:B5:1596:C:N4    | 2.41                     | 0.54              |
| 7:AD:41:LYS:NZ     | 22:AT:30:TYR:O     | 2.37                     | 0.54              |
| 51:BG:193:LEU:O    | 51:BG:197:ASN:HB2  | 2.08                     | 0.54              |
| 53:BI:57:ALA:HB2   | 53:BI:177:GLY:HA2  | 1.89                     | 0.54              |
| 1:A1:358:G:N2      | 1:A1:361:A:OP2     | 2.36                     | 0.54              |
| 29:Aa:104:THR:HG22 | 29:Aa:109:TYR:HB2  | 1.89                     | 0.54              |
| 54:BJ:59:LEU:HD22  | 54:BJ:69:ARG:HA    | 1.90                     | 0.54              |
| 58:BN:54:LEU:HB3   | 58:BN:60:VAL:HB    | 1.90                     | 0.54              |
| 1:A1:1302:A:N7     | 1:A1:2857:C:O2'    | 2.41                     | 0.53              |
| 7:AD:146:LEU:HD22  | 7:AD:163:LEU:HD13  | 1.89                     | 0.53              |
| 49:BE:21:ASP:OD1   | 49:BE:21:ASP:N     | 2.40                     | 0.53              |
| 61:BQ:10:PHE:HA    | 61:BQ:18:ALA:O     | 2.09                     | 0.53              |
| 69:BY:89:TYR:OH    | 69:BY:90:ARG:NH2   | 2.42                     | 0.53              |
| 1:A1:351:A:N6      | 40:Al:37:TYR:O     | 2.38                     | 0.53              |
| 18:AP:126:ARG:HA   | 18:AP:140:GLU:HG2  | 1.89                     | 0.53              |
| 26:AX:47:ALA:HB3   | 26:AX:50:ALA:HB2   | 1.90                     | 0.53              |
| 45:BA:119:ARG:NH1  | 47:BC:241:ASP:OD1  | 2.41                     | 0.53              |
| 52:BH:11:GLN:HG3   | 52:BH:13:PRO:HD2   | 1.90                     | 0.53              |
| 1:A1:824:C:H5''    | 4:AA:21:ARG:HD3    | 1.90                     | 0.53              |
| 12:AI:12:GLN:HG2   | 12:AI:128:ARG:HG2  | 1.91                     | 0.53              |
| 51:BG:131:LYS:HD2  | 79:B5:166:C:H4'    | 1.89                     | 0.53              |
| 59:BO:90:ARG:NH1   | 79:B5:902:G:OP1    | 2.42                     | 0.53              |
| 64:BT:6:VAL:HG22   | 64:BT:136:ALA:HB2  | 1.89                     | 0.53              |
| 77:Bg:240:VAL:HG22 | 77:Bg:256:THR:HG22 | 1.90                     | 0.53              |
| 79:B5:1267:G:HO2'  | 79:B5:1448:G:HO2'  | 1.55                     | 0.53              |
| 6:AC:325:LEU:O     | 9:AF:41:ARG:NH2    | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AH:22:SER:OG    | 11:AH:23:ARG:N     | 2.41                     | 0.53              |
| 73:Bc:42:ARG:NH2   | 73:Bc:58:GLU:O     | 2.37                     | 0.53              |
| 79:B5:1229:G:O2'   | 79:B5:1255:G:N2    | 2.37                     | 0.53              |
| 1:A1:297:G:O2'     | 37:Ai:32:ALA:O     | 2.27                     | 0.53              |
| 1:A1:1149:G:OP2    | 34:Af:21:ARG:NH2   | 2.42                     | 0.53              |
| 1:A1:1348:U:OP2    | 19:AQ:38:ARG:NH2   | 2.41                     | 0.53              |
| 1:A1:2193:U:H5''   | 1:A1:2194:G:H5'    | 1.91                     | 0.53              |
| 9:AF:118:LYS:HG3   | 9:AF:191:VAL:HG11  | 1.90                     | 0.53              |
| 13:AJ:60:ARG:NH2   | 43:Ao:104:LEU:O    | 2.41                     | 0.53              |
| 52:BH:112:ARG:NH2  | 79:B5:639:U:OP1    | 2.40                     | 0.53              |
| 67:BW:81:VAL:HB    | 67:BW:123:GLY:O    | 2.08                     | 0.53              |
| 74:Bd:31:ILE:HG22  | 79:B5:1199:G:H1    | 1.74                     | 0.53              |
| 1:A1:1565:G:N2     | 1:A1:1811:G:OP1    | 2.41                     | 0.53              |
| 1:A1:2836:C:H5     | 1:A1:2852:C:H42    | 1.56                     | 0.53              |
| 24:AV:18:PRO:HA    | 24:AV:51:ALA:HA    | 1.89                     | 0.53              |
| 46:BB:168:ILE:HG12 | 46:BB:197:ILE:HD12 | 1.89                     | 0.53              |
| 61:BQ:95:LYS:O     | 77:Bg:59:ARG:NH1   | 2.41                     | 0.53              |
| 1:A1:449:U:O2'     | 1:A1:450:G:N2      | 2.42                     | 0.53              |
| 64:BT:40:SER:HB3   | 64:BT:43:ASN:HB2   | 1.90                     | 0.53              |
| 68:BX:60:GLU:HG2   | 75:Be:3:LYS:HB2    | 1.91                     | 0.53              |
| 72:Bb:53:ALA:HB1   | 72:Bb:62:ILE:HD12  | 1.91                     | 0.53              |
| 79:B5:1171:A:H2'   | 79:B5:1172:G:C8    | 2.44                     | 0.53              |
| 79:B5:1561:U:H2'   | 79:B5:1562:G:H8    | 1.73                     | 0.53              |
| 79:B5:1600:A:O2'   | 79:B5:1602:C:N4    | 2.41                     | 0.53              |
| 1:A1:797:U:O2      | 14:AL:12:ASN:ND2   | 2.41                     | 0.53              |
| 22:AT:17:ARG:HE    | 22:AT:47:SER:HB3   | 1.74                     | 0.53              |
| 53:BI:5:ARG:NH1    | 79:B5:332:U:O2'    | 2.41                     | 0.53              |
| 60:BP:40:ARG:NH2   | 79:B5:1551:U:O4    | 2.42                     | 0.53              |
| 77:Bg:126:SER:OG   | 77:Bg:127:ARG:N    | 2.38                     | 0.53              |
| 1:A1:165:A:H62     | 1:A1:257:U:H3      | 1.57                     | 0.53              |
| 1:A1:289:A:O2'     | 16:AN:93:LYS:O     | 2.26                     | 0.53              |
| 1:A1:2969:A:N7     | 4:AA:215:ASN:ND2   | 2.56                     | 0.53              |
| 24:AV:38:ALA:HB3   | 24:AV:59:MET:HB2   | 1.90                     | 0.53              |
| 54:BJ:144:PRO:HD2  | 79:B5:474:A:H5''   | 1.89                     | 0.53              |
| 56:BL:133:LYS:HB2  | 79:B5:337:G:H3'    | 1.91                     | 0.53              |
| 1:A1:1132:C:H2'    | 1:A1:1133:A2M:H8   | 1.90                     | 0.52              |
| 1:A1:2700:G:H5''   | 22:AT:17:ARG:HB2   | 1.91                     | 0.52              |
| 48:BD:40:ARG:HG2   | 65:BU:110:PRO:HB3  | 1.90                     | 0.52              |
| 48:BD:138:VAL:HG22 | 48:BD:184:ILE:HG22 | 1.91                     | 0.52              |
| 79:B5:1474:G:H2'   | 79:B5:1475:A:H8    | 1.74                     | 0.52              |
| 51:BG:70:PRO:HA    | 51:BG:98:ARG:HH22  | 1.74                     | 0.52              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 67:BW:112:ASP:OD1 | 67:BW:112:ASP:N     | 2.40                     | 0.52              |
| 1:A1:503:C:O2     | 8:AE:23:LYS:NZ      | 2.40                     | 0.52              |
| 1:A1:728:G:H5''   | 19:AQ:43:PRO:HB2    | 1.90                     | 0.52              |
| 11:AH:129:ARG:NH1 | 11:AH:160:ASP:OD2   | 2.38                     | 0.52              |
| 37:AI:25:LYS:O    | 37:AI:29:LYS:NZ     | 2.42                     | 0.52              |
| 41:Am:127:LEU:HG  | 41:Am:128:LYS:HG3   | 1.91                     | 0.52              |
| 50:BF:96:SER:HB3  | 50:BF:176:THR:HG21  | 1.91                     | 0.52              |
| 61:BQ:136:SER:HB3 | 79:B5:1586:A:H5''   | 1.91                     | 0.52              |
| 63:BS:126:ARG:HB2 | 63:BS:133:VAL:HG12  | 1.92                     | 0.52              |
| 74:Bd:13:ARG:NH2  | 79:B5:1554:U:OP1    | 2.38                     | 0.52              |
| 21:AS:12:ARG:HD2  | 21:AS:22:PRO:HD2    | 1.91                     | 0.52              |
| 45:BA:140:ASN:ND2 | 66:BV:31:SER:O      | 2.36                     | 0.52              |
| 51:BG:32:ILE:HD12 | 51:BG:65:GLN:HA     | 1.90                     | 0.52              |
| 64:BT:109:GLU:OE1 | 64:BT:122:ARG:NH1   | 2.42                     | 0.52              |
| 1:A1:444:U:H3     | 1:A1:491:A:H61      | 1.58                     | 0.52              |
| 1:A1:938:C:O2     | 1:A1:2813:A:O2'     | 2.28                     | 0.52              |
| 4:AA:92:LYS:HE3   | 4:AA:93:LYS:HE3     | 1.91                     | 0.52              |
| 62:BR:14:LYS:HG3  | 62:BR:69:ILE:HD13   | 1.90                     | 0.52              |
| 1:A1:733:G:N2     | 1:A1:736:A:OP2      | 2.42                     | 0.52              |
| 1:A1:824:C:O2'    | 1:A1:1534:A:N3      | 2.40                     | 0.52              |
| 1:A1:2383:C:OP2   | 17:AO:85[A]:ARG:NH2 | 2.43                     | 0.52              |
| 1:A1:3070:A:OP1   | 20:AR:62:ARG:NH2    | 2.39                     | 0.52              |
| 9:AF:83:LEU:HD11  | 9:AF:116:PHE:HB3    | 1.91                     | 0.52              |
| 12:AI:82:ARG:NH2  | 12:AI:83:ASP:OD1    | 2.39                     | 0.52              |
| 1:A1:450:G:N7     | 1:A1:487:U:O2'      | 2.42                     | 0.52              |
| 1:A1:1174:G:N2    | 17:AO:87[A]:MET:SD  | 2.83                     | 0.52              |
| 5:AB:187:SER:O    | 5:AB:190:GLU:N      | 2.43                     | 0.52              |
| 7:AD:107:ARG:NH1  | 7:AD:169:GLY:O      | 2.40                     | 0.52              |
| 49:BE:95:THR:HG22 | 69:BY:16:PRO:HD2    | 1.90                     | 0.52              |
| 77:Bg:10:ARG:NH1  | 77:Bg:314:GLN:OE1   | 2.42                     | 0.52              |
| 1:A1:1315:U:OP1   | 17:AO:18[A]:ARG:NE  | 2.33                     | 0.52              |
| 1:A1:3119:U:H4'   | 41:Am:104:PRO:HG3   | 1.92                     | 0.52              |
| 3:A4:37:A:OP1     | 36:Ah:89:ARG:NH2    | 2.43                     | 0.52              |
| 46:BB:39:GLU:HG3  | 46:BB:40:ASN:H      | 1.74                     | 0.52              |
| 53:BI:5:ARG:NH2   | 79:B5:334:G:O6      | 2.43                     | 0.52              |
| 53:BI:8:ARG:HE    | 53:BI:22:ARG:HH21   | 1.58                     | 0.52              |
| 66:BV:4:ASP:N     | 66:BV:4:ASP:OD1     | 2.43                     | 0.52              |
| 71:Ba:3:LYS:HE2   | 71:Ba:6:ALA:HA      | 1.92                     | 0.52              |
| 1:A1:2727:A:OP2   | 1:A1:2728:G:N2      | 2.38                     | 0.52              |
| 2:A3:101:G:N7     | 21:AS:52:LYS:NZ     | 2.57                     | 0.52              |
| 10:AG:162:LEU:HA  | 16:AN:7:LEU:HD11    | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:Am:98:LYS:HD3   | 41:Am:118:THR:HG21 | 1.91                     | 0.52              |
| 44:Ap:38:ASP:HA    | 44:Ap:45:LYS:HA    | 1.92                     | 0.52              |
| 46:BB:180:THR:O    | 46:BB:183:GLN:N    | 2.43                     | 0.52              |
| 47:BC:79:GLU:HG3   | 47:BC:186:LYS:HE3  | 1.91                     | 0.52              |
| 79:B5:720:G:N2     | 79:B5:722:G:OP2    | 2.43                     | 0.52              |
| 1:A1:3313:U:H4'    | 5:AB:173:GLN:HG3   | 1.91                     | 0.51              |
| 14:AL:48:PRO:HB2   | 36:Ah:117:ALA:HB2  | 1.92                     | 0.51              |
| 18:AP:64:ASN:O     | 18:AP:80:LYS:NZ    | 2.43                     | 0.51              |
| 46:BB:60:ALA:O     | 46:BB:64:ARG:NH1   | 2.43                     | 0.51              |
| 48:BD:172:THR:HG23 | 48:BD:185:LYS:HG2  | 1.92                     | 0.51              |
| 64:BT:105:LEU:HD22 | 64:BT:122:ARG:HG3  | 1.92                     | 0.51              |
| 70:BZ:46:LYS:HE3   | 70:BZ:49:ARG:HH11  | 1.75                     | 0.51              |
| 1:A1:649:A2M:OP2   | 1:A1:2868:U:O2'    | 2.28                     | 0.51              |
| 1:A1:1232:C:N4     | 1:A1:1262:G:OP2    | 2.43                     | 0.51              |
| 1:A1:1729:A:O4'    | 31:Ac:52:ARG:NH1   | 2.40                     | 0.51              |
| 7:AD:30:TYR:HA     | 7:AD:33:ARG:HB3    | 1.92                     | 0.51              |
| 13:AJ:28:ASP:OD1   | 13:AJ:28:ASP:N     | 2.40                     | 0.51              |
| 65:BU:22:ILE:HG22  | 65:BU:118:VAL:HG12 | 1.92                     | 0.51              |
| 65:BU:59:PRO:HG3   | 79:B5:1381:U:H4'   | 1.92                     | 0.51              |
| 77:Bg:73:LEU:HD23  | 77:Bg:77:GLY:HA2   | 1.91                     | 0.51              |
| 77:Bg:255:ALA:HB2  | 77:Bg:292:LEU:HD22 | 1.91                     | 0.51              |
| 79:B5:472:U:O2'    | 79:B5:769:A:N3     | 2.37                     | 0.51              |
| 79:B5:701:U:O2     | 79:B5:738:G:O6     | 2.28                     | 0.51              |
| 79:B5:1027:A:OP1   | 79:B5:1789:G:O2'   | 2.28                     | 0.51              |
| 1:A1:873:C:H3'     | 1:A1:874:U:H4'     | 1.93                     | 0.51              |
| 1:A1:1468:A:N1     | 1:A1:1880:U:O2'    | 2.37                     | 0.51              |
| 12:AI:52:LEU:HB3   | 12:AI:136:PHE:HB2  | 1.91                     | 0.51              |
| 21:AS:24:LEU:HD21  | 22:AT:141:VAL:HG11 | 1.93                     | 0.51              |
| 27:AY:55:GLU:HB2   | 27:AY:108:LYS:HB3  | 1.91                     | 0.51              |
| 53:BI:16:ALA:HB2   | 79:B5:354:C:H5''   | 1.92                     | 0.51              |
| 54:BJ:173:ALA:HB2  | 79:B5:511:A:H5'    | 1.91                     | 0.51              |
| 1:A1:115:A:H2'     | 1:A1:265:A:H2      | 1.75                     | 0.51              |
| 1:A1:2157:G:N7     | 4:AA:152:SER:OG    | 2.39                     | 0.51              |
| 31:Ac:27:TYR:OH    | 31:Ac:55:GLU:OE2   | 2.28                     | 0.51              |
| 60:BP:77:ARG:HG3   | 79:B5:1241:G:H5''  | 1.91                     | 0.51              |
| 65:BU:106:ILE:HG13 | 65:BU:107:THR:HG23 | 1.91                     | 0.51              |
| 72:Bb:42:ASN:C     | 72:Bb:42:ASN:HD22  | 2.17                     | 0.51              |
| 72:Bb:67:THR:OG1   | 72:Bb:70:LYS:O     | 2.29                     | 0.51              |
| 1:A1:3042:U:OP2    | 1:A1:3092:C:N4     | 2.41                     | 0.51              |
| 28:AZ:33:SER:OG    | 28:AZ:35:SER:O     | 2.25                     | 0.51              |
| 66:BV:21:ASN:HB3   | 67:BW:67:GLY:HA3   | 1.92                     | 0.51              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:A1:292:U:OP2     | 16:AN:68:ARG:NH2     | 2.41                     | 0.51              |
| 7:AD:215:ASP:OD1   | 7:AD:215:ASP:N       | 2.44                     | 0.51              |
| 11:AH:22:SER:OG    | 11:AH:39:LYS:NZ      | 2.43                     | 0.51              |
| 12:AI:192:ASP:HA   | 12:AI:197:VAL:HG23   | 1.92                     | 0.51              |
| 29:Aa:72:VAL:HG12  | 29:Aa:111:LYS:HB3    | 1.91                     | 0.51              |
| 55:BK:44:LYS:HD2   | 79:B5:1217:A:H5'     | 1.93                     | 0.51              |
| 60:BP:53:PRO:HB2   | 60:BP:57:MET:HE2     | 1.92                     | 0.51              |
| 61:BQ:16:ALA:HB2   | 61:BQ:72:GLY:HA3     | 1.92                     | 0.51              |
| 78:Bh:93:ARG:NH1   | 79:B5:1636:C:OP1     | 2.43                     | 0.51              |
| 4:AA:180:LEU:HD11  | 44:Ap:26:VAL:HG11    | 1.93                     | 0.51              |
| 47:BC:83:ILE:HD11  | 47:BC:125:ILE:HD11   | 1.92                     | 0.51              |
| 1:A1:412:G:OP1     | 18:AP:62:ARG:NH1     | 2.43                     | 0.51              |
| 3:A4:143:U:OP1     | 16:AN:38:ARG:NH2     | 2.38                     | 0.51              |
| 6:AC:334:PHE:HA    | 6:AC:339:LEU:HD12    | 1.92                     | 0.51              |
| 13:AJ:49:LYS:HG2   | 13:AJ:64:LYS:HG2     | 1.93                     | 0.51              |
| 79:B5:428:A:N3     | 79:B5:440:U:O2'      | 2.38                     | 0.51              |
| 1:A1:2146:C:OP1    | 4:AA:200:ARG:NH1     | 2.40                     | 0.51              |
| 3:A4:142:C:OP1     | 16:AN:38:ARG:NH1     | 2.43                     | 0.51              |
| 11:AH:5:GLN:NE2    | 11:AH:7:GLU:OE1      | 2.37                     | 0.51              |
| 22:AT:14:MET:HE1   | 22:AT:55:LYS:HB2     | 1.93                     | 0.51              |
| 51:BG:164:LYS:NZ   | 79:B5:71:A:OP2       | 2.38                     | 0.51              |
| 4:AA:168:VAL:HG13  | 44:Ap:79:VAL:HG21    | 1.93                     | 0.51              |
| 51:BG:21:GLU:OE2   | 51:BG:25:ARG:NH2     | 2.44                     | 0.51              |
| 51:BG:92:ARG:NH2   | 79:B5:1674:C:OP1     | 2.42                     | 0.51              |
| 64:BT:41:SER:O     | 64:BT:84:LYS:NZ      | 2.44                     | 0.51              |
| 17:AO:27[A]:LEU:O  | 17:AO:101[A]:ARG:NH1 | 2.42                     | 0.50              |
| 77:Bg:42:LEU:HB2   | 77:Bg:61:PHE:HB2     | 1.92                     | 0.50              |
| 79:B5:480:G:O6     | 79:B5:508:U:O2       | 2.29                     | 0.50              |
| 79:B5:1280:4AC:H2' | 79:B5:1281:G:H8      | 1.76                     | 0.50              |
| 1:A1:286:U:O2'     | 16:AN:179:LYS:O      | 2.29                     | 0.50              |
| 1:A1:1410:U:O2'    | 33:Ae:95:GLU:OE1     | 2.27                     | 0.50              |
| 51:BG:94:ARG:NH2   | 79:B5:1673:G:OP1     | 2.44                     | 0.50              |
| 51:BG:159:ARG:NH2  | 79:B5:79:C:OP1       | 2.41                     | 0.50              |
| 57:BM:60:VAL:HG22  | 57:BM:122:VAL:HG12   | 1.93                     | 0.50              |
| 4:AA:177:LYS:NZ    | 44:Ap:33:GLN:OE1     | 2.44                     | 0.50              |
| 45:BA:125:ASP:O    | 45:BA:129:ASP:HB2    | 2.11                     | 0.50              |
| 54:BJ:113:VAL:HG12 | 54:BJ:119:ALA:HB2    | 1.93                     | 0.50              |
| 55:BK:86:ILE:HG23  | 55:BK:87:VAL:HG23    | 1.94                     | 0.50              |
| 61:BQ:94:GLN:HB2   | 61:BQ:102:LYS:HD3    | 1.93                     | 0.50              |
| 64:BT:65:ILE:HD13  | 64:BT:71:VAL:HB      | 1.93                     | 0.50              |
| 65:BU:100:VAL:HA   | 65:BU:103:ILE:HG12   | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:BY:34:ASN:O     | 79:B5:521:A:O2'    | 2.24                     | 0.50              |
| 79:B5:1525:A:N3    | 79:B5:1589:C:O2'   | 2.44                     | 0.50              |
| 12:AI:76:MET:HE2   | 12:AI:148:VAL:HG22 | 1.92                     | 0.50              |
| 1:A1:114:A:OP1     | 16:AN:54:LYS:NZ    | 2.41                     | 0.50              |
| 1:A1:591:G:O2'     | 8:AE:17:ALA:O      | 2.27                     | 0.50              |
| 1:A1:664:U:H5'     | 6:AC:107:ARG:HA    | 1.94                     | 0.50              |
| 1:A1:2209:U:H3     | 1:A1:2230:C:H5''   | 1.76                     | 0.50              |
| 4:AA:113:VAL:HG12  | 4:AA:166:ILE:HD13  | 1.93                     | 0.50              |
| 20:AR:13:SER:OG    | 20:AR:38:ARG:NH2   | 2.40                     | 0.50              |
| 66:BV:15:ARG:NH1   | 66:BV:33:GLN:OE1   | 2.44                     | 0.50              |
| 79:B5:514:G:H1     | 79:B5:543:C:H5     | 1.58                     | 0.50              |
| 79:B5:1687:U:OP1   | 79:B5:1707:A:O2'   | 2.29                     | 0.50              |
| 1:A1:775:A:OP1     | 30:Ab:44:LYS:NZ    | 2.44                     | 0.50              |
| 28:AZ:50:PRO:HD3   | 28:AZ:68:ILE:HG12  | 1.94                     | 0.50              |
| 46:BB:118:GLN:OE1  | 46:BB:208:GLN:NE2  | 2.44                     | 0.50              |
| 49:BE:100:ARG:HB2  | 49:BE:114:ILE:HD13 | 1.93                     | 0.50              |
| 77:Bg:116:ASP:OD1  | 77:Bg:116:ASP:N    | 2.44                     | 0.50              |
| 77:Bg:200:ASN:H    | 77:Bg:215:GLY:HA2  | 1.76                     | 0.50              |
| 1:A1:520:U:OP2     | 9:AF:70:LYS:NZ     | 2.44                     | 0.50              |
| 1:A1:2799:A:O2'    | 29:Aa:42:ARG:NH1   | 2.45                     | 0.50              |
| 14:AL:57:VAL:HG22  | 14:AL:147:ILE:HG23 | 1.93                     | 0.50              |
| 1:A1:1873:U:OP1    | 20:AR:21:LYS:NZ    | 2.34                     | 0.50              |
| 4:AA:117:GLU:HB2   | 4:AA:162:ALA:HB1   | 1.94                     | 0.50              |
| 6:AC:315:LYS:HB3   | 6:AC:320:ASN:HD22  | 1.76                     | 0.50              |
| 10:AG:74:THR:HG22  | 10:AG:164:VAL:HG22 | 1.93                     | 0.50              |
| 31:Ac:30:THR:HG23  | 31:Ac:91:SER:HB2   | 1.92                     | 0.50              |
| 48:BD:105:MET:HE1  | 48:BD:136:VAL:HG11 | 1.92                     | 0.50              |
| 55:BK:5:LYS:NZ     | 55:BK:79:TYR:OH    | 2.44                     | 0.50              |
| 65:BU:68:ARG:HH22  | 65:BU:77:LYS:HG3   | 1.76                     | 0.50              |
| 75:Be:55:ARG:NH2   | 79:B5:558:U:OP2    | 2.40                     | 0.50              |
| 1:A1:996:A:N3      | 2:A3:80:G:O2'      | 2.45                     | 0.50              |
| 4:AA:45:VAL:HG22   | 4:AA:61:VAL:HG22   | 1.93                     | 0.50              |
| 11:AH:101:VAL:HG22 | 11:AH:114:VAL:HG22 | 1.92                     | 0.50              |
| 32:Ad:20:LEU:HD11  | 32:Ad:32:ALA:HB2   | 1.94                     | 0.50              |
| 52:BH:49:ILE:HB    | 52:BH:57:ALA:HB3   | 1.94                     | 0.50              |
| 58:BN:124:ARG:NH2  | 79:B5:967:A:OP2    | 2.44                     | 0.50              |
| 79:B5:192:U:H4'    | 79:B5:195:G:H1     | 1.75                     | 0.50              |
| 79:B5:1235:C:H2'   | 79:B5:1236:A:C8    | 2.47                     | 0.50              |
| 1:A1:718:G:OP1     | 29:Aa:117:ARG:NH2  | 2.45                     | 0.49              |
| 1:A1:1613:A:OP1    | 39:Ak:2:ALA:N      | 2.45                     | 0.49              |
| 1:A1:1825:G:H5''   | 39:Ak:48:SER:HB3   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AB:122:TRP:O    | 5:AB:127:LYS:NZ    | 2.45                     | 0.49              |
| 79:B5:319:U:H4'   | 79:B5:323:A:C8     | 2.46                     | 0.49              |
| 46:BB:154:SER:O   | 46:BB:154:SER:OG   | 2.26                     | 0.49              |
| 53:BI:10:LYS:NZ   | 79:B5:322:G:O2'    | 2.45                     | 0.49              |
| 65:BU:97:VAL:HG13 | 65:BU:98:GLN:HG2   | 1.93                     | 0.49              |
| 69:BY:55:VAL:HG22 | 69:BY:75:VAL:HG22  | 1.93                     | 0.49              |
| 79:B5:869:A:H61   | 79:B5:958:U:H3     | 1.60                     | 0.49              |
| 1:A1:815:G:OP2    | 38:Aj:31:LYS:NZ    | 2.40                     | 0.49              |
| 1:A1:1795:U:OP2   | 4:AA:50:HIS:NE2    | 2.45                     | 0.49              |
| 60:BP:81:ARG:NH2  | 60:BP:117:GLY:O    | 2.45                     | 0.49              |
| 79:B5:1591:C:H2'  | 79:B5:1592:A:H8    | 1.77                     | 0.49              |
| 3:A4:29:U:H5''    | 14:AL:27:ASP:HB3   | 1.95                     | 0.49              |
| 7:AD:119:TYR:OH   | 7:AD:139:PRO:O     | 2.28                     | 0.49              |
| 8:AE:62:THR:HG21  | 8:AE:78:ARG:HD2    | 1.93                     | 0.49              |
| 9:AF:116:PHE:O    | 9:AF:199:ASN:ND2   | 2.37                     | 0.49              |
| 45:BA:118:PRO:HG2 | 45:BA:141:ILE:HD13 | 1.95                     | 0.49              |
| 58:BN:3:ARG:HB3   | 58:BN:6:SER:HB3    | 1.94                     | 0.49              |
| 68:BX:30:LYS:NZ   | 79:B5:1132:A:OP1   | 2.38                     | 0.49              |
| 75:Be:54:ARG:HE   | 75:Be:56:MET:HE2   | 1.77                     | 0.49              |
| 1:A1:847:A:OP1    | 58:BN:140:LYS:NZ   | 2.40                     | 0.49              |
| 5:AB:77:THR:OG1   | 5:AB:326:GLY:O     | 2.29                     | 0.49              |
| 39:Ak:8:ILE:HD12  | 39:Ak:65:LEU:HD11  | 1.94                     | 0.49              |
| 49:BE:200:ARG:NH2 | 79:B5:737:A:OP1    | 2.46                     | 0.49              |
| 50:BF:63:GLN:HB3  | 50:BF:88:PRO:HA    | 1.95                     | 0.49              |
| 79:B5:162:A:H3'   | 79:B5:163:G:H21    | 1.77                     | 0.49              |
| 79:B5:1164:G:O2'  | 79:B5:1612:U:O2    | 2.29                     | 0.49              |
| 1:A1:874:U:N3     | 1:A1:2978:U:OP1    | 2.38                     | 0.49              |
| 1:A1:2618:G:O2'   | 1:A1:2865:U:OP1    | 2.30                     | 0.49              |
| 50:BF:166:ARG:NH2 | 79:B5:1163:A:O3'   | 2.45                     | 0.49              |
| 58:BN:64:ARG:O    | 58:BN:64:ARG:NH1   | 2.40                     | 0.49              |
| 61:BQ:143:ARG:NH2 | 79:B5:1464:G:OP1   | 2.46                     | 0.49              |
| 18:AP:47:TYR:OH   | 18:AP:57:ALA:O     | 2.28                     | 0.49              |
| 46:BB:138:PHE:O   | 46:BB:212:VAL:O    | 2.30                     | 0.49              |
| 48:BD:124:ARG:NH2 | 78:Bh:124:GLN:OE1  | 2.46                     | 0.49              |
| 52:BH:150:GLN:HB3 | 52:BH:181:ILE:HG13 | 1.95                     | 0.49              |
| 73:Bc:19:THR:HG21 | 73:Bc:66:LEU:HA    | 1.95                     | 0.49              |
| 1:A1:3094:A:OP1   | 24:AV:14:SER:OG    | 2.31                     | 0.49              |
| 1:A1:3275:U:O2'   | 34:Af:99:ARG:NH1   | 2.46                     | 0.49              |
| 3:A4:97:A:OP1     | 36:Ah:67:ARG:NH2   | 2.42                     | 0.49              |
| 4:AA:180:LEU:HD22 | 44:Ap:18:TYR:HB3   | 1.95                     | 0.49              |
| 18:AP:29:THR:HA   | 18:AP:32:THR:HG22  | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:BK:1:MET:HE3    | 79:B5:1219:A:H4'   | 1.95                     | 0.49              |
| 58:BN:119:GLU:HG2  | 58:BN:141:TYR:HE2  | 1.78                     | 0.49              |
| 59:BO:132:ARG:NH2  | 79:B5:1789:G:OP2   | 2.43                     | 0.49              |
| 1:A1:1746:U:O2'    | 39:Ak:4:GLU:OE2    | 2.24                     | 0.49              |
| 13:AJ:32:ARG:HD2   | 13:AJ:120:ILE:HG12 | 1.95                     | 0.49              |
| 26:AX:108:LEU:HD23 | 26:AX:125:ARG:HD3  | 1.95                     | 0.49              |
| 29:Aa:112:ILE:HB   | 29:Aa:130:VAL:HG12 | 1.95                     | 0.49              |
| 64:BT:106:GLN:NE2  | 79:B5:1500:C:OP1   | 2.46                     | 0.49              |
| 70:BZ:61:SER:OG    | 70:BZ:62:VAL:N     | 2.46                     | 0.49              |
| 71:Ba:57:SER:OG    | 71:Ba:58:VAL:O     | 2.29                     | 0.49              |
| 79:B5:647:G:H21    | 79:B5:687:G:H1     | 1.61                     | 0.49              |
| 1:A1:2697:A:H2'    | 1:A1:2698:G:C8     | 2.48                     | 0.49              |
| 4:AA:33:ASP:OD1    | 4:AA:33:ASP:N      | 2.46                     | 0.49              |
| 22:AT:136:ARG:HD2  | 22:AT:139:ARG:HH12 | 1.77                     | 0.49              |
| 24:AV:59:MET:HE1   | 24:AV:75:PRO:HG3   | 1.94                     | 0.49              |
| 49:BE:181:VAL:HG13 | 49:BE:225:VAL:HG13 | 1.95                     | 0.49              |
| 61:BQ:15:SER:O     | 61:BQ:15:SER:OG    | 2.31                     | 0.49              |
| 63:BS:26:ILE:HG23  | 63:BS:31:ALA:HB2   | 1.94                     | 0.49              |
| 79:B5:1356:U:O4    | 79:B5:1367:G:O6    | 2.31                     | 0.49              |
| 1:A1:879:U:O2'     | 18:AP:135:ARG:NH2  | 2.38                     | 0.48              |
| 21:AS:77:VAL:HG11  | 21:AS:106:LEU:HD22 | 1.95                     | 0.48              |
| 39:Ak:14:LEU:HD12  | 39:Ak:17:ARG:HD3   | 1.95                     | 0.48              |
| 53:BI:191:PHE:O    | 53:BI:195:ARG:HB2  | 2.12                     | 0.48              |
| 63:BS:30:TYR:HE1   | 63:BS:40:ARG:HD3   | 1.77                     | 0.48              |
| 79:B5:1297:G:N2    | 79:B5:1300:A:OP2   | 2.36                     | 0.48              |
| 79:B5:1533:C:H4'   | 79:B5:1539:G:C6    | 2.48                     | 0.48              |
| 34:Af:37:THR:HG22  | 34:Af:39:GLN:H     | 1.78                     | 0.48              |
| 64:BT:39:THR:HA    | 64:BT:100:ILE:HD12 | 1.95                     | 0.48              |
| 71:Ba:88:SER:HA    | 79:B5:1628:U:H5'   | 1.95                     | 0.48              |
| 74:Bd:30:LEU:O     | 79:B5:1199:G:N2    | 2.46                     | 0.48              |
| 77:Bg:12:THR:HG22  | 77:Bg:311:ARG:HG3  | 1.94                     | 0.48              |
| 77:Bg:89:LEU:HB2   | 77:Bg:103:PHE:HB2  | 1.95                     | 0.48              |
| 1:A1:1805:C:H2'    | 1:A1:1806:A:H8     | 1.77                     | 0.48              |
| 1:A1:2940:A:OP2    | 5:AB:2:SER:N       | 2.47                     | 0.48              |
| 48:BD:54:ARG:HB3   | 48:BD:57:ASP:HB2   | 1.95                     | 0.48              |
| 49:BE:122:LYS:HD2  | 49:BE:164:LEU:HD21 | 1.95                     | 0.48              |
| 65:BU:66:SER:HA    | 65:BU:80:GLU:O     | 2.14                     | 0.48              |
| 67:BW:41:MET:HG2   | 67:BW:129:VAL:HG21 | 1.94                     | 0.48              |
| 1:A1:2176:U:OP1    | 4:AA:54:ARG:NH2    | 2.38                     | 0.48              |
| 1:A1:2947:G:N3     | 5:AB:250:ALA:HB1   | 2.29                     | 0.48              |
| 12:AI:19:LYS:HD2   | 12:AI:26:VAL:HB    | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:Ao:61:LYS:NZ    | 43:Ao:63:LYS:O     | 2.45                     | 0.48              |
| 57:BM:33:ARG:HH21  | 57:BM:36:LEU:HD22  | 1.78                     | 0.48              |
| 1:A1:907:G:H4'     | 1:A1:908:OMG:H5'   | 1.96                     | 0.48              |
| 4:AA:116:VAL:HG13  | 4:AA:126:LEU:HB2   | 1.96                     | 0.48              |
| 29:Aa:101:VAL:HA   | 29:Aa:124:ILE:HB   | 1.94                     | 0.48              |
| 47:BC:81:MET:HB2   | 47:BC:101:VAL:HG23 | 1.94                     | 0.48              |
| 53:BI:166:TYR:HB3  | 53:BI:184:LEU:HD12 | 1.95                     | 0.48              |
| 64:BT:89:ARG:NH1   | 79:B5:1562:G:OP1   | 2.44                     | 0.48              |
| 64:BT:97:SER:OG    | 79:B5:1504:G:OP1   | 2.31                     | 0.48              |
| 1:A1:1334:U:HO2'   | 9:AF:151:ARG:HH12  | 1.59                     | 0.48              |
| 1:A1:3050:U:O2'    | 25:AW:16:GLY:O     | 2.29                     | 0.48              |
| 5:AB:85:VAL:HG22   | 5:AB:202:THR:HG22  | 1.95                     | 0.48              |
| 12:AI:153:ARG:HA   | 12:AI:156:ARG:HD2  | 1.94                     | 0.48              |
| 39:Ak:7:ASP:HB3    | 39:Ak:10:GLN:HB3   | 1.95                     | 0.48              |
| 1:A1:1863:G:N1     | 1:A1:1866:C:OP2    | 2.38                     | 0.48              |
| 4:AA:47:GLN:HB3    | 4:AA:49:VAL:HG13   | 1.95                     | 0.48              |
| 13:AJ:23:VAL:HG11  | 13:AJ:29:ARG:HG2   | 1.95                     | 0.48              |
| 28:AZ:97:SER:O     | 28:AZ:100:THR:OG1  | 2.29                     | 0.48              |
| 52:BH:97:ARG:NH1   | 79:B5:856:A:OP1    | 2.46                     | 0.48              |
| 59:BO:125:SER:HB3  | 79:B5:926:A:H2     | 1.78                     | 0.48              |
| 77:Bg:69:GLN:OE1   | 77:Bg:85:TRP:NE1   | 2.38                     | 0.48              |
| 79:B5:1290:U:H2'   | 79:B5:1291:G:C8    | 2.49                     | 0.48              |
| 79:B5:1682:U:O4    | 79:B5:1720:G:N2    | 2.47                     | 0.48              |
| 1:A1:2185:G:O2'    | 1:A1:2314:U:OP2    | 2.31                     | 0.48              |
| 1:A1:2767:U:O2'    | 43:Ao:30:ALA:O     | 2.30                     | 0.48              |
| 9:AF:86:VAL:O      | 9:AF:114:GLY:HA2   | 2.13                     | 0.48              |
| 25:AW:6:ASP:HB3    | 25:AW:11:ALA:H     | 1.78                     | 0.48              |
| 64:BT:48:GLN:OE1   | 79:B5:1531:G:N2    | 2.41                     | 0.48              |
| 64:BT:71:VAL:HG13  | 64:BT:75:LYS:HB2   | 1.96                     | 0.48              |
| 79:B5:1280:4AC:H2' | 79:B5:1281:G:C8    | 2.49                     | 0.48              |
| 1:A1:339:C:OP1     | 1:A1:1380:G:O2'    | 2.32                     | 0.48              |
| 12:AI:5:PRO:HB2    | 12:AI:7:ARG:HG2    | 1.96                     | 0.48              |
| 13:AJ:49:LYS:HB3   | 13:AJ:62:ASN:HA    | 1.96                     | 0.48              |
| 14:AL:46:ILE:HD11  | 14:AL:51:LEU:HA    | 1.95                     | 0.48              |
| 38:Aj:54:LYS:O     | 38:Aj:58:THR:HB    | 2.14                     | 0.48              |
| 46:BB:27:LYS:NZ    | 46:BB:49:ASN:OD1   | 2.41                     | 0.48              |
| 55:BK:64:TYR:OH    | 79:B5:1435:G:O6    | 2.31                     | 0.48              |
| 58:BN:109:LYS:HD2  | 79:B5:975:C:H5''   | 1.95                     | 0.48              |
| 62:BR:34:LEU:HB3   | 77:Bg:150:TRP:HH2  | 1.78                     | 0.48              |
| 71:Ba:32:LYS:O     | 71:Ba:37:LYS:NZ    | 2.37                     | 0.48              |
| 1:A1:1352:A:H1'    | 1:A1:1353:U:H4'    | 1.96                     | 0.48              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 28:AZ:46:ILE:HG23    | 28:AZ:68:ILE:HG23    | 1.96                     | 0.48              |
| 70:BZ:74:SER:OG      | 79:B5:1534:G:OP2     | 2.32                     | 0.48              |
| 77:Bg:211:ILE:HB     | 77:Bg:223:TRP:HB2    | 1.96                     | 0.48              |
| 79:B5:1474:G:H2'     | 79:B5:1475:A:C8      | 2.48                     | 0.48              |
| 8:AE:40:LEU:HD11     | 8:AE:54:TYR:HB2      | 1.95                     | 0.47              |
| 36:Ah:12:LYS:NZ      | 36:Ah:20:GLN:OE1     | 2.38                     | 0.47              |
| 45:BA:73:VAL:HG13    | 45:BA:120:LEU:HD23   | 1.96                     | 0.47              |
| 46:BB:138:PHE:C      | 46:BB:212:VAL:O      | 2.57                     | 0.47              |
| 64:BT:57:ARG:NH1     | 64:BT:101:ASN:OD1    | 2.47                     | 0.47              |
| 68:BX:19:ARG:O       | 68:BX:23:ARG:HB2     | 2.14                     | 0.47              |
| 71:Ba:44:ILE:HG23    | 71:Ba:45:VAL:HG13    | 1.96                     | 0.47              |
| 79:B5:1483:A:OP2     | 79:B5:1521:G:N2      | 2.47                     | 0.47              |
| 1:A1:2559:U:OP1      | 10:AG:32:LYS:NZ      | 2.47                     | 0.47              |
| 1:A1:3140:G:N7       | 5:AB:28:ARG:NH2      | 2.55                     | 0.47              |
| 7:AD:163:LEU:HD11    | 7:AD:175:HIS:HB3     | 1.96                     | 0.47              |
| 51:BG:74:LYS:HA      | 51:BG:96:SER:HA      | 1.96                     | 0.47              |
| 52:BH:96:ARG:NH1     | 52:BH:128:ASP:OD2    | 2.46                     | 0.47              |
| 1:A1:490:C:O2'       | 1:A1:491:A:N7        | 2.43                     | 0.47              |
| 1:A1:1157:G:O2'      | 1:A1:1169:A:N3       | 2.46                     | 0.47              |
| 10:AG:133:LYS:HD2    | 10:AG:138:HIS:HE1    | 1.79                     | 0.47              |
| 17:AO:177[A]:LYS:HE2 | 17:AO:177[A]:LYS:HB3 | 1.70                     | 0.47              |
| 46:BB:125:VAL:O      | 46:BB:136:ARG:HA     | 2.14                     | 0.47              |
| 49:BE:104:ASP:HB3    | 49:BE:110:ALA:HB2    | 1.97                     | 0.47              |
| 53:BI:49:ARG:O       | 53:BI:52:ASN:ND2     | 2.46                     | 0.47              |
| 57:BM:46:ARG:HD3     | 76:Bf:99:LYS:HD3     | 1.96                     | 0.47              |
| 64:BT:131:ASP:OD1    | 64:BT:134:ARG:NH2    | 2.48                     | 0.47              |
| 1:A1:1347:U:H5''     | 6:AC:303:GLY:H       | 1.79                     | 0.47              |
| 1:A1:2880:U:OP1      | 24:AV:47:ASN:ND2     | 2.38                     | 0.47              |
| 5:AB:41:VAL:HA       | 5:AB:185:GLY:HA3     | 1.97                     | 0.47              |
| 27:AY:11:ASP:HB3     | 27:AY:14:LYS:HB2     | 1.95                     | 0.47              |
| 47:BC:156:THR:HG23   | 67:BW:95:PRO:HB2     | 1.96                     | 0.47              |
| 48:BD:195:SER:OG     | 48:BD:196:ARG:N      | 2.47                     | 0.47              |
| 60:BP:59:LYS:HB3     | 60:BP:76:VAL:HG21    | 1.95                     | 0.47              |
| 1:A1:874:U:OP2       | 5:AB:240:ARG:NH2     | 2.47                     | 0.47              |
| 7:AD:182:GLY:HA2     | 7:AD:194:LEU:HD23    | 1.97                     | 0.47              |
| 51:BG:126:ASP:OD1    | 51:BG:126:ASP:N      | 2.47                     | 0.47              |
| 53:BI:22:ARG:HG3     | 79:B5:385:A:H5''     | 1.97                     | 0.47              |
| 59:BO:121:VAL:O      | 79:B5:886:U:O2'      | 2.33                     | 0.47              |
| 68:BX:30:LYS:HE2     | 68:BX:34:LEU:HD11    | 1.97                     | 0.47              |
| 5:AB:211:GLN:NE2     | 5:AB:283:TYR:O       | 2.48                     | 0.47              |
| 6:AC:92:ASN:OD1      | 6:AC:92:ASN:N        | 2.48                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AF:155:LYS:HG3   | 9:AF:158:LYS:HA    | 1.96                     | 0.47              |
| 19:AQ:147:ARG:HB3  | 19:AQ:150:VAL:HG23 | 1.96                     | 0.47              |
| 48:BD:192:PRO:HB2  | 48:BD:201:ALA:HA   | 1.97                     | 0.47              |
| 51:BG:120:GLU:HG3  | 51:BG:125:THR:HB   | 1.97                     | 0.47              |
| 67:BW:31:SER:HB2   | 79:B5:636:A:H5''   | 1.96                     | 0.47              |
| 79:B5:31:C:O2'     | 79:B5:547:U:OP1    | 2.32                     | 0.47              |
| 79:B5:580:A:O2'    | 79:B5:582:U:OP1    | 2.33                     | 0.47              |
| 79:B5:1114:G:O2'   | 79:B5:1130:G:O6    | 2.31                     | 0.47              |
| 79:B5:1785:U:H2'   | 79:B5:1786:G:H8    | 1.80                     | 0.47              |
| 1:A1:655:C:H2'     | 1:A1:656:A:C8      | 2.49                     | 0.47              |
| 1:A1:1686:U:O4     | 23:AU:82:LYS:NZ    | 2.43                     | 0.47              |
| 1:A1:1721:U:OP2    | 20:AR:124:TYR:OH   | 2.27                     | 0.47              |
| 1:A1:2617:U:H3'    | 30:Ab:3:LYS:HD3    | 1.97                     | 0.47              |
| 1:A1:3003:G:HO2'   | 5:AB:92:TYR:HH     | 1.57                     | 0.47              |
| 3:A4:58:G:O6       | 38:Aj:63:ARG:NH2   | 2.47                     | 0.47              |
| 7:AD:277:LEU:HD22  | 7:AD:281:GLU:HG3   | 1.96                     | 0.47              |
| 16:AN:80:THR:HB    | 16:AN:87:GLN:HG2   | 1.96                     | 0.47              |
| 21:AS:81:TYR:CE1   | 21:AS:90:MET:HE3   | 2.50                     | 0.47              |
| 45:BA:197:ILE:HG23 | 45:BA:201:LEU:HD21 | 1.96                     | 0.47              |
| 49:BE:22:LYS:N     | 79:B5:773:C:OP1    | 2.44                     | 0.47              |
| 58:BN:49:GLN:HA    | 58:BN:52:VAL:HG12  | 1.95                     | 0.47              |
| 63:BS:140:THR:O    | 63:BS:143:ARG:NH1  | 2.47                     | 0.47              |
| 68:BX:126:LYS:HE2  | 68:BX:129:GLY:HA2  | 1.96                     | 0.47              |
| 1:A1:908:OMG:HN1   | 1:A1:2414:G:H5''   | 1.80                     | 0.47              |
| 1:A1:1809:A:OP2    | 28:AZ:65:ARG:NH1   | 2.47                     | 0.47              |
| 1:A1:2588:U:OP1    | 10:AG:241:LYS:NZ   | 2.47                     | 0.47              |
| 1:A1:3086:A:H4'    | 5:AB:366:GLY:HA2   | 1.95                     | 0.47              |
| 1:A1:3164:C:O2'    | 1:A1:3165:A:O4'    | 2.33                     | 0.47              |
| 11:AH:186:PHE:HB2  | 11:AH:189:GLU:HB2  | 1.97                     | 0.47              |
| 49:BE:131:LEU:HD12 | 79:B5:251:A:H2     | 1.80                     | 0.47              |
| 57:BM:86:VAL:HG13  | 57:BM:140:PHE:HE1  | 1.80                     | 0.47              |
| 76:Bf:120:GLU:HB3  | 76:Bf:129:GLY:HA2  | 1.97                     | 0.47              |
| 79:B5:1553:G:N1    | 79:B5:1556:A:OP2   | 2.46                     | 0.47              |
| 1:A1:269:G:H5''    | 16:AN:14:LYS:HE2   | 1.97                     | 0.47              |
| 1:A1:896:A:H5''    | 4:AA:183:GLY:HA2   | 1.97                     | 0.47              |
| 1:A1:1324:U:H4'    | 21:AS:2:ALA:HB2    | 1.95                     | 0.47              |
| 6:AC:208:VAL:HA    | 6:AC:228:ALA:O     | 2.14                     | 0.47              |
| 16:AN:18:VAL:HG13  | 16:AN:19:LEU:HD12  | 1.97                     | 0.47              |
| 31:Ac:9:SER:OG     | 31:Ac:10:ILE:N     | 2.45                     | 0.47              |
| 49:BE:30:ARG:NH2   | 79:B5:298:C:O3'    | 2.48                     | 0.47              |
| 79:B5:34:G:O2'     | 79:B5:515:A:O2'    | 2.32                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:1312:C:O2'    | 17:AO:83[A]:ALA:O  | 2.32                     | 0.47              |
| 1:A1:1386:A:O4'    | 6:AC:141:ARG:NH2   | 2.48                     | 0.47              |
| 10:AG:25:PRO:HB2   | 28:AZ:125:GLY:H    | 1.80                     | 0.47              |
| 12:AI:30:LYS:HD3   | 12:AI:63:GLU:HG3   | 1.97                     | 0.47              |
| 27:AY:23:PRO:HG2   | 27:AY:26:GLN:HG3   | 1.97                     | 0.47              |
| 34:Af:6:ARG:NH1    | 34:Af:8:TYR:O      | 2.48                     | 0.47              |
| 45:BA:20:ALA:HB2   | 62:BR:91:LEU:HD21  | 1.96                     | 0.47              |
| 48:BD:109:LEU:HD22 | 48:BD:115:ILE:HD13 | 1.97                     | 0.47              |
| 1:A1:950:G:N1      | 1:A1:1368:U:OP2    | 2.39                     | 0.46              |
| 1:A1:2896:A:OP1    | 41:Am:124:LYS:NZ   | 2.45                     | 0.46              |
| 1:A1:3352:U:O2'    | 53:BI:162:ALA:O    | 2.29                     | 0.46              |
| 25:AW:18:GLY:HA3   | 25:AW:31:PHE:O     | 2.15                     | 0.46              |
| 45:BA:156:VAL:O    | 66:BV:65:SER:OG    | 2.31                     | 0.46              |
| 48:BD:23:GLU:OE1   | 55:BK:61:TRP:NE1   | 2.33                     | 0.46              |
| 67:BW:81:VAL:O     | 67:BW:122:SER:OG   | 2.29                     | 0.46              |
| 1:A1:911:C:OP1     | 4:AA:14:SER:OG     | 2.33                     | 0.46              |
| 1:A1:1864:A:OP1    | 20:AR:88:ARG:NH1   | 2.46                     | 0.46              |
| 1:A1:3016:A:H2'    | 1:A1:3017:A:C8     | 2.50                     | 0.46              |
| 6:AC:138:ARG:HE    | 6:AC:240:PRO:HD2   | 1.79                     | 0.46              |
| 7:AD:211:LEU:HD12  | 7:AD:223:PHE:HE2   | 1.80                     | 0.46              |
| 45:BA:31:VAL:HA    | 45:BA:34:GLU:HG3   | 1.96                     | 0.46              |
| 45:BA:123:VAL:HG21 | 45:BA:133:ILE:HD11 | 1.97                     | 0.46              |
| 63:BS:138:THR:N    | 79:B5:1458:G:OP1   | 2.47                     | 0.46              |
| 78:Bh:55:SER:HA    | 78:Bh:59:GLY:HA3   | 1.97                     | 0.46              |
| 79:B5:816:G:H2'    | 79:B5:817:A:H8     | 1.81                     | 0.46              |
| 79:B5:1716:C:O2'   | 79:B5:1717:G:O4'   | 2.28                     | 0.46              |
| 1:A1:1724:U:H1'    | 1:A1:1725:C:C6     | 2.50                     | 0.46              |
| 3:A4:27:U:H4'      | 6:AC:51:ALA:HB3    | 1.97                     | 0.46              |
| 5:AB:219:ALA:HB2   | 5:AB:336:VAL:HG23  | 1.98                     | 0.46              |
| 6:AC:31:ARG:HG3    | 6:AC:120:TYR:HE2   | 1.80                     | 0.46              |
| 6:AC:361:HIS:O     | 21:AS:28:ARG:NH2   | 2.47                     | 0.46              |
| 15:AM:121:MET:HB3  | 15:AM:121:MET:HE2  | 1.78                     | 0.46              |
| 20:AR:21:LYS:HE2   | 20:AR:55:VAL:HA    | 1.98                     | 0.46              |
| 47:BC:67:GLN:HA    | 47:BC:70:ASP:HB2   | 1.96                     | 0.46              |
| 60:BP:49:MET:SD    | 60:BP:49:MET:N     | 2.89                     | 0.46              |
| 65:BU:87:HIS:ND1   | 79:B5:1383:G:OP1   | 2.48                     | 0.46              |
| 74:Bd:32:ARG:NH1   | 79:B5:1597:A:OP2   | 2.46                     | 0.46              |
| 77:Bg:70:ASP:HB3   | 77:Bg:113:VAL:HG12 | 1.97                     | 0.46              |
| 1:A1:1497:C:O2'    | 1:A1:1602:A:N3     | 2.43                     | 0.46              |
| 1:A1:1915:A:H5''   | 20:AR:84:THR:HG22  | 1.98                     | 0.46              |
| 1:A1:2768:U:H2'    | 1:A1:2769:A:H8     | 1.79                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:3109:G:N2     | 11:AH:156:GLN:OE1  | 2.47                     | 0.46              |
| 12:AI:145:LYS:HD2  | 12:AI:167:LEU:HD11 | 1.96                     | 0.46              |
| 24:AV:101:VAL:HG11 | 24:AV:114:ILE:HG12 | 1.97                     | 0.46              |
| 46:BB:137:ILE:HG21 | 46:BB:172:LEU:HD22 | 1.96                     | 0.46              |
| 47:BC:116:LYS:HG2  | 47:BC:127:ALA:HB3  | 1.97                     | 0.46              |
| 51:BG:12:SER:OG    | 51:BG:124:LEU:O    | 2.33                     | 0.46              |
| 63:BS:82:PRO:HD3   | 64:BT:36:ILE:HD11  | 1.98                     | 0.46              |
| 65:BU:60:THR:HG23  | 79:B5:1382:A:H5''  | 1.97                     | 0.46              |
| 79:B5:392:G:O2'    | 79:B5:1673:G:N3    | 2.47                     | 0.46              |
| 1:A1:3068:U:OP2    | 20:AR:62:ARG:NH1   | 2.38                     | 0.46              |
| 13:AJ:108:GLU:HA   | 13:AJ:122:ILE:HG13 | 1.98                     | 0.46              |
| 16:AN:11:GLN:HA    | 16:AN:19:LEU:HD21  | 1.97                     | 0.46              |
| 20:AR:105:LEU:HD13 | 20:AR:135:LYS:HE3  | 1.98                     | 0.46              |
| 24:AV:87:ARG:HH22  | 24:AV:137:VAL:HG21 | 1.80                     | 0.46              |
| 41:Am:99:CYS:HB2   | 41:Am:114:LYS:HE3  | 1.97                     | 0.46              |
| 52:BH:49:ILE:HG13  | 52:BH:172:VAL:HG23 | 1.97                     | 0.46              |
| 79:B5:1688:U:H1'   | 79:B5:1713:G:H22   | 1.80                     | 0.46              |
| 1:A1:860:G:C5      | 4:AA:181:LYS:HB2   | 2.50                     | 0.46              |
| 1:A1:1446:A:H5''   | 18:AP:65:SER:HB2   | 1.97                     | 0.46              |
| 2:A3:7:G:OP1       | 7:AD:33:ARG:NH1    | 2.48                     | 0.46              |
| 5:AB:346:THR:HG22  | 5:AB:351:LEU:HD11  | 1.98                     | 0.46              |
| 11:AH:23:ARG:HE    | 11:AH:39:LYS:HA    | 1.80                     | 0.46              |
| 15:AM:17:VAL:HG11  | 15:AM:74:ARG:HA    | 1.96                     | 0.46              |
| 24:AV:28:ASN:HD21  | 24:AV:112:SER:HB2  | 1.80                     | 0.46              |
| 29:Aa:74:ASN:HB3   | 29:Aa:115:LYS:HB3  | 1.98                     | 0.46              |
| 57:BM:52:LEU:HG    | 57:BM:122:VAL:HG13 | 1.97                     | 0.46              |
| 58:BN:61:THR:OG1   | 58:BN:62:GLN:N     | 2.49                     | 0.46              |
| 63:BS:123:ARG:HG3  | 63:BS:133:VAL:HB   | 1.98                     | 0.46              |
| 1:A1:67:A:O2'      | 1:A1:315:C:O2      | 2.30                     | 0.46              |
| 1:A1:448:U:O2'     | 1:A1:489:U:OP1     | 2.30                     | 0.46              |
| 1:A1:1412:G:OP1    | 33:Ae:105:ARG:NH1  | 2.48                     | 0.46              |
| 1:A1:2512:C:H5''   | 10:AG:249:ARG:HH22 | 1.80                     | 0.46              |
| 1:A1:3058:U:O4     | 32:Ad:65:LYS:NZ    | 2.41                     | 0.46              |
| 38:Aj:72:ARG:HA    | 38:Aj:75:LYS:HE2   | 1.97                     | 0.46              |
| 45:BA:111:ILE:HD11 | 79:B5:1292:G:H21   | 1.80                     | 0.46              |
| 47:BC:188:LEU:HD13 | 47:BC:196:VAL:HG11 | 1.98                     | 0.46              |
| 48:BD:75:LYS:NZ    | 55:BK:18:GLU:OE2   | 2.48                     | 0.46              |
| 79:B5:217:A:N1     | 79:B5:844:A:O2'    | 2.47                     | 0.46              |
| 79:B5:513:U:H2'    | 79:B5:514:G:C8     | 2.50                     | 0.46              |
| 79:B5:1591:C:H2'   | 79:B5:1592:A:C8    | 2.50                     | 0.46              |
| 1:A1:115:A:OP2     | 16:AN:49:ARG:NE    | 2.38                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:651:G:O2'     | 1:A1:1435:A:OP1    | 2.26                     | 0.46              |
| 1:A1:1813:A:H4'    | 1:A1:1817:G:H1'    | 1.98                     | 0.46              |
| 1:A1:1914:G:O2'    | 20:AR:82:LYS:O     | 2.30                     | 0.46              |
| 1:A1:2357:A:H2'    | 1:A1:2358:A:C8     | 2.51                     | 0.46              |
| 8:AE:66:SER:HB2    | 8:AE:76:LEU:HD23   | 1.97                     | 0.46              |
| 45:BA:79:ARG:HH12  | 45:BA:164:ASN:HB3  | 1.81                     | 0.46              |
| 45:BA:83:GLN:HE22  | 45:BA:100:GLY:HA2  | 1.81                     | 0.46              |
| 48:BD:163:PRO:HA   | 48:BD:166:ASP:HB2  | 1.98                     | 0.46              |
| 79:B5:800:U:H2'    | 79:B5:801:G:C8     | 2.51                     | 0.46              |
| 1:A1:683:U:H5'     | 16:AN:204:LYS:HE3  | 1.97                     | 0.46              |
| 12:AI:49:CYS:HB3   | 12:AI:168:SER:HB3  | 1.97                     | 0.46              |
| 46:BB:100:PHE:HB3  | 46:BB:181:LEU:HD21 | 1.97                     | 0.46              |
| 71:Ba:12:LYS:HZ2   | 71:Ba:16:GLY:H     | 1.64                     | 0.46              |
| 79:B5:65:A:H2      | 79:B5:84:A:H62     | 1.63                     | 0.46              |
| 1:A1:1795:U:C2     | 44:Ap:51:ALA:HB2   | 2.51                     | 0.46              |
| 3:A4:110:C:O2'     | 3:A4:112:U:OP2     | 2.28                     | 0.46              |
| 29:Aa:24:LYS:O     | 29:Aa:26:ARG:HG2   | 2.16                     | 0.46              |
| 59:BO:72:LYS:HA    | 59:BO:72:LYS:HD3   | 1.80                     | 0.46              |
| 77:Bg:159:ASN:ND2  | 77:Bg:163:ASP:OD1  | 2.42                     | 0.46              |
| 79:B5:1592:A:H2'   | 79:B5:1593:A:C8    | 2.52                     | 0.46              |
| 1:A1:1019:G:N2     | 1:A1:1034:U:OP1    | 2.49                     | 0.45              |
| 1:A1:2253:G:H22    | 1:A1:2264:U:H5     | 1.62                     | 0.45              |
| 5:AB:292:ALA:HB1   | 5:AB:295:ALA:HB3   | 1.98                     | 0.45              |
| 11:AH:90:MET:HB2   | 11:AH:144:ILE:HG23 | 1.97                     | 0.45              |
| 46:BB:88:VAL:HG11  | 46:BB:96:LEU:HD13  | 1.99                     | 0.45              |
| 46:BB:117:TRP:HE1  | 79:B5:1799:U:H5'   | 1.81                     | 0.45              |
| 49:BE:72:VAL:HG22  | 49:BE:90:ILE:HG12  | 1.98                     | 0.45              |
| 49:BE:148:ARG:HD2  | 79:B5:125:U:H5'    | 1.97                     | 0.45              |
| 52:BH:14:THR:OG1   | 52:BH:15:GLU:N     | 2.38                     | 0.45              |
| 54:BJ:134:ILE:HD12 | 54:BJ:134:ILE:H    | 1.80                     | 0.45              |
| 63:BS:86:LEU:HD22  | 63:BS:99:HIS:HB2   | 1.98                     | 0.45              |
| 1:A1:1522:U:OP1    | 26:AX:123:TYR:OH   | 2.31                     | 0.45              |
| 1:A1:1696:A:H2'    | 1:A1:1697:A:C8     | 2.51                     | 0.45              |
| 1:A1:2827:U:O2'    | 1:A1:2829:U:O4     | 2.31                     | 0.45              |
| 1:A1:3016:A:H2'    | 1:A1:3017:A:H8     | 1.81                     | 0.45              |
| 58:BN:5:HIS:HD2    | 79:B5:627:C:H5''   | 1.80                     | 0.45              |
| 64:BT:117:SER:HB2  | 64:BT:123:ARG:HG3  | 1.97                     | 0.45              |
| 67:BW:24:GLN:HA    | 67:BW:63:VAL:O     | 2.15                     | 0.45              |
| 79:B5:906:A:H2     | 79:B5:998:A:H1'    | 1.81                     | 0.45              |
| 1:A1:571:U:H2'     | 1:A1:572:A:H8      | 1.82                     | 0.45              |
| 1:A1:2815:OMG:N2   | 1:A1:2818:U:O2     | 2.41                     | 0.45              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 33:Ae:9:ILE:HG12   | 33:Ae:63:THR:HB      | 1.98                     | 0.45              |
| 48:BD:113:LEU:HD22 | 48:BD:118:ALA:HB2    | 1.99                     | 0.45              |
| 65:BU:53:LYS:HB2   | 65:BU:92:ASP:HB2     | 1.98                     | 0.45              |
| 1:A1:26:A:N3       | 1:A1:328:U:O2'       | 2.44                     | 0.45              |
| 1:A1:1836:C:O2'    | 1:A1:1842:A:N1       | 2.43                     | 0.45              |
| 3:A4:26:U:O2'      | 6:AC:51:ALA:O        | 2.33                     | 0.45              |
| 16:AN:45:PRO:O     | 16:AN:49:ARG:HG3     | 2.17                     | 0.45              |
| 17:AO:115[A]:LYS:O | 17:AO:117[A]:ARG:NH1 | 2.46                     | 0.45              |
| 48:BD:196:ARG:HH11 | 48:BD:200:LYS:HD3    | 1.81                     | 0.45              |
| 49:BE:79:ASP:HB3   | 49:BE:82:TYR:HB2     | 1.98                     | 0.45              |
| 50:BF:103:ASN:HA   | 50:BF:106:LYS:HD2    | 1.98                     | 0.45              |
| 74:Bd:34:TYR:OH    | 79:B5:1487:A:OP1     | 2.31                     | 0.45              |
| 79:B5:781:U:O2'    | 79:B5:782:U:O4'      | 2.31                     | 0.45              |
| 1:A1:1778:G:O2'    | 1:A1:1780:G:OP2      | 2.31                     | 0.45              |
| 16:AN:84:PRO:HA    | 16:AN:87:GLN:HG3     | 1.99                     | 0.45              |
| 17:AO:126[A]:VAL:O | 21:AS:154:HIS:NE2    | 2.48                     | 0.45              |
| 34:Af:16:TYR:OH    | 34:Af:89:LEU:O       | 2.28                     | 0.45              |
| 47:BC:39:THR:O     | 47:BC:42:GLY:N       | 2.44                     | 0.45              |
| 56:BL:46:LYS:HB2   | 56:BL:46:LYS:HE2     | 1.84                     | 0.45              |
| 74:Bd:20:GLN:HB2   | 74:Bd:25:SER:HA      | 1.98                     | 0.45              |
| 74:Bd:42:CYS:SG    | 79:B5:1433:G:N2      | 2.80                     | 0.45              |
| 79:B5:1171:A:H2'   | 79:B5:1172:G:H8      | 1.82                     | 0.45              |
| 1:A1:52:A:N3       | 1:A1:811:U:O2'       | 2.50                     | 0.45              |
| 1:A1:2555:G:O6     | 35:Ag:99:LYS:NZ      | 2.42                     | 0.45              |
| 4:AA:80:GLU:HG3    | 44:Ap:66:GLY:HA2     | 1.99                     | 0.45              |
| 6:AC:156:LEU:HD12  | 6:AC:159:ILE:HD12    | 1.98                     | 0.45              |
| 10:AG:91:PHE:O     | 10:AG:95:ASN:ND2     | 2.49                     | 0.45              |
| 10:AG:162:LEU:HD21 | 16:AN:45:PRO:HG2     | 1.98                     | 0.45              |
| 22:AT:46:GLY:O     | 22:AT:49:GLN:NE2     | 2.50                     | 0.45              |
| 27:AY:116:LYS:HG2  | 27:AY:126:LEU:HD11   | 1.99                     | 0.45              |
| 56:BL:101:GLU:OE1  | 68:BX:16:ARG:NH1     | 2.46                     | 0.45              |
| 63:BS:65:GLU:HG2   | 63:BS:68:ARG:HH21    | 1.81                     | 0.45              |
| 68:BX:92:CYS:HA    | 68:BX:95:PHE:HD2     | 1.81                     | 0.45              |
| 68:BX:96:VAL:HA    | 68:BX:127:VAL:HG21   | 1.99                     | 0.45              |
| 72:Bb:15:GLU:OE1   | 72:Bb:18:LYS:NZ      | 2.47                     | 0.45              |
| 79:B5:1592:A:H2'   | 79:B5:1593:A:H8      | 1.82                     | 0.45              |
| 79:B5:1672:G:H2'   | 79:B5:1673:G:C8      | 2.52                     | 0.45              |
| 79:B5:1717:G:H2'   | 79:B5:1718:G:C8      | 2.51                     | 0.45              |
| 1:A1:957:C:H1'     | 29:Aa:43:ILE:HD11    | 1.99                     | 0.45              |
| 1:A1:2814:G:OP1    | 6:AC:73:ARG:NH1      | 2.45                     | 0.45              |
| 46:BB:166:LYS:HB2  | 46:BB:166:LYS:HE2    | 1.76                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 51:BG:74:LYS:HG2   | 51:BG:96:SER:HB3    | 1.99                     | 0.45              |
| 60:BP:97:TYR:OH    | 79:B5:1211:A:N3     | 2.41                     | 0.45              |
| 1:A1:505:G:H5''    | 6:AC:315:LYS:HA     | 1.99                     | 0.45              |
| 1:A1:1686:U:OP1    | 23:AU:42:LYS:NZ     | 2.38                     | 0.45              |
| 11:AH:21:LYS:HG3   | 11:AH:22:SER:H      | 1.82                     | 0.45              |
| 23:AU:49:ASN:HD22  | 23:AU:49:ASN:C      | 2.23                     | 0.45              |
| 45:BA:90:ALA:HA    | 45:BA:95:ALA:HB3    | 1.99                     | 0.45              |
| 53:BI:169:ILE:HD12 | 53:BI:179:CYS:HB3   | 1.99                     | 0.45              |
| 63:BS:37:GLY:O     | 63:BS:99:HIS:NE2    | 2.45                     | 0.45              |
| 77:Bg:74:THR:HA    | 77:Bg:115:ILE:HD11  | 1.98                     | 0.45              |
| 77:Bg:112:SER:HB3  | 77:Bg:154:VAL:HG22  | 1.99                     | 0.45              |
| 79:B5:1240:U:H3    | 79:B5:1242:A:HO2'   | 1.65                     | 0.45              |
| 1:A1:1333:C:OP1    | 19:AQ:2:GLY:N       | 2.49                     | 0.45              |
| 1:A1:1378:U:H2'    | 1:A1:1379:G:H8      | 1.82                     | 0.45              |
| 1:A1:2809:C:H5''   | 1:A1:2956:A:H5''    | 1.99                     | 0.45              |
| 1:A1:2989:U:O2'    | 5:AB:267:ALA:O      | 2.26                     | 0.45              |
| 27:AY:51:ARG:HG2   | 27:AY:52:ARG:H      | 1.81                     | 0.45              |
| 47:BC:139:ILE:HD13 | 47:BC:191:ALA:HB1   | 1.99                     | 0.45              |
| 52:BH:64:VAL:HG22  | 52:BH:94:ALA:HB1    | 1.98                     | 0.45              |
| 53:BI:3:ILE:O      | 53:BI:30:GLY:N      | 2.50                     | 0.45              |
| 59:BO:20:TYR:HB3   | 59:BO:27:PHE:HB2    | 1.99                     | 0.45              |
| 59:BO:21:ALA:HB2   | 59:BO:98:GLY:HA3    | 1.99                     | 0.45              |
| 68:BX:130:VAL:HG11 | 68:BX:142:LYS:HA    | 1.99                     | 0.45              |
| 75:Be:13:LYS:NZ    | 75:Be:17:GLN:OE1    | 2.49                     | 0.45              |
| 1:A1:2402:A:H2'    | 6:AC:67:THR:HG21    | 1.99                     | 0.45              |
| 1:A1:2880:U:H5''   | 5:AB:236:LYS:HD3    | 1.99                     | 0.45              |
| 6:AC:42:VAL:HG12   | 6:AC:236:LEU:HD21   | 1.99                     | 0.45              |
| 46:BB:53:GLY:HA2   | 46:BB:54:LEU:HA     | 1.58                     | 0.45              |
| 52:BH:78:THR:HG23  | 52:BH:90:VAL:HG13   | 1.99                     | 0.45              |
| 55:BK:60:SER:HB3   | 55:BK:65:TYR:HE2    | 1.82                     | 0.45              |
| 57:BM:65:SER:HB3   | 57:BM:91:VAL:HB     | 1.99                     | 0.45              |
| 79:B5:1466:G:O2'   | 79:B5:1602:C:OP1    | 2.31                     | 0.45              |
| 1:A1:1175:C:H1'    | 17:AO:87[A]:MET:HG2 | 1.99                     | 0.44              |
| 1:A1:1661:G:H2'    | 1:A1:1662:G:C8      | 2.52                     | 0.44              |
| 9:AF:54:GLU:OE2    | 9:AF:186:HIS:NE2    | 2.48                     | 0.44              |
| 18:AP:33:ALA:HB1   | 18:AP:117:ILE:HG12  | 1.98                     | 0.44              |
| 27:AY:3:LYS:HD2    | 27:AY:8:VAL:HG13    | 1.98                     | 0.44              |
| 48:BD:141:LYS:O    | 48:BD:179:GLN:NE2   | 2.43                     | 0.44              |
| 49:BE:141:THR:OG1  | 49:BE:143:ASP:OD1   | 2.35                     | 0.44              |
| 51:BG:2:LYS:HG2    | 51:BG:17:GLU:HG3    | 1.99                     | 0.44              |
| 54:BJ:114:TYR:HA   | 54:BJ:119:ALA:HB3   | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BM:44:GLY:HA2   | 79:B5:1227:A:C2    | 2.51                     | 0.44              |
| 58:BN:6:SER:OG     | 58:BN:7:ALA:N      | 2.50                     | 0.44              |
| 64:BT:86:ARG:NH1   | 64:BT:90:PRO:O     | 2.45                     | 0.44              |
| 67:BW:14:ILE:HA    | 67:BW:25:VAL:HG11  | 1.98                     | 0.44              |
| 71:Ba:46:GLU:HB3   | 71:Ba:48:ALA:H     | 1.81                     | 0.44              |
| 79:B5:1717:G:H2'   | 79:B5:1718:G:H8    | 1.82                     | 0.44              |
| 1:A1:664:U:H2'     | 1:A1:665:A:C8      | 2.53                     | 0.44              |
| 1:A1:1747:G:OP1    | 39:Ak:42:LYS:NZ    | 2.43                     | 0.44              |
| 27:AY:5:SER:HB3    | 27:AY:8:VAL:HG12   | 1.99                     | 0.44              |
| 49:BE:54:TYR:O     | 69:BY:15:ASN:ND2   | 2.51                     | 0.44              |
| 53:BI:76:THR:HG21  | 53:BI:104:ILE:HD12 | 1.98                     | 0.44              |
| 71:Ba:70:LYS:NZ    | 79:B5:933:A:OP1    | 2.35                     | 0.44              |
| 79:B5:1294:G:O2'   | 79:B5:1321:A:N1    | 2.50                     | 0.44              |
| 1:A1:904:A:OP2     | 38:Aj:30:GLN:NE2   | 2.45                     | 0.44              |
| 1:A1:1739:U:O2'    | 35:Ag:56:THR:OG1   | 2.32                     | 0.44              |
| 51:BG:27:PHE:HE1   | 51:BG:36:VAL:HG21  | 1.82                     | 0.44              |
| 57:BM:141:SER:OG   | 57:BM:142:GLN:OE1  | 2.35                     | 0.44              |
| 79:B5:924:A:H2'    | 79:B5:925:G:C8     | 2.53                     | 0.44              |
| 1:A1:715:A:C8      | 29:Aa:115:LYS:HD3  | 2.52                     | 0.44              |
| 1:A1:1129:A:N3     | 1:A1:2826:U:O2'    | 2.44                     | 0.44              |
| 1:A1:2768:U:H2'    | 1:A1:2769:A:C8     | 2.53                     | 0.44              |
| 1:A1:3275:U:H5'    | 34:Af:68:TRP:HZ2   | 1.82                     | 0.44              |
| 2:A3:121:U:H5''    | 7:AD:265:TYR:HE1   | 1.83                     | 0.44              |
| 21:AS:26:ARG:H     | 22:AT:150:THR:HB   | 1.83                     | 0.44              |
| 31:Ac:24:THR:HG22  | 31:Ac:91:SER:HB3   | 1.99                     | 0.44              |
| 44:Ap:36:ARG:HB3   | 44:Ap:45:LYS:HG2   | 1.98                     | 0.44              |
| 51:BG:92:ARG:O     | 79:B5:405:C:O2'    | 2.27                     | 0.44              |
| 69:BY:112:LYS:NZ   | 79:B5:55:A:OP1     | 2.42                     | 0.44              |
| 77:Bg:266:ASP:OD1  | 77:Bg:267:PRO:HD3  | 2.18                     | 0.44              |
| 79:B5:1175:U:H2'   | 79:B5:1176:G:C8    | 2.52                     | 0.44              |
| 5:AB:385:LYS:O     | 5:AB:387:LEU:N     | 2.50                     | 0.44              |
| 9:AF:92:ILE:HD12   | 19:AQ:4:ASP:HB2    | 1.99                     | 0.44              |
| 9:AF:156:ILE:HD12  | 9:AF:161:VAL:HB    | 1.99                     | 0.44              |
| 52:BH:13:PRO:HA    | 52:BH:14:THR:HA    | 1.81                     | 0.44              |
| 53:BI:138:ASN:OD1  | 79:B5:197:A:N6     | 2.51                     | 0.44              |
| 54:BJ:143:ILE:HG21 | 79:B5:768:C:H1'    | 1.99                     | 0.44              |
| 69:BY:44:LEU:HA    | 69:BY:47:VAL:HG12  | 2.00                     | 0.44              |
| 76:Bf:119:ARG:HH22 | 76:Bf:152:ALA:HA   | 1.81                     | 0.44              |
| 77:Bg:275:ARG:HA   | 77:Bg:275:ARG:HD3  | 1.81                     | 0.44              |
| 1:A1:1203:A:H2'    | 1:A1:1204:A:C8     | 2.53                     | 0.44              |
| 1:A1:2592:G:H4'    | 1:A1:2594:C:C2     | 2.53                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 7:AD:68:THR:OG1      | 7:AD:71:GLY:O        | 2.30                     | 0.44              |
| 9:AF:120:THR:HB      | 22:AT:132:PRO:HB2    | 1.99                     | 0.44              |
| 17:AO:155[A]:LYS:HB3 | 17:AO:155[A]:LYS:HE3 | 1.78                     | 0.44              |
| 47:BC:101:VAL:HG12   | 47:BC:115:ILE:HG12   | 1.99                     | 0.44              |
| 50:BF:93:LEU:HD12    | 50:BF:172:ILE:HG23   | 2.00                     | 0.44              |
| 54:BJ:39:LYS:HA      | 54:BJ:42:ILE:HD12    | 2.00                     | 0.44              |
| 69:BY:37:LYS:HG3     | 79:B5:522:U:H5''     | 1.99                     | 0.44              |
| 77:Bg:124:SER:OG     | 77:Bg:134:TRP:NE1    | 2.43                     | 0.44              |
| 79:B5:1174:C:O2'     | 79:B5:1196:A:N6      | 2.51                     | 0.44              |
| 79:B5:1201:G:H21     | 79:B5:1600:A:H5'     | 1.83                     | 0.44              |
| 79:B5:1687:U:N3      | 79:B5:1709:C:OP1     | 2.51                     | 0.44              |
| 1:A1:655:C:H2'       | 1:A1:656:A:H8        | 1.82                     | 0.44              |
| 1:A1:715:A:H8        | 29:Aa:115:LYS:HD3    | 1.82                     | 0.44              |
| 1:A1:1003:A:N1       | 1:A1:1049:C:O2'      | 2.50                     | 0.44              |
| 1:A1:1604:G:H4'      | 1:A1:1835:A:H4'      | 1.99                     | 0.44              |
| 1:A1:2261:G:H1'      | 1:A1:2262:A:H2       | 1.82                     | 0.44              |
| 1:A1:3258:U:O2'      | 1:A1:3260:G:OP1      | 2.31                     | 0.44              |
| 5:AB:73:VAL:O        | 24:AV:86:ARG:NH2     | 2.51                     | 0.44              |
| 12:AI:51:HIS:CD2     | 12:AI:168:SER:HB2    | 2.52                     | 0.44              |
| 31:Ac:92:ILE:HG21    | 31:Ac:100:ILE:HD11   | 1.99                     | 0.44              |
| 44:Ap:23:ARG:HA      | 44:Ap:26:VAL:HG12    | 1.99                     | 0.44              |
| 50:BF:95:ASN:O       | 79:B5:1611:A:O2'     | 2.35                     | 0.44              |
| 79:B5:800:U:H2'      | 79:B5:801:G:H8       | 1.82                     | 0.44              |
| 1:A1:76:G:N7         | 14:AL:101:ARG:HB3    | 2.33                     | 0.44              |
| 1:A1:1376:C:O2'      | 1:A1:1408:G:O2'      | 2.29                     | 0.44              |
| 1:A1:1831:U:O2'      | 3:A4:114:G:OP1       | 2.27                     | 0.44              |
| 1:A1:2955:U:H2'      | 1:A1:2956:A:C8       | 2.53                     | 0.44              |
| 5:AB:287:LYS:HB3     | 5:AB:287:LYS:HE3     | 1.76                     | 0.44              |
| 7:AD:60:ILE:HB       | 7:AD:80:SER:HB3      | 2.00                     | 0.44              |
| 13:AJ:20:ASN:HB2     | 13:AJ:126:ASP:HB2    | 1.99                     | 0.44              |
| 21:AS:132:THR:HG23   | 21:AS:144:LEU:HD13   | 2.00                     | 0.44              |
| 22:AT:101:CYS:SG     | 22:AT:102:ARG:N      | 2.90                     | 0.44              |
| 45:BA:126:PRO:HG3    | 45:BA:147:THR:HG22   | 1.98                     | 0.44              |
| 46:BB:187:LYS:HB3    | 46:BB:193:ILE:HD11   | 2.00                     | 0.44              |
| 52:BH:114:ARG:NH1    | 79:B5:637:C:O2       | 2.45                     | 0.44              |
| 53:BI:48:THR:OG1     | 53:BI:52:ASN:O       | 2.35                     | 0.44              |
| 62:BR:23:LYS:HD3     | 62:BR:23:LYS:HA      | 1.78                     | 0.44              |
| 68:BX:107:PHE:CE2    | 68:BX:114:LYS:HB3    | 2.53                     | 0.44              |
| 79:B5:1354:G:N1      | 79:B5:1369:U:N3      | 2.64                     | 0.44              |
| 1:A1:63:A:H5''       | 16:AN:174:ILE:HG21   | 1.98                     | 0.44              |
| 1:A1:1315:U:H4'      | 1:A1:1317:A:H1'      | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:2218:G:H2'    | 1:A1:2219:A:C8     | 2.53                     | 0.44              |
| 4:AA:127:ALA:HB2   | 4:AA:134:VAL:HG23  | 1.98                     | 0.44              |
| 9:AF:178:ILE:HG23  | 9:AF:183:ASP:HB2   | 1.99                     | 0.44              |
| 12:AI:43:VAL:HG21  | 12:AI:197:VAL:HB   | 1.99                     | 0.44              |
| 13:AJ:92:ARG:HA    | 13:AJ:172:LEU:H    | 1.82                     | 0.44              |
| 16:AN:149:ASN:HB2  | 36:Ah:92:LEU:HD11  | 2.00                     | 0.44              |
| 45:BA:74:VAL:HA    | 45:BA:96:THR:O     | 2.18                     | 0.44              |
| 46:BB:130:SER:HB2  | 46:BB:180:THR:HG22 | 2.00                     | 0.44              |
| 48:BD:204:ASP:OD1  | 48:BD:204:ASP:N    | 2.50                     | 0.44              |
| 53:BI:84:HIS:NE2   | 53:BI:97:THR:OG1   | 2.34                     | 0.44              |
| 60:BP:111:MET:HA   | 63:BS:119:ILE:HD11 | 2.00                     | 0.44              |
| 79:B5:1681:A:N6    | 79:B5:1720:G:O2'   | 2.51                     | 0.44              |
| 1:A1:307:A:H2'     | 1:A1:308:A:C8      | 2.53                     | 0.43              |
| 1:A1:417:A:H2'     | 1:A1:418:A:C8      | 2.53                     | 0.43              |
| 8:AE:14:ASP:OD1    | 8:AE:14:ASP:N      | 2.48                     | 0.43              |
| 10:AG:98:ARG:NH2   | 10:AG:188:THR:O    | 2.51                     | 0.43              |
| 52:BH:9:LEU:HD21   | 52:BH:17:GLU:HG3   | 2.00                     | 0.43              |
| 1:A1:860:G:H5'     | 1:A1:861:C:H5''    | 2.00                     | 0.43              |
| 1:A1:1222:G:H21    | 1:A1:1286:A:H62    | 1.67                     | 0.43              |
| 2:A3:81:U:H2'      | 2:A3:82:G:H8       | 1.82                     | 0.43              |
| 4:AA:80:GLU:HB2    | 4:AA:170:ALA:HA    | 2.01                     | 0.43              |
| 17:AO:21[A]:SER:OG | 17:AO:87[A]:MET:SD | 2.75                     | 0.43              |
| 22:AT:77:ASN:HB3   | 22:AT:84:TYR:HD2   | 1.83                     | 0.43              |
| 29:Aa:34:MET:HB3   | 29:Aa:34:MET:HE3   | 1.81                     | 0.43              |
| 43:Ao:26:THR:HA    | 43:Ao:93:LEU:HD21  | 2.00                     | 0.43              |
| 48:BD:117:ARG:HA   | 78:Bh:123:ALA:HB2  | 2.00                     | 0.43              |
| 49:BE:45:ILE:HG13  | 49:BE:61:VAL:HG21  | 1.99                     | 0.43              |
| 51:BG:188:ARG:HD3  | 79:B5:283:U:H5''   | 1.99                     | 0.43              |
| 54:BJ:83:VAL:HA    | 54:BJ:149:ARG:HA   | 2.00                     | 0.43              |
| 77:Bg:10:ARG:HA    | 77:Bg:10:ARG:HD3   | 1.79                     | 0.43              |
| 79:B5:209:U:H2'    | 79:B5:210:A:C8     | 2.53                     | 0.43              |
| 79:B5:497:G:OP2    | 79:B5:498:G:N2     | 2.48                     | 0.43              |
| 79:B5:1511:U:H2'   | 79:B5:1512:G:C8    | 2.54                     | 0.43              |
| 1:A1:3319:U:H5'    | 1:A1:3320:A:H5'    | 2.00                     | 0.43              |
| 5:AB:187:SER:HB3   | 5:AB:190:GLU:HB2   | 2.01                     | 0.43              |
| 7:AD:33:ARG:HH12   | 7:AD:50:ARG:NH2    | 2.16                     | 0.43              |
| 7:AD:65:ILE:HG12   | 7:AD:74:VAL:HG22   | 2.00                     | 0.43              |
| 46:BB:134:VAL:HB   | 46:BB:219:LYS:HB2  | 2.00                     | 0.43              |
| 48:BD:115:ILE:HG13 | 48:BD:142:LEU:HD11 | 1.99                     | 0.43              |
| 49:BE:160:VAL:HB   | 49:BE:169:ILE:HD12 | 2.00                     | 0.43              |
| 68:BX:73:ARG:NH1   | 68:BX:84:THR:OG1   | 2.52                     | 0.43              |

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| Atom-1              | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 79:B5:1496:U:O2'    | 79:B5:1519:U:O2'      | 2.31                     | 0.43              |
| 1:A1:1247:U:O4      | 1:A1:1270:A:O2'       | 2.29                     | 0.43              |
| 1:A1:3182:G:H4'     | 17:AO:161[A]:LYS:HG2  | 2.01                     | 0.43              |
| 4:AA:111:THR:HB     | 4:AA:136:ILE:HD12     | 1.99                     | 0.43              |
| 6:AC:22:LEU:HA      | 6:AC:23:PRO:HD3       | 1.84                     | 0.43              |
| 14:AL:76:THR:OG1    | 14:AL:101:ARG:NH1     | 2.51                     | 0.43              |
| 45:BA:56:LYS:HE3    | 45:BA:56:LYS:HB3      | 1.86                     | 0.43              |
| 53:BI:25:ARG:HA     | 79:B5:400:A:H5''      | 1.99                     | 0.43              |
| 77:Bg:83:ALA:HB2    | 77:Bg:113:VAL:HB      | 2.00                     | 0.43              |
| 79:B5:92:A:H5''     | 79:B5:93:A:H5''       | 2.01                     | 0.43              |
| 1:A1:19:U:H2'       | 1:A1:20:A:C8          | 2.53                     | 0.43              |
| 1:A1:737:G:H2'      | 1:A1:738:A:H8         | 1.84                     | 0.43              |
| 1:A1:1596:C:H2'     | 1:A1:1597:C:C6        | 2.53                     | 0.43              |
| 1:A1:3121:U:H1'     | 1:A1:3122:A:H5''      | 2.00                     | 0.43              |
| 14:AL:76:THR:O      | 14:AL:79:GLU:N        | 2.42                     | 0.43              |
| 17:AO:37[A]:ARG:HG3 | 17:AO:108[A]:ILE:HG13 | 2.01                     | 0.43              |
| 22:AT:100:LYS:O     | 22:AT:104:GLU:HG2     | 2.18                     | 0.43              |
| 49:BE:88:ASP:OD1    | 49:BE:122:LYS:NZ      | 2.51                     | 0.43              |
| 53:BI:104:ILE:HG13  | 53:BI:105:ASP:H       | 1.83                     | 0.43              |
| 54:BJ:147:MET:HE2   | 54:BJ:147:MET:HB2     | 1.80                     | 0.43              |
| 60:BP:22:LEU:HA     | 60:BP:25:LEU:HG       | 1.99                     | 0.43              |
| 61:BQ:46:PHE:HA     | 61:BQ:49:TYR:HB2      | 1.99                     | 0.43              |
| 61:BQ:48:VAL:HG13   | 61:BQ:78:VAL:HG13     | 2.00                     | 0.43              |
| 68:BX:41:SER:O      | 68:BX:41:SER:OG       | 2.28                     | 0.43              |
| 71:Ba:2:PRO:HB3     | 79:B5:1142:A:H5''     | 1.99                     | 0.43              |
| 74:Bd:7:TRP:O       | 79:B5:1450:U:O2'      | 2.24                     | 0.43              |
| 1:A1:3092:C:O2'     | 1:A1:3094:A:OP2       | 2.26                     | 0.43              |
| 5:AB:106:TRP:O      | 5:AB:137:TYR:OH       | 2.33                     | 0.43              |
| 5:AB:257:PRO:HG2    | 5:AB:261:MET:HE2      | 1.99                     | 0.43              |
| 44:Ap:53:GLY:O      | 44:Ap:65:ALA:HA       | 2.19                     | 0.43              |
| 46:BB:27:LYS:HD3    | 46:BB:47:LEU:HB3      | 2.01                     | 0.43              |
| 53:BI:86:SER:OG     | 79:B5:328:A:N3        | 2.49                     | 0.43              |
| 54:BJ:37:LYS:NZ     | 79:B5:594:A:OP2       | 2.49                     | 0.43              |
| 58:BN:4:MET:HE3     | 58:BN:4:MET:HB2       | 1.87                     | 0.43              |
| 1:A1:727:G:OP2      | 1:A1:742:G:N2         | 2.46                     | 0.43              |
| 1:A1:2160:G:H2'     | 1:A1:2161:G:C8        | 2.54                     | 0.43              |
| 4:AA:52:SER:HB3     | 4:AA:191:LEU:HD23     | 2.01                     | 0.43              |
| 8:AE:150:LYS:HE3    | 8:AE:150:LYS:HB3      | 1.85                     | 0.43              |
| 31:Ac:103:THR:HG22  | 31:Ac:105:ALA:H       | 1.84                     | 0.43              |
| 49:BE:92:LEU:HD13   | 69:BY:17:LEU:HD11     | 2.00                     | 0.43              |
| 57:BM:60:VAL:HG23   | 57:BM:86:VAL:HG21     | 2.01                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 58:BN:46:THR:HB    | 58:BN:49:GLN:HG3    | 2.01                     | 0.43              |
| 61:BQ:44:LEU:HB3   | 61:BQ:78:VAL:HG11   | 2.01                     | 0.43              |
| 69:BY:109:LYS:NZ   | 79:B5:459:G:OP1     | 2.51                     | 0.43              |
| 79:B5:1291:G:H22   | 79:B5:1324:G:N2     | 2.17                     | 0.43              |
| 1:A1:158:G:H2'     | 1:A1:159:A:H8       | 1.84                     | 0.43              |
| 1:A1:2666:C:OP2    | 1:A1:2687:G:N1      | 2.42                     | 0.43              |
| 1:A1:2714:G:OP1    | 43:Ao:20:HIS:NE2    | 2.50                     | 0.43              |
| 3:A4:103:G:OP2     | 3:A4:105:A:O2'      | 2.28                     | 0.43              |
| 19:AQ:158:HIS:H    | 19:AQ:186:VAL:HG12  | 1.83                     | 0.43              |
| 19:AQ:176:ARG:NH1  | 29:Aa:46:ASP:OD2    | 2.46                     | 0.43              |
| 20:AR:159:ALA:HB1  | 20:AR:163:ARG:HH11  | 1.84                     | 0.43              |
| 27:AY:73:VAL:HG13  | 27:AY:80:VAL:HG12   | 2.00                     | 0.43              |
| 29:Aa:77:LYS:O     | 29:Aa:79:TRP:N      | 2.42                     | 0.43              |
| 47:BC:119:LYS:HE3  | 79:B5:1291:G:H5'    | 1.99                     | 0.43              |
| 48:BD:141:LYS:HA   | 78:Bh:110:TRP:HE1   | 1.84                     | 0.43              |
| 51:BG:74:LYS:HE3   | 51:BG:94:ARG:HG3    | 2.00                     | 0.43              |
| 58:BN:22:ALA:HB3   | 58:BN:65:VAL:HG11   | 2.00                     | 0.43              |
| 1:A1:29:C:H4'      | 1:A1:62:A:H4'       | 2.01                     | 0.43              |
| 1:A1:1144:U:OP1    | 1:A1:1367:G:O2'     | 2.29                     | 0.43              |
| 1:A1:2681:U:H2'    | 1:A1:2682:C:H6      | 1.84                     | 0.43              |
| 1:A1:3008:A:OP2    | 17:AO:74[A]:ARG:NH1 | 2.52                     | 0.43              |
| 1:A1:3116:G:N2     | 1:A1:3116:G:OP1     | 2.51                     | 0.43              |
| 2:A3:81:U:H2'      | 2:A3:82:G:C8        | 2.54                     | 0.43              |
| 12:AI:48:LEU:HD11  | 12:AI:167:LEU:HD12  | 2.01                     | 0.43              |
| 19:AQ:20:LYS:HE3   | 19:AQ:20:LYS:HB3    | 1.90                     | 0.43              |
| 31:Ac:99:ASP:OD1   | 31:Ac:99:ASP:N      | 2.52                     | 0.43              |
| 35:Ag:19:LYS:HA    | 35:Ag:19:LYS:HD3    | 1.83                     | 0.43              |
| 43:Ao:25:VAL:HG12  | 43:Ao:93:LEU:HD11   | 2.00                     | 0.43              |
| 54:BJ:105:LEU:HD13 | 54:BJ:108:ARG:HD2   | 2.01                     | 0.43              |
| 57:BM:42:ALA:HB1   | 57:BM:51:ALA:HB1    | 2.01                     | 0.43              |
| 79:B5:980:G:H4'    | 79:B5:1776:A:H4'    | 2.00                     | 0.43              |
| 1:A1:1145:G:O2'    | 33:Ae:45:ARG:O      | 2.34                     | 0.43              |
| 1:A1:2557:A:OP1    | 4:AA:69:TYR:OH      | 2.27                     | 0.43              |
| 1:A1:3002:C:OP1    | 5:AB:26:ARG:NH2     | 2.49                     | 0.43              |
| 1:A1:3252:G:H2'    | 1:A1:3253:G:C8      | 2.54                     | 0.43              |
| 13:AJ:80:LEU:HD21  | 13:AJ:129:VAL:HG21  | 2.01                     | 0.43              |
| 43:Ao:2:VAL:N      | 43:Ao:90:HIS:O      | 2.52                     | 0.43              |
| 45:BA:201:LEU:HB3  | 62:BR:85:VAL:HG22   | 2.00                     | 0.43              |
| 49:BE:107:GLY:HA2  | 49:BE:189:LEU:HG    | 2.01                     | 0.43              |
| 52:BH:177:THR:HG22 | 52:BH:179:LYS:HG3   | 2.01                     | 0.43              |
| 56:BL:99:ARG:HG2   | 68:BX:9:LEU:HA      | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:BQ:68:ARG:HD3   | 61:BQ:68:ARG:HA    | 1.93                     | 0.43              |
| 63:BS:35:ILE:H     | 63:BS:35:ILE:HG13  | 1.68                     | 0.43              |
| 66:BV:44:ARG:HA    | 66:BV:44:ARG:HD3   | 1.85                     | 0.43              |
| 71:Ba:35:ALA:O     | 71:Ba:73:TYR:O     | 2.36                     | 0.43              |
| 73:Bc:41:VAL:HG12  | 73:Bc:63:ALA:HB3   | 2.01                     | 0.43              |
| 79:B5:1279:C:H2'   | 79:B5:1280:4AC:H6  | 2.01                     | 0.43              |
| 1:A1:911:C:H42     | 4:AA:3:ARG:HD3     | 1.84                     | 0.42              |
| 3:A4:8:C:H2'       | 3:A4:9:A:C8        | 2.54                     | 0.42              |
| 5:AB:228:GLY:O     | 5:AB:232:ARG:HB2   | 2.19                     | 0.42              |
| 7:AD:34:LYS:HA     | 22:AT:27:LEU:HD11  | 2.00                     | 0.42              |
| 16:AN:80:THR:HG22  | 16:AN:82:GLY:N     | 2.33                     | 0.42              |
| 31:Ac:17:VAL:HG21  | 31:Ac:100:ILE:HD13 | 2.00                     | 0.42              |
| 46:BB:207:LEU:HD23 | 46:BB:207:LEU:HA   | 1.87                     | 0.42              |
| 49:BE:127:LYS:HD2  | 49:BE:127:LYS:HA   | 1.79                     | 0.42              |
| 51:BG:15:THR:OG1   | 79:B5:153:G:OP1    | 2.31                     | 0.42              |
| 52:BH:23:ALA:HB1   | 52:BH:84:LYS:HD2   | 2.01                     | 0.42              |
| 53:BI:7:SER:O      | 53:BI:18:ARG:NH1   | 2.52                     | 0.42              |
| 54:BJ:115:LYS:HD3  | 54:BJ:115:LYS:HA   | 1.85                     | 0.42              |
| 55:BK:59:PHE:CZ    | 55:BK:62:GLN:HA    | 2.54                     | 0.42              |
| 68:BX:43:PHE:O     | 68:BX:45:GLY:N     | 2.51                     | 0.42              |
| 77:Bg:37:SER:OG    | 77:Bg:38:ARG:N     | 2.50                     | 0.42              |
| 1:A1:148:G:OP2     | 16:AN:4:TYR:OH     | 2.28                     | 0.42              |
| 1:A1:155:G:N1      | 1:A1:265:A:OP2     | 2.40                     | 0.42              |
| 1:A1:422:A:C2      | 1:A1:2363:A:H4'    | 2.54                     | 0.42              |
| 1:A1:2183:A:H5''   | 4:AA:7:ASN:HB2     | 2.00                     | 0.42              |
| 1:A1:2727:A:C2     | 29:Aa:43:ILE:HG23  | 2.54                     | 0.42              |
| 1:A1:3309:G:O6     | 5:AB:21:ARG:NH2    | 2.52                     | 0.42              |
| 12:AI:48:LEU:O     | 12:AI:139:ARG:HA   | 2.19                     | 0.42              |
| 32:Ad:84:ASP:OD1   | 32:Ad:84:ASP:N     | 2.51                     | 0.42              |
| 51:BG:7:TYR:HE2    | 51:BG:10:ASN:ND2   | 2.17                     | 0.42              |
| 77:Bg:109:ASP:OD2  | 77:Bg:127:ARG:NH1  | 2.46                     | 0.42              |
| 77:Bg:260:ILE:O    | 77:Bg:274:LEU:N    | 2.52                     | 0.42              |
| 1:A1:737:G:H2'     | 1:A1:738:A:C8      | 2.54                     | 0.42              |
| 1:A1:1786:G:H2'    | 1:A1:1787:A:C8     | 2.54                     | 0.42              |
| 13:AJ:93:ASP:HB3   | 13:AJ:172:LEU:HD22 | 2.02                     | 0.42              |
| 21:AS:10:ILE:HD12  | 21:AS:60:SER:HB3   | 1.99                     | 0.42              |
| 34:Af:42:GLN:HA    | 34:Af:45:LEU:HG    | 2.00                     | 0.42              |
| 41:Am:110:CYS:SG   | 41:Am:111:ARG:N    | 2.91                     | 0.42              |
| 46:BB:142:PHE:HB2  | 46:BB:208:GLN:HG3  | 2.01                     | 0.42              |
| 49:BE:105:VAL:HG21 | 49:BE:245:LYS:H    | 1.84                     | 0.42              |
| 52:BH:81:LEU:O     | 52:BH:85:PHE:HB2   | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:BK:56:LYS:HE2   | 55:BK:69:THR:HG22  | 2.00                     | 0.42              |
| 59:BO:17:ALA:HB3   | 59:BO:81:VAL:HA    | 2.00                     | 0.42              |
| 61:BQ:13:LYS:HD2   | 61:BQ:13:LYS:HA    | 1.92                     | 0.42              |
| 71:Ba:35:ALA:C     | 71:Ba:73:TYR:O     | 2.62                     | 0.42              |
| 72:Bb:50:ALA:O     | 72:Bb:52:THR:N     | 2.52                     | 0.42              |
| 77:Bg:20:VAL:HB    | 77:Bg:304:GLY:HA3  | 2.01                     | 0.42              |
| 77:Bg:88:THR:HG22  | 77:Bg:104:VAL:HG12 | 2.01                     | 0.42              |
| 79:B5:436:A2M:O5'  | 79:B5:436:A2M:H8   | 2.19                     | 0.42              |
| 79:B5:591:A:H2'    | 79:B5:592:A:C8     | 2.54                     | 0.42              |
| 1:A1:114:A:N1      | 1:A1:266:A:O2'     | 2.44                     | 0.42              |
| 1:A1:1456:A:N1     | 1:A1:1476:G:O2'    | 2.44                     | 0.42              |
| 1:A1:2129:U:H2'    | 1:A1:2130:G:C8     | 2.54                     | 0.42              |
| 1:A1:2895:G:O2'    | 41:Am:100:TYR:O    | 2.30                     | 0.42              |
| 1:A1:3295:A:H2'    | 1:A1:3296:A:C8     | 2.54                     | 0.42              |
| 4:AA:20:THR:HG22   | 4:AA:23:ARG:HD2    | 2.01                     | 0.42              |
| 23:AU:33:TYR:HD2   | 23:AU:63:VAL:HG21  | 1.84                     | 0.42              |
| 28:AZ:90:GLU:HG3   | 28:AZ:93:LYS:HE3   | 2.01                     | 0.42              |
| 45:BA:70:PRO:HB2   | 45:BA:94:GLY:HA3   | 2.01                     | 0.42              |
| 45:BA:120:LEU:HD12 | 45:BA:142:PRO:HB2  | 2.01                     | 0.42              |
| 53:BI:38:ILE:HG12  | 53:BI:96:LEU:HD11  | 2.01                     | 0.42              |
| 59:BO:40:ALA:HB2   | 59:BO:70:LYS:HD3   | 2.01                     | 0.42              |
| 64:BT:77:ASN:HB3   | 64:BT:95:ASP:HB3   | 2.00                     | 0.42              |
| 77:Bg:211:ILE:HD11 | 77:Bg:225:LEU:HD22 | 2.01                     | 0.42              |
| 79:B5:505:A:H2'    | 79:B5:507:U:C2     | 2.55                     | 0.42              |
| 79:B5:753:A:H2     | 79:B5:796:A2M:H62  | 1.67                     | 0.42              |
| 1:A1:528:U:H2'     | 1:A1:529:A:C8      | 2.54                     | 0.42              |
| 1:A1:2728:G:N7     | 22:AT:87:LYS:NZ    | 2.46                     | 0.42              |
| 28:AZ:81:LEU:HD22  | 35:Ag:90:ILE:HG12  | 2.01                     | 0.42              |
| 39:Ak:8:ILE:HG23   | 39:Ak:65:LEU:HD11  | 2.02                     | 0.42              |
| 51:BG:187:LYS:NZ   | 79:B5:139:C:O2'    | 2.52                     | 0.42              |
| 57:BM:50:LYS:HZ2   | 79:B5:1254:U:H3    | 1.67                     | 0.42              |
| 65:BU:103:ILE:HA   | 65:BU:106:ILE:HG12 | 2.02                     | 0.42              |
| 73:Bc:10:ALA:HB1   | 73:Bc:30:VAL:HB    | 2.02                     | 0.42              |
| 77:Bg:48:THR:OG1   | 77:Bg:50:ASP:OD2   | 2.25                     | 0.42              |
| 79:B5:871:G:H2'    | 79:B5:872:G:C8     | 2.54                     | 0.42              |
| 1:A1:2115:G:H22    | 1:A1:2120:A:H1'    | 1.85                     | 0.42              |
| 7:AD:38:THR:HG23   | 22:AT:30:TYR:HB3   | 2.00                     | 0.42              |
| 14:AL:75:PHE:H     | 14:AL:97:VAL:HA    | 1.83                     | 0.42              |
| 22:AT:143:THR:HG23 | 22:AT:148:PRO:HD3  | 2.02                     | 0.42              |
| 23:AU:80:THR:HG21  | 23:AU:95:PHE:CD1   | 2.54                     | 0.42              |
| 27:AY:70:ILE:HA    | 27:AY:82:VAL:HA    | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:Ad:77:ARG:HD2   | 32:Ad:89:LEU:HD13  | 2.00                     | 0.42              |
| 38:Aj:27:PHE:HA    | 38:Aj:34:CYS:HA    | 2.01                     | 0.42              |
| 57:BM:31:VAL:HG11  | 57:BM:136:ILE:HG21 | 2.02                     | 0.42              |
| 63:BS:83:ALA:HA    | 63:BS:86:LEU:HG    | 2.00                     | 0.42              |
| 76:Bf:99:LYS:NZ    | 79:B5:1229:G:N7    | 2.63                     | 0.42              |
| 78:Bh:83:LYS:HD3   | 78:Bh:83:LYS:HA    | 1.88                     | 0.42              |
| 79:B5:209:U:H2'    | 79:B5:210:A:H8     | 1.85                     | 0.42              |
| 1:A1:2228:A:H2'    | 1:A1:2229:A:C8     | 2.55                     | 0.42              |
| 1:A1:2423:U:H2'    | 1:A1:2424:A:C8     | 2.55                     | 0.42              |
| 4:AA:41:ILE:HG12   | 4:AA:63:PHE:HD2    | 1.85                     | 0.42              |
| 9:AF:239:LEU:HG    | 9:AF:243:MET:HE2   | 2.01                     | 0.42              |
| 11:AH:150:SER:HB3  | 11:AH:153:ASP:HB2  | 2.01                     | 0.42              |
| 32:Ad:55:LEU:HB2   | 32:Ad:95:PRO:HD3   | 2.01                     | 0.42              |
| 45:BA:84:ARG:NH2   | 62:BR:84:TYR:O     | 2.43                     | 0.42              |
| 52:BH:91:ILE:HG12  | 52:BH:169:PHE:HE1  | 1.84                     | 0.42              |
| 58:BN:102:LEU:HD23 | 58:BN:102:LEU:HA   | 1.92                     | 0.42              |
| 59:BO:136:ARG:O    | 79:B5:1006:C:O2'   | 2.33                     | 0.42              |
| 63:BS:127:HIS:CD2  | 63:BS:133:VAL:HG11 | 2.55                     | 0.42              |
| 79:B5:58:U:O2'     | 79:B5:451:A:N3     | 2.52                     | 0.42              |
| 79:B5:884:A:H2'    | 79:B5:885:G:C8     | 2.54                     | 0.42              |
| 5:AB:53:MET:HE2    | 5:AB:53:MET:HB3    | 1.96                     | 0.42              |
| 5:AB:113:GLU:OE2   | 5:AB:167:ARG:HG2   | 2.20                     | 0.42              |
| 9:AF:84:VAL:HG23   | 9:AF:117:VAL:HB    | 2.01                     | 0.42              |
| 9:AF:216:VAL:HA    | 9:AF:217:PRO:HD2   | 1.89                     | 0.42              |
| 12:AI:53:VAL:HG21  | 12:AI:166:ILE:HD12 | 2.02                     | 0.42              |
| 19:AQ:161:LYS:HD2  | 19:AQ:161:LYS:HA   | 1.82                     | 0.42              |
| 47:BC:233:GLN:HA   | 47:BC:234:PRO:HD3  | 1.91                     | 0.42              |
| 49:BE:141:THR:HG21 | 49:BE:162:ILE:HD11 | 2.02                     | 0.42              |
| 77:Bg:82:SER:HB3   | 77:Bg:92:TRP:HE1   | 1.85                     | 0.42              |
| 79:B5:29:U:H2'     | 79:B5:30:G:H8      | 1.83                     | 0.42              |
| 79:B5:1397:U:O2'   | 79:B5:1400:A:N6    | 2.53                     | 0.42              |
| 79:B5:1650:U:H2'   | 79:B5:1651:A:C8    | 2.54                     | 0.42              |
| 1:A1:710:A:H2'     | 1:A1:711:A:C8      | 2.55                     | 0.42              |
| 1:A1:1724:U:O4     | 20:AR:125:LYS:NZ   | 2.52                     | 0.42              |
| 1:A1:2960:C:H2'    | 1:A1:2961:G:C8     | 2.55                     | 0.42              |
| 1:A1:3139:A:OP2    | 5:AB:30:LYS:NZ     | 2.36                     | 0.42              |
| 5:AB:83:PRO:O      | 5:AB:165:GLN:NE2   | 2.50                     | 0.42              |
| 6:AC:26:PHE:HA     | 6:AC:127:ALA:HA    | 2.01                     | 0.42              |
| 10:AG:82:LEU:HG    | 10:AG:86:THR:HG23  | 2.02                     | 0.42              |
| 14:AL:62:THR:O     | 14:AL:64:LYS:N     | 2.53                     | 0.42              |
| 14:AL:171:ARG:HA   | 14:AL:171:ARG:HD2  | 1.92                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AS:27:MET:HE2   | 21:AS:27:MET:HB3   | 1.90                     | 0.42              |
| 27:AY:42:GLN:NE2   | 27:AY:127:GLU:O    | 2.47                     | 0.42              |
| 32:Ad:46:THR:HA    | 32:Ad:87:ASN:HD21  | 1.84                     | 0.42              |
| 48:BD:21:LEU:HD12  | 48:BD:21:LEU:HA    | 1.91                     | 0.42              |
| 61:BQ:47:LYS:HB3   | 61:BQ:82:ARG:HD2   | 2.02                     | 0.42              |
| 64:BT:31:PRO:HD2   | 64:BT:34:VAL:HG13  | 2.02                     | 0.42              |
| 69:BY:60:PHE:O     | 79:B5:522:U:O2'    | 2.37                     | 0.42              |
| 72:Bb:18:LYS:O     | 72:Bb:29:ARG:NH2   | 2.43                     | 0.42              |
| 79:B5:538:A:H5'    | 79:B5:543:C:H42    | 1.84                     | 0.42              |
| 79:B5:1359:C:H2'   | 79:B5:1360:A:C8    | 2.55                     | 0.42              |
| 79:B5:1561:U:H4'   | 79:B5:1599:C:H4'   | 2.02                     | 0.42              |
| 1:A1:87:U:H2'      | 1:A1:88:A:C8       | 2.54                     | 0.42              |
| 1:A1:302:U:H5''    | 16:AN:179:LYS:HE3  | 2.01                     | 0.42              |
| 1:A1:2423:U:H2'    | 1:A1:2424:A:H8     | 1.84                     | 0.42              |
| 1:A1:2683:U:H2'    | 1:A1:2684:C:C6     | 2.55                     | 0.42              |
| 6:AC:181:VAL:HG22  | 6:AC:202:ARG:HB2   | 2.01                     | 0.42              |
| 14:AL:5:LYS:H      | 14:AL:5:LYS:HG3    | 1.68                     | 0.42              |
| 29:Aa:36:GLY:HA3   | 29:Aa:40:HIS:CE1   | 2.54                     | 0.42              |
| 33:Ae:126:LEU:HD23 | 33:Ae:126:LEU:HA   | 1.87                     | 0.42              |
| 35:Ag:57:LEU:HB3   | 35:Ag:61:GLN:HB2   | 2.02                     | 0.42              |
| 46:BB:174:LYS:HB3  | 46:BB:174:LYS:HE2  | 1.83                     | 0.42              |
| 48:BD:136:VAL:HG22 | 48:BD:186:VAL:HG22 | 2.00                     | 0.42              |
| 70:BZ:55:PRO:HD3   | 70:BZ:88:ILE:HD12  | 2.01                     | 0.42              |
| 79:B5:1760:G:H1'   | 79:B5:1781:MA6:H2  | 2.02                     | 0.42              |
| 1:A1:848:A:C8      | 79:B5:973:A:H4'    | 2.55                     | 0.41              |
| 1:A1:1794:G:O2'    | 1:A1:1796:G:N2     | 2.53                     | 0.41              |
| 1:A1:1886:A:O2'    | 5:AB:226:PHE:O     | 2.29                     | 0.41              |
| 1:A1:2218:G:H2'    | 1:A1:2219:A:H8     | 1.85                     | 0.41              |
| 1:A1:2759:U:H5''   | 1:A1:2760:C:H5'    | 2.02                     | 0.41              |
| 5:AB:27:ALA:HB2    | 5:AB:220:VAL:HG23  | 2.01                     | 0.41              |
| 9:AF:208:SER:OG    | 9:AF:209:ASN:N     | 2.51                     | 0.41              |
| 10:AG:189:LEU:HD12 | 10:AG:190:VAL:HG13 | 2.02                     | 0.41              |
| 13:AJ:80:LEU:HA    | 13:AJ:80:LEU:HD23  | 1.82                     | 0.41              |
| 14:AL:116:LEU:HD23 | 14:AL:116:LEU:HA   | 1.85                     | 0.41              |
| 38:Aj:29:VAL:O     | 38:Aj:32:LYS:NZ    | 2.51                     | 0.41              |
| 52:BH:113:PRO:HG2  | 52:BH:116:ARG:HD3  | 2.02                     | 0.41              |
| 66:BV:64:GLU:HG2   | 72:Bb:3:LEU:HB2    | 2.00                     | 0.41              |
| 79:B5:565:C:H4'    | 79:B5:566:C:H5''   | 2.02                     | 0.41              |
| 1:A1:40:A:H5''     | 29:Aa:35:ALA:HB1   | 2.02                     | 0.41              |
| 1:A1:627:U:H4'     | 1:A1:1399:A:H1'    | 2.01                     | 0.41              |
| 1:A1:629:U:H2'     | 1:A1:630:A:C8      | 2.55                     | 0.41              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:A1:1497:C:H2'     | 1:A1:1498:A:C8       | 2.54                     | 0.41              |
| 2:A3:112:G:H2'      | 2:A3:113:C:C6        | 2.55                     | 0.41              |
| 15:AM:23:ILE:O      | 15:AM:30:GLY:N       | 2.52                     | 0.41              |
| 27:AY:63:LYS:HD2    | 27:AY:85:VAL:HG13    | 2.02                     | 0.41              |
| 28:AZ:26:VAL:HG11   | 28:AZ:96:VAL:HB      | 2.01                     | 0.41              |
| 29:Aa:56:VAL:HG12   | 29:Aa:57:GLY:H       | 1.84                     | 0.41              |
| 34:Af:49:ILE:HD11   | 34:Af:71:VAL:HG22    | 2.02                     | 0.41              |
| 35:Ag:58:ARG:HD2    | 35:Ag:58:ARG:HA      | 1.86                     | 0.41              |
| 38:Aj:21:ARG:NH2    | 38:Aj:41:ALA:O       | 2.28                     | 0.41              |
| 44:Ap:36:ARG:HG3    | 44:Ap:48:LYS:HD3     | 2.01                     | 0.41              |
| 50:BF:166:ARG:HB2   | 73:Bc:46:GLY:HA3     | 2.02                     | 0.41              |
| 53:BI:121:LEU:HD22  | 53:BI:157:GLU:HG3    | 2.01                     | 0.41              |
| 69:BY:60:PHE:HA     | 69:BY:70:VAL:O       | 2.20                     | 0.41              |
| 79:B5:273:G:O6      | 79:B5:283:U:O2       | 2.37                     | 0.41              |
| 1:A1:345:G:O2'      | 3:A4:25:G:N3         | 2.52                     | 0.41              |
| 1:A1:532:A:H2'      | 1:A1:533:A:C8        | 2.56                     | 0.41              |
| 1:A1:675:C:O2'      | 1:A1:679:U:OP1       | 2.32                     | 0.41              |
| 1:A1:900:G:H1'      | 1:A1:1589:A:N6       | 2.35                     | 0.41              |
| 1:A1:911:C:N4       | 4:AA:3:ARG:HD3       | 2.35                     | 0.41              |
| 1:A1:943:U:H3'      | 29:Aa:13:GLY:HA2     | 2.01                     | 0.41              |
| 1:A1:1646:G:O2'     | 1:A1:1808:G:N2       | 2.37                     | 0.41              |
| 4:AA:3:ARG:HB2      | 4:AA:207:VAL:HG22    | 2.02                     | 0.41              |
| 9:AF:92:ILE:HD11    | 9:AF:110:ARG:HA      | 2.02                     | 0.41              |
| 49:BE:171:ASP:OD2   | 49:BE:171:ASP:N      | 2.52                     | 0.41              |
| 54:BJ:108:ARG:NH1   | 54:BJ:110:GLN:OE1    | 2.51                     | 0.41              |
| 62:BR:34:LEU:HB3    | 77:Bg:150:TRP:CH2    | 2.54                     | 0.41              |
| 62:BR:116:LYS:HA    | 62:BR:116:LYS:HD2    | 1.82                     | 0.41              |
| 67:BW:56:HIS:O      | 79:B5:861:U:O2'      | 2.29                     | 0.41              |
| 79:B5:1188:G:O2'    | 79:B5:1430:U:OP1     | 2.31                     | 0.41              |
| 1:A1:49:A:OP1       | 14:AL:16:LYS:NZ      | 2.38                     | 0.41              |
| 1:A1:1095:U:H4'     | 1:A1:1096:U:H5''     | 2.02                     | 0.41              |
| 1:A1:1497:C:H2'     | 1:A1:1498:A:H8       | 1.86                     | 0.41              |
| 1:A1:1621:A:H2'     | 1:A1:1622:U:C6       | 2.55                     | 0.41              |
| 1:A1:2213:A:H2'     | 1:A1:2214:A:C8       | 2.55                     | 0.41              |
| 6:AC:120:TYR:CE1    | 6:AC:277:PRO:HB3     | 2.55                     | 0.41              |
| 13:AJ:16:LYS:HE3    | 13:AJ:130:VAL:HG21   | 2.03                     | 0.41              |
| 17:AO:64[A]:PHE:HE2 | 17:AO:68[A]:ARG:HH11 | 1.68                     | 0.41              |
| 26:AX:73:MET:HE2    | 26:AX:142:ILE:HB     | 2.02                     | 0.41              |
| 28:AZ:72:ILE:HG22   | 28:AZ:101:PHE:CZ     | 2.55                     | 0.41              |
| 29:Aa:75:LEU:HD11   | 29:Aa:134:ALA:HA     | 2.03                     | 0.41              |
| 35:Ag:3:GLN:HE22    | 35:Ag:29:ILE:HB      | 1.86                     | 0.41              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 46:BB:219:LYS:HB3    | 46:BB:219:LYS:HE3   | 1.76                     | 0.41              |
| 61:BQ:50:GLU:OE1     | 61:BQ:82:ARG:NH2    | 2.53                     | 0.41              |
| 79:B5:968:U:O3'      | 79:B5:1032:G:N2     | 2.53                     | 0.41              |
| 3:A4:74:U:O2'        | 3:A4:76:C:OP2       | 2.37                     | 0.41              |
| 15:AM:19:ARG:NH1     | 15:AM:66:THR:O      | 2.46                     | 0.41              |
| 20:AR:15:VAL:HG23    | 20:AR:17:VAL:HG22   | 2.00                     | 0.41              |
| 43:Ao:100:LYS:HE3    | 43:Ao:100:LYS:HB2   | 1.82                     | 0.41              |
| 48:BD:64:ARG:NH1     | 55:BK:91:TYR:HB2    | 2.35                     | 0.41              |
| 50:BF:80:LYS:HB2     | 50:BF:83:ARG:HG3    | 2.03                     | 0.41              |
| 50:BF:136:ALA:O      | 50:BF:140:THR:HG22  | 2.21                     | 0.41              |
| 53:BI:83:TYR:HB3     | 53:BI:101:ILE:HB    | 2.02                     | 0.41              |
| 53:BI:112:TRP:O      | 53:BI:116:HIS:HB2   | 2.21                     | 0.41              |
| 61:BQ:22:VAL:HG22    | 61:BQ:65:ILE:HG23   | 2.02                     | 0.41              |
| 61:BQ:136:SER:HA     | 79:B5:1581:C:H5'    | 2.03                     | 0.41              |
| 63:BS:101:LEU:HB3    | 63:BS:102:ALA:H     | 1.80                     | 0.41              |
| 65:BU:69:LYS:HG2     | 79:B5:1280:4AC:H5'' | 2.02                     | 0.41              |
| 67:BW:51:GLU:HG2     | 72:Bb:8:LEU:HD11    | 2.03                     | 0.41              |
| 77:Bg:292:LEU:HD12   | 77:Bg:301:LEU:HD11  | 2.02                     | 0.41              |
| 79:B5:17:C:H2'       | 79:B5:18:C:C6       | 2.56                     | 0.41              |
| 1:A1:411:U:H2'       | 1:A1:412:G:H8       | 1.84                     | 0.41              |
| 1:A1:2941:A:OP1      | 1:A1:2943:G:O2'     | 2.35                     | 0.41              |
| 1:A1:3113:A:H4'      | 11:AH:69:ARG:HG3    | 2.02                     | 0.41              |
| 1:A1:3280:U:O2'      | 1:A1:3281:U:O5'     | 2.34                     | 0.41              |
| 1:A1:3348:G:O6       | 1:A1:3357:U:O4      | 2.38                     | 0.41              |
| 14:AL:59:ARG:HA      | 14:AL:59:ARG:HD3    | 1.93                     | 0.41              |
| 17:AO:189[A]:ASP:OD1 | 17:AO:189[A]:ASP:N  | 2.52                     | 0.41              |
| 28:AZ:25:ILE:HG23    | 28:AZ:41:ALA:HB1    | 2.03                     | 0.41              |
| 46:BB:33:LYS:O       | 46:BB:98:THR:OG1    | 2.29                     | 0.41              |
| 49:BE:3:ARG:HG3      | 79:B5:399:A:H4'     | 2.01                     | 0.41              |
| 49:BE:27:TYR:O       | 79:B5:447:U:O2'     | 2.30                     | 0.41              |
| 64:BT:36:ILE:HG23    | 64:BT:37:VAL:HG23   | 2.02                     | 0.41              |
| 64:BT:68:ARG:NE      | 79:B5:1521:G:O6     | 2.51                     | 0.41              |
| 75:Be:31:LYS:HD2     | 79:B5:545:A:H2'     | 2.03                     | 0.41              |
| 79:B5:97:C:O2        | 79:B5:425:A:O2'     | 2.37                     | 0.41              |
| 1:A1:76:G:O2'        | 14:AL:100:ARG:NH1   | 2.44                     | 0.41              |
| 1:A1:662:U:H2'       | 1:A1:663:OMC:C6     | 2.56                     | 0.41              |
| 1:A1:673:U:H2'       | 1:A1:674:G:C8       | 2.56                     | 0.41              |
| 1:A1:804:C:OP1       | 6:AC:98:ARG:NH2     | 2.32                     | 0.41              |
| 1:A1:1750:A:OP1      | 39:Ak:44:LYS:NZ     | 2.36                     | 0.41              |
| 7:AD:52:VAL:HG21     | 7:AD:65:ILE:HD12    | 2.03                     | 0.41              |
| 27:AY:74:TYR:HD2     | 27:AY:77:LYS:HB2    | 1.84                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BA:52:LYS:HE3   | 66:BV:82:VAL:HA    | 2.01                     | 0.41              |
| 60:BP:51:SER:O     | 60:BP:51:SER:OG    | 2.31                     | 0.41              |
| 69:BY:35:VAL:HG23  | 69:BY:36:SER:H     | 1.85                     | 0.41              |
| 79:B5:139:C:N4     | 79:B5:175:G:O2'    | 2.53                     | 0.41              |
| 79:B5:702:G:O6     | 79:B5:737:A:N6     | 2.52                     | 0.41              |
| 79:B5:1175:U:H2'   | 79:B5:1176:G:H8    | 1.85                     | 0.41              |
| 1:A1:746:A:OP1     | 19:AQ:145:ASN:ND2  | 2.53                     | 0.41              |
| 1:A1:1119:C:H2'    | 1:A1:1120:A:C8     | 2.56                     | 0.41              |
| 1:A1:2413:A:H2'    | 1:A1:2414:G:H8     | 1.86                     | 0.41              |
| 1:A1:2683:U:H5'    | 13:AJ:18:VAL:HG11  | 2.02                     | 0.41              |
| 1:A1:3322:A:H2'    | 1:A1:3323:A:C8     | 2.56                     | 0.41              |
| 5:AB:380:MET:HE2   | 5:AB:383:LEU:HD21  | 2.03                     | 0.41              |
| 10:AG:82:LEU:HD13  | 10:AG:222:PHE:HE2  | 1.86                     | 0.41              |
| 10:AG:140:VAL:HG22 | 10:AG:166:LEU:HD21 | 2.03                     | 0.41              |
| 60:BP:103:ASN:OD1  | 60:BP:120:SER:OG   | 2.39                     | 0.41              |
| 67:BW:85:ASP:OD2   | 67:BW:85:ASP:N     | 2.53                     | 0.41              |
| 69:BY:62:THR:HA    | 69:BY:69:SER:HA    | 2.03                     | 0.41              |
| 71:Ba:13:LYS:O     | 71:Ba:15:ARG:NH2   | 2.54                     | 0.41              |
| 74:Bd:15:GLY:O     | 74:Bd:19:ARG:NH1   | 2.54                     | 0.41              |
| 79:B5:818:C:O2'    | 79:B5:819:G:O5'    | 2.34                     | 0.41              |
| 79:B5:1241:G:OP1   | 79:B5:1241:G:N2    | 2.45                     | 0.41              |
| 1:A1:107:A:O2'     | 1:A1:324:A:N3      | 2.50                     | 0.41              |
| 1:A1:609:G:O6      | 6:AC:308:LYS:NZ    | 2.48                     | 0.41              |
| 1:A1:656:A:H2'     | 1:A1:657:A:C8      | 2.56                     | 0.41              |
| 1:A1:985:U:H2'     | 1:A1:986:U:H6      | 1.85                     | 0.41              |
| 1:A1:1190:A:H4'    | 41:Am:113:ARG:NH2  | 2.35                     | 0.41              |
| 1:A1:1351:U:O2     | 1:A1:1355:A:N7     | 2.54                     | 0.41              |
| 1:A1:1466:G:N2     | 1:A1:1510:G:H5''   | 2.36                     | 0.41              |
| 1:A1:2284:C:N4     | 1:A1:2308:C:OP2    | 2.52                     | 0.41              |
| 1:A1:2618:G:H5''   | 12:AI:116:ARG:HB2  | 2.02                     | 0.41              |
| 1:A1:2632:G:H5''   | 22:AT:12:ARG:HB2   | 2.01                     | 0.41              |
| 1:A1:3214:U:C4     | 15:AM:121:MET:HG3  | 2.56                     | 0.41              |
| 1:A1:3294:A:H2'    | 1:A1:3295:A:O4'    | 2.21                     | 0.41              |
| 2:A3:64:A:N7       | 12:AI:209:ASN:ND2  | 2.67                     | 0.41              |
| 5:AB:331:ASN:OD1   | 5:AB:331:ASN:N     | 2.50                     | 0.41              |
| 34:Af:89:LEU:HD23  | 34:Af:89:LEU:HA    | 1.87                     | 0.41              |
| 37:Ai:66:GLU:O     | 37:Ai:70:ARG:HB2   | 2.21                     | 0.41              |
| 45:BA:206:ASP:HA   | 45:BA:207:PRO:HA   | 1.88                     | 0.41              |
| 48:BD:151:LYS:NZ   | 79:B5:1423:U:OP1   | 2.45                     | 0.41              |
| 51:BG:177:ARG:NH2  | 79:B5:143:G:O6     | 2.44                     | 0.41              |
| 52:BH:91:ILE:HG21  | 52:BH:129:LEU:HD12 | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BL:124:THR:HB   | 56:BL:141:LYS:HB3  | 2.03                     | 0.41              |
| 57:BM:106:ILE:HG22 | 57:BM:115:VAL:HG21 | 2.02                     | 0.41              |
| 59:BO:17:ALA:HA    | 59:BO:30:VAL:HG22  | 2.02                     | 0.41              |
| 59:BO:114:ARG:HD3  | 59:BO:114:ARG:HA   | 1.87                     | 0.41              |
| 65:BU:63:LEU:O     | 65:BU:83:GLU:HA    | 2.20                     | 0.41              |
| 71:Ba:17:HIS:NE2   | 79:B5:1789:G:OP1   | 2.41                     | 0.41              |
| 76:Bf:98:VAL:HG23  | 76:Bf:100:LEU:HD23 | 2.01                     | 0.41              |
| 77:Bg:302:PHE:HD1  | 77:Bg:312:VAL:HG22 | 1.86                     | 0.41              |
| 79:B5:1041:G:H2'   | 79:B5:1042:G:C8    | 2.56                     | 0.41              |
| 79:B5:1354:G:C6    | 79:B5:1369:U:N3    | 2.89                     | 0.41              |
| 1:A1:268:A:N1      | 1:A1:295:A:H5'     | 2.36                     | 0.41              |
| 1:A1:1432:C:O2'    | 1:A1:1434:G:OP2    | 2.39                     | 0.41              |
| 1:A1:2819:A:OP1    | 1:A1:2866:U:O2'    | 2.34                     | 0.41              |
| 2:A3:84:A:H2'      | 2:A3:85:G:C8       | 2.55                     | 0.41              |
| 8:AE:72:ASN:HB3    | 8:AE:160:SER:HA    | 2.03                     | 0.41              |
| 16:AN:138:GLN:HA   | 16:AN:143:ARG:HH11 | 1.86                     | 0.41              |
| 37:Ai:56:ARG:HH12  | 37:Ai:76:ARG:HD2   | 1.86                     | 0.41              |
| 46:BB:119:THR:HG21 | 46:BB:161:ILE:HD11 | 2.03                     | 0.41              |
| 48:BD:142:LEU:HB2  | 78:Bh:110:TRP:CD1  | 2.56                     | 0.41              |
| 52:BH:67:LEU:HD11  | 52:BH:94:ALA:HB2   | 2.02                     | 0.41              |
| 53:BI:4:SER:OG     | 53:BI:6:ASP:OD1    | 2.38                     | 0.41              |
| 55:BK:31:LYS:HD3   | 55:BK:31:LYS:HA    | 1.96                     | 0.41              |
| 58:BN:16:ILE:O     | 67:BW:57:ARG:NH2   | 2.50                     | 0.41              |
| 64:BT:5:SER:OG     | 64:BT:6:VAL:N      | 2.53                     | 0.41              |
| 65:BU:57:ARG:HG2   | 65:BU:89:ARG:HG2   | 2.03                     | 0.41              |
| 67:BW:42:GLN:NE2   | 67:BW:48:GLY:O     | 2.50                     | 0.41              |
| 69:BY:82:ALA:O     | 69:BY:86:GLU:HB2   | 2.20                     | 0.41              |
| 71:Ba:53:LEU:O     | 71:Ba:57:SER:CB    | 2.68                     | 0.41              |
| 73:Bc:27:GLN:OE1   | 73:Bc:65:ARG:O     | 2.39                     | 0.41              |
| 1:A1:1490:A:O2'    | 38:Aj:12:HIS:O     | 2.34                     | 0.40              |
| 1:A1:1899:G:O2'    | 1:A1:2334:U:O4     | 2.30                     | 0.40              |
| 11:AH:99:ILE:HG22  | 11:AH:101:VAL:HG23 | 2.02                     | 0.40              |
| 13:AJ:110:ILE:HG13 | 13:AJ:111:ASP:H    | 1.86                     | 0.40              |
| 15:AM:46:ILE:HD11  | 15:AM:56:GLN:HE21  | 1.86                     | 0.40              |
| 18:AP:116:HIS:HB3  | 18:AP:149:VAL:HB   | 2.04                     | 0.40              |
| 27:AY:106:ILE:HG21 | 27:AY:109:LEU:HD23 | 2.03                     | 0.40              |
| 28:AZ:61:LYS:O     | 28:AZ:65:ARG:HG2   | 2.21                     | 0.40              |
| 36:Ah:100:VAL:HG22 | 36:Ah:104:GLN:HB3  | 2.03                     | 0.40              |
| 47:BC:121:VAL:O    | 47:BC:125:ILE:HG12 | 2.21                     | 0.40              |
| 49:BE:31:PRO:HD2   | 49:BE:38:LEU:HG    | 2.03                     | 0.40              |
| 52:BH:30:SER:OG    | 52:BH:33:GLU:OE2   | 2.29                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:BI:56:ARG:HH22 | 79:B5:332:U:P      | 2.44                     | 0.40              |
| 58:BN:127:ARG:O   | 58:BN:131:THR:HG23 | 2.21                     | 0.40              |
| 63:BS:80:LYS:HA   | 63:BS:80:LYS:HD3   | 1.84                     | 0.40              |
| 70:BZ:60:VAL:HB   | 70:BZ:101:TYR:HB2  | 2.03                     | 0.40              |
| 71:Ba:7:SER:O     | 71:Ba:7:SER:OG     | 2.36                     | 0.40              |
| 79:B5:5:U:H2'     | 79:B5:6:G:H8       | 1.86                     | 0.40              |
| 79:B5:509:G:H2'   | 79:B5:510:G:C8     | 2.57                     | 0.40              |
| 79:B5:1344:A:O2'  | 79:B5:1345:A:O4'   | 2.39                     | 0.40              |
| 79:B5:1515:A:O2'  | 79:B5:1517:U:OP2   | 2.28                     | 0.40              |
| 1:A1:75:G:H1'     | 14:AL:61:PRO:HG3   | 2.03                     | 0.40              |
| 1:A1:282:G:O2'    | 1:A1:283:G:OP2     | 2.37                     | 0.40              |
| 1:A1:963:G:O2'    | 29:Aa:29:PRO:O     | 2.36                     | 0.40              |
| 1:A1:1389:G:OP1   | 33:Ae:104:ASN:ND2  | 2.49                     | 0.40              |
| 1:A1:1495:U:H5    | 1:A1:1835:A:N1     | 2.19                     | 0.40              |
| 6:AC:178:LEU:HD23 | 6:AC:178:LEU:HA    | 1.90                     | 0.40              |
| 7:AD:164:LYS:NZ   | 7:AD:168:ASP:OD1   | 2.54                     | 0.40              |
| 50:BF:29:ILE:O    | 50:BF:34:GLN:NE2   | 2.49                     | 0.40              |
| 51:BG:136:LYS:HD3 | 79:B5:168:A:H4'    | 2.03                     | 0.40              |
| 51:BG:216:LEU:HG  | 51:BG:220:LYS:HE3  | 2.03                     | 0.40              |
| 69:BY:15:ASN:OD1  | 69:BY:18:LEU:N     | 2.43                     | 0.40              |
| 79:B5:891:A:H2'   | 79:B5:892:A:C8     | 2.56                     | 0.40              |
| 79:B5:1216:C:O2'  | 79:B5:1444:A:N1    | 2.47                     | 0.40              |
| 1:A1:1447:G:N7    | 18:AP:25:SER:OG    | 2.47                     | 0.40              |
| 1:A1:2219:A:H2'   | 1:A1:2220:A2M:C8   | 2.51                     | 0.40              |
| 1:A1:2697:A:H2'   | 1:A1:2698:G:H8     | 1.87                     | 0.40              |
| 1:A1:2948:OMC:H5' | 5:AB:243:HIC:HB2   | 2.03                     | 0.40              |
| 5:AB:232:ARG:HD3  | 5:AB:233:TRP:NE1   | 2.36                     | 0.40              |
| 9:AF:77:VAL:HB    | 22:AT:139:ARG:HB2  | 2.02                     | 0.40              |
| 11:AH:93:VAL:HG22 | 41:Am:82:LEU:HB3   | 2.03                     | 0.40              |
| 12:AI:146:ASP:HA  | 12:AI:149:VAL:HG22 | 2.04                     | 0.40              |
| 14:AL:36:ARG:HG2  | 14:AL:39:ARG:HH21  | 1.87                     | 0.40              |
| 55:BK:40:LEU:HD11 | 79:B5:1217:A:C5    | 2.57                     | 0.40              |
| 61:BQ:77:GLN:O    | 61:BQ:81:ILE:HG12  | 2.21                     | 0.40              |
| 63:BS:108:LYS:HA  | 63:BS:108:LYS:HD2  | 1.88                     | 0.40              |
| 64:BT:22:LEU:HD13 | 64:BT:28:LEU:HD22  | 2.03                     | 0.40              |
| 68:BX:87:VAL:HA   | 68:BX:88:PRO:HD3   | 1.97                     | 0.40              |
| 78:Bh:88:ARG:HH22 | 78:Bh:91:THR:HG1   | 1.61                     | 0.40              |
| 79:B5:1171:A:O2'  | 79:B5:1570:A:N3    | 2.49                     | 0.40              |
| 79:B5:1561:U:H2'  | 79:B5:1562:G:C8    | 2.54                     | 0.40              |
| 79:B5:1585:U:N3   | 79:B5:1611:A:H2    | 2.18                     | 0.40              |
| 1:A1:965:A:H2     | 29:Aa:43:ILE:HD12  | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A1:1127:G:H5'    | 12:AI:118:ALA:O    | 2.21                     | 0.40              |
| 1:A1:2424:A:OP1    | 16:AN:90:ASN:ND2   | 2.40                     | 0.40              |
| 2:A3:9:C:OP1       | 22:AT:26:HIS:ND1   | 2.54                     | 0.40              |
| 4:AA:195:SER:O     | 4:AA:198:LYS:NZ    | 2.43                     | 0.40              |
| 6:AC:2:SER:OG      | 6:AC:3:ARG:N       | 2.54                     | 0.40              |
| 12:AI:54:SER:HB2   | 12:AI:135:ILE:HD11 | 2.02                     | 0.40              |
| 12:AI:76:MET:O     | 12:AI:80:SER:OG    | 2.36                     | 0.40              |
| 18:AP:16:SER:O     | 18:AP:101:ASN:ND2  | 2.51                     | 0.40              |
| 18:AP:25:SER:O     | 18:AP:29:THR:OG1   | 2.30                     | 0.40              |
| 19:AQ:67:ILE:HG12  | 19:AQ:81:VAL:HG11  | 2.02                     | 0.40              |
| 25:AW:12:LYS:HB2   | 25:AW:12:LYS:HE2   | 1.85                     | 0.40              |
| 29:Aa:94:ALA:HA    | 29:Aa:121:VAL:HG13 | 2.02                     | 0.40              |
| 36:Ah:31:LEU:HB3   | 36:Ah:44:ILE:HD13  | 2.04                     | 0.40              |
| 45:BA:122:ILE:HA   | 45:BA:144:ILE:O    | 2.22                     | 0.40              |
| 48:BD:45:LYS:HA    | 48:BD:83:THR:O     | 2.21                     | 0.40              |
| 56:BL:26:LYS:HE3   | 56:BL:26:LYS:HB3   | 1.91                     | 0.40              |
| 57:BM:28:LEU:HD23  | 57:BM:28:LEU:HA    | 1.97                     | 0.40              |
| 67:BW:79:PHE:O     | 67:BW:124:LYS:HA   | 2.22                     | 0.40              |
| 73:Bc:30:VAL:O     | 73:Bc:39:THR:HA    | 2.22                     | 0.40              |
| 79:B5:874:C:H2'    | 79:B5:875:G:C8     | 2.57                     | 0.40              |
| 1:A1:66:A:H3'      | 1:A1:316:U:H5''    | 2.03                     | 0.40              |
| 1:A1:187:A:N3      | 1:A1:208:C:O2'     | 2.43                     | 0.40              |
| 1:A1:267:G:OP2     | 1:A1:318:A:N6      | 2.54                     | 0.40              |
| 1:A1:816:A:H5'     | 1:A1:906:A:N6      | 2.35                     | 0.40              |
| 1:A1:1643:A:H2'    | 1:A1:1644:C:C2     | 2.55                     | 0.40              |
| 1:A1:1793:C:OP2    | 44:Ap:49:ARG:NH2   | 2.36                     | 0.40              |
| 1:A1:2216:G:H22    | 1:A1:2229:A:H2     | 1.69                     | 0.40              |
| 4:AA:248:GLY:O     | 79:B5:1011:G:O2'   | 2.40                     | 0.40              |
| 8:AE:40:LEU:O      | 8:AE:51:ARG:HA     | 2.21                     | 0.40              |
| 9:AF:88:ARG:HA     | 9:AF:134:VAL:HG12  | 2.04                     | 0.40              |
| 10:AG:148:ALA:HA   | 10:AG:201:THR:HG22 | 2.03                     | 0.40              |
| 12:AI:206:LEU:HD23 | 12:AI:206:LEU:HA   | 1.93                     | 0.40              |
| 16:AN:73:ARG:HB2   | 16:AN:92:LEU:HD12  | 2.03                     | 0.40              |
| 21:AS:71:LYS:NZ    | 21:AS:128:GLU:OE2  | 2.55                     | 0.40              |
| 47:BC:178:ILE:HG21 | 47:BC:185:LYS:HA   | 2.03                     | 0.40              |
| 50:BF:212:LYS:HE3  | 50:BF:212:LYS:HB2  | 1.89                     | 0.40              |
| 51:BG:187:LYS:O    | 51:BG:191:ARG:HG3  | 2.22                     | 0.40              |
| 56:BL:109:VAL:HG21 | 56:BL:125:VAL:HG11 | 2.02                     | 0.40              |
| 58:BN:132:VAL:HG13 | 58:BN:134:VAL:HG23 | 2.03                     | 0.40              |
| 60:BP:98:ASN:ND2   | 60:BP:121:ILE:O    | 2.32                     | 0.40              |
| 67:BW:16:ASN:ND2   | 79:B5:1037:C:O2    | 2.54                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 71:Ba:13:LYS:O    | 79:B5:1075:C:O2'   | 2.34                     | 0.40              |
| 77:Bg:84:SER:OG   | 77:Bg:85:TRP:N     | 2.53                     | 0.40              |
| 77:Bg:221:MET:HG2 | 77:Bg:233:THR:HG23 | 2.04                     | 0.40              |
| 79:B5:1645:G:H2'  | 79:B5:1646:C:H6    | 1.86                     | 0.40              |
| 79:B5:1688:U:H3   | 79:B5:1712:A:N6    | 2.18                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | AA    | 245/247 (99%) | 232 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 5   | AB    | 383/386 (99%) | 363 (95%) | 20 (5%)  | 0        | 100         | 100 |
| 6   | AC    | 359/361 (99%) | 326 (91%) | 31 (9%)  | 2 (1%)   | 21          | 48  |
| 7   | AD    | 290/292 (99%) | 272 (94%) | 17 (6%)  | 1 (0%)   | 36          | 63  |
| 8   | AE    | 152/156 (97%) | 139 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 9   | AF    | 220/222 (99%) | 207 (94%) | 11 (5%)  | 2 (1%)   | 14          | 39  |
| 10  | AG    | 228/230 (99%) | 216 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 11  | AH    | 188/190 (99%) | 171 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 12  | AI    | 201/205 (98%) | 187 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 13  | AJ    | 167/169 (99%) | 147 (88%) | 20 (12%) | 0        | 100         | 100 |
| 14  | AL    | 191/193 (99%) | 165 (86%) | 22 (12%) | 4 (2%)   | 5           | 21  |
| 15  | AM    | 134/136 (98%) | 128 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 16  | AN    | 201/203 (99%) | 186 (92%) | 14 (7%)  | 1 (0%)   | 24          | 52  |
| 17  | AO    | 195/197 (99%) | 191 (98%) | 2 (1%)   | 2 (1%)   | 12          | 37  |
| 18  | AP    | 171/175 (98%) | 163 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 19  | AQ    | 183/185 (99%) | 177 (97%) | 6 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 20  | AR    | 186/188 (99%) | 176 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 21  | AS    | 170/172 (99%) | 161 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 22  | AT    | 157/159 (99%) | 146 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 23  | AU    | 98/100 (98%)  | 94 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 24  | AV    | 134/136 (98%) | 132 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 25  | AW    | 61/63 (97%)   | 60 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 26  | AX    | 119/121 (98%) | 115 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 27  | AY    | 124/126 (98%) | 116 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 28  | AZ    | 133/135 (98%) | 123 (92%) | 9 (7%)   | 1 (1%)   | 16          | 42  |
| 29  | Aa    | 146/148 (99%) | 126 (86%) | 18 (12%) | 2 (1%)   | 9           | 29  |
| 30  | Ab    | 56/58 (97%)   | 49 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 31  | Ac    | 95/97 (98%)   | 94 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 32  | Ad    | 107/109 (98%) | 103 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 33  | Ae    | 125/127 (98%) | 120 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 34  | Af    | 104/106 (98%) | 100 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 35  | Ag    | 110/112 (98%) | 107 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 36  | Ah    | 117/119 (98%) | 107 (92%) | 9 (8%)   | 1 (1%)   | 14          | 39  |
| 37  | Ai    | 97/99 (98%)   | 89 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 38  | Aj    | 85/87 (98%)   | 82 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 39  | Ak    | 75/77 (97%)   | 74 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 40  | Al    | 48/50 (96%)   | 46 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 41  | Am    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 42  | An    | 23/25 (92%)   | 23 (100%) | 0        | 0        | 100         | 100 |
| 43  | Ao    | 103/105 (98%) | 93 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 44  | Ap    | 89/91 (98%)   | 82 (92%)  | 6 (7%)   | 1 (1%)   | 11          | 34  |
| 45  | BA    | 204/206 (99%) | 185 (91%) | 18 (9%)  | 1 (0%)   | 24          | 52  |
| 46  | BB    | 212/214 (99%) | 186 (88%) | 24 (11%) | 2 (1%)   | 14          | 39  |
| 47  | BC    | 215/217 (99%) | 197 (92%) | 17 (8%)  | 1 (0%)   | 24          | 52  |
| 48  | BD    | 221/223 (99%) | 207 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 49  | BE    | 258/260 (99%) | 240 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 50  | BF    | 204/206 (99%) | 185 (91%) | 19 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 51  | BG    | 224/226 (99%)     | 209 (93%)   | 13 (6%)  | 2 (1%)   | 14          | 39  |
| 52  | BH    | 182/184 (99%)     | 166 (91%)   | 14 (8%)  | 2 (1%)   | 11          | 34  |
| 53  | BI    | 184/188 (98%)     | 156 (85%)   | 28 (15%) | 0        | 100         | 100 |
| 54  | BJ    | 183/185 (99%)     | 168 (92%)   | 14 (8%)  | 1 (0%)   | 24          | 52  |
| 55  | BK    | 94/96 (98%)       | 77 (82%)    | 17 (18%) | 0        | 100         | 100 |
| 56  | BL    | 153/155 (99%)     | 145 (95%)   | 8 (5%)   | 0        | 100         | 100 |
| 57  | BM    | 119/121 (98%)     | 93 (78%)    | 26 (22%) | 0        | 100         | 100 |
| 58  | BN    | 148/150 (99%)     | 140 (95%)   | 8 (5%)   | 0        | 100         | 100 |
| 59  | BO    | 125/127 (98%)     | 110 (88%)   | 15 (12%) | 0        | 100         | 100 |
| 60  | BP    | 122/124 (98%)     | 101 (83%)   | 19 (16%) | 2 (2%)   | 7           | 26  |
| 61  | BQ    | 139/141 (99%)     | 131 (94%)   | 7 (5%)   | 1 (1%)   | 18          | 45  |
| 62  | BR    | 117/121 (97%)     | 106 (91%)   | 10 (8%)  | 1 (1%)   | 14          | 39  |
| 63  | BS    | 143/145 (99%)     | 128 (90%)   | 13 (9%)  | 2 (1%)   | 9           | 29  |
| 64  | BT    | 139/141 (99%)     | 125 (90%)   | 14 (10%) | 0        | 100         | 100 |
| 65  | BU    | 105/107 (98%)     | 100 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 66  | BV    | 83/87 (95%)       | 78 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 67  | BW    | 127/129 (98%)     | 117 (92%)   | 9 (7%)   | 1 (1%)   | 16          | 42  |
| 68  | BX    | 142/144 (99%)     | 120 (84%)   | 20 (14%) | 2 (1%)   | 9           | 29  |
| 69  | BY    | 132/134 (98%)     | 124 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 70  | BZ    | 67/69 (97%)       | 61 (91%)    | 6 (9%)   | 0        | 100         | 100 |
| 71  | Ba    | 95/97 (98%)       | 76 (80%)    | 16 (17%) | 3 (3%)   | 3           | 14  |
| 72  | Bb    | 79/81 (98%)       | 72 (91%)    | 7 (9%)   | 0        | 100         | 100 |
| 73  | Bc    | 61/63 (97%)       | 57 (93%)    | 4 (7%)   | 0        | 100         | 100 |
| 74  | Bd    | 51/53 (96%)       | 47 (92%)    | 4 (8%)   | 0        | 100         | 100 |
| 75  | Be    | 58/60 (97%)       | 53 (91%)    | 5 (9%)   | 0        | 100         | 100 |
| 76  | Bf    | 53/57 (93%)       | 39 (74%)    | 14 (26%) | 0        | 100         | 100 |
| 77  | Bg    | 310/312 (99%)     | 275 (89%)   | 35 (11%) | 0        | 100         | 100 |
| 78  | Bh    | 87/89 (98%)       | 81 (93%)    | 6 (7%)   | 0        | 100         | 100 |
| All | All   | 10956/11121 (98%) | 10091 (92%) | 827 (8%) | 38 (0%)  | 37          | 63  |

All (38) Ramachandran outliers are listed below:



| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 6   | AC    | 339    | LEU  |
| 9   | AF    | 159    | GLN  |
| 14  | AL    | 48     | PRO  |
| 14  | AL    | 63     | VAL  |
| 16  | AN    | 81     | TYR  |
| 17  | AO    | 111[A] | PRO  |
| 29  | Aa    | 78     | LEU  |
| 51  | BG    | 68     | LEU  |
| 68  | BX    | 97     | ASP  |
| 46  | BB    | 206    | PRO  |
| 46  | BB    | 207    | LEU  |
| 47  | BC    | 40     | LYS  |
| 51  | BG    | 173    | PRO  |
| 52  | BH    | 111    | LYS  |
| 54  | BJ    | 134    | ILE  |
| 63  | BS    | 91     | ASP  |
| 71  | Ba    | 36     | ILE  |
| 7   | AD    | 20     | PHE  |
| 14  | AL    | 76     | THR  |
| 14  | AL    | 77     | LEU  |
| 45  | BA    | 4      | PRO  |
| 60  | BP    | 125    | PRO  |
| 62  | BR    | 24     | LEU  |
| 71  | Ba    | 35     | ALA  |
| 71  | Ba    | 62     | TYR  |
| 36  | Ah    | 91     | ALA  |
| 44  | Ap    | 52     | ALA  |
| 6   | AC    | 268    | ALA  |
| 68  | BX    | 96     | VAL  |
| 28  | AZ    | 17     | ARG  |
| 29  | Aa    | 47     | LYS  |
| 61  | BQ    | 33     | GLY  |
| 60  | BP    | 107    | ILE  |
| 9   | AF    | 216    | VAL  |
| 63  | BS    | 92     | ILE  |
| 52  | BH    | 65     | PRO  |
| 17  | AO    | 110[A] | PRO  |
| 67  | BW    | 67     | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | AA    | 189/189 (100%) | 189 (100%) | 0        | 100         | 100 |
| 5   | AB    | 321/321 (100%) | 321 (100%) | 0        | 100         | 100 |
| 6   | AC    | 288/288 (100%) | 288 (100%) | 0        | 100         | 100 |
| 7   | AD    | 241/241 (100%) | 241 (100%) | 0        | 100         | 100 |
| 8   | AE    | 134/134 (100%) | 134 (100%) | 0        | 100         | 100 |
| 9   | AF    | 186/186 (100%) | 186 (100%) | 0        | 100         | 100 |
| 10  | AG    | 189/189 (100%) | 189 (100%) | 0        | 100         | 100 |
| 11  | AH    | 170/170 (100%) | 170 (100%) | 0        | 100         | 100 |
| 12  | AI    | 176/176 (100%) | 176 (100%) | 0        | 100         | 100 |
| 13  | AJ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 14  | AL    | 154/154 (100%) | 154 (100%) | 0        | 100         | 100 |
| 15  | AM    | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 16  | AN    | 175/175 (100%) | 175 (100%) | 0        | 100         | 100 |
| 17  | AO    | 160/160 (100%) | 160 (100%) | 0        | 100         | 100 |
| 18  | AP    | 141/141 (100%) | 141 (100%) | 0        | 100         | 100 |
| 19  | AQ    | 150/150 (100%) | 150 (100%) | 0        | 100         | 100 |
| 20  | AR    | 153/153 (100%) | 153 (100%) | 0        | 100         | 100 |
| 21  | AS    | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |
| 22  | AT    | 136/136 (100%) | 136 (100%) | 0        | 100         | 100 |
| 23  | AU    | 87/87 (100%)   | 86 (99%)   | 1 (1%)   | 65          | 76  |
| 24  | AV    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 25  | AW    | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 26  | AX    | 105/105 (100%) | 105 (100%) | 0        | 100         | 100 |
| 27  | AY    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 28  | AZ    | 115/115 (100%) | 115 (100%) | 0        | 100         | 100 |
| 29  | Aa    | 118/118 (100%) | 118 (100%) | 0        | 100         | 100 |
| 30  | Ab    | 46/46 (100%)   | 46 (100%)  | 0        | 100         | 100 |
| 31  | Ac    | 81/81 (100%)   | 81 (100%)  | 0        | 100         | 100 |
| 32  | Ad    | 96/96 (100%)   | 96 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 33  | Ae    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 34  | Af    | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 35  | Ag    | 95/95 (100%)   | 95 (100%)  | 0        | 100         | 100 |
| 36  | Ah    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 37  | Ai    | 81/81 (100%)   | 81 (100%)  | 0        | 100         | 100 |
| 38  | Aj    | 70/70 (100%)   | 70 (100%)  | 0        | 100         | 100 |
| 39  | Ak    | 68/68 (100%)   | 68 (100%)  | 0        | 100         | 100 |
| 40  | Al    | 45/45 (100%)   | 45 (100%)  | 0        | 100         | 100 |
| 41  | Am    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 42  | An    | 23/23 (100%)   | 23 (100%)  | 0        | 100         | 100 |
| 43  | Ao    | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 44  | Ap    | 71/71 (100%)   | 71 (100%)  | 0        | 100         | 100 |
| 45  | BA    | 173/173 (100%) | 173 (100%) | 0        | 100         | 100 |
| 46  | BB    | 191/191 (100%) | 190 (100%) | 1 (0%)   | 81          | 82  |
| 47  | BC    | 176/176 (100%) | 176 (100%) | 0        | 100         | 100 |
| 48  | BD    | 182/182 (100%) | 182 (100%) | 0        | 100         | 100 |
| 49  | BE    | 221/221 (100%) | 221 (100%) | 0        | 100         | 100 |
| 50  | BF    | 173/173 (100%) | 173 (100%) | 0        | 100         | 100 |
| 51  | BG    | 193/193 (100%) | 193 (100%) | 0        | 100         | 100 |
| 52  | BH    | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 53  | BI    | 150/150 (100%) | 150 (100%) | 0        | 100         | 100 |
| 54  | BJ    | 158/158 (100%) | 158 (100%) | 0        | 100         | 100 |
| 55  | BK    | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 56  | BL    | 136/136 (100%) | 136 (100%) | 0        | 100         | 100 |
| 57  | BM    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 58  | BN    | 127/127 (100%) | 127 (100%) | 0        | 100         | 100 |
| 59  | BO    | 96/96 (100%)   | 96 (100%)  | 0        | 100         | 100 |
| 60  | BP    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 61  | BQ    | 117/117 (100%) | 117 (100%) | 0        | 100         | 100 |
| 62  | BR    | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 63  | BS    | 128/128 (100%) | 128 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 64  | BT    | 113/113 (100%)   | 113 (100%)  | 0        | 100         | 100 |
| 65  | BU    | 100/100 (100%)   | 100 (100%)  | 0        | 100         | 100 |
| 66  | BV    | 74/74 (100%)     | 74 (100%)   | 0        | 100         | 100 |
| 67  | BW    | 110/110 (100%)   | 110 (100%)  | 0        | 100         | 100 |
| 68  | BX    | 119/119 (100%)   | 119 (100%)  | 0        | 100         | 100 |
| 69  | BY    | 112/112 (100%)   | 112 (100%)  | 0        | 100         | 100 |
| 70  | BZ    | 61/61 (100%)     | 61 (100%)   | 0        | 100         | 100 |
| 71  | Ba    | 83/83 (100%)     | 83 (100%)   | 0        | 100         | 100 |
| 72  | Bb    | 70/70 (100%)     | 69 (99%)    | 1 (1%)   | 59          | 73  |
| 73  | Bc    | 56/56 (100%)     | 56 (100%)   | 0        | 100         | 100 |
| 74  | Bd    | 47/47 (100%)     | 46 (98%)    | 1 (2%)   | 47          | 68  |
| 75  | Be    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 76  | Bf    | 49/49 (100%)     | 49 (100%)   | 0        | 100         | 100 |
| 77  | Bg    | 256/257 (100%)   | 256 (100%)  | 0        | 100         | 100 |
| 78  | Bh    | 68/68 (100%)     | 68 (100%)   | 0        | 100         | 100 |
| All | All   | 9338/9339 (100%) | 9334 (100%) | 4 (0%)   | 100         | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | AU    | 49  | ASN  |
| 46  | BB    | 146 | GLN  |
| 72  | Bb    | 42  | ASN  |
| 74  | Bd    | 28  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AA    | 97  | ASN  |
| 4   | AA    | 132 | ASN  |
| 5   | AB    | 68  | HIS  |
| 5   | AB    | 121 | ASN  |
| 6   | AC    | 213 | ASN  |
| 6   | AC    | 260 | GLN  |
| 7   | AD    | 90  | HIS  |
| 9   | AF    | 194 | HIS  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 10  | AG    | 95    | ASN  |
| 11  | AH    | 96    | HIS  |
| 11  | AH    | 163   | GLN  |
| 14  | AL    | 105   | ASN  |
| 14  | AL    | 120   | GLN  |
| 14  | AL    | 137   | GLN  |
| 15  | AM    | 56    | GLN  |
| 16  | AN    | 95    | GLN  |
| 17  | AO    | 26[A] | GLN  |
| 17  | AO    | 31[A] | GLN  |
| 18  | AP    | 54    | HIS  |
| 19  | AQ    | 23    | ASN  |
| 20  | AR    | 66    | HIS  |
| 22  | AT    | 49    | GLN  |
| 22  | AT    | 98    | HIS  |
| 23  | AU    | 49    | ASN  |
| 27  | AY    | 110   | HIS  |
| 28  | AZ    | 78    | ASN  |
| 28  | AZ    | 122   | HIS  |
| 29  | Aa    | 120   | ASN  |
| 31  | Ac    | 11    | ASN  |
| 35  | Ag    | 3     | GLN  |
| 36  | Ah    | 16    | GLN  |
| 36  | Ah    | 76    | GLN  |
| 36  | Ah    | 113   | GLN  |
| 38  | Aj    | 69    | HIS  |
| 40  | Al    | 32    | ASN  |
| 40  | Al    | 33    | ASN  |
| 41  | Am    | 90    | ASN  |
| 46  | BB    | 146   | GLN  |
| 46  | BB    | 183   | GLN  |
| 46  | BB    | 194   | ASN  |
| 46  | BB    | 208   | GLN  |
| 46  | BB    | 209   | ASN  |
| 47  | BC    | 201   | ASN  |
| 48  | BD    | 165   | ASN  |
| 49  | BE    | 17    | HIS  |
| 49  | BE    | 50    | ASN  |
| 49  | BE    | 157   | ASN  |
| 50  | BF    | 63    | GLN  |
| 51  | BG    | 190   | GLN  |
| 51  | BG    | 197   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | BH    | 11  | GLN  |
| 52  | BH    | 22  | GLN  |
| 52  | BH    | 42  | GLN  |
| 52  | BH    | 161 | GLN  |
| 53  | BI    | 103 | GLN  |
| 55  | BK    | 93  | GLN  |
| 56  | BL    | 14  | GLN  |
| 56  | BL    | 21  | ASN  |
| 56  | BL    | 92  | HIS  |
| 57  | BM    | 84  | ASN  |
| 58  | BN    | 78  | ASN  |
| 62  | BR    | 62  | GLN  |
| 63  | BS    | 8   | GLN  |
| 63  | BS    | 25  | ASN  |
| 63  | BS    | 75  | ASN  |
| 65  | BU    | 17  | GLN  |
| 65  | BU    | 105 | GLN  |
| 67  | BW    | 39  | GLN  |
| 67  | BW    | 70  | ASN  |
| 72  | Bb    | 5   | GLN  |
| 72  | Bb    | 9   | HIS  |
| 74  | Bd    | 48  | ASN  |
| 77  | Bg    | 237 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A1    | 3150/3156 (99%) | 695 (22%)         | 13 (0%)         |
| 2   | A3    | 120/121 (99%)   | 15 (12%)          | 0               |
| 3   | A4    | 156/158 (98%)   | 34 (21%)          | 2 (1%)          |
| 79  | B5    | 1781/1783 (99%) | 459 (25%)         | 14 (0%)         |
| All | All   | 5207/5218 (99%) | 1203 (23%)        | 29 (0%)         |

All (1203) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 14  | U    |
| 1   | A1    | 18  | G    |
| 1   | A1    | 21  | G    |
| 1   | A1    | 26  | A    |
| 1   | A1    | 34  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 40  | A    |
| 1   | A1    | 43  | A    |
| 1   | A1    | 49  | A    |
| 1   | A1    | 57  | A    |
| 1   | A1    | 59  | G    |
| 1   | A1    | 60  | A    |
| 1   | A1    | 65  | A    |
| 1   | A1    | 66  | A    |
| 1   | A1    | 72  | C    |
| 1   | A1    | 75  | G    |
| 1   | A1    | 76  | G    |
| 1   | A1    | 85  | A    |
| 1   | A1    | 92  | G    |
| 1   | A1    | 109 | A    |
| 1   | A1    | 110 | G    |
| 1   | A1    | 111 | C    |
| 1   | A1    | 115 | A    |
| 1   | A1    | 116 | A    |
| 1   | A1    | 117 | U    |
| 1   | A1    | 120 | G    |
| 1   | A1    | 121 | A    |
| 1   | A1    | 122 | A    |
| 1   | A1    | 134 | U    |
| 1   | A1    | 135 | C    |
| 1   | A1    | 136 | G    |
| 1   | A1    | 143 | G    |
| 1   | A1    | 148 | G    |
| 1   | A1    | 150 | A    |
| 1   | A1    | 154 | U    |
| 1   | A1    | 156 | G    |
| 1   | A1    | 157 | A    |
| 1   | A1    | 164 | A    |
| 1   | A1    | 165 | A    |
| 1   | A1    | 166 | C    |
| 1   | A1    | 170 | G    |
| 1   | A1    | 187 | A    |
| 1   | A1    | 190 | U    |
| 1   | A1    | 191 | U    |
| 1   | A1    | 200 | C    |
| 1   | A1    | 206 | G    |
| 1   | A1    | 210 | U    |
| 1   | A1    | 211 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 219 | A    |
| 1   | A1    | 220 | G    |
| 1   | A1    | 231 | G    |
| 1   | A1    | 239 | G    |
| 1   | A1    | 240 | U    |
| 1   | A1    | 242 | C    |
| 1   | A1    | 243 | G    |
| 1   | A1    | 244 | G    |
| 1   | A1    | 249 | U    |
| 1   | A1    | 250 | U    |
| 1   | A1    | 251 | G    |
| 1   | A1    | 252 | U    |
| 1   | A1    | 266 | A    |
| 1   | A1    | 267 | G    |
| 1   | A1    | 268 | A    |
| 1   | A1    | 269 | G    |
| 1   | A1    | 281 | G    |
| 1   | A1    | 283 | G    |
| 1   | A1    | 285 | A    |
| 1   | A1    | 286 | U    |
| 1   | A1    | 295 | A    |
| 1   | A1    | 297 | G    |
| 1   | A1    | 299 | G    |
| 1   | A1    | 305 | U    |
| 1   | A1    | 315 | C    |
| 1   | A1    | 316 | U    |
| 1   | A1    | 329 | U    |
| 1   | A1    | 337 | G    |
| 1   | A1    | 339 | C    |
| 1   | A1    | 352 | A    |
| 1   | A1    | 359 | U    |
| 1   | A1    | 371 | G    |
| 1   | A1    | 372 | A    |
| 1   | A1    | 374 | A    |
| 1   | A1    | 375 | A    |
| 1   | A1    | 376 | G    |
| 1   | A1    | 384 | A    |
| 1   | A1    | 387 | A    |
| 1   | A1    | 398 | A    |
| 1   | A1    | 399 | A    |
| 1   | A1    | 400 | G    |
| 1   | A1    | 401 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 402 | A    |
| 1   | A1    | 403 | C    |
| 1   | A1    | 420 | G    |
| 1   | A1    | 421 | G    |
| 1   | A1    | 422 | A    |
| 1   | A1    | 429 | U    |
| 1   | A1    | 439 | C    |
| 1   | A1    | 440 | A    |
| 1   | A1    | 441 | U    |
| 1   | A1    | 442 | G    |
| 1   | A1    | 443 | G    |
| 1   | A1    | 446 | U    |
| 1   | A1    | 447 | U    |
| 1   | A1    | 448 | U    |
| 1   | A1    | 450 | G    |
| 1   | A1    | 451 | U    |
| 1   | A1    | 487 | U    |
| 1   | A1    | 488 | U    |
| 1   | A1    | 489 | U    |
| 1   | A1    | 491 | A    |
| 1   | A1    | 493 | U    |
| 1   | A1    | 494 | G    |
| 1   | A1    | 498 | A    |
| 1   | A1    | 520 | U    |
| 1   | A1    | 521 | A    |
| 1   | A1    | 523 | A    |
| 1   | A1    | 535 | G    |
| 1   | A1    | 542 | G    |
| 1   | A1    | 543 | C    |
| 1   | A1    | 545 | U    |
| 1   | A1    | 546 | C    |
| 1   | A1    | 547 | G    |
| 1   | A1    | 548 | G    |
| 1   | A1    | 550 | A    |
| 1   | A1    | 551 | A    |
| 1   | A1    | 552 | G    |
| 1   | A1    | 555 | U    |
| 1   | A1    | 557 | A    |
| 1   | A1    | 558 | U    |
| 1   | A1    | 559 | A    |
| 1   | A1    | 560 | G    |
| 1   | A1    | 569 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 578 | A    |
| 1   | A1    | 579 | G    |
| 1   | A1    | 588 | G    |
| 1   | A1    | 589 | A    |
| 1   | A1    | 592 | A    |
| 1   | A1    | 602 | A    |
| 1   | A1    | 604 | G    |
| 1   | A1    | 611 | A    |
| 1   | A1    | 620 | U    |
| 1   | A1    | 621 | A    |
| 1   | A1    | 637 | C    |
| 1   | A1    | 647 | A    |
| 1   | A1    | 649 | A2M  |
| 1   | A1    | 660 | A    |
| 1   | A1    | 677 | A    |
| 1   | A1    | 681 | U    |
| 1   | A1    | 690 | A    |
| 1   | A1    | 691 | A    |
| 1   | A1    | 705 | A    |
| 1   | A1    | 719 | U    |
| 1   | A1    | 725 | G    |
| 1   | A1    | 736 | A    |
| 1   | A1    | 765 | C    |
| 1   | A1    | 766 | U    |
| 1   | A1    | 767 | U    |
| 1   | A1    | 774 | G    |
| 1   | A1    | 775 | A    |
| 1   | A1    | 780 | A    |
| 1   | A1    | 781 | G    |
| 1   | A1    | 784 | A    |
| 1   | A1    | 785 | G    |
| 1   | A1    | 786 | A    |
| 1   | A1    | 799 | G    |
| 1   | A1    | 801 | A    |
| 1   | A1    | 806 | A    |
| 1   | A1    | 813 | G    |
| 1   | A1    | 817 | A2M  |
| 1   | A1    | 826 | G    |
| 1   | A1    | 830 | A    |
| 1   | A1    | 844 | G    |
| 1   | A1    | 845 | G    |
| 1   | A1    | 849 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 861  | C    |
| 1   | A1    | 862  | U    |
| 1   | A1    | 871  | U    |
| 1   | A1    | 874  | U    |
| 1   | A1    | 879  | U    |
| 1   | A1    | 896  | A    |
| 1   | A1    | 897  | U    |
| 1   | A1    | 907  | G    |
| 1   | A1    | 914  | A    |
| 1   | A1    | 916  | G    |
| 1   | A1    | 917  | A    |
| 1   | A1    | 921  | A    |
| 1   | A1    | 923  | C    |
| 1   | A1    | 924  | G    |
| 1   | A1    | 925  | A    |
| 1   | A1    | 934  | G    |
| 1   | A1    | 937  | G    |
| 1   | A1    | 944  | C    |
| 1   | A1    | 959  | C    |
| 1   | A1    | 960  | U    |
| 1   | A1    | 963  | G    |
| 1   | A1    | 970  | A    |
| 1   | A1    | 974  | G    |
| 1   | A1    | 979  | U    |
| 1   | A1    | 981  | U    |
| 1   | A1    | 994  | G    |
| 1   | A1    | 1000 | C    |
| 1   | A1    | 1002 | A    |
| 1   | A1    | 1006 | A    |
| 1   | A1    | 1010 | G    |
| 1   | A1    | 1014 | U    |
| 1   | A1    | 1016 | C    |
| 1   | A1    | 1017 | C    |
| 1   | A1    | 1018 | G    |
| 1   | A1    | 1019 | G    |
| 1   | A1    | 1021 | G    |
| 1   | A1    | 1032 | C    |
| 1   | A1    | 1033 | U    |
| 1   | A1    | 1034 | U    |
| 1   | A1    | 1035 | G    |
| 1   | A1    | 1047 | A    |
| 1   | A1    | 1049 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 1052 | U    |
| 1   | A1    | 1064 | A    |
| 1   | A1    | 1072 | G    |
| 1   | A1    | 1075 | A    |
| 1   | A1    | 1081 | U    |
| 1   | A1    | 1087 | G    |
| 1   | A1    | 1094 | U    |
| 1   | A1    | 1095 | U    |
| 1   | A1    | 1096 | U    |
| 1   | A1    | 1097 | G    |
| 1   | A1    | 1098 | A    |
| 1   | A1    | 1103 | A    |
| 1   | A1    | 1104 | G    |
| 1   | A1    | 1117 | G    |
| 1   | A1    | 1131 | G    |
| 1   | A1    | 1132 | C    |
| 1   | A1    | 1143 | A    |
| 1   | A1    | 1144 | U    |
| 1   | A1    | 1153 | A    |
| 1   | A1    | 1155 | C    |
| 1   | A1    | 1156 | C    |
| 1   | A1    | 1159 | A    |
| 1   | A1    | 1160 | C    |
| 1   | A1    | 1177 | G    |
| 1   | A1    | 1179 | A    |
| 1   | A1    | 1180 | A    |
| 1   | A1    | 1181 | U    |
| 1   | A1    | 1182 | A    |
| 1   | A1    | 1186 | G    |
| 1   | A1    | 1190 | A    |
| 1   | A1    | 1192 | C    |
| 1   | A1    | 1193 | A    |
| 1   | A1    | 1201 | C    |
| 1   | A1    | 1207 | G    |
| 1   | A1    | 1208 | U    |
| 1   | A1    | 1219 | C    |
| 1   | A1    | 1222 | G    |
| 1   | A1    | 1223 | A    |
| 1   | A1    | 1225 | A    |
| 1   | A1    | 1227 | C    |
| 1   | A1    | 1228 | C    |
| 1   | A1    | 1231 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 1232 | C    |
| 1   | A1    | 1233 | G    |
| 1   | A1    | 1235 | U    |
| 1   | A1    | 1236 | G    |
| 1   | A1    | 1237 | G    |
| 1   | A1    | 1239 | C    |
| 1   | A1    | 1240 | A    |
| 1   | A1    | 1241 | U    |
| 1   | A1    | 1242 | G    |
| 1   | A1    | 1243 | G    |
| 1   | A1    | 1244 | A    |
| 1   | A1    | 1246 | G    |
| 1   | A1    | 1247 | U    |
| 1   | A1    | 1248 | C    |
| 1   | A1    | 1249 | G    |
| 1   | A1    | 1250 | G    |
| 1   | A1    | 1251 | A    |
| 1   | A1    | 1252 | A    |
| 1   | A1    | 1263 | A    |
| 1   | A1    | 1264 | G    |
| 1   | A1    | 1266 | G    |
| 1   | A1    | 1268 | G    |
| 1   | A1    | 1270 | A    |
| 1   | A1    | 1271 | A    |
| 1   | A1    | 1272 | C    |
| 1   | A1    | 1276 | U    |
| 1   | A1    | 1277 | C    |
| 1   | A1    | 1278 | A    |
| 1   | A1    | 1281 | G    |
| 1   | A1    | 1283 | C    |
| 1   | A1    | 1286 | A    |
| 1   | A1    | 1287 | A    |
| 1   | A1    | 1306 | G    |
| 1   | A1    | 1307 | G    |
| 1   | A1    | 1309 | U    |
| 1   | A1    | 1315 | U    |
| 1   | A1    | 1317 | A    |
| 1   | A1    | 1318 | A    |
| 1   | A1    | 1325 | U    |
| 1   | A1    | 1330 | A    |
| 1   | A1    | 1331 | U    |
| 1   | A1    | 1345 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 1348 | U    |
| 1   | A1    | 1350 | A    |
| 1   | A1    | 1351 | U    |
| 1   | A1    | 1352 | A    |
| 1   | A1    | 1353 | U    |
| 1   | A1    | 1354 | G    |
| 1   | A1    | 1355 | A    |
| 1   | A1    | 1356 | U    |
| 1   | A1    | 1357 | G    |
| 1   | A1    | 1386 | A    |
| 1   | A1    | 1391 | C    |
| 1   | A1    | 1392 | G    |
| 1   | A1    | 1399 | A    |
| 1   | A1    | 1400 | G    |
| 1   | A1    | 1417 | G    |
| 1   | A1    | 1418 | A    |
| 1   | A1    | 1419 | A    |
| 1   | A1    | 1434 | G    |
| 1   | A1    | 1437 | OMC  |
| 1   | A1    | 1443 | G    |
| 1   | A1    | 1446 | A    |
| 1   | A1    | 1450 | OMG  |
| 1   | A1    | 1465 | A    |
| 1   | A1    | 1469 | C    |
| 1   | A1    | 1475 | A    |
| 1   | A1    | 1477 | A    |
| 1   | A1    | 1481 | A    |
| 1   | A1    | 1487 | G    |
| 1   | A1    | 1494 | U    |
| 1   | A1    | 1508 | C    |
| 1   | A1    | 1522 | U    |
| 1   | A1    | 1523 | U    |
| 1   | A1    | 1524 | A    |
| 1   | A1    | 1525 | G    |
| 1   | A1    | 1526 | U    |
| 1   | A1    | 1533 | U    |
| 1   | A1    | 1536 | G    |
| 1   | A1    | 1539 | A    |
| 1   | A1    | 1555 | U    |
| 1   | A1    | 1556 | C    |
| 1   | A1    | 1562 | C    |
| 1   | A1    | 1564 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 1565 | G    |
| 1   | A1    | 1566 | A    |
| 1   | A1    | 1567 | U    |
| 1   | A1    | 1569 | U    |
| 1   | A1    | 1570 | U    |
| 1   | A1    | 1572 | U    |
| 1   | A1    | 1574 | C    |
| 1   | A1    | 1576 | G    |
| 1   | A1    | 1583 | A    |
| 1   | A1    | 1587 | A    |
| 1   | A1    | 1589 | A    |
| 1   | A1    | 1590 | G    |
| 1   | A1    | 1593 | A    |
| 1   | A1    | 1596 | C    |
| 1   | A1    | 1605 | A    |
| 1   | A1    | 1628 | C    |
| 1   | A1    | 1629 | U    |
| 1   | A1    | 1630 | U    |
| 1   | A1    | 1642 | A    |
| 1   | A1    | 1643 | A    |
| 1   | A1    | 1657 | C    |
| 1   | A1    | 1683 | A    |
| 1   | A1    | 1717 | U    |
| 1   | A1    | 1722 | U    |
| 1   | A1    | 1724 | U    |
| 1   | A1    | 1730 | G    |
| 1   | A1    | 1736 | G    |
| 1   | A1    | 1741 | A    |
| 1   | A1    | 1742 | U    |
| 1   | A1    | 1750 | A    |
| 1   | A1    | 1751 | G    |
| 1   | A1    | 1756 | C    |
| 1   | A1    | 1761 | C    |
| 1   | A1    | 1762 | C    |
| 1   | A1    | 1763 | U    |
| 1   | A1    | 1764 | U    |
| 1   | A1    | 1765 | U    |
| 1   | A1    | 1766 | G    |
| 1   | A1    | 1775 | G    |
| 1   | A1    | 1778 | G    |
| 1   | A1    | 1780 | G    |
| 1   | A1    | 1794 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 1795 | U    |
| 1   | A1    | 1796 | G    |
| 1   | A1    | 1797 | A    |
| 1   | A1    | 1813 | A    |
| 1   | A1    | 1814 | A    |
| 1   | A1    | 1815 | U    |
| 1   | A1    | 1821 | U    |
| 1   | A1    | 1825 | G    |
| 1   | A1    | 1839 | A    |
| 1   | A1    | 1840 | U    |
| 1   | A1    | 1842 | A    |
| 1   | A1    | 1846 | C    |
| 1   | A1    | 1848 | G    |
| 1   | A1    | 1849 | C    |
| 1   | A1    | 1850 | A    |
| 1   | A1    | 1858 | A    |
| 1   | A1    | 1866 | C    |
| 1   | A1    | 1871 | U    |
| 1   | A1    | 1878 | G    |
| 1   | A1    | 1880 | U    |
| 1   | A1    | 1886 | A    |
| 1   | A1    | 1893 | A    |
| 1   | A1    | 1899 | G    |
| 1   | A1    | 1906 | G    |
| 1   | A1    | 1943 | C    |
| 1   | A1    | 1948 | G    |
| 1   | A1    | 1951 | C    |
| 1   | A1    | 1952 | G    |
| 1   | A1    | 1953 | G    |
| 1   | A1    | 1954 | G    |
| 1   | A1    | 2094 | C    |
| 1   | A1    | 2095 | G    |
| 1   | A1    | 2096 | A    |
| 1   | A1    | 2110 | G    |
| 1   | A1    | 2112 | U    |
| 1   | A1    | 2114 | C    |
| 1   | A1    | 2115 | G    |
| 1   | A1    | 2121 | G    |
| 1   | A1    | 2122 | G    |
| 1   | A1    | 2131 | A    |
| 1   | A1    | 2140 | U    |
| 1   | A1    | 2142 | 1MA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 2144 | A    |
| 1   | A1    | 2145 | A    |
| 1   | A1    | 2158 | A    |
| 1   | A1    | 2169 | G    |
| 1   | A1    | 2176 | U    |
| 1   | A1    | 2188 | A    |
| 1   | A1    | 2194 | G    |
| 1   | A1    | 2197 | OMC  |
| 1   | A1    | 2205 | U    |
| 1   | A1    | 2207 | A    |
| 1   | A1    | 2208 | A    |
| 1   | A1    | 2209 | U    |
| 1   | A1    | 2210 | G    |
| 1   | A1    | 2244 | A    |
| 1   | A1    | 2249 | G    |
| 1   | A1    | 2253 | G    |
| 1   | A1    | 2256 | A    |
| 1   | A1    | 2257 | C    |
| 1   | A1    | 2258 | U    |
| 1   | A1    | 2260 | U    |
| 1   | A1    | 2268 | U    |
| 1   | A1    | 2269 | U    |
| 1   | A1    | 2270 | A    |
| 1   | A1    | 2272 | G    |
| 1   | A1    | 2273 | G    |
| 1   | A1    | 2281 | A2M  |
| 1   | A1    | 2288 | OMG  |
| 1   | A1    | 2298 | U    |
| 1   | A1    | 2306 | C    |
| 1   | A1    | 2307 | G    |
| 1   | A1    | 2308 | C    |
| 1   | A1    | 2310 | U    |
| 1   | A1    | 2313 | A    |
| 1   | A1    | 2314 | U    |
| 1   | A1    | 2315 | G    |
| 1   | A1    | 2334 | U    |
| 1   | A1    | 2336 | U    |
| 1   | A1    | 2340 | U    |
| 1   | A1    | 2366 | C    |
| 1   | A1    | 2373 | A    |
| 1   | A1    | 2374 | C    |
| 1   | A1    | 2375 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 2376 | G    |
| 1   | A1    | 2383 | C    |
| 1   | A1    | 2388 | U    |
| 1   | A1    | 2391 | G    |
| 1   | A1    | 2393 | G    |
| 1   | A1    | 2397 | A    |
| 1   | A1    | 2401 | A    |
| 1   | A1    | 2402 | A    |
| 1   | A1    | 2403 | G    |
| 1   | A1    | 2404 | A    |
| 1   | A1    | 2411 | U    |
| 1   | A1    | 2418 | G    |
| 1   | A1    | 2422 | C    |
| 1   | A1    | 2435 | G    |
| 1   | A1    | 2437 | G    |
| 1   | A1    | 2441 | A    |
| 1   | A1    | 2442 | G    |
| 1   | A1    | 2444 | C    |
| 1   | A1    | 2502 | A    |
| 1   | A1    | 2503 | G    |
| 1   | A1    | 2504 | U    |
| 1   | A1    | 2506 | U    |
| 1   | A1    | 2507 | C    |
| 1   | A1    | 2508 | U    |
| 1   | A1    | 2514 | U    |
| 1   | A1    | 2515 | A    |
| 1   | A1    | 2523 | A    |
| 1   | A1    | 2524 | A    |
| 1   | A1    | 2531 | C    |
| 1   | A1    | 2532 | U    |
| 1   | A1    | 2536 | A    |
| 1   | A1    | 2537 | U    |
| 1   | A1    | 2538 | U    |
| 1   | A1    | 2539 | C    |
| 1   | A1    | 2540 | A    |
| 1   | A1    | 2541 | U    |
| 1   | A1    | 2542 | U    |
| 1   | A1    | 2543 | U    |
| 1   | A1    | 2544 | U    |
| 1   | A1    | 2545 | C    |
| 1   | A1    | 2548 | C    |
| 1   | A1    | 2552 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 2553 | U    |
| 1   | A1    | 2561 | A    |
| 1   | A1    | 2568 | C    |
| 1   | A1    | 2569 | A    |
| 1   | A1    | 2570 | U    |
| 1   | A1    | 2571 | U    |
| 1   | A1    | 2572 | C    |
| 1   | A1    | 2573 | G    |
| 1   | A1    | 2580 | A    |
| 1   | A1    | 2585 | G    |
| 1   | A1    | 2586 | G    |
| 1   | A1    | 2593 | A    |
| 1   | A1    | 2606 | G    |
| 1   | A1    | 2607 | G    |
| 1   | A1    | 2614 | G    |
| 1   | A1    | 2629 | U    |
| 1   | A1    | 2635 | A    |
| 1   | A1    | 2648 | G    |
| 1   | A1    | 2651 | G    |
| 1   | A1    | 2652 | U    |
| 1   | A1    | 2656 | A    |
| 1   | A1    | 2666 | C    |
| 1   | A1    | 2672 | G    |
| 1   | A1    | 2674 | A    |
| 1   | A1    | 2676 | A    |
| 1   | A1    | 2677 | G    |
| 1   | A1    | 2678 | A    |
| 1   | A1    | 2679 | A    |
| 1   | A1    | 2681 | U    |
| 1   | A1    | 2688 | U    |
| 1   | A1    | 2689 | A    |
| 1   | A1    | 2690 | G    |
| 1   | A1    | 2691 | A    |
| 1   | A1    | 2703 | A    |
| 1   | A1    | 2704 | A    |
| 1   | A1    | 2705 | A    |
| 1   | A1    | 2712 | U    |
| 1   | A1    | 2714 | G    |
| 1   | A1    | 2723 | U    |
| 1   | A1    | 2726 | C    |
| 1   | A1    | 2727 | A    |
| 1   | A1    | 2728 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 2729 | OMU  |
| 1   | A1    | 2737 | C    |
| 1   | A1    | 2739 | A    |
| 1   | A1    | 2740 | A    |
| 1   | A1    | 2752 | U    |
| 1   | A1    | 2753 | G    |
| 1   | A1    | 2755 | C    |
| 1   | A1    | 2772 | C    |
| 1   | A1    | 2777 | G    |
| 1   | A1    | 2778 | G    |
| 1   | A1    | 2796 | G    |
| 1   | A1    | 2797 | C    |
| 1   | A1    | 2799 | A    |
| 1   | A1    | 2800 | G    |
| 1   | A1    | 2801 | A    |
| 1   | A1    | 2802 | A    |
| 1   | A1    | 2803 | A    |
| 1   | A1    | 2810 | C    |
| 1   | A1    | 2816 | G    |
| 1   | A1    | 2817 | A    |
| 1   | A1    | 2828 | G    |
| 1   | A1    | 2838 | A    |
| 1   | A1    | 2839 | G    |
| 1   | A1    | 2842 | U    |
| 1   | A1    | 2843 | U    |
| 1   | A1    | 2845 | A    |
| 1   | A1    | 2858 | U    |
| 1   | A1    | 2860 | U    |
| 1   | A1    | 2861 | U    |
| 1   | A1    | 2867 | C    |
| 1   | A1    | 2872 | A    |
| 1   | A1    | 2873 | U    |
| 1   | A1    | 2875 | U    |
| 1   | A1    | 2887 | A    |
| 1   | A1    | 2889 | C    |
| 1   | A1    | 2898 | G    |
| 1   | A1    | 2911 | A    |
| 1   | A1    | 2923 | U    |
| 1   | A1    | 2933 | A    |
| 1   | A1    | 2935 | U    |
| 1   | A1    | 2936 | A    |
| 1   | A1    | 2938 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 2941 | A    |
| 1   | A1    | 2942 | C    |
| 1   | A1    | 2947 | G    |
| 1   | A1    | 2948 | OMC  |
| 1   | A1    | 2951 | G    |
| 1   | A1    | 2955 | U    |
| 1   | A1    | 2956 | A    |
| 1   | A1    | 2983 | C    |
| 1   | A1    | 2990 | G    |
| 1   | A1    | 2992 | U    |
| 1   | A1    | 2997 | G    |
| 1   | A1    | 3011 | A    |
| 1   | A1    | 3012 | A    |
| 1   | A1    | 3021 | A    |
| 1   | A1    | 3022 | G    |
| 1   | A1    | 3032 | A    |
| 1   | A1    | 3056 | U    |
| 1   | A1    | 3057 | U    |
| 1   | A1    | 3059 | G    |
| 1   | A1    | 3078 | U    |
| 1   | A1    | 3079 | U    |
| 1   | A1    | 3080 | G    |
| 1   | A1    | 3086 | A    |
| 1   | A1    | 3087 | A    |
| 1   | A1    | 3092 | C    |
| 1   | A1    | 3095 | U    |
| 1   | A1    | 3109 | G    |
| 1   | A1    | 3116 | G    |
| 1   | A1    | 3129 | A    |
| 1   | A1    | 3130 | A    |
| 1   | A1    | 3131 | U    |
| 1   | A1    | 3142 | A    |
| 1   | A1    | 3143 | C    |
| 1   | A1    | 3153 | U    |
| 1   | A1    | 3154 | C    |
| 1   | A1    | 3155 | U    |
| 1   | A1    | 3156 | U    |
| 1   | A1    | 3157 | U    |
| 1   | A1    | 3165 | A    |
| 1   | A1    | 3170 | A    |
| 1   | A1    | 3172 | A    |
| 1   | A1    | 3173 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 3174 | A    |
| 1   | A1    | 3175 | U    |
| 1   | A1    | 3176 | G    |
| 1   | A1    | 3179 | U    |
| 1   | A1    | 3181 | C    |
| 1   | A1    | 3186 | A    |
| 1   | A1    | 3187 | A    |
| 1   | A1    | 3196 | U    |
| 1   | A1    | 3198 | U    |
| 1   | A1    | 3199 | G    |
| 1   | A1    | 3206 | C    |
| 1   | A1    | 3207 | U    |
| 1   | A1    | 3210 | A    |
| 1   | A1    | 3215 | A    |
| 1   | A1    | 3216 | G    |
| 1   | A1    | 3217 | C    |
| 1   | A1    | 3218 | A    |
| 1   | A1    | 3219 | G    |
| 1   | A1    | 3234 | A    |
| 1   | A1    | 3243 | A    |
| 1   | A1    | 3244 | A    |
| 1   | A1    | 3247 | G    |
| 1   | A1    | 3251 | U    |
| 1   | A1    | 3259 | U    |
| 1   | A1    | 3260 | G    |
| 1   | A1    | 3263 | G    |
| 1   | A1    | 3270 | U    |
| 1   | A1    | 3273 | A    |
| 1   | A1    | 3275 | U    |
| 1   | A1    | 3276 | G    |
| 1   | A1    | 3277 | U    |
| 1   | A1    | 3278 | C    |
| 1   | A1    | 3281 | U    |
| 1   | A1    | 3282 | U    |
| 1   | A1    | 3283 | U    |
| 1   | A1    | 3284 | G    |
| 1   | A1    | 3289 | G    |
| 1   | A1    | 3294 | A    |
| 1   | A1    | 3303 | G    |
| 1   | A1    | 3304 | U    |
| 1   | A1    | 3309 | G    |
| 1   | A1    | 3313 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 3316 | A    |
| 1   | A1    | 3320 | A    |
| 1   | A1    | 3342 | A    |
| 1   | A1    | 3345 | G    |
| 1   | A1    | 3351 | U    |
| 1   | A1    | 3352 | U    |
| 1   | A1    | 3353 | G    |
| 1   | A1    | 3354 | U    |
| 1   | A1    | 3355 | U    |
| 1   | A1    | 3356 | G    |
| 1   | A1    | 3363 | U    |
| 1   | A1    | 3369 | G    |
| 1   | A1    | 3375 | A    |
| 1   | A1    | 3378 | C    |
| 1   | A1    | 3382 | U    |
| 1   | A1    | 3383 | G    |
| 1   | A1    | 3389 | U    |
| 1   | A1    | 3390 | G    |
| 2   | A3    | 7    | G    |
| 2   | A3    | 10   | C    |
| 2   | A3    | 22   | A    |
| 2   | A3    | 38   | U    |
| 2   | A3    | 41   | G    |
| 2   | A3    | 43   | U    |
| 2   | A3    | 49   | G    |
| 2   | A3    | 54   | U    |
| 2   | A3    | 55   | A    |
| 2   | A3    | 65   | G    |
| 2   | A3    | 74   | C    |
| 2   | A3    | 76   | A    |
| 2   | A3    | 99   | G    |
| 2   | A3    | 102  | A    |
| 2   | A3    | 112  | G    |
| 3   | A4    | 13   | A    |
| 3   | A4    | 25   | G    |
| 3   | A4    | 34   | U    |
| 3   | A4    | 35   | C    |
| 3   | A4    | 51   | G    |
| 3   | A4    | 52   | A    |
| 3   | A4    | 59   | A    |
| 3   | A4    | 62   | C    |
| 3   | A4    | 63   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A4    | 68  | G    |
| 3   | A4    | 75  | G    |
| 3   | A4    | 76  | C    |
| 3   | A4    | 80  | A    |
| 3   | A4    | 81  | U    |
| 3   | A4    | 82  | U    |
| 3   | A4    | 84  | C    |
| 3   | A4    | 86  | U    |
| 3   | A4    | 87  | G    |
| 3   | A4    | 88  | A    |
| 3   | A4    | 90  | U    |
| 3   | A4    | 95  | G    |
| 3   | A4    | 97  | A    |
| 3   | A4    | 104 | A    |
| 3   | A4    | 105 | A    |
| 3   | A4    | 106 | C    |
| 3   | A4    | 111 | A    |
| 3   | A4    | 112 | U    |
| 3   | A4    | 113 | U    |
| 3   | A4    | 116 | G    |
| 3   | A4    | 125 | U    |
| 3   | A4    | 126 | A    |
| 3   | A4    | 152 | G    |
| 3   | A4    | 157 | U    |
| 3   | A4    | 158 | U    |
| 79  | B5    | 4   | C    |
| 79  | B5    | 25  | C    |
| 79  | B5    | 26  | A    |
| 79  | B5    | 34  | G    |
| 79  | B5    | 42  | G    |
| 79  | B5    | 46  | A    |
| 79  | B5    | 47  | A    |
| 79  | B5    | 57  | G    |
| 79  | B5    | 60  | U    |
| 79  | B5    | 67  | A    |
| 79  | B5    | 68  | A    |
| 79  | B5    | 72  | A    |
| 79  | B5    | 75  | U    |
| 79  | B5    | 76  | A    |
| 79  | B5    | 77  | U    |
| 79  | B5    | 78  | A    |
| 79  | B5    | 81  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | B5    | 94  | U    |
| 79  | B5    | 104 | A    |
| 79  | B5    | 114 | C    |
| 79  | B5    | 115 | G    |
| 79  | B5    | 126 | A    |
| 79  | B5    | 127 | G    |
| 79  | B5    | 130 | C    |
| 79  | B5    | 133 | U    |
| 79  | B5    | 134 | U    |
| 79  | B5    | 135 | A    |
| 79  | B5    | 136 | C    |
| 79  | B5    | 137 | U    |
| 79  | B5    | 138 | A    |
| 79  | B5    | 141 | U    |
| 79  | B5    | 145 | A    |
| 79  | B5    | 158 | U    |
| 79  | B5    | 161 | U    |
| 79  | B5    | 166 | C    |
| 79  | B5    | 168 | A    |
| 79  | B5    | 171 | A    |
| 79  | B5    | 178 | U    |
| 79  | B5    | 179 | A    |
| 79  | B5    | 188 | A    |
| 79  | B5    | 189 | C    |
| 79  | B5    | 190 | C    |
| 79  | B5    | 191 | C    |
| 79  | B5    | 192 | U    |
| 79  | B5    | 193 | U    |
| 79  | B5    | 195 | G    |
| 79  | B5    | 196 | G    |
| 79  | B5    | 198 | A    |
| 79  | B5    | 200 | A    |
| 79  | B5    | 207 | U    |
| 79  | B5    | 217 | A    |
| 79  | B5    | 218 | A    |
| 79  | B5    | 224 | C    |
| 79  | B5    | 225 | A    |
| 79  | B5    | 227 | U    |
| 79  | B5    | 228 | G    |
| 79  | B5    | 229 | U    |
| 79  | B5    | 230 | C    |
| 79  | B5    | 232 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | B5    | 233 | C    |
| 79  | B5    | 234 | G    |
| 79  | B5    | 239 | C    |
| 79  | B5    | 240 | U    |
| 79  | B5    | 241 | U    |
| 79  | B5    | 257 | A    |
| 79  | B5    | 260 | U    |
| 79  | B5    | 261 | U    |
| 79  | B5    | 265 | A    |
| 79  | B5    | 273 | G    |
| 79  | B5    | 278 | U    |
| 79  | B5    | 280 | U    |
| 79  | B5    | 299 | A    |
| 79  | B5    | 314 | C    |
| 79  | B5    | 316 | A    |
| 79  | B5    | 322 | G    |
| 79  | B5    | 333 | A    |
| 79  | B5    | 337 | G    |
| 79  | B5    | 338 | C    |
| 79  | B5    | 352 | A    |
| 79  | B5    | 359 | A    |
| 79  | B5    | 360 | A    |
| 79  | B5    | 361 | C    |
| 79  | B5    | 365 | G    |
| 79  | B5    | 369 | A    |
| 79  | B5    | 380 | U    |
| 79  | B5    | 388 | G    |
| 79  | B5    | 390 | G    |
| 79  | B5    | 393 | C    |
| 79  | B5    | 399 | A    |
| 79  | B5    | 400 | A    |
| 79  | B5    | 401 | A    |
| 79  | B5    | 402 | C    |
| 79  | B5    | 404 | G    |
| 79  | B5    | 417 | A    |
| 79  | B5    | 419 | G    |
| 79  | B5    | 423 | G    |
| 79  | B5    | 424 | C    |
| 79  | B5    | 425 | A    |
| 79  | B5    | 426 | G    |
| 79  | B5    | 434 | G    |
| 79  | B5    | 439 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | B5    | 444 | C    |
| 79  | B5    | 448 | C    |
| 79  | B5    | 452 | A    |
| 79  | B5    | 459 | G    |
| 79  | B5    | 460 | A    |
| 79  | B5    | 468 | A    |
| 79  | B5    | 475 | A    |
| 79  | B5    | 477 | A    |
| 79  | B5    | 481 | A    |
| 79  | B5    | 484 | C    |
| 79  | B5    | 485 | A    |
| 79  | B5    | 486 | G    |
| 79  | B5    | 487 | G    |
| 79  | B5    | 489 | C    |
| 79  | B5    | 490 | C    |
| 79  | B5    | 491 | C    |
| 79  | B5    | 492 | A    |
| 79  | B5    | 493 | U    |
| 79  | B5    | 494 | U    |
| 79  | B5    | 495 | C    |
| 79  | B5    | 496 | G    |
| 79  | B5    | 497 | G    |
| 79  | B5    | 498 | G    |
| 79  | B5    | 499 | U    |
| 79  | B5    | 500 | C    |
| 79  | B5    | 501 | U    |
| 79  | B5    | 503 | G    |
| 79  | B5    | 505 | A    |
| 79  | B5    | 506 | A    |
| 79  | B5    | 507 | U    |
| 79  | B5    | 515 | A    |
| 79  | B5    | 519 | C    |
| 79  | B5    | 525 | A    |
| 79  | B5    | 527 | A    |
| 79  | B5    | 538 | A    |
| 79  | B5    | 539 | G    |
| 79  | B5    | 540 | G    |
| 79  | B5    | 541 | A2M  |
| 79  | B5    | 542 | A    |
| 79  | B5    | 556 | A    |
| 79  | B5    | 557 | G    |
| 79  | B5    | 558 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | B5    | 559 | C    |
| 79  | B5    | 565 | C    |
| 79  | B5    | 566 | C    |
| 79  | B5    | 568 | G    |
| 79  | B5    | 577 | G    |
| 79  | B5    | 579 | A    |
| 79  | B5    | 580 | A    |
| 79  | B5    | 582 | U    |
| 79  | B5    | 594 | A    |
| 79  | B5    | 595 | G    |
| 79  | B5    | 606 | A    |
| 79  | B5    | 611 | U    |
| 79  | B5    | 613 | G    |
| 79  | B5    | 614 | C    |
| 79  | B5    | 617 | U    |
| 79  | B5    | 619 | A2M  |
| 79  | B5    | 620 | A    |
| 79  | B5    | 621 | A    |
| 79  | B5    | 622 | A    |
| 79  | B5    | 623 | A    |
| 79  | B5    | 635 | A    |
| 79  | B5    | 639 | U    |
| 79  | B5    | 650 | U    |
| 79  | B5    | 651 | G    |
| 79  | B5    | 652 | G    |
| 79  | B5    | 655 | G    |
| 79  | B5    | 656 | G    |
| 79  | B5    | 657 | U    |
| 79  | B5    | 658 | C    |
| 79  | B5    | 677 | G    |
| 79  | B5    | 678 | A    |
| 79  | B5    | 679 | U    |
| 79  | B5    | 681 | U    |
| 79  | B5    | 683 | C    |
| 79  | B5    | 694 | U    |
| 79  | B5    | 696 | C    |
| 79  | B5    | 697 | C    |
| 79  | B5    | 698 | U    |
| 79  | B5    | 700 | C    |
| 79  | B5    | 702 | G    |
| 79  | B5    | 703 | G    |
| 79  | B5    | 704 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | B5    | 705 | U    |
| 79  | B5    | 706 | A    |
| 79  | B5    | 707 | A    |
| 79  | B5    | 708 | C    |
| 79  | B5    | 709 | C    |
| 79  | B5    | 710 | U    |
| 79  | B5    | 711 | U    |
| 79  | B5    | 714 | G    |
| 79  | B5    | 715 | U    |
| 79  | B5    | 716 | C    |
| 79  | B5    | 717 | C    |
| 79  | B5    | 718 | U    |
| 79  | B5    | 719 | U    |
| 79  | B5    | 720 | G    |
| 79  | B5    | 721 | U    |
| 79  | B5    | 722 | G    |
| 79  | B5    | 724 | C    |
| 79  | B5    | 725 | U    |
| 79  | B5    | 727 | U    |
| 79  | B5    | 729 | G    |
| 79  | B5    | 731 | C    |
| 79  | B5    | 732 | G    |
| 79  | B5    | 733 | A    |
| 79  | B5    | 734 | A    |
| 79  | B5    | 735 | C    |
| 79  | B5    | 736 | C    |
| 79  | B5    | 738 | G    |
| 79  | B5    | 740 | A    |
| 79  | B5    | 741 | C    |
| 79  | B5    | 742 | U    |
| 79  | B5    | 743 | U    |
| 79  | B5    | 745 | U    |
| 79  | B5    | 753 | A    |
| 79  | B5    | 755 | A    |
| 79  | B5    | 765 | G    |
| 79  | B5    | 766 | U    |
| 79  | B5    | 774 | A    |
| 79  | B5    | 775 | G    |
| 79  | B5    | 778 | G    |
| 79  | B5    | 779 | U    |
| 79  | B5    | 780 | A    |
| 79  | B5    | 781 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 782  | U    |
| 79  | B5    | 783  | G    |
| 79  | B5    | 784  | C    |
| 79  | B5    | 787  | G    |
| 79  | B5    | 789  | A    |
| 79  | B5    | 794  | U    |
| 79  | B5    | 812  | A    |
| 79  | B5    | 814  | A    |
| 79  | B5    | 815  | G    |
| 79  | B5    | 820  | U    |
| 79  | B5    | 821  | U    |
| 79  | B5    | 823  | G    |
| 79  | B5    | 829  | A    |
| 79  | B5    | 833  | U    |
| 79  | B5    | 836  | U    |
| 79  | B5    | 837  | G    |
| 79  | B5    | 838  | G    |
| 79  | B5    | 840  | U    |
| 79  | B5    | 846  | G    |
| 79  | B5    | 857  | U    |
| 79  | B5    | 859  | A    |
| 79  | B5    | 863  | A    |
| 79  | B5    | 873  | U    |
| 79  | B5    | 876  | G    |
| 79  | B5    | 886  | U    |
| 79  | B5    | 898  | A    |
| 79  | B5    | 906  | A    |
| 79  | B5    | 914  | G    |
| 79  | B5    | 932  | U    |
| 79  | B5    | 933  | A    |
| 79  | B5    | 935  | U    |
| 79  | B5    | 945  | U    |
| 79  | B5    | 951  | A    |
| 79  | B5    | 960  | U    |
| 79  | B5    | 964  | U    |
| 79  | B5    | 966  | A    |
| 79  | B5    | 973  | A    |
| 79  | B5    | 987  | G    |
| 79  | B5    | 992  | A    |
| 79  | B5    | 993  | A    |
| 79  | B5    | 1003 | A    |
| 79  | B5    | 1004 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 1005 | A    |
| 79  | B5    | 1021 | C    |
| 79  | B5    | 1025 | A    |
| 79  | B5    | 1026 | A    |
| 79  | B5    | 1028 | C    |
| 79  | B5    | 1030 | A    |
| 79  | B5    | 1032 | G    |
| 79  | B5    | 1039 | A    |
| 79  | B5    | 1052 | U    |
| 79  | B5    | 1056 | U    |
| 79  | B5    | 1058 | U    |
| 79  | B5    | 1060 | U    |
| 79  | B5    | 1061 | A    |
| 79  | B5    | 1062 | A    |
| 79  | B5    | 1076 | A    |
| 79  | B5    | 1082 | C    |
| 79  | B5    | 1083 | G    |
| 79  | B5    | 1086 | A    |
| 79  | B5    | 1092 | A    |
| 79  | B5    | 1097 | U    |
| 79  | B5    | 1098 | U    |
| 79  | B5    | 1100 | G    |
| 79  | B5    | 1101 | G    |
| 79  | B5    | 1111 | G    |
| 79  | B5    | 1113 | A    |
| 79  | B5    | 1126 | OMG  |
| 79  | B5    | 1138 | A    |
| 79  | B5    | 1150 | G    |
| 79  | B5    | 1158 | C    |
| 79  | B5    | 1166 | A    |
| 79  | B5    | 1185 | U    |
| 79  | B5    | 1194 | A    |
| 79  | B5    | 1196 | A    |
| 79  | B5    | 1199 | G    |
| 79  | B5    | 1200 | G    |
| 79  | B5    | 1201 | G    |
| 79  | B5    | 1202 | A    |
| 79  | B5    | 1203 | A    |
| 79  | B5    | 1207 | C    |
| 79  | B5    | 1214 | U    |
| 79  | B5    | 1217 | A    |
| 79  | B5    | 1218 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 1225 | U    |
| 79  | B5    | 1226 | A    |
| 79  | B5    | 1227 | A    |
| 79  | B5    | 1228 | G    |
| 79  | B5    | 1229 | G    |
| 79  | B5    | 1230 | A    |
| 79  | B5    | 1235 | C    |
| 79  | B5    | 1237 | G    |
| 79  | B5    | 1238 | A    |
| 79  | B5    | 1239 | U    |
| 79  | B5    | 1240 | U    |
| 79  | B5    | 1241 | G    |
| 79  | B5    | 1242 | A    |
| 79  | B5    | 1243 | G    |
| 79  | B5    | 1244 | A    |
| 79  | B5    | 1245 | G    |
| 79  | B5    | 1247 | U    |
| 79  | B5    | 1248 | C    |
| 79  | B5    | 1249 | U    |
| 79  | B5    | 1251 | U    |
| 79  | B5    | 1252 | C    |
| 79  | B5    | 1255 | G    |
| 79  | B5    | 1256 | A    |
| 79  | B5    | 1257 | U    |
| 79  | B5    | 1270 | G    |
| 79  | B5    | 1284 | C    |
| 79  | B5    | 1285 | U    |
| 79  | B5    | 1286 | U    |
| 79  | B5    | 1314 | U    |
| 79  | B5    | 1315 | U    |
| 79  | B5    | 1316 | G    |
| 79  | B5    | 1321 | A    |
| 79  | B5    | 1340 | U    |
| 79  | B5    | 1344 | A    |
| 79  | B5    | 1345 | A    |
| 79  | B5    | 1355 | C    |
| 79  | B5    | 1356 | U    |
| 79  | B5    | 1359 | C    |
| 79  | B5    | 1362 | U    |
| 79  | B5    | 1363 | U    |
| 79  | B5    | 1364 | G    |
| 79  | B5    | 1369 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 1371 | A    |
| 79  | B5    | 1372 | U    |
| 79  | B5    | 1373 | C    |
| 79  | B5    | 1378 | U    |
| 79  | B5    | 1382 | A    |
| 79  | B5    | 1390 | U    |
| 79  | B5    | 1399 | C    |
| 79  | B5    | 1400 | A    |
| 79  | B5    | 1413 | U    |
| 79  | B5    | 1415 | U    |
| 79  | B5    | 1418 | G    |
| 79  | B5    | 1425 | A    |
| 79  | B5    | 1427 | A    |
| 79  | B5    | 1428 | OMG  |
| 79  | B5    | 1432 | U    |
| 79  | B5    | 1435 | G    |
| 79  | B5    | 1436 | A    |
| 79  | B5    | 1445 | G    |
| 79  | B5    | 1446 | A    |
| 79  | B5    | 1447 | C    |
| 79  | B5    | 1458 | G    |
| 79  | B5    | 1459 | C    |
| 79  | B5    | 1461 | C    |
| 79  | B5    | 1471 | A    |
| 79  | B5    | 1477 | G    |
| 79  | B5    | 1486 | G    |
| 79  | B5    | 1491 | U    |
| 79  | B5    | 1492 | A    |
| 79  | B5    | 1493 | A    |
| 79  | B5    | 1496 | U    |
| 79  | B5    | 1503 | A    |
| 79  | B5    | 1506 | G    |
| 79  | B5    | 1514 | U    |
| 79  | B5    | 1516 | A    |
| 79  | B5    | 1520 | U    |
| 79  | B5    | 1521 | G    |
| 79  | B5    | 1523 | G    |
| 79  | B5    | 1524 | A    |
| 79  | B5    | 1537 | C    |
| 79  | B5    | 1542 | G    |
| 79  | B5    | 1557 | U    |
| 79  | B5    | 1559 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 1563 | C    |
| 79  | B5    | 1575 | G7M  |
| 79  | B5    | 1576 | A    |
| 79  | B5    | 1577 | A    |
| 79  | B5    | 1582 | U    |
| 79  | B5    | 1584 | G    |
| 79  | B5    | 1590 | G    |
| 79  | B5    | 1596 | C    |
| 79  | B5    | 1597 | A    |
| 79  | B5    | 1601 | G    |
| 79  | B5    | 1607 | G    |
| 79  | B5    | 1619 | C    |
| 79  | B5    | 1631 | A    |
| 79  | B5    | 1634 | C    |
| 79  | B5    | 1637 | C    |
| 79  | B5    | 1642 | G    |
| 79  | B5    | 1646 | C    |
| 79  | B5    | 1651 | A    |
| 79  | B5    | 1657 | U    |
| 79  | B5    | 1658 | G    |
| 79  | B5    | 1663 | G    |
| 79  | B5    | 1680 | G    |
| 79  | B5    | 1681 | A    |
| 79  | B5    | 1682 | U    |
| 79  | B5    | 1683 | C    |
| 79  | B5    | 1684 | U    |
| 79  | B5    | 1688 | U    |
| 79  | B5    | 1689 | A    |
| 79  | B5    | 1690 | G    |
| 79  | B5    | 1691 | A    |
| 79  | B5    | 1692 | G    |
| 79  | B5    | 1693 | A    |
| 79  | B5    | 1694 | A    |
| 79  | B5    | 1695 | G    |
| 79  | B5    | 1697 | G    |
| 79  | B5    | 1698 | G    |
| 79  | B5    | 1699 | G    |
| 79  | B5    | 1701 | A    |
| 79  | B5    | 1702 | A    |
| 79  | B5    | 1703 | C    |
| 79  | B5    | 1704 | U    |
| 79  | B5    | 1706 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 1708 | U    |
| 79  | B5    | 1709 | C    |
| 79  | B5    | 1710 | U    |
| 79  | B5    | 1711 | C    |
| 79  | B5    | 1713 | G    |
| 79  | B5    | 1714 | A    |
| 79  | B5    | 1716 | C    |
| 79  | B5    | 1717 | G    |
| 79  | B5    | 1730 | A    |
| 79  | B5    | 1750 | A    |
| 79  | B5    | 1766 | A    |
| 79  | B5    | 1767 | G    |
| 79  | B5    | 1768 | G    |
| 79  | B5    | 1769 | U    |
| 79  | B5    | 1780 | G    |
| 79  | B5    | 1782 | MA6  |
| 79  | B5    | 1792 | G    |
| 79  | B5    | 1793 | G    |
| 79  | B5    | 1794 | A    |
| 79  | B5    | 1795 | U    |
| 79  | B5    | 1796 | C    |
| 79  | B5    | 1799 | U    |

All (29) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A1    | 267  | G    |
| 1   | A1    | 282  | G    |
| 1   | A1    | 588  | G    |
| 1   | A1    | 916  | G    |
| 1   | A1    | 1032 | C    |
| 1   | A1    | 1280 | C    |
| 1   | A1    | 1314 | C    |
| 1   | A1    | 1385 | C    |
| 1   | A1    | 1575 | A    |
| 1   | A1    | 2093 | A    |
| 1   | A1    | 2401 | A    |
| 1   | A1    | 2585 | G    |
| 1   | A1    | 3164 | C    |
| 3   | A4    | 67   | U    |
| 3   | A4    | 81   | U    |
| 79  | B5    | 187  | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | B5    | 224  | C    |
| 79  | B5    | 272  | U    |
| 79  | B5    | 488  | G    |
| 79  | B5    | 489  | C    |
| 79  | B5    | 819  | G    |
| 79  | B5    | 950  | C    |
| 79  | B5    | 1059 | U    |
| 79  | B5    | 1285 | U    |
| 79  | B5    | 1344 | A    |
| 79  | B5    | 1358 | G    |
| 79  | B5    | 1572 | OMG  |
| 79  | B5    | 1633 | A    |
| 79  | B5    | 1645 | G    |

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

66 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 |
| 79  | OMG  | B5    | 1428 | 81,79 | 23,26,27     | 1.25 | 4 (17%)  | 32,38,41    | 1.85 | 5 (15%)  |
| 1   | A2M  | A1    | 876  | 1     | 22,25,26     | 1.52 | 5 (22%)  | 30,36,39    | 2.13 | 7 (23%)  |
| 1   | OMU  | A1    | 2724 | 1     | 19,22,23     | 1.34 | 4 (21%)  | 25,31,34    | 1.85 | 5 (20%)  |
| 1   | A2M  | A1    | 817  | 1,81  | 22,25,26     | 1.48 | 4 (18%)  | 30,36,39    | 2.16 | 9 (30%)  |
| 1   | A2M  | A1    | 1449 | 1,81  | 22,25,26     | 1.50 | 4 (18%)  | 30,36,39    | 2.01 | 7 (23%)  |
| 1   | OMG  | A1    | 908  | 1,81  | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 2.07 | 7 (21%)  |
| 79  | A2M  | B5    | 974  | 79    | 22,25,26     | 1.49 | 5 (22%)  | 30,36,39    | 2.03 | 10 (33%) |
| 1   | 1MA  | A1    | 645  | 1,81  | 21,25,26     | 1.39 | 4 (19%)  | 30,37,40    | 1.79 | 6 (20%)  |
| 79  | OMG  | B5    | 1572 | 79    | 23,26,27     | 1.24 | 3 (13%)  | 32,38,41    | 2.14 | 6 (18%)  |
| 79  | A2M  | B5    | 619  | 81,79 | 22,25,26     | 1.49 | 6 (27%)  | 30,36,39    | 2.08 | 9 (30%)  |
| 79  | OMC  | B5    | 1007 | 79    | 19,22,23     | 0.83 | 1 (5%)   | 25,31,34    | 0.97 | 1 (4%)   |
| 1   | OMG  | A1    | 2619 | 1     | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.00 | 6 (18%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 79  | OMU  | B5    | 1269 | 81,79 | 19,22,23     | 1.40 | 4 (21%)  | 25,31,34    | 1.95 | 6 (24%)  |
| 1   | OMG  | A1    | 2791 | 1     | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.07 | 7 (21%)  |
| 1   | OMG  | A1    | 805  | 1     | 23,26,27     | 1.26 | 4 (17%)  | 32,38,41    | 1.93 | 5 (15%)  |
| 1   | OMC  | A1    | 2197 | 1     | 19,22,23     | 0.81 | 0        | 25,31,34    | 0.79 | 0        |
| 1   | OMC  | A1    | 663  | 1     | 19,22,23     | 0.90 | 2 (10%)  | 25,31,34    | 0.85 | 0        |
| 79  | MA6  | B5    | 1782 | 79    | 23,26,27     | 1.48 | 4 (17%)  | 33,38,41    | 2.06 | 9 (27%)  |
| 1   | A2M  | A1    | 2280 | 1     | 22,25,26     | 1.50 | 5 (22%)  | 30,36,39    | 2.03 | 8 (26%)  |
| 1   | A2M  | A1    | 2281 | 1     | 22,25,26     | 1.42 | 4 (18%)  | 30,36,39    | 2.36 | 10 (33%) |
| 1   | A2M  | A1    | 1133 | 1     | 22,25,26     | 1.48 | 5 (22%)  | 30,36,39    | 2.16 | 8 (26%)  |
| 79  | A2M  | B5    | 436  | 79    | 22,25,26     | 1.49 | 4 (18%)  | 30,36,39    | 1.96 | 6 (20%)  |
| 1   | OMU  | A1    | 898  | 1     | 19,22,23     | 1.42 | 4 (21%)  | 25,31,34    | 1.77 | 4 (16%)  |
| 1   | OMC  | A1    | 1437 | 1,81  | 19,22,23     | 0.91 | 1 (5%)   | 25,31,34    | 1.49 | 5 (20%)  |
| 1   | OMC  | A1    | 2959 | 1     | 19,22,23     | 0.89 | 1 (5%)   | 25,31,34    | 0.99 | 1 (4%)   |
| 79  | OMG  | B5    | 562  | 79    | 23,26,27     | 1.23 | 3 (13%)  | 32,38,41    | 2.03 | 7 (21%)  |
| 79  | OMU  | B5    | 578  | 79    | 19,22,23     | 1.24 | 4 (21%)  | 25,31,34    | 1.85 | 6 (24%)  |
| 79  | OMC  | B5    | 1639 | 79    | 19,22,23     | 0.82 | 0        | 25,31,34    | 0.79 | 0        |
| 1   | UR3  | A1    | 2634 | 1,81  | 19,22,23     | 0.96 | 2 (10%)  | 26,32,35    | 1.92 | 4 (15%)  |
| 1   | OMU  | A1    | 2921 | 1     | 19,22,23     | 1.34 | 4 (21%)  | 25,31,34    | 1.87 | 5 (20%)  |
| 5   | HIC  | AB    | 243  | 5     | 10,11,12     | 1.27 | 1 (10%)  | 9,14,16     | 4.58 | 3 (33%)  |
| 1   | A2M  | A1    | 649  | 1     | 22,25,26     | 1.43 | 5 (22%)  | 30,36,39    | 2.08 | 10 (33%) |
| 1   | OMG  | A1    | 2288 | 1     | 23,26,27     | 1.25 | 3 (13%)  | 32,38,41    | 2.07 | 7 (21%)  |
| 1   | 1MA  | A1    | 2142 | 1,81  | 21,25,26     | 1.31 | 4 (19%)  | 30,37,40    | 1.69 | 6 (20%)  |
| 79  | OMC  | B5    | 414  | 79    | 19,22,23     | 0.82 | 0        | 25,31,34    | 0.88 | 1 (4%)   |
| 79  | A2M  | B5    | 420  | 79    | 22,25,26     | 1.48 | 5 (22%)  | 30,36,39    | 2.15 | 10 (33%) |
| 1   | 5MC  | A1    | 2870 | 1,81  | 19,22,23     | 1.07 | 3 (15%)  | 26,32,35    | 1.35 | 3 (11%)  |
| 79  | MA6  | B5    | 1781 | 79    | 23,26,27     | 1.53 | 4 (17%)  | 33,38,41    | 2.12 | 10 (30%) |
| 1   | OMG  | A1    | 1450 | 1     | 23,26,27     | 1.28 | 5 (21%)  | 32,38,41    | 1.99 | 7 (21%)  |
| 1   | OMU  | A1    | 2421 | 1     | 19,22,23     | 1.34 | 3 (15%)  | 25,31,34    | 1.87 | 4 (16%)  |
| 1   | OMU  | A1    | 2347 | 1     | 19,22,23     | 1.46 | 4 (21%)  | 25,31,34    | 1.92 | 7 (28%)  |
| 1   | OMG  | A1    | 2815 | 1     | 23,26,27     | 1.24 | 4 (17%)  | 32,38,41    | 2.11 | 8 (25%)  |
| 1   | 5MC  | A1    | 2278 | 1,81  | 19,22,23     | 1.31 | 3 (15%)  | 26,32,35    | 1.32 | 4 (15%)  |
| 1   | A2M  | A1    | 2640 | 1     | 22,25,26     | 1.47 | 5 (22%)  | 30,36,39    | 2.09 | 7 (23%)  |
| 1   | A2M  | A1    | 2946 | 1,81  | 22,25,26     | 1.50 | 5 (22%)  | 30,36,39    | 2.10 | 11 (36%) |
| 1   | OMG  | A1    | 2793 | 1     | 23,26,27     | 1.23 | 4 (17%)  | 32,38,41    | 1.99 | 6 (18%)  |
| 79  | 3AU  | B5    | 1191 | 79    | 24,28,29     | 0.48 | 0        | 30,40,43    | 0.70 | 0        |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMU  | A1    | 2729 | 1     | 19,22,23     | 1.40 | 3 (15%)  | 25,31,34    | 1.72 | 6 (24%)  |
| 79  | 4AC  | B5    | 1280 | 79    | 21,24,25     | 1.16 | 3 (14%)  | 28,34,37    | 1.71 | 3 (10%)  |
| 79  | 4AC  | B5    | 1773 | 79    | 21,24,25     | 1.01 | 1 (4%)   | 28,34,37    | 1.38 | 6 (21%)  |
| 79  | OMG  | B5    | 1126 | 79    | 23,26,27     | 1.25 | 4 (17%)  | 32,38,41    | 1.96 | 5 (15%)  |
| 79  | G7M  | B5    | 1575 | 79    | 23,26,27     | 2.42 | 5 (21%)  | 34,39,42    | 3.10 | 13 (38%) |
| 1   | OMG  | A1    | 867  | 1,81  | 23,26,27     | 1.22 | 4 (17%)  | 32,38,41    | 2.05 | 7 (21%)  |
| 1   | OMC  | A1    | 650  | 1     | 19,22,23     | 0.87 | 2 (10%)  | 25,31,34    | 0.89 | 1 (4%)   |
| 1   | OMG  | A1    | 2922 | 1     | 23,26,27     | 1.23 | 4 (17%)  | 32,38,41    | 1.97 | 6 (18%)  |
| 1   | A2M  | A1    | 2220 | 1     | 22,25,26     | 1.54 | 4 (18%)  | 30,36,39    | 2.02 | 9 (30%)  |
| 1   | OMC  | A1    | 2948 | 1     | 19,22,23     | 0.92 | 2 (10%)  | 25,31,34    | 1.01 | 2 (8%)   |
| 79  | A2M  | B5    | 28   | 81,79 | 22,25,26     | 1.54 | 5 (22%)  | 30,36,39    | 2.10 | 9 (30%)  |
| 79  | A2M  | B5    | 541  | 79    | 22,25,26     | 1.50 | 4 (18%)  | 30,36,39    | 2.17 | 7 (23%)  |
| 1   | A2M  | A1    | 807  | 1     | 22,25,26     | 1.55 | 5 (22%)  | 30,36,39    | 2.11 | 9 (30%)  |
| 1   | OMU  | A1    | 2417 | 1     | 19,22,23     | 1.34 | 4 (21%)  | 25,31,34    | 1.77 | 5 (20%)  |
| 79  | A2M  | B5    | 796  | 79    | 22,25,26     | 1.45 | 6 (27%)  | 30,36,39    | 2.18 | 10 (33%) |
| 79  | A2M  | B5    | 100  | 81,79 | 22,25,26     | 1.48 | 5 (22%)  | 30,36,39    | 2.15 | 8 (26%)  |
| 1   | OMC  | A1    | 2337 | 1     | 19,22,23     | 0.94 | 2 (10%)  | 25,31,34    | 1.03 | 1 (4%)   |
| 1   | OMU  | A1    | 1888 | 1     | 19,22,23     | 1.41 | 4 (21%)  | 25,31,34    | 1.98 | 5 (20%)  |
| 79  | OMG  | B5    | 1271 | 79    | 23,26,27     | 1.24 | 3 (13%)  | 32,38,41    | 2.06 | 7 (21%)  |

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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 79  | OMG  | B5    | 1428 | 81,79 | -       | 3/9/27/28 | 0/3/3/3 |
| 1   | A2M  | A1    | 876  | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMU  | A1    | 2724 | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | A2M  | A1    | 817  | 1,81  | -       | 2/9/27/28 | 0/3/3/3 |
| 1   | A2M  | A1    | 1449 | 1,81  | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMG  | A1    | 908  | 1,81  | -       | 3/9/27/28 | 0/3/3/3 |
| 79  | A2M  | B5    | 974  | 79    | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | 1MA  | A1    | 645  | 1,81  | -       | 1/7/25/26 | 0/3/3/3 |
| 79  | OMG  | B5    | 1572 | 79    | -       | 1/9/27/28 | 0/3/3/3 |
| 79  | A2M  | B5    | 619  | 81,79 | -       | 3/9/27/28 | 0/3/3/3 |
| 79  | OMC  | B5    | 1007 | 79    | -       | 0/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | OMG  | A1    | 2619 | 1     | -       | 1/9/27/28  | 0/3/3/3 |
| 79  | OMU  | B5    | 1269 | 81,79 | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMG  | A1    | 2791 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | A1    | 805  | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | A1    | 2197 | 1     | -       | 6/9/27/28  | 0/2/2/2 |
| 1   | OMC  | A1    | 663  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | MA6  | B5    | 1782 | 79    | -       | 5/11/29/30 | 0/3/3/3 |
| 1   | A2M  | A1    | 2280 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | A1    | 2281 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | A2M  | A1    | 1133 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | A2M  | B5    | 436  | 79    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMU  | A1    | 898  | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMC  | A1    | 1437 | 1,81  | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMC  | A1    | 2959 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | OMG  | B5    | 562  | 79    | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | OMU  | B5    | 578  | 79    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | OMC  | B5    | 1639 | 79    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | UR3  | A1    | 2634 | 1,81  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | A1    | 2921 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 5   | HIC  | AB    | 243  | 5     | -       | 1/5/6/8    | 0/1/1/1 |
| 1   | A2M  | A1    | 649  | 1     | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | OMG  | A1    | 2288 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | 1MA  | A1    | 2142 | 1,81  | -       | 2/7/25/26  | 0/3/3/3 |
| 79  | OMC  | B5    | 414  | 79    | -       | 0/9/27/28  | 0/2/2/2 |
| 79  | A2M  | B5    | 420  | 79    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 5MC  | A1    | 2870 | 1,81  | -       | 6/7/25/26  | 0/2/2/2 |
| 79  | MA6  | B5    | 1781 | 79    | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | OMG  | A1    | 1450 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMU  | A1    | 2421 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | A1    | 2347 | 1     | -       | 2/9/27/28  | 0/2/2/2 |
| 1   | OMG  | A1    | 2815 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 5MC  | A1    | 2278 | 1,81  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | A1    | 2640 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 79  | 3AU  | B5    | 1191 | 79    | 1/1/7/7 | 3/16/34/35 | 0/2/2/2 |
| 1   | OMG  | A1    | 2793 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | A1    | 2946 | 1,81  | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMU  | A1    | 2729 | 1     | -       | 2/9/27/28  | 0/2/2/2 |
| 79  | 4AC  | B5    | 1280 | 79    | -       | 4/11/29/30 | 0/2/2/2 |
| 79  | 4AC  | B5    | 1773 | 79    | -       | 2/11/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 79  | OMG  | B5    | 1126 | 79    | -       | 2/9/27/28 | 0/3/3/3 |
| 79  | G7M  | B5    | 1575 | 79    | 3/3/5/5 | 3/7/25/26 | 0/3/3/3 |
| 1   | OMG  | A1    | 867  | 1,81  | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMC  | A1    | 650  | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 1   | OMG  | A1    | 2922 | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | A2M  | A1    | 2220 | 1     | -       | 0/9/27/28 | 0/3/3/3 |
| 1   | OMC  | A1    | 2948 | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | A2M  | B5    | 28   | 81,79 | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | A2M  | B5    | 541  | 79    | -       | 3/9/27/28 | 0/3/3/3 |
| 1   | A2M  | A1    | 807  | 1     | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | OMU  | A1    | 2417 | 1     | -       | 2/9/27/28 | 0/2/2/2 |
| 79  | A2M  | B5    | 796  | 79    | -       | 0/9/27/28 | 0/3/3/3 |
| 79  | A2M  | B5    | 100  | 81,79 | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | OMC  | A1    | 2337 | 1     | -       | 1/9/27/28 | 0/2/2/2 |
| 1   | OMU  | A1    | 1888 | 1     | -       | 0/9/27/28 | 0/2/2/2 |
| 79  | OMG  | B5    | 1271 | 79    | -       | 1/9/27/28 | 0/3/3/3 |

All (228) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 79  | B5    | 1575 | G7M  | C8-N7 | 6.93  | 1.44        | 1.33     |
| 79  | B5    | 1575 | G7M  | C5-N7 | -5.67 | 1.32        | 1.39     |
| 79  | B5    | 1781 | MA6  | C5-C4 | 4.89  | 1.47        | 1.39     |
| 79  | B5    | 1575 | G7M  | C8-N9 | 4.52  | 1.47        | 1.35     |
| 79  | B5    | 1782 | MA6  | C5-C4 | 4.41  | 1.47        | 1.39     |
| 79  | B5    | 541  | A2M  | C5-C4 | 4.34  | 1.46        | 1.39     |
| 1   | A1    | 807  | A2M  | C5-C4 | 4.23  | 1.46        | 1.39     |
| 1   | A1    | 2280 | A2M  | C5-C4 | 4.19  | 1.46        | 1.39     |
| 1   | A1    | 2640 | A2M  | C5-C4 | 4.15  | 1.46        | 1.39     |
| 79  | B5    | 974  | A2M  | C5-C4 | 4.13  | 1.46        | 1.39     |
| 1   | A1    | 2220 | A2M  | C5-C4 | 4.09  | 1.46        | 1.39     |
| 1   | A1    | 1133 | A2M  | C5-C4 | 4.05  | 1.46        | 1.39     |
| 79  | B5    | 420  | A2M  | C5-C4 | 4.05  | 1.46        | 1.39     |
| 79  | B5    | 436  | A2M  | C5-C4 | 4.02  | 1.46        | 1.39     |
| 1   | A1    | 2278 | 5MC  | C5-C4 | 3.98  | 1.47        | 1.44     |
| 79  | B5    | 28   | A2M  | C5-C4 | 3.97  | 1.46        | 1.39     |
| 79  | B5    | 619  | A2M  | C5-C4 | 3.97  | 1.46        | 1.39     |
| 79  | B5    | 100  | A2M  | C5-C4 | 3.86  | 1.46        | 1.39     |
| 79  | B5    | 796  | A2M  | C5-C4 | 3.85  | 1.46        | 1.39     |
| 79  | B5    | 1575 | G7M  | C5-C4 | 3.76  | 1.47        | 1.38     |
| 1   | A1    | 649  | A2M  | C5-C4 | 3.72  | 1.45        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A1    | 2281 | A2M  | C5-C4   | 3.68  | 1.45        | 1.39     |
| 1   | A1    | 2946 | A2M  | C5-C4   | 3.68  | 1.45        | 1.39     |
| 1   | A1    | 876  | A2M  | C5-C4   | 3.64  | 1.45        | 1.39     |
| 1   | A1    | 1449 | A2M  | C5-C4   | 3.53  | 1.45        | 1.39     |
| 1   | A1    | 817  | A2M  | C5-C4   | 3.52  | 1.45        | 1.39     |
| 1   | A1    | 898  | OMU  | C4-N3   | -3.45 | 1.32        | 1.38     |
| 1   | A1    | 2347 | OMU  | C4-N3   | -3.42 | 1.32        | 1.38     |
| 79  | B5    | 1269 | OMU  | C4-N3   | -3.31 | 1.32        | 1.38     |
| 1   | A1    | 1888 | OMU  | C4-N3   | -3.27 | 1.33        | 1.38     |
| 1   | A1    | 2921 | OMU  | C4-N3   | -3.26 | 1.33        | 1.38     |
| 1   | A1    | 2729 | OMU  | C4-N3   | -3.25 | 1.33        | 1.38     |
| 79  | B5    | 1781 | MA6  | C5-C6   | 3.25  | 1.49        | 1.41     |
| 79  | B5    | 1572 | OMG  | C5-C4   | 3.24  | 1.47        | 1.38     |
| 1   | A1    | 2421 | OMU  | C4-N3   | -3.19 | 1.33        | 1.38     |
| 1   | A1    | 2815 | OMG  | C6-N1   | -3.15 | 1.33        | 1.38     |
| 1   | A1    | 2417 | OMU  | C4-N3   | -3.13 | 1.33        | 1.38     |
| 1   | A1    | 817  | A2M  | C5-N7   | -3.11 | 1.33        | 1.39     |
| 1   | A1    | 1449 | A2M  | C5-N7   | -3.11 | 1.33        | 1.39     |
| 79  | B5    | 436  | A2M  | C5-N7   | -3.10 | 1.33        | 1.39     |
| 1   | A1    | 805  | OMG  | C6-N1   | -3.10 | 1.33        | 1.38     |
| 1   | A1    | 908  | OMG  | C5-C4   | 3.08  | 1.47        | 1.38     |
| 79  | B5    | 100  | A2M  | C5-N7   | -3.07 | 1.33        | 1.39     |
| 1   | A1    | 2347 | OMU  | C2-N3   | -3.06 | 1.32        | 1.38     |
| 1   | A1    | 2220 | A2M  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 1   | A1    | 876  | A2M  | C5-N7   | -3.03 | 1.33        | 1.39     |
| 79  | B5    | 1126 | OMG  | C6-N1   | -3.03 | 1.33        | 1.38     |
| 1   | A1    | 2724 | OMU  | C4-N3   | -3.03 | 1.33        | 1.38     |
| 1   | A1    | 2220 | A2M  | C4-N9   | -3.02 | 1.31        | 1.37     |
| 79  | B5    | 1280 | 4AC  | C4-N4   | -3.02 | 1.35        | 1.39     |
| 1   | A1    | 2729 | OMU  | C5-C4   | -2.99 | 1.37        | 1.43     |
| 1   | A1    | 2288 | OMG  | C6-N1   | -2.98 | 1.33        | 1.38     |
| 1   | A1    | 2619 | OMG  | C5-C4   | 2.97  | 1.46        | 1.38     |
| 1   | A1    | 2791 | OMG  | C6-N1   | -2.95 | 1.33        | 1.38     |
| 5   | AB    | 243  | HIC  | CD2-NE2 | -2.95 | 1.32        | 1.37     |
| 79  | B5    | 1271 | OMG  | C5-C4   | 2.91  | 1.46        | 1.38     |
| 79  | B5    | 1271 | OMG  | C6-N1   | -2.91 | 1.33        | 1.38     |
| 1   | A1    | 2870 | 5MC  | C5-C4   | 2.89  | 1.46        | 1.44     |
| 79  | B5    | 562  | OMG  | C6-N1   | -2.89 | 1.33        | 1.38     |
| 1   | A1    | 2278 | 5MC  | C6-N1   | -2.88 | 1.33        | 1.38     |
| 79  | B5    | 541  | A2M  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 1   | A1    | 2288 | OMG  | C5-C4   | 2.87  | 1.46        | 1.38     |
| 1   | A1    | 867  | OMG  | C6-N1   | -2.87 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 79  | B5    | 562  | OMG  | C5-C4 | 2.86  | 1.46        | 1.38     |
| 1   | A1    | 2793 | OMG  | C6-N1 | -2.86 | 1.33        | 1.38     |
| 1   | A1    | 2724 | OMU  | C2-N3 | -2.83 | 1.33        | 1.38     |
| 1   | A1    | 898  | OMU  | C5-C4 | -2.83 | 1.37        | 1.43     |
| 79  | B5    | 1428 | OMG  | C5-C4 | 2.82  | 1.46        | 1.38     |
| 1   | A1    | 2922 | OMG  | C6-N1 | -2.82 | 1.33        | 1.38     |
| 79  | B5    | 1572 | OMG  | C6-N1 | -2.82 | 1.33        | 1.38     |
| 79  | B5    | 28   | A2M  | C5-N7 | -2.81 | 1.34        | 1.39     |
| 1   | A1    | 2921 | OMU  | C2-N3 | -2.81 | 1.33        | 1.38     |
| 1   | A1    | 1450 | OMG  | C6-N1 | -2.81 | 1.33        | 1.38     |
| 79  | B5    | 1782 | MA6  | C5-C6 | 2.80  | 1.48        | 1.41     |
| 79  | B5    | 1575 | G7M  | C6-N1 | -2.79 | 1.33        | 1.38     |
| 1   | A1    | 2946 | A2M  | C5-N7 | -2.79 | 1.34        | 1.39     |
| 1   | A1    | 898  | OMU  | C2-N3 | -2.78 | 1.33        | 1.38     |
| 1   | A1    | 807  | A2M  | C5-N7 | -2.77 | 1.34        | 1.39     |
| 1   | A1    | 2946 | A2M  | C4-N9 | -2.77 | 1.31        | 1.37     |
| 1   | A1    | 2421 | OMU  | C2-N3 | -2.76 | 1.33        | 1.38     |
| 1   | A1    | 649  | A2M  | C5-N7 | -2.76 | 1.34        | 1.39     |
| 1   | A1    | 1450 | OMG  | C4-N9 | -2.76 | 1.31        | 1.38     |
| 79  | B5    | 1269 | OMU  | C2-N3 | -2.75 | 1.33        | 1.38     |
| 1   | A1    | 2724 | OMU  | C5-C4 | -2.75 | 1.37        | 1.43     |
| 1   | A1    | 2281 | A2M  | C5-N7 | -2.74 | 1.34        | 1.39     |
| 79  | B5    | 796  | A2M  | C5-N7 | -2.74 | 1.34        | 1.39     |
| 1   | A1    | 817  | A2M  | C4-N9 | -2.73 | 1.32        | 1.37     |
| 1   | A1    | 1133 | A2M  | C5-N7 | -2.72 | 1.34        | 1.39     |
| 1   | A1    | 645  | 1MA  | C6-N6 | 2.72  | 1.34        | 1.28     |
| 1   | A1    | 2417 | OMU  | C2-N3 | -2.71 | 1.33        | 1.38     |
| 1   | A1    | 2922 | OMG  | C5-C4 | 2.71  | 1.46        | 1.38     |
| 1   | A1    | 2347 | OMU  | C5-C4 | -2.71 | 1.37        | 1.43     |
| 79  | B5    | 578  | OMU  | C4-N3 | -2.70 | 1.34        | 1.38     |
| 79  | B5    | 1126 | OMG  | C5-C4 | 2.70  | 1.46        | 1.38     |
| 79  | B5    | 974  | A2M  | C5-N7 | -2.70 | 1.34        | 1.39     |
| 1   | A1    | 2280 | A2M  | C5-N7 | -2.68 | 1.34        | 1.39     |
| 1   | A1    | 2729 | OMU  | C2-N3 | -2.67 | 1.33        | 1.38     |
| 79  | B5    | 420  | A2M  | C5-N7 | -2.66 | 1.34        | 1.39     |
| 1   | A1    | 1888 | OMU  | C2-N3 | -2.66 | 1.33        | 1.38     |
| 79  | B5    | 1428 | OMG  | C6-N1 | -2.65 | 1.33        | 1.38     |
| 1   | A1    | 1888 | OMU  | C5-C4 | -2.64 | 1.38        | 1.43     |
| 1   | A1    | 2640 | A2M  | C5-N7 | -2.64 | 1.34        | 1.39     |
| 1   | A1    | 876  | A2M  | C8-N9 | -2.63 | 1.33        | 1.37     |
| 1   | A1    | 867  | OMG  | C5-C4 | 2.63  | 1.45        | 1.38     |
| 79  | B5    | 1428 | OMG  | C5-N7 | -2.63 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 79  | B5    | 1773 | 4AC  | C4-N4 | -2.61 | 1.36        | 1.39     |
| 1   | A1    | 908  | OMG  | C6-N1 | -2.61 | 1.34        | 1.38     |
| 1   | A1    | 2793 | OMG  | C5-C4 | 2.59  | 1.45        | 1.38     |
| 1   | A1    | 645  | 1MA  | C5-N7 | -2.58 | 1.33        | 1.39     |
| 79  | B5    | 541  | A2M  | C5-C6 | 2.58  | 1.48        | 1.41     |
| 1   | A1    | 2948 | OMC  | C5-C4 | -2.58 | 1.36        | 1.42     |
| 1   | A1    | 2421 | OMU  | C5-C4 | -2.57 | 1.38        | 1.43     |
| 79  | B5    | 1572 | OMG  | C5-N7 | -2.57 | 1.33        | 1.39     |
| 1   | A1    | 2619 | OMG  | C6-N1 | -2.55 | 1.34        | 1.38     |
| 79  | B5    | 100  | A2M  | C8-N9 | -2.55 | 1.33        | 1.37     |
| 79  | B5    | 619  | A2M  | C5-N7 | -2.54 | 1.34        | 1.39     |
| 1   | A1    | 1437 | OMC  | C5-C4 | -2.54 | 1.37        | 1.42     |
| 1   | A1    | 649  | A2M  | C4-N9 | -2.54 | 1.32        | 1.37     |
| 1   | A1    | 2815 | OMG  | C5-C4 | 2.54  | 1.45        | 1.38     |
| 1   | A1    | 805  | OMG  | C5-N7 | -2.53 | 1.34        | 1.39     |
| 1   | A1    | 2280 | A2M  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 1   | A1    | 1449 | A2M  | C8-N9 | -2.53 | 1.33        | 1.37     |
| 1   | A1    | 2288 | OMG  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 1   | A1    | 2142 | 1MA  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 79  | B5    | 974  | A2M  | C4-N9 | -2.52 | 1.32        | 1.37     |
| 1   | A1    | 2791 | OMG  | C5-C4 | 2.51  | 1.45        | 1.38     |
| 1   | A1    | 807  | A2M  | C5-C6 | 2.50  | 1.48        | 1.41     |
| 1   | A1    | 2142 | 1MA  | C4-N9 | -2.50 | 1.31        | 1.38     |
| 1   | A1    | 805  | OMG  | C5-C4 | 2.50  | 1.45        | 1.38     |
| 1   | A1    | 2791 | OMG  | C5-N7 | -2.50 | 1.34        | 1.39     |
| 1   | A1    | 2281 | A2M  | C4-N9 | -2.49 | 1.32        | 1.37     |
| 1   | A1    | 2417 | OMU  | C5-C4 | -2.49 | 1.38        | 1.43     |
| 79  | B5    | 1782 | MA6  | C5-N7 | -2.49 | 1.34        | 1.39     |
| 79  | B5    | 619  | A2M  | C4-N9 | -2.49 | 1.32        | 1.37     |
| 1   | A1    | 2142 | 1MA  | C5-C4 | 2.49  | 1.45        | 1.38     |
| 79  | B5    | 28   | A2M  | C4-N9 | -2.49 | 1.32        | 1.37     |
| 79  | B5    | 1126 | OMG  | C5-N7 | -2.48 | 1.34        | 1.39     |
| 1   | A1    | 1449 | A2M  | C4-N9 | -2.48 | 1.32        | 1.37     |
| 1   | A1    | 807  | A2M  | C4-N9 | -2.47 | 1.32        | 1.37     |
| 1   | A1    | 2619 | OMG  | C5-N7 | -2.47 | 1.34        | 1.39     |
| 1   | A1    | 645  | 1MA  | C5-C4 | 2.44  | 1.45        | 1.38     |
| 79  | B5    | 28   | A2M  | C5-C6 | 2.44  | 1.47        | 1.41     |
| 1   | A1    | 2922 | OMG  | C5-N7 | -2.44 | 1.34        | 1.39     |
| 1   | A1    | 805  | OMG  | C4-N9 | -2.43 | 1.31        | 1.38     |
| 1   | A1    | 867  | OMG  | C5-N7 | -2.43 | 1.34        | 1.39     |
| 1   | A1    | 645  | 1MA  | C4-N9 | -2.42 | 1.31        | 1.38     |
| 1   | A1    | 1450 | OMG  | C5-N7 | -2.42 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A1    | 2959 | OMC  | C5-C4 | -2.41 | 1.37        | 1.42     |
| 1   | A1    | 817  | A2M  | C8-N9 | -2.41 | 1.33        | 1.37     |
| 1   | A1    | 663  | OMC  | C5-C4 | -2.41 | 1.37        | 1.42     |
| 1   | A1    | 650  | OMC  | C5-C4 | -2.41 | 1.37        | 1.42     |
| 1   | A1    | 2870 | 5MC  | C6-C5 | 2.39  | 1.38        | 1.34     |
| 1   | A1    | 908  | OMG  | C5-N7 | -2.39 | 1.34        | 1.39     |
| 79  | B5    | 578  | OMU  | C2-N3 | -2.39 | 1.33        | 1.38     |
| 79  | B5    | 420  | A2M  | C5-C6 | 2.39  | 1.47        | 1.41     |
| 1   | A1    | 2815 | OMG  | C5-N7 | -2.39 | 1.34        | 1.39     |
| 79  | B5    | 562  | OMG  | C5-N7 | -2.38 | 1.34        | 1.39     |
| 1   | A1    | 2793 | OMG  | C5-N7 | -2.38 | 1.34        | 1.39     |
| 1   | A1    | 2142 | 1MA  | C6-N6 | 2.37  | 1.33        | 1.28     |
| 79  | B5    | 436  | A2M  | C5-C6 | 2.36  | 1.47        | 1.41     |
| 1   | A1    | 2337 | OMC  | C5-C4 | -2.34 | 1.37        | 1.42     |
| 1   | A1    | 1133 | A2M  | C4-N9 | -2.34 | 1.32        | 1.37     |
| 79  | B5    | 619  | A2M  | C5-C6 | 2.33  | 1.47        | 1.41     |
| 79  | B5    | 436  | A2M  | C4-N9 | -2.33 | 1.32        | 1.37     |
| 79  | B5    | 974  | A2M  | C5-C6 | 2.33  | 1.47        | 1.41     |
| 1   | A1    | 876  | A2M  | C4-N9 | -2.32 | 1.32        | 1.37     |
| 1   | A1    | 2220 | A2M  | C8-N9 | -2.32 | 1.33        | 1.37     |
| 79  | B5    | 420  | A2M  | C4-N9 | -2.31 | 1.32        | 1.37     |
| 1   | A1    | 2640 | A2M  | C5-C6 | 2.31  | 1.47        | 1.41     |
| 79  | B5    | 1428 | OMG  | C4-N9 | -2.31 | 1.32        | 1.38     |
| 1   | A1    | 2921 | OMU  | C5-C4 | -2.31 | 1.38        | 1.43     |
| 79  | B5    | 1271 | OMG  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 79  | B5    | 619  | A2M  | C8-N9 | -2.30 | 1.33        | 1.37     |
| 79  | B5    | 28   | A2M  | C8-N9 | -2.29 | 1.33        | 1.37     |
| 1   | A1    | 2946 | A2M  | C8-N9 | -2.28 | 1.33        | 1.37     |
| 1   | A1    | 2948 | OMC  | C6-N1 | -2.28 | 1.32        | 1.38     |
| 79  | B5    | 1269 | OMU  | C2-N1 | 2.27  | 1.42        | 1.38     |
| 1   | A1    | 2280 | A2M  | C4-N9 | -2.27 | 1.33        | 1.37     |
| 79  | B5    | 1782 | MA6  | C4-N9 | -2.26 | 1.33        | 1.37     |
| 79  | B5    | 578  | OMU  | C5-C4 | -2.26 | 1.38        | 1.43     |
| 79  | B5    | 796  | A2M  | C5-C6 | 2.25  | 1.47        | 1.41     |
| 79  | B5    | 1280 | 4AC  | C7-N4 | -2.24 | 1.32        | 1.37     |
| 1   | A1    | 1888 | OMU  | C6-N1 | -2.24 | 1.32        | 1.38     |
| 79  | B5    | 100  | A2M  | C5-C6 | 2.23  | 1.47        | 1.41     |
| 1   | A1    | 2640 | A2M  | C8-N9 | -2.22 | 1.33        | 1.37     |
| 1   | A1    | 2793 | OMG  | C4-N9 | -2.20 | 1.32        | 1.38     |
| 1   | A1    | 2640 | A2M  | C4-N9 | -2.20 | 1.33        | 1.37     |
| 1   | A1    | 1133 | A2M  | C5-C6 | 2.20  | 1.47        | 1.41     |
| 1   | A1    | 2634 | UR3  | C5-C4 | -2.19 | 1.38        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 79  | B5    | 796  | A2M  | C4-N9 | -2.19 | 1.33        | 1.37     |
| 1   | A1    | 2634 | UR3  | C6-N1 | -2.19 | 1.32        | 1.38     |
| 79  | B5    | 100  | A2M  | C4-N9 | -2.19 | 1.33        | 1.37     |
| 1   | A1    | 2281 | A2M  | C5-C6 | 2.18  | 1.47        | 1.41     |
| 1   | A1    | 807  | A2M  | C8-N9 | -2.18 | 1.33        | 1.37     |
| 1   | A1    | 1450 | OMG  | C5-C4 | 2.17  | 1.44        | 1.38     |
| 79  | B5    | 1280 | 4AC  | C6-N1 | -2.17 | 1.32        | 1.38     |
| 1   | A1    | 876  | A2M  | C5-C6 | 2.16  | 1.47        | 1.41     |
| 79  | B5    | 1269 | OMU  | C5-C4 | -2.16 | 1.39        | 1.43     |
| 1   | A1    | 898  | OMU  | C6-N1 | -2.15 | 1.33        | 1.38     |
| 1   | A1    | 2946 | A2M  | C5-C6 | 2.13  | 1.46        | 1.41     |
| 1   | A1    | 2278 | 5MC  | C6-C5 | 2.13  | 1.38        | 1.34     |
| 1   | A1    | 1133 | A2M  | C8-N9 | -2.13 | 1.33        | 1.37     |
| 1   | A1    | 2870 | 5MC  | C6-N1 | -2.11 | 1.34        | 1.38     |
| 79  | B5    | 1007 | OMC  | C5-C4 | -2.09 | 1.38        | 1.42     |
| 1   | A1    | 2347 | OMU  | C6-N1 | -2.09 | 1.33        | 1.38     |
| 79  | B5    | 1781 | MA6  | C4-N9 | -2.08 | 1.33        | 1.37     |
| 1   | A1    | 663  | OMC  | C6-N1 | -2.07 | 1.33        | 1.38     |
| 79  | B5    | 420  | A2M  | C8-N9 | -2.07 | 1.34        | 1.37     |
| 1   | A1    | 649  | A2M  | C5-C6 | 2.05  | 1.46        | 1.41     |
| 1   | A1    | 2815 | OMG  | C4-N9 | -2.05 | 1.32        | 1.38     |
| 1   | A1    | 1450 | OMG  | C8-N9 | -2.05 | 1.32        | 1.37     |
| 1   | A1    | 2417 | OMU  | C6-N1 | -2.05 | 1.33        | 1.38     |
| 1   | A1    | 2280 | A2M  | C8-N7 | 2.05  | 1.35        | 1.31     |
| 1   | A1    | 650  | OMC  | C6-N1 | -2.04 | 1.33        | 1.38     |
| 1   | A1    | 2337 | OMC  | C6-N1 | -2.04 | 1.33        | 1.38     |
| 79  | B5    | 541  | A2M  | C8-N9 | -2.03 | 1.34        | 1.37     |
| 1   | A1    | 2921 | OMU  | C6-N1 | -2.03 | 1.33        | 1.38     |
| 79  | B5    | 974  | A2M  | C8-N9 | -2.03 | 1.34        | 1.37     |
| 79  | B5    | 1781 | MA6  | C5-N7 | -2.03 | 1.35        | 1.39     |
| 1   | A1    | 2724 | OMU  | C6-N1 | -2.02 | 1.33        | 1.38     |
| 79  | B5    | 796  | A2M  | C8-N9 | -2.02 | 1.34        | 1.37     |
| 79  | B5    | 578  | OMU  | C6-N1 | -2.02 | 1.33        | 1.38     |
| 1   | A1    | 2922 | OMG  | C4-N9 | -2.02 | 1.32        | 1.38     |
| 79  | B5    | 619  | A2M  | C8-N7 | 2.01  | 1.35        | 1.31     |
| 79  | B5    | 1126 | OMG  | C4-N9 | -2.01 | 1.33        | 1.38     |
| 1   | A1    | 867  | OMG  | C4-N9 | -2.01 | 1.33        | 1.38     |
| 79  | B5    | 796  | A2M  | C8-N7 | 2.00  | 1.35        | 1.31     |
| 1   | A1    | 649  | A2M  | C8-N9 | -2.00 | 1.34        | 1.37     |

All (392) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5   | AB    | 243  | HIC  | NE2-CE1-ND1 | -11.91 | 108.10      | 112.66   |
| 79  | B5    | 1575 | G7M  | CN7-N7-C8   | -8.56  | 111.82      | 124.79   |
| 1   | A1    | 2634 | UR3  | C4-N3-C2    | -7.58  | 118.48      | 124.58   |
| 79  | B5    | 1572 | OMG  | C5-C4-N3    | -7.19  | 116.94      | 128.39   |
| 79  | B5    | 541  | A2M  | C5-C4-N3    | -6.63  | 117.58      | 126.72   |
| 79  | B5    | 1271 | OMG  | C5-C4-N3    | -6.61  | 117.87      | 128.39   |
| 1   | A1    | 2288 | OMG  | C5-C4-N3    | -6.58  | 117.91      | 128.39   |
| 1   | A1    | 2619 | OMG  | C5-C4-N3    | -6.51  | 118.02      | 128.39   |
| 79  | B5    | 1280 | 4AC  | N4-C4-N3    | 6.49   | 124.41      | 113.87   |
| 79  | B5    | 562  | OMG  | C5-C4-N3    | -6.40  | 118.21      | 128.39   |
| 1   | A1    | 2815 | OMG  | C5-C4-N3    | -6.32  | 118.33      | 128.39   |
| 1   | A1    | 867  | OMG  | C5-C4-N3    | -6.28  | 118.39      | 128.39   |
| 1   | A1    | 2640 | A2M  | C5-C4-N3    | -6.26  | 118.09      | 126.72   |
| 1   | A1    | 876  | A2M  | C5-C4-N3    | -6.24  | 118.12      | 126.72   |
| 79  | B5    | 1575 | G7M  | C8-N7-C5    | 6.23   | 115.58      | 107.78   |
| 1   | A1    | 2791 | OMG  | C5-C4-N3    | -6.23  | 118.47      | 128.39   |
| 79  | B5    | 1575 | G7M  | C5-C4-N3    | -6.22  | 116.41      | 128.15   |
| 79  | B5    | 100  | A2M  | C5-C4-N3    | -6.17  | 118.22      | 126.72   |
| 1   | A1    | 2922 | OMG  | C5-C4-N3    | -6.16  | 118.58      | 128.39   |
| 79  | B5    | 1126 | OMG  | C5-C4-N3    | -6.15  | 118.60      | 128.39   |
| 1   | A1    | 908  | OMG  | C5-C4-N3    | -6.11  | 118.66      | 128.39   |
| 1   | A1    | 807  | A2M  | C5-C4-N3    | -6.09  | 118.34      | 126.72   |
| 79  | B5    | 436  | A2M  | C5-C4-N3    | -5.98  | 118.48      | 126.72   |
| 79  | B5    | 796  | A2M  | C5-C4-N3    | -5.98  | 118.48      | 126.72   |
| 1   | A1    | 2280 | A2M  | C5-C4-N3    | -5.96  | 118.52      | 126.72   |
| 1   | A1    | 1449 | A2M  | C5-C4-N3    | -5.92  | 118.56      | 126.72   |
| 5   | AB    | 243  | HIC  | CD2-NE2-CE1 | 5.81   | 109.01      | 106.71   |
| 79  | B5    | 28   | A2M  | C5-C4-N3    | -5.80  | 118.72      | 126.72   |
| 79  | B5    | 1428 | OMG  | C5-C4-N3    | -5.75  | 119.24      | 128.39   |
| 79  | B5    | 1575 | G7M  | N9-C4-N3    | 5.75   | 137.44      | 125.95   |
| 1   | A1    | 817  | A2M  | C5-C4-N3    | -5.73  | 118.83      | 126.72   |
| 1   | A1    | 2793 | OMG  | C5-C4-N3    | -5.66  | 119.38      | 128.39   |
| 79  | B5    | 1575 | G7M  | N9-C8-N7    | -5.63  | 98.82       | 112.48   |
| 1   | A1    | 805  | OMG  | C5-C4-N3    | -5.61  | 119.45      | 128.39   |
| 79  | B5    | 974  | A2M  | C5-C4-N3    | -5.60  | 119.01      | 126.72   |
| 1   | A1    | 1133 | A2M  | C5-C4-N3    | -5.60  | 119.01      | 126.72   |
| 79  | B5    | 1572 | OMG  | C2-N3-C4    | 5.58   | 121.90      | 112.30   |
| 79  | B5    | 420  | A2M  | C5-C4-N3    | -5.57  | 119.05      | 126.72   |
| 79  | B5    | 619  | A2M  | C5-C4-N3    | -5.51  | 119.13      | 126.72   |
| 1   | A1    | 2281 | A2M  | C5-C4-N3    | -5.41  | 119.27      | 126.72   |
| 79  | B5    | 1572 | OMG  | N9-C4-N3    | 5.40   | 136.76      | 125.95   |
| 1   | A1    | 1450 | OMG  | C5-C4-N3    | -5.40  | 119.80      | 128.39   |
| 1   | A1    | 2791 | OMG  | C2-N3-C4    | 5.36   | 121.53      | 112.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A1    | 2946 | A2M  | C5-C4-N3  | -5.35 | 119.35      | 126.72   |
| 1   | A1    | 645  | 1MA  | C5-C4-N3  | -5.32 | 119.44      | 127.27   |
| 79  | B5    | 541  | A2M  | N3-C4-N9  | 5.28  | 136.14      | 127.17   |
| 1   | A1    | 2288 | OMG  | C2-N3-C4  | 5.27  | 121.38      | 112.30   |
| 1   | A1    | 649  | A2M  | C5-C4-N3  | -5.27 | 119.46      | 126.72   |
| 79  | B5    | 1271 | OMG  | C2-N3-C4  | 5.26  | 121.35      | 112.30   |
| 79  | B5    | 1781 | MA6  | C5-C4-N3  | -5.23 | 119.52      | 126.72   |
| 1   | A1    | 2815 | OMG  | C2-N3-C4  | 5.22  | 121.30      | 112.30   |
| 1   | A1    | 867  | OMG  | C2-N3-C4  | 5.22  | 121.28      | 112.30   |
| 79  | B5    | 1782 | MA6  | C5-C4-N3  | -5.20 | 119.56      | 126.72   |
| 1   | A1    | 1450 | OMG  | C2-N3-C4  | 5.17  | 121.20      | 112.30   |
| 1   | A1    | 2640 | A2M  | N3-C4-N9  | 5.16  | 135.95      | 127.17   |
| 1   | A1    | 2288 | OMG  | N9-C4-N3  | 5.16  | 136.26      | 125.95   |
| 1   | A1    | 876  | A2M  | N3-C4-N9  | 5.15  | 135.93      | 127.17   |
| 1   | A1    | 2922 | OMG  | C2-N3-C4  | 5.13  | 121.14      | 112.30   |
| 1   | A1    | 2619 | OMG  | C2-N3-C4  | 5.12  | 121.12      | 112.30   |
| 79  | B5    | 562  | OMG  | C2-N3-C4  | 5.10  | 121.08      | 112.30   |
| 1   | A1    | 908  | OMG  | C2-N3-C4  | 5.02  | 120.94      | 112.30   |
| 1   | A1    | 1888 | OMU  | C4-N3-C2  | -5.01 | 120.39      | 126.61   |
| 79  | B5    | 100  | A2M  | N3-C4-N9  | 5.00  | 135.68      | 127.17   |
| 1   | A1    | 2793 | OMG  | C2-N3-C4  | 4.95  | 120.83      | 112.30   |
| 1   | A1    | 645  | 1MA  | C2-N3-C4  | 4.92  | 122.19      | 112.53   |
| 1   | A1    | 1449 | A2M  | N3-C4-N9  | 4.91  | 135.52      | 127.17   |
| 1   | A1    | 805  | OMG  | C2-N3-C4  | 4.91  | 120.75      | 112.30   |
| 1   | A1    | 2619 | OMG  | N9-C4-N3  | 4.90  | 135.75      | 125.95   |
| 79  | B5    | 1428 | OMG  | C2-N3-C4  | 4.88  | 120.71      | 112.30   |
| 79  | B5    | 1575 | G7M  | C2-N3-C4  | 4.88  | 120.70      | 112.30   |
| 79  | B5    | 1271 | OMG  | N9-C4-N3  | 4.85  | 135.65      | 125.95   |
| 79  | B5    | 578  | OMU  | C4-N3-C2  | -4.84 | 120.60      | 126.61   |
| 1   | A1    | 2142 | 1MA  | C5-C4-N3  | -4.81 | 120.19      | 127.27   |
| 1   | A1    | 2921 | OMU  | C4-N3-C2  | -4.81 | 120.65      | 126.61   |
| 79  | B5    | 1126 | OMG  | C2-N3-C4  | 4.80  | 120.57      | 112.30   |
| 1   | A1    | 817  | A2M  | N3-C4-N9  | 4.76  | 135.26      | 127.17   |
| 79  | B5    | 1126 | OMG  | N9-C4-N3  | 4.74  | 135.44      | 125.95   |
| 1   | A1    | 2724 | OMU  | C4-N3-C2  | -4.69 | 120.79      | 126.61   |
| 1   | A1    | 2921 | OMU  | N3-C2-N1  | 4.69  | 120.99      | 114.89   |
| 1   | A1    | 2421 | OMU  | C4-N3-C2  | -4.67 | 120.82      | 126.61   |
| 79  | B5    | 1575 | G7M  | CN7-N7-C5 | 4.66  | 132.60      | 126.80   |
| 1   | A1    | 2281 | A2M  | N3-C4-N9  | 4.64  | 135.06      | 127.17   |
| 79  | B5    | 1575 | G7M  | C1'-N9-C8 | -4.63 | 111.11      | 126.74   |
| 79  | B5    | 1781 | MA6  | C4-C5-N7  | -4.60 | 105.33      | 110.58   |
| 1   | A1    | 2220 | A2M  | C5-C4-N3  | -4.59 | 120.40      | 126.72   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A1    | 807  | A2M  | N3-C4-N9   | 4.59  | 134.97      | 127.17   |
| 1   | A1    | 2922 | OMG  | N9-C4-N3   | 4.58  | 135.11      | 125.95   |
| 1   | A1    | 867  | OMG  | N9-C4-N3   | 4.58  | 135.10      | 125.95   |
| 79  | B5    | 1781 | MA6  | C2-N1-C6   | 4.56  | 122.98      | 111.83   |
| 79  | B5    | 796  | A2M  | N3-C4-N9   | 4.54  | 134.89      | 127.17   |
| 1   | A1    | 2815 | OMG  | N9-C4-N3   | 4.54  | 135.02      | 125.95   |
| 1   | A1    | 1133 | A2M  | N3-C4-N9   | 4.52  | 134.85      | 127.17   |
| 1   | A1    | 2417 | OMU  | C4-N3-C2   | -4.52 | 121.01      | 126.61   |
| 79  | B5    | 562  | OMG  | N9-C4-N3   | 4.51  | 134.98      | 125.95   |
| 79  | B5    | 28   | A2M  | N3-C4-N9   | 4.51  | 134.83      | 127.17   |
| 79  | B5    | 974  | A2M  | N3-C4-N9   | 4.49  | 134.80      | 127.17   |
| 1   | A1    | 2142 | 1MA  | C2-N3-C4   | 4.47  | 121.30      | 112.53   |
| 1   | A1    | 2791 | OMG  | N9-C4-N3   | 4.47  | 134.89      | 125.95   |
| 1   | A1    | 2946 | A2M  | N3-C4-N9   | 4.46  | 134.76      | 127.17   |
| 79  | B5    | 1782 | MA6  | C2-N1-C6   | 4.45  | 122.70      | 111.83   |
| 79  | B5    | 420  | A2M  | N3-C4-N9   | 4.44  | 134.71      | 127.17   |
| 1   | A1    | 898  | OMU  | C4-N3-C2   | -4.42 | 121.12      | 126.61   |
| 1   | A1    | 2280 | A2M  | N3-C4-N9   | 4.41  | 134.66      | 127.17   |
| 79  | B5    | 436  | A2M  | N3-C4-N9   | 4.40  | 134.66      | 127.17   |
| 79  | B5    | 619  | A2M  | N3-C4-N9   | 4.37  | 134.61      | 127.17   |
| 79  | B5    | 1269 | OMU  | C4-N3-C2   | -4.37 | 121.19      | 126.61   |
| 1   | A1    | 2421 | OMU  | N3-C2-N1   | 4.35  | 120.55      | 114.89   |
| 1   | A1    | 2347 | OMU  | C4-N3-C2   | -4.34 | 121.22      | 126.61   |
| 1   | A1    | 908  | OMG  | N9-C4-N3   | 4.32  | 134.58      | 125.95   |
| 1   | A1    | 2220 | A2M  | N3-C2-N1   | -4.31 | 122.06      | 128.58   |
| 1   | A1    | 2724 | OMU  | C5-C4-N3   | 4.31  | 120.83      | 114.80   |
| 1   | A1    | 649  | A2M  | N3-C4-N9   | 4.29  | 134.46      | 127.17   |
| 1   | A1    | 1888 | OMU  | N3-C2-N1   | 4.28  | 120.47      | 114.89   |
| 1   | A1    | 2347 | OMU  | N3-C2-N1   | 4.27  | 120.44      | 114.89   |
| 1   | A1    | 2281 | A2M  | O4'-C1'-N9 | 4.25  | 116.25      | 108.09   |
| 79  | B5    | 1269 | OMU  | N3-C2-N1   | 4.22  | 120.39      | 114.89   |
| 1   | A1    | 2793 | OMG  | N9-C4-N3   | 4.18  | 134.32      | 125.95   |
| 1   | A1    | 1888 | OMU  | C5-C4-N3   | 4.18  | 120.66      | 114.80   |
| 1   | A1    | 1450 | OMG  | N9-C4-N3   | 4.16  | 134.28      | 125.95   |
| 79  | B5    | 1782 | MA6  | C4-C5-N7   | -4.15 | 105.84      | 110.58   |
| 1   | A1    | 1437 | OMC  | O2-C2-N3   | -4.15 | 115.79      | 122.33   |
| 79  | B5    | 541  | A2M  | C2-N3-C4   | 4.12  | 121.90      | 111.83   |
| 1   | A1    | 898  | OMU  | N3-C2-N1   | 4.10  | 120.22      | 114.89   |
| 1   | A1    | 2281 | A2M  | C2'-C1'-N9 | -4.09 | 107.03      | 113.75   |
| 1   | A1    | 2421 | OMU  | C5-C4-N3   | 4.06  | 120.48      | 114.80   |
| 1   | A1    | 2417 | OMU  | C5-C4-N3   | 4.02  | 120.44      | 114.80   |
| 1   | A1    | 2417 | OMU  | N3-C2-N1   | 3.95  | 120.03      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 79  | B5    | 578  | OMU  | C5-C4-N3   | 3.94  | 120.32      | 114.80   |
| 1   | A1    | 805  | OMG  | N9-C4-N3   | 3.94  | 133.82      | 125.95   |
| 1   | A1    | 2724 | OMU  | N3-C2-N1   | 3.93  | 120.01      | 114.89   |
| 1   | A1    | 2347 | OMU  | C5-C4-N3   | 3.92  | 120.29      | 114.80   |
| 1   | A1    | 898  | OMU  | C5-C4-N3   | 3.90  | 120.27      | 114.80   |
| 79  | B5    | 578  | OMU  | N3-C2-N1   | 3.90  | 119.97      | 114.89   |
| 79  | B5    | 796  | A2M  | C2'-C1'-N9 | -3.90 | 107.34      | 113.75   |
| 1   | A1    | 2921 | OMU  | C5-C4-N3   | 3.86  | 120.21      | 114.80   |
| 79  | B5    | 1280 | 4AC  | C5-C4-N4   | -3.84 | 116.48      | 122.94   |
| 1   | A1    | 876  | A2M  | C2-N3-C4   | 3.82  | 121.17      | 111.83   |
| 1   | A1    | 2280 | A2M  | C2-N3-C4   | 3.82  | 121.16      | 111.83   |
| 79  | B5    | 28   | A2M  | C2-N3-C4   | 3.81  | 121.14      | 111.83   |
| 79  | B5    | 1269 | OMU  | C5-C4-N3   | 3.78  | 120.10      | 114.80   |
| 79  | B5    | 796  | A2M  | C2-N3-C4   | 3.77  | 121.05      | 111.83   |
| 1   | A1    | 817  | A2M  | C2-N3-C4   | 3.77  | 121.05      | 111.83   |
| 1   | A1    | 649  | A2M  | N3-C2-N1   | -3.75 | 122.91      | 128.58   |
| 79  | B5    | 1428 | OMG  | N9-C4-N3   | 3.74  | 133.44      | 125.95   |
| 79  | B5    | 100  | A2M  | C2-N3-C4   | 3.73  | 120.95      | 111.83   |
| 79  | B5    | 1782 | MA6  | N3-C4-N9   | 3.73  | 133.51      | 127.17   |
| 1   | A1    | 2347 | OMU  | C1'-N1-C2  | 3.71  | 124.26      | 117.59   |
| 1   | A1    | 2640 | A2M  | C2-N3-C4   | 3.71  | 120.89      | 111.83   |
| 1   | A1    | 2729 | OMU  | C4-N3-C2   | -3.71 | 122.01      | 126.61   |
| 79  | B5    | 1781 | MA6  | C2-N3-C4   | 3.69  | 120.86      | 111.83   |
| 1   | A1    | 2946 | A2M  | C2-N3-C4   | 3.69  | 120.85      | 111.83   |
| 1   | A1    | 1133 | A2M  | C2'-C1'-N9 | -3.68 | 107.70      | 113.75   |
| 1   | A1    | 807  | A2M  | C2-N3-C4   | 3.67  | 120.81      | 111.83   |
| 1   | A1    | 1450 | OMG  | C6-C5-N7   | 3.67  | 136.97      | 130.29   |
| 79  | B5    | 436  | A2M  | C2-N3-C4   | 3.66  | 120.77      | 111.83   |
| 1   | A1    | 2946 | A2M  | N3-C2-N1   | -3.65 | 123.05      | 128.58   |
| 1   | A1    | 2729 | OMU  | N3-C2-N1   | 3.65  | 119.65      | 114.89   |
| 79  | B5    | 420  | A2M  | C2-N3-C4   | 3.65  | 120.74      | 111.83   |
| 1   | A1    | 649  | A2M  | C2-N3-C4   | 3.63  | 120.70      | 111.83   |
| 1   | A1    | 1133 | A2M  | C2-N3-C4   | 3.63  | 120.69      | 111.83   |
| 1   | A1    | 2281 | A2M  | C2-N3-C4   | 3.62  | 120.67      | 111.83   |
| 1   | A1    | 807  | A2M  | C4-C5-N7   | -3.62 | 106.45      | 110.58   |
| 1   | A1    | 2729 | OMU  | C5-C4-N3   | 3.62  | 119.86      | 114.80   |
| 1   | A1    | 2220 | A2M  | C2-N1-C6   | 3.61  | 124.67      | 118.73   |
| 79  | B5    | 1781 | MA6  | N3-C4-N9   | 3.61  | 133.30      | 127.17   |
| 79  | B5    | 619  | A2M  | C4-C5-N7   | -3.61 | 106.46      | 110.58   |
| 1   | A1    | 2220 | A2M  | C2'-C1'-N9 | -3.61 | 107.82      | 113.75   |
| 79  | B5    | 974  | A2M  | C2-N3-C4   | 3.60  | 120.62      | 111.83   |
| 1   | A1    | 2220 | A2M  | N3-C4-N9   | 3.60  | 133.28      | 127.17   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A1    | 1449 | A2M  | C2-N3-C4   | 3.58  | 120.58      | 111.83   |
| 1   | A1    | 2280 | A2M  | C4-C5-N7   | -3.58 | 106.49      | 110.58   |
| 1   | A1    | 2793 | OMG  | C6-C5-N7   | 3.57  | 136.78      | 130.29   |
| 79  | B5    | 1781 | MA6  | N1-C2-N3   | -3.57 | 123.18      | 128.58   |
| 79  | B5    | 28   | A2M  | C4-C5-N7   | -3.54 | 106.54      | 110.58   |
| 79  | B5    | 1269 | OMU  | C1'-N1-C2  | 3.50  | 123.89      | 117.59   |
| 1   | A1    | 2634 | UR3  | C5-C4-N3   | 3.48  | 119.63      | 115.04   |
| 79  | B5    | 1782 | MA6  | C2-N3-C4   | 3.48  | 120.33      | 111.83   |
| 1   | A1    | 2281 | A2M  | C4-N9-C8   | 3.47  | 109.38      | 105.74   |
| 1   | A1    | 805  | OMG  | C6-C5-N7   | 3.47  | 136.60      | 130.29   |
| 1   | A1    | 817  | A2M  | N3-C2-N1   | -3.46 | 123.34      | 128.58   |
| 1   | A1    | 2791 | OMG  | C6-C5-N7   | 3.46  | 136.58      | 130.29   |
| 79  | B5    | 420  | A2M  | C2'-C1'-N9 | -3.44 | 108.09      | 113.75   |
| 79  | B5    | 28   | A2M  | N3-C2-N1   | -3.42 | 123.40      | 128.58   |
| 79  | B5    | 420  | A2M  | C4-C5-N7   | -3.42 | 106.68      | 110.58   |
| 79  | B5    | 796  | A2M  | C4-C5-N7   | -3.40 | 106.69      | 110.58   |
| 79  | B5    | 100  | A2M  | C4-C5-N7   | -3.40 | 106.69      | 110.58   |
| 1   | A1    | 2142 | 1MA  | N9-C4-N3   | 3.40  | 134.65      | 126.90   |
| 1   | A1    | 2815 | OMG  | C6-C5-N7   | 3.39  | 136.46      | 130.29   |
| 1   | A1    | 1133 | A2M  | N3-C2-N1   | -3.39 | 123.46      | 128.58   |
| 1   | A1    | 2421 | OMU  | O4-C4-C5   | -3.38 | 119.33      | 125.16   |
| 79  | B5    | 436  | A2M  | C4-C5-N7   | -3.38 | 106.71      | 110.58   |
| 79  | B5    | 541  | A2M  | N3-C2-N1   | -3.38 | 123.47      | 128.58   |
| 1   | A1    | 2870 | 5MC  | O2-C2-N3   | -3.37 | 117.01      | 122.33   |
| 79  | B5    | 974  | A2M  | N3-C2-N1   | -3.37 | 123.48      | 128.58   |
| 79  | B5    | 420  | A2M  | N3-C2-N1   | -3.36 | 123.49      | 128.58   |
| 1   | A1    | 2724 | OMU  | O4-C4-C5   | -3.36 | 119.36      | 125.16   |
| 79  | B5    | 619  | A2M  | C2-N3-C4   | 3.36  | 120.03      | 111.83   |
| 1   | A1    | 645  | 1MA  | N9-C4-N3   | 3.34  | 134.52      | 126.90   |
| 79  | B5    | 1782 | MA6  | N1-C2-N3   | -3.34 | 123.53      | 128.58   |
| 1   | A1    | 2280 | A2M  | N3-C2-N1   | -3.33 | 123.55      | 128.58   |
| 79  | B5    | 541  | A2M  | C4-C5-N7   | -3.32 | 106.78      | 110.58   |
| 1   | A1    | 867  | OMG  | C6-C5-N7   | 3.32  | 136.33      | 130.29   |
| 79  | B5    | 1428 | OMG  | C6-C5-N7   | 3.30  | 136.30      | 130.29   |
| 1   | A1    | 2220 | A2M  | C2-N3-C4   | 3.30  | 119.90      | 111.83   |
| 1   | A1    | 2281 | A2M  | N3-C2-N1   | -3.30 | 123.59      | 128.58   |
| 79  | B5    | 562  | OMG  | C6-C5-N7   | 3.29  | 136.28      | 130.29   |
| 1   | A1    | 876  | A2M  | C4-C5-N7   | -3.28 | 106.83      | 110.58   |
| 79  | B5    | 578  | OMU  | O4-C4-C5   | -3.27 | 119.52      | 125.16   |
| 79  | B5    | 1773 | 4AC  | O2-C2-N3   | -3.27 | 117.17      | 122.33   |
| 79  | B5    | 1271 | OMG  | C6-C5-N7   | 3.26  | 136.22      | 130.29   |
| 1   | A1    | 2640 | A2M  | C4-C5-N7   | -3.25 | 106.87      | 110.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A1    | 649  | A2M  | C4-C5-N7    | -3.25 | 106.87      | 110.58   |
| 1   | A1    | 2278 | 5MC  | O2-C2-N3    | -3.24 | 117.22      | 122.33   |
| 1   | A1    | 1437 | OMC  | C1'-N1-C2   | 3.24  | 125.59      | 118.44   |
| 79  | B5    | 619  | A2M  | C4-N9-C8    | 3.23  | 109.13      | 105.74   |
| 1   | A1    | 876  | A2M  | N3-C2-N1    | -3.23 | 123.70      | 128.58   |
| 1   | A1    | 2870 | 5MC  | C5-C6-N1    | -3.21 | 119.83      | 123.31   |
| 79  | B5    | 974  | A2M  | C4-C5-N7    | -3.20 | 106.92      | 110.58   |
| 1   | A1    | 2278 | 5MC  | C5-C4-N3    | -3.20 | 118.48      | 121.75   |
| 79  | B5    | 796  | A2M  | N3-C2-N1    | -3.18 | 123.76      | 128.58   |
| 1   | A1    | 908  | OMG  | C6-C5-N7    | 3.18  | 136.07      | 130.29   |
| 1   | A1    | 2946 | A2M  | C4-N9-C8    | 3.17  | 109.06      | 105.74   |
| 79  | B5    | 100  | A2M  | N3-C2-N1    | -3.16 | 123.80      | 128.58   |
| 1   | A1    | 898  | OMU  | O4-C4-C5    | -3.16 | 119.72      | 125.16   |
| 1   | A1    | 1888 | OMU  | O4-C4-C5    | -3.15 | 119.73      | 125.16   |
| 1   | A1    | 908  | OMG  | O2'-C2'-C1' | 3.14  | 114.95      | 108.99   |
| 1   | A1    | 2417 | OMU  | O4-C4-C5    | -3.13 | 119.76      | 125.16   |
| 1   | A1    | 1133 | A2M  | C4-C5-N7    | -3.12 | 107.01      | 110.58   |
| 1   | A1    | 2946 | A2M  | C4-C5-N7    | -3.12 | 107.02      | 110.58   |
| 1   | A1    | 1449 | A2M  | N3-C2-N1    | -3.11 | 123.87      | 128.58   |
| 1   | A1    | 2922 | OMG  | C6-C5-N7    | 3.11  | 135.95      | 130.29   |
| 1   | A1    | 2729 | OMU  | O4-C4-C5    | -3.09 | 119.83      | 125.16   |
| 1   | A1    | 649  | A2M  | C4-N9-C8    | 3.09  | 108.98      | 105.74   |
| 79  | B5    | 1781 | MA6  | C5-N7-C8    | 3.07  | 108.28      | 103.45   |
| 1   | A1    | 2640 | A2M  | N3-C2-N1    | -3.00 | 124.04      | 128.58   |
| 79  | B5    | 1781 | MA6  | C6-C5-N7    | 2.99  | 138.20      | 133.43   |
| 1   | A1    | 908  | OMG  | CM2-O2'-C2' | 2.98  | 122.14      | 114.47   |
| 1   | A1    | 2815 | OMG  | CM2-O2'-C2' | -2.98 | 106.83      | 114.47   |
| 79  | B5    | 436  | A2M  | N3-C2-N1    | -2.97 | 124.08      | 128.58   |
| 1   | A1    | 2870 | 5MC  | C5-C4-N3    | -2.95 | 118.73      | 121.75   |
| 1   | A1    | 2220 | A2M  | C4-C5-N7    | -2.95 | 107.21      | 110.58   |
| 79  | B5    | 1575 | G7M  | C1'-N9-C4   | 2.94  | 135.17      | 126.49   |
| 1   | A1    | 2347 | OMU  | O4-C4-C5    | -2.91 | 120.15      | 125.16   |
| 1   | A1    | 1449 | A2M  | C4-C5-N7    | -2.90 | 107.26      | 110.58   |
| 79  | B5    | 420  | A2M  | C4-N9-C8    | 2.90  | 108.78      | 105.74   |
| 1   | A1    | 817  | A2M  | C4-N9-C8    | 2.90  | 108.78      | 105.74   |
| 79  | B5    | 1126 | OMG  | C6-C5-N7    | 2.88  | 135.54      | 130.29   |
| 1   | A1    | 2337 | OMC  | O2-C2-N3    | -2.87 | 117.81      | 122.33   |
| 1   | A1    | 2281 | A2M  | C4-C5-N7    | -2.86 | 107.31      | 110.58   |
| 1   | A1    | 817  | A2M  | C4-C5-N7    | -2.85 | 107.32      | 110.58   |
| 1   | A1    | 2288 | OMG  | C6-C5-N7    | 2.84  | 135.46      | 130.29   |
| 1   | A1    | 2948 | OMC  | O2-C2-N3    | -2.83 | 117.87      | 122.33   |
| 1   | A1    | 2921 | OMU  | O4-C4-C5    | -2.82 | 120.30      | 125.16   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A1    | 2619 | OMG  | C6-C5-N7   | 2.81  | 135.41      | 130.29   |
| 79  | B5    | 974  | A2M  | C4-N9-C8   | 2.81  | 108.69      | 105.74   |
| 1   | A1    | 876  | A2M  | C4-N9-C8   | 2.81  | 108.68      | 105.74   |
| 1   | A1    | 817  | A2M  | O4'-C1'-N9 | -2.80 | 102.70      | 108.09   |
| 79  | B5    | 1782 | MA6  | C5-N7-C8   | 2.80  | 107.86      | 103.45   |
| 1   | A1    | 1437 | OMC  | O2-C2-N1   | 2.80  | 124.39      | 118.90   |
| 1   | A1    | 1449 | A2M  | C4-N9-C8   | 2.80  | 108.67      | 105.74   |
| 1   | A1    | 807  | A2M  | O4'-C1'-N9 | 2.79  | 113.44      | 108.09   |
| 1   | A1    | 645  | 1MA  | N1-C2-N3   | -2.77 | 122.70      | 126.00   |
| 79  | B5    | 1007 | OMC  | O2-C2-N3   | -2.77 | 117.97      | 122.33   |
| 79  | B5    | 28   | A2M  | C2'-C1'-N9 | -2.74 | 109.24      | 113.75   |
| 79  | B5    | 562  | OMG  | C4-C5-N7   | -2.73 | 106.34      | 110.67   |
| 79  | B5    | 1271 | OMG  | C4-C5-N7   | -2.71 | 106.38      | 110.67   |
| 1   | A1    | 2791 | OMG  | C4-C5-N7   | -2.70 | 106.39      | 110.67   |
| 1   | A1    | 807  | A2M  | N3-C2-N1   | -2.69 | 124.51      | 128.58   |
| 1   | A1    | 2640 | A2M  | C4-N9-C8   | 2.68  | 108.55      | 105.74   |
| 79  | B5    | 619  | A2M  | N3-C2-N1   | -2.68 | 124.53      | 128.58   |
| 79  | B5    | 100  | A2M  | C4-N9-C8   | 2.66  | 108.53      | 105.74   |
| 79  | B5    | 1269 | OMU  | O2-C2-N3   | -2.66 | 116.59      | 121.49   |
| 1   | A1    | 2815 | OMG  | C4-C5-N7   | -2.66 | 106.46      | 110.67   |
| 79  | B5    | 28   | A2M  | C4-N9-C8   | 2.65  | 108.52      | 105.74   |
| 1   | A1    | 1133 | A2M  | C4-N9-C8   | 2.65  | 108.52      | 105.74   |
| 79  | B5    | 1428 | OMG  | C4-C5-N7   | -2.64 | 106.49      | 110.67   |
| 79  | B5    | 1269 | OMU  | O4-C4-C5   | -2.64 | 120.62      | 125.16   |
| 79  | B5    | 1773 | 4AC  | O7-C7-N4   | 2.64  | 126.05      | 121.90   |
| 79  | B5    | 100  | A2M  | C2'-C1'-N9 | -2.62 | 109.44      | 113.75   |
| 1   | A1    | 2959 | OMC  | O2-C2-N3   | -2.61 | 118.22      | 122.33   |
| 79  | B5    | 619  | A2M  | C5-N7-C8   | 2.56  | 107.47      | 103.45   |
| 1   | A1    | 867  | OMG  | C4-C5-N7   | -2.56 | 106.62      | 110.67   |
| 79  | B5    | 100  | A2M  | C5-N7-C8   | 2.56  | 107.47      | 103.45   |
| 1   | A1    | 2793 | OMG  | C4-C5-N7   | -2.56 | 106.62      | 110.67   |
| 79  | B5    | 1773 | 4AC  | C6-C5-C4   | 2.53  | 120.05      | 117.00   |
| 1   | A1    | 2729 | OMU  | C1'-N1-C2  | 2.53  | 122.14      | 117.59   |
| 1   | A1    | 2142 | 1MA  | N1-C2-N3   | -2.52 | 123.00      | 126.00   |
| 1   | A1    | 649  | A2M  | C5-N7-C8   | 2.51  | 107.40      | 103.45   |
| 79  | B5    | 420  | A2M  | C5-N7-C8   | 2.51  | 107.39      | 103.45   |
| 79  | B5    | 1773 | 4AC  | C5-C4-N3   | -2.47 | 118.73      | 122.60   |
| 1   | A1    | 876  | A2M  | C5-N7-C8   | 2.47  | 107.33      | 103.45   |
| 1   | A1    | 2724 | OMU  | O2-C2-N1   | -2.47 | 119.59      | 122.80   |
| 1   | A1    | 805  | OMG  | C4-C5-N7   | -2.46 | 106.77      | 110.67   |
| 1   | A1    | 2281 | A2M  | N9-C8-N7   | -2.45 | 110.46      | 113.94   |
| 1   | A1    | 908  | OMG  | C4-C5-N7   | -2.44 | 106.80      | 110.67   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A1    | 1437 | OMC  | CM2-O2'-C2' | 2.44  | 120.73      | 114.47   |
| 79  | B5    | 28   | A2M  | C5-N7-C8    | 2.44  | 107.28      | 103.45   |
| 1   | A1    | 2921 | OMU  | O2-C2-N1    | -2.44 | 119.62      | 122.80   |
| 79  | B5    | 1575 | G7M  | C8-N9-C4    | 2.43  | 113.12      | 107.09   |
| 79  | B5    | 1575 | G7M  | C2'-C1'-N9  | 2.40  | 119.94      | 113.25   |
| 79  | B5    | 796  | A2M  | C5-N7-C8    | 2.40  | 107.23      | 103.45   |
| 79  | B5    | 1782 | MA6  | C4-N9-C8    | 2.40  | 108.26      | 105.74   |
| 1   | A1    | 867  | OMG  | O6-C6-C5    | -2.40 | 120.19      | 126.53   |
| 79  | B5    | 541  | A2M  | C5-N7-C8    | 2.40  | 107.22      | 103.45   |
| 1   | A1    | 2922 | OMG  | C4-C5-N7    | -2.40 | 106.87      | 110.67   |
| 1   | A1    | 2347 | OMU  | O2-C2-N3    | -2.40 | 117.07      | 121.49   |
| 1   | A1    | 2619 | OMG  | C4-C5-N7    | -2.39 | 106.88      | 110.67   |
| 79  | B5    | 1782 | MA6  | C6-C5-N7    | 2.38  | 137.23      | 133.43   |
| 1   | A1    | 2220 | A2M  | C4-N9-C8    | 2.37  | 108.23      | 105.74   |
| 1   | A1    | 2281 | A2M  | C5-N7-C8    | 2.37  | 107.17      | 103.45   |
| 1   | A1    | 645  | 1MA  | C6-C5-N7    | 2.37  | 136.34      | 132.16   |
| 1   | A1    | 1450 | OMG  | C4-C5-N7    | -2.36 | 106.93      | 110.67   |
| 1   | A1    | 2729 | OMU  | C6-N1-C2    | -2.35 | 118.13      | 121.00   |
| 1   | A1    | 2142 | 1MA  | C6-C5-N7    | 2.35  | 136.31      | 132.16   |
| 1   | A1    | 2280 | A2M  | C5-N7-C8    | 2.35  | 107.14      | 103.45   |
| 1   | A1    | 1450 | OMG  | O6-C6-C5    | -2.33 | 120.37      | 126.53   |
| 79  | B5    | 1126 | OMG  | C4-C5-N7    | -2.33 | 106.98      | 110.67   |
| 1   | A1    | 807  | A2M  | C5-N7-C8    | 2.33  | 107.11      | 103.45   |
| 1   | A1    | 645  | 1MA  | C4-C5-N7    | -2.32 | 106.99      | 110.67   |
| 79  | B5    | 1781 | MA6  | C4-N9-C8    | 2.31  | 108.16      | 105.74   |
| 1   | A1    | 2640 | A2M  | C5-N7-C8    | 2.31  | 107.08      | 103.45   |
| 1   | A1    | 649  | A2M  | N9-C8-N7    | -2.30 | 110.67      | 113.94   |
| 79  | B5    | 796  | A2M  | C4-N9-C8    | 2.30  | 108.16      | 105.74   |
| 79  | B5    | 619  | A2M  | N9-C8-N7    | -2.30 | 110.67      | 113.94   |
| 1   | A1    | 649  | A2M  | C6-C5-N7    | 2.29  | 136.51      | 132.09   |
| 79  | B5    | 1773 | 4AC  | N4-C4-N3    | 2.29  | 117.58      | 113.87   |
| 1   | A1    | 2946 | A2M  | C5-N7-C8    | 2.29  | 107.05      | 103.45   |
| 79  | B5    | 1572 | OMG  | C6-C5-N7    | 2.29  | 134.45      | 130.29   |
| 79  | B5    | 414  | OMC  | O2-C2-N3    | -2.28 | 118.74      | 122.33   |
| 79  | B5    | 578  | OMU  | O2-C2-N1    | -2.27 | 119.84      | 122.80   |
| 1   | A1    | 807  | A2M  | C4-N9-C8    | 2.27  | 108.12      | 105.74   |
| 79  | B5    | 1575 | G7M  | O6-C6-C5    | -2.26 | 122.97      | 128.01   |
| 79  | B5    | 436  | A2M  | C5-N7-C8    | 2.26  | 107.00      | 103.45   |
| 1   | A1    | 2922 | OMG  | O6-C6-C5    | -2.25 | 120.60      | 126.53   |
| 79  | B5    | 28   | A2M  | C6-C5-N7    | 2.24  | 136.41      | 132.09   |
| 79  | B5    | 1280 | 4AC  | C5-C4-N3    | -2.24 | 119.09      | 122.60   |
| 79  | B5    | 1572 | OMG  | O6-C6-C5    | -2.24 | 120.63      | 126.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | B5    | 974  | A2M  | C5-N7-C8    | 2.23  | 106.95      | 103.45   |
| 1   | A1    | 2634 | UR3  | C1'-N1-C2   | 2.23  | 120.68      | 117.04   |
| 1   | A1    | 2347 | OMU  | C6-N1-C2    | -2.22 | 118.29      | 121.00   |
| 1   | A1    | 2288 | OMG  | C4-C5-N7    | -2.22 | 107.15      | 110.67   |
| 1   | A1    | 2288 | OMG  | O6-C6-C5    | -2.22 | 120.67      | 126.53   |
| 79  | B5    | 974  | A2M  | C2'-C1'-N9  | -2.21 | 110.12      | 113.75   |
| 1   | A1    | 2946 | A2M  | O4'-C4'-C3' | -2.20 | 100.78      | 105.15   |
| 79  | B5    | 619  | A2M  | C6-C5-N7    | 2.19  | 136.31      | 132.09   |
| 1   | A1    | 2619 | OMG  | O6-C6-C5    | -2.19 | 120.75      | 126.53   |
| 1   | A1    | 649  | A2M  | C2-N1-C6    | 2.19  | 122.32      | 118.73   |
| 1   | A1    | 1133 | A2M  | C5-N7-C8    | 2.19  | 106.89      | 103.45   |
| 1   | A1    | 1449 | A2M  | C5-N7-C8    | 2.18  | 106.87      | 103.45   |
| 1   | A1    | 2793 | OMG  | O6-C6-C5    | -2.18 | 120.78      | 126.53   |
| 1   | A1    | 2634 | UR3  | C3U-N3-C4   | 2.18  | 120.89      | 117.87   |
| 79  | B5    | 974  | A2M  | C2-N1-C6    | 2.17  | 122.30      | 118.73   |
| 1   | A1    | 2815 | OMG  | O6-C6-C5    | -2.17 | 120.80      | 126.53   |
| 1   | A1    | 2948 | OMC  | C1'-N1-C2   | 2.15  | 123.19      | 118.44   |
| 1   | A1    | 2417 | OMU  | C1'-N1-C2   | 2.15  | 121.45      | 117.59   |
| 79  | B5    | 796  | A2M  | C6-C5-N7    | 2.13  | 136.20      | 132.09   |
| 1   | A1    | 2220 | A2M  | C6-C5-N7    | 2.13  | 136.20      | 132.09   |
| 79  | B5    | 420  | A2M  | N9-C8-N7    | -2.13 | 110.92      | 113.94   |
| 1   | A1    | 2278 | 5MC  | C1'-N1-C6   | -2.13 | 117.65      | 121.15   |
| 1   | A1    | 2278 | 5MC  | C5-C6-N1    | -2.12 | 121.01      | 123.31   |
| 1   | A1    | 650  | OMC  | CM2-O2'-C2' | -2.12 | 109.02      | 114.47   |
| 1   | A1    | 2280 | A2M  | C6-C5-N7    | 2.12  | 136.18      | 132.09   |
| 1   | A1    | 817  | A2M  | C5-N7-C8    | 2.11  | 106.77      | 103.45   |
| 1   | A1    | 2791 | OMG  | O6-C6-C5    | -2.10 | 120.98      | 126.53   |
| 79  | B5    | 420  | A2M  | C6-C5-N7    | 2.10  | 136.14      | 132.09   |
| 1   | A1    | 2280 | A2M  | C4-N9-C8    | 2.09  | 107.93      | 105.74   |
| 1   | A1    | 2946 | A2M  | N9-C8-N7    | -2.08 | 110.98      | 113.94   |
| 1   | A1    | 867  | OMG  | C5-C6-N1    | 2.08  | 118.55      | 113.25   |
| 1   | A1    | 817  | A2M  | O3'-C3'-C4' | -2.08 | 105.12      | 111.08   |
| 79  | B5    | 578  | OMU  | C1'-N1-C2   | 2.07  | 121.32      | 117.59   |
| 79  | B5    | 1572 | OMG  | C4-C5-N7    | -2.07 | 107.39      | 110.67   |
| 1   | A1    | 2946 | A2M  | C2-N1-C6    | 2.06  | 122.12      | 118.73   |
| 79  | B5    | 796  | A2M  | O4'-C1'-N9  | 2.06  | 112.04      | 108.09   |
| 5   | AB    | 243  | HIC  | CB-CG-ND1   | 2.05  | 127.87      | 121.74   |
| 1   | A1    | 2815 | OMG  | C5-C6-N1    | 2.05  | 118.47      | 113.25   |
| 1   | A1    | 2142 | 1MA  | C8-N9-C4    | 2.05  | 109.86      | 106.03   |
| 1   | A1    | 807  | A2M  | C6-C5-N7    | 2.04  | 136.02      | 132.09   |
| 79  | B5    | 1781 | MA6  | N9-C8-N7    | -2.04 | 111.04      | 113.94   |
| 79  | B5    | 541  | A2M  | C4-N9-C8    | 2.03  | 107.87      | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 79  | B5    | 1271 | OMG  | C5-C6-N1    | 2.03  | 118.42      | 113.25   |
| 79  | B5    | 562  | OMG  | O6-C6-C5    | -2.03 | 121.19      | 126.53   |
| 79  | B5    | 1271 | OMG  | O6-C6-C5    | -2.02 | 121.19      | 126.53   |
| 1   | A1    | 2946 | A2M  | C6-C5-N7    | 2.02  | 135.99      | 132.09   |
| 1   | A1    | 1888 | OMU  | C2'-C1'-N1  | -2.02 | 110.41      | 114.24   |
| 79  | B5    | 1773 | 4AC  | O2-C2-N1    | 2.02  | 122.85      | 118.90   |
| 1   | A1    | 1437 | OMC  | C6-N1-C2    | -2.01 | 117.06      | 120.46   |
| 79  | B5    | 974  | A2M  | C6-C5-N7    | 2.01  | 135.97      | 132.09   |
| 1   | A1    | 2791 | OMG  | C8-N7-C5    | 2.01  | 107.84      | 104.26   |
| 79  | B5    | 562  | OMG  | CM2-O2'-C2' | -2.01 | 109.31      | 114.47   |
| 1   | A1    | 2288 | OMG  | C5-C6-N1    | 2.01  | 118.36      | 113.25   |
| 1   | A1    | 1450 | OMG  | C5-C6-N1    | 2.00  | 118.36      | 113.25   |
| 79  | B5    | 1575 | G7M  | C5-C6-N1    | 2.00  | 115.98      | 111.84   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 79  | B5    | 1191 | 3AU  | C12  |
| 79  | B5    | 1575 | G7M  | C2'  |
| 79  | B5    | 1575 | G7M  | C4'  |
| 79  | B5    | 1575 | G7M  | C3'  |

All (72) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A1    | 908  | OMG  | C1'-C2'-O2'-CM2 |
| 1   | A1    | 1437 | OMC  | C1'-C2'-O2'-CM2 |
| 1   | A1    | 1450 | OMG  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2197 | OMC  | C2'-C1'-N1-C6   |
| 1   | A1    | 2197 | OMC  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2288 | OMG  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2417 | OMU  | C1'-C2'-O2'-CM2 |
| 1   | A1    | 2619 | OMG  | C1'-C2'-O2'-CM2 |
| 1   | A1    | 2870 | 5MC  | C2'-C1'-N1-C2   |
| 1   | A1    | 2870 | 5MC  | C2'-C1'-N1-C6   |
| 79  | B5    | 619  | A2M  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1280 | 4AC  | N3-C4-N4-C7     |
| 79  | B5    | 1280 | 4AC  | C5-C4-N4-C7     |
| 79  | B5    | 1280 | 4AC  | O7-C7-N4-C4     |
| 79  | B5    | 1280 | 4AC  | CM7-C7-N4-C4    |
| 79  | B5    | 1773 | 4AC  | N3-C4-N4-C7     |
| 79  | B5    | 1782 | MA6  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 79  | B5    | 1782 | MA6  | C5-C6-N6-C9     |
| 1   | A1    | 2197 | OMC  | C2'-C1'-N1-C2   |
| 1   | A1    | 908  | OMG  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2197 | OMC  | C3'-C4'-C5'-O5' |
| 1   | A1    | 2288 | OMG  | C3'-C4'-C5'-O5' |
| 1   | A1    | 2729 | OMU  | C3'-C4'-C5'-O5' |
| 1   | A1    | 2729 | OMU  | O4'-C4'-C5'-O5' |
| 79  | B5    | 1575 | G7M  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1269 | OMU  | O4'-C1'-N1-C2   |
| 1   | A1    | 2142 | 1MA  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2142 | 1MA  | C3'-C4'-C5'-O5' |
| 79  | B5    | 541  | A2M  | O4'-C4'-C5'-O5' |
| 79  | B5    | 619  | A2M  | O4'-C4'-C5'-O5' |
| 79  | B5    | 1782 | MA6  | N1-C6-N6-C9     |
| 1   | A1    | 1450 | OMG  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1782 | MA6  | C3'-C4'-C5'-O5' |
| 1   | A1    | 2347 | OMU  | C3'-C4'-C5'-O5' |
| 79  | B5    | 541  | A2M  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1428 | OMG  | O4'-C4'-C5'-O5' |
| 79  | B5    | 1191 | 3AU  | N40-C12-C13-O31 |
| 1   | A1    | 908  | OMG  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1575 | G7M  | O4'-C4'-C5'-O5' |
| 79  | B5    | 1782 | MA6  | C5-C6-N6-C10    |
| 1   | A1    | 2870 | 5MC  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2870 | 5MC  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1269 | OMU  | O4'-C1'-N1-C6   |
| 1   | A1    | 2347 | OMU  | O4'-C4'-C5'-O5' |
| 79  | B5    | 1271 | OMG  | C1'-C2'-O2'-CM2 |
| 1   | A1    | 2870 | 5MC  | O4'-C1'-N1-C6   |
| 79  | B5    | 1773 | 4AC  | C5-C4-N4-C7     |
| 79  | B5    | 1428 | OMG  | C3'-C4'-C5'-O5' |
| 79  | B5    | 1191 | 3AU  | N3-C10-C11-C12  |
| 1   | A1    | 817  | A2M  | C4'-C5'-O5'-P   |
| 1   | A1    | 2281 | A2M  | C3'-C2'-O2'-CM' |
| 1   | A1    | 2870 | 5MC  | O4'-C1'-N1-C2   |
| 79  | B5    | 100  | A2M  | O4'-C4'-C5'-O5' |
| 79  | B5    | 1126 | OMG  | C4'-C5'-O5'-P   |
| 1   | A1    | 2197 | OMC  | O4'-C1'-N1-C6   |
| 1   | A1    | 2417 | OMU  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2197 | OMC  | O4'-C1'-N1-C2   |
| 1   | A1    | 649  | A2M  | C4'-C5'-O5'-P   |
| 79  | B5    | 1428 | OMG  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | AB    | 243  | HIC  | CA-CB-CG-CD2    |
| 79  | B5    | 1575 | G7M  | C2'-C1'-N9-C8   |
| 1   | A1    | 807  | A2M  | C3'-C2'-O2'-CM' |
| 1   | A1    | 817  | A2M  | O4'-C4'-C5'-O5' |
| 1   | A1    | 2337 | OMC  | O4'-C4'-C5'-O5' |
| 79  | B5    | 541  | A2M  | O4'-C1'-N9-C8   |
| 79  | B5    | 1126 | OMG  | C3'-C4'-C5'-O5' |
| 1   | A1    | 2281 | A2M  | O4'-C4'-C5'-O5' |
| 1   | A1    | 645  | 1MA  | C2'-C1'-N9-C8   |
| 79  | B5    | 1572 | OMG  | C2'-C1'-N9-C4   |
| 1   | A1    | 1437 | OMC  | C2'-C1'-N1-C2   |
| 79  | B5    | 619  | A2M  | C2'-C1'-N9-C8   |
| 79  | B5    | 1191 | 3AU  | N40-C12-C13-O30 |

There are no ring outliers.

15 monomers are involved in 20 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | A1    | 1449 | A2M  | 1       | 0            |
| 1   | A1    | 908  | OMG  | 2       | 0            |
| 1   | A1    | 2619 | OMG  | 1       | 0            |
| 1   | A1    | 663  | OMC  | 1       | 0            |
| 1   | A1    | 1133 | A2M  | 1       | 0            |
| 79  | B5    | 436  | A2M  | 1       | 0            |
| 5   | AB    | 243  | HIC  | 1       | 0            |
| 1   | A1    | 649  | A2M  | 1       | 0            |
| 79  | B5    | 1781 | MA6  | 1       | 0            |
| 1   | A1    | 2815 | OMG  | 1       | 0            |
| 79  | B5    | 1280 | 4AC  | 4       | 0            |
| 79  | B5    | 1126 | OMG  | 2       | 0            |
| 1   | A1    | 2220 | A2M  | 2       | 0            |
| 1   | A1    | 2948 | OMC  | 1       | 0            |
| 79  | B5    | 796  | A2M  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 377 ligands modelled in this entry, 376 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 80  | 3HE  | A1    | 3401 | -    | 21,21,21     | 0.43 | 0           | 23,30,30    | 0.76 | 0           |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 80  | 3HE  | A1    | 3401 | -    | -       | 0/8/36/36 | 0/2/2/2 |

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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A1    | 6                |
| 79  | B5    | 2                |
| 18  | AP    | 1                |
| 53  | BI    | 1                |
| 8   | AE    | 1                |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 12  | AI    | 1                |
| 62  | BR    | 1                |
| 76  | Bf    | 1                |
| 3   | A4    | 1                |
| 66  | BV    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A1    | 1253:U    | O3'    | 1260:A    | P      | 26.34        |
| 1     | AP    | 155:GLU   | C      | 164:LYS   | N      | 24.32        |
| 1     | BI    | 123:LYS   | C      | 135:LYS   | N      | 18.64        |
| 1     | A1    | 1955:U    | O3'    | 2093:A    | P      | 18.09        |
| 1     | B5    | 658:C     | O3'    | 676:G     | P      | 17.61        |
| 1     | A1    | 1023:C    | O3'    | 1030:A    | P      | 17.20        |
| 1     | AE    | 109:GLU   | C      | 129:GLU   | N      | 14.45        |
| 1     | A1    | 2445:A    | O3'    | 2501:U    | P      | 13.63        |
| 1     | AI    | 101:LYS   | C      | 114:GLY   | N      | 10.06        |
| 1     | A1    | 451:U     | O3'    | 486:A     | P      | 9.84         |
| 1     | BR    | 95:ARG    | C      | 100:LEU   | N      | 6.89         |
| 1     | Bf    | 125:THR   | C      | 129:GLY   | N      | 6.42         |
| 1     | A4    | 73:U      | O3'    | 74:U      | P      | 5.20         |
| 1     | BV    | 11:LEU    | C      | 12:TYR    | N      | 5.14         |
| 1     | A1    | 444:U     | O3'    | 445:G     | P      | 3.94         |
| 1     | B5    | 1798:U    | O3'    | 1799:U    | P      | 3.20         |

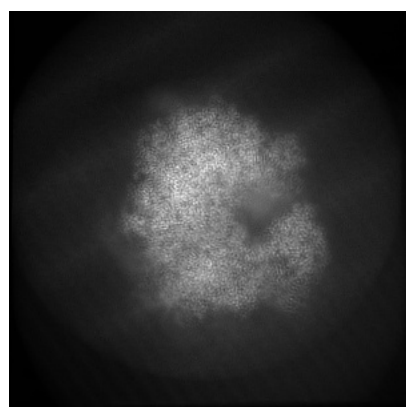
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24235. These allow visual inspection of the internal detail of the map and identification of artifacts.

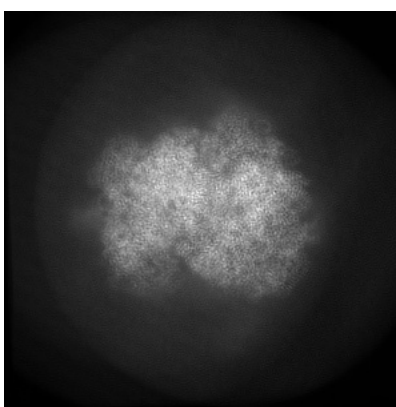
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

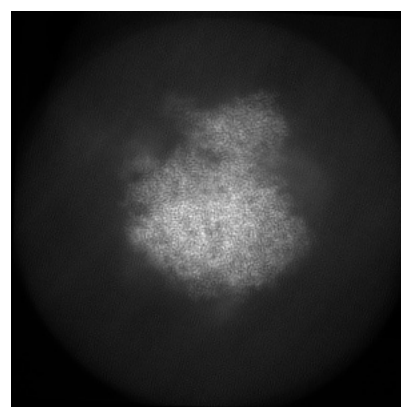
#### 6.1.1 Primary map



X



Y

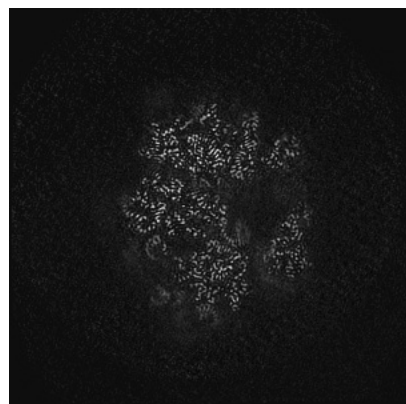


Z

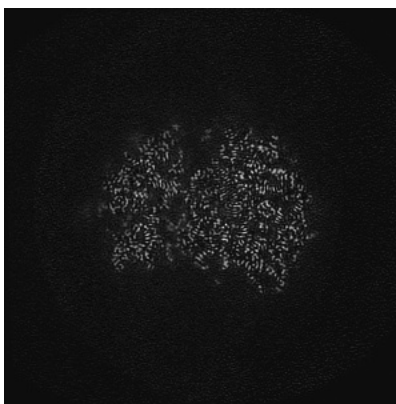
The images above show the map projected in three orthogonal directions.

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

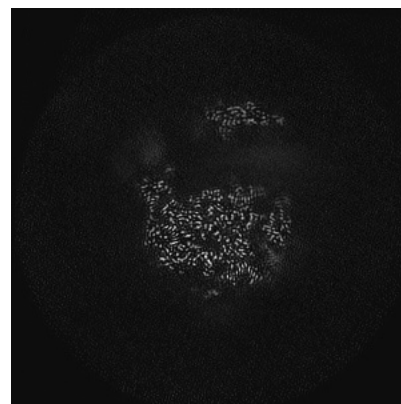
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

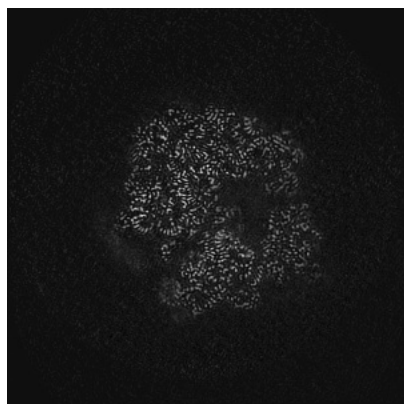


Z Index: 216

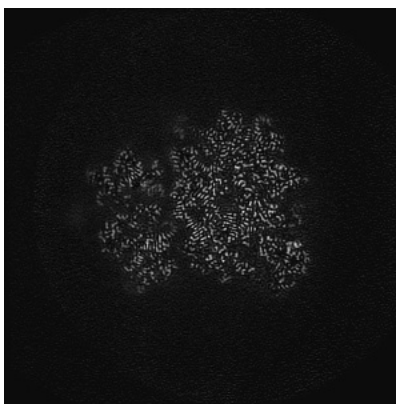
The images above show central slices of the map in three orthogonal directions.

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

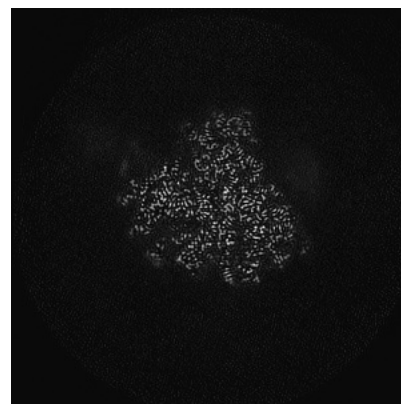
### 6.3.1 Primary map



X Index: 240



Y Index: 199

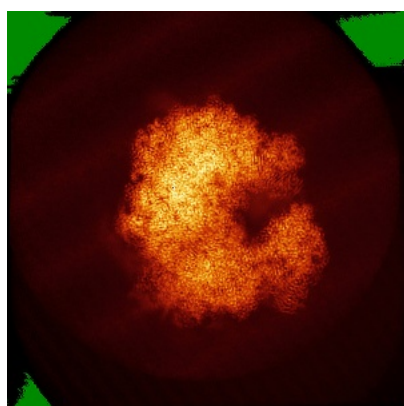


Z Index: 265

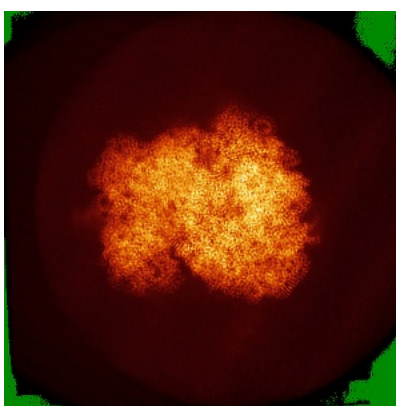
The images above show the largest variance slices of the map in three orthogonal directions.

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

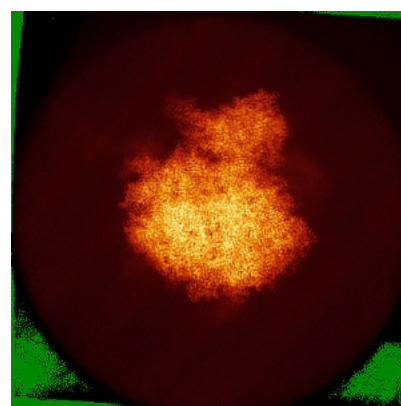
### 6.4.1 Primary map



X



Y



Z

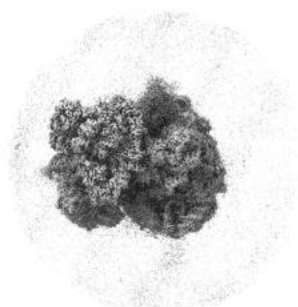
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

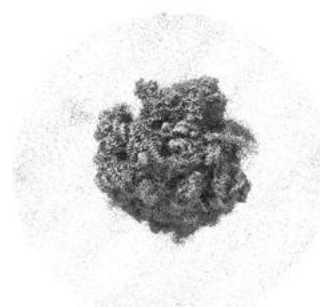
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

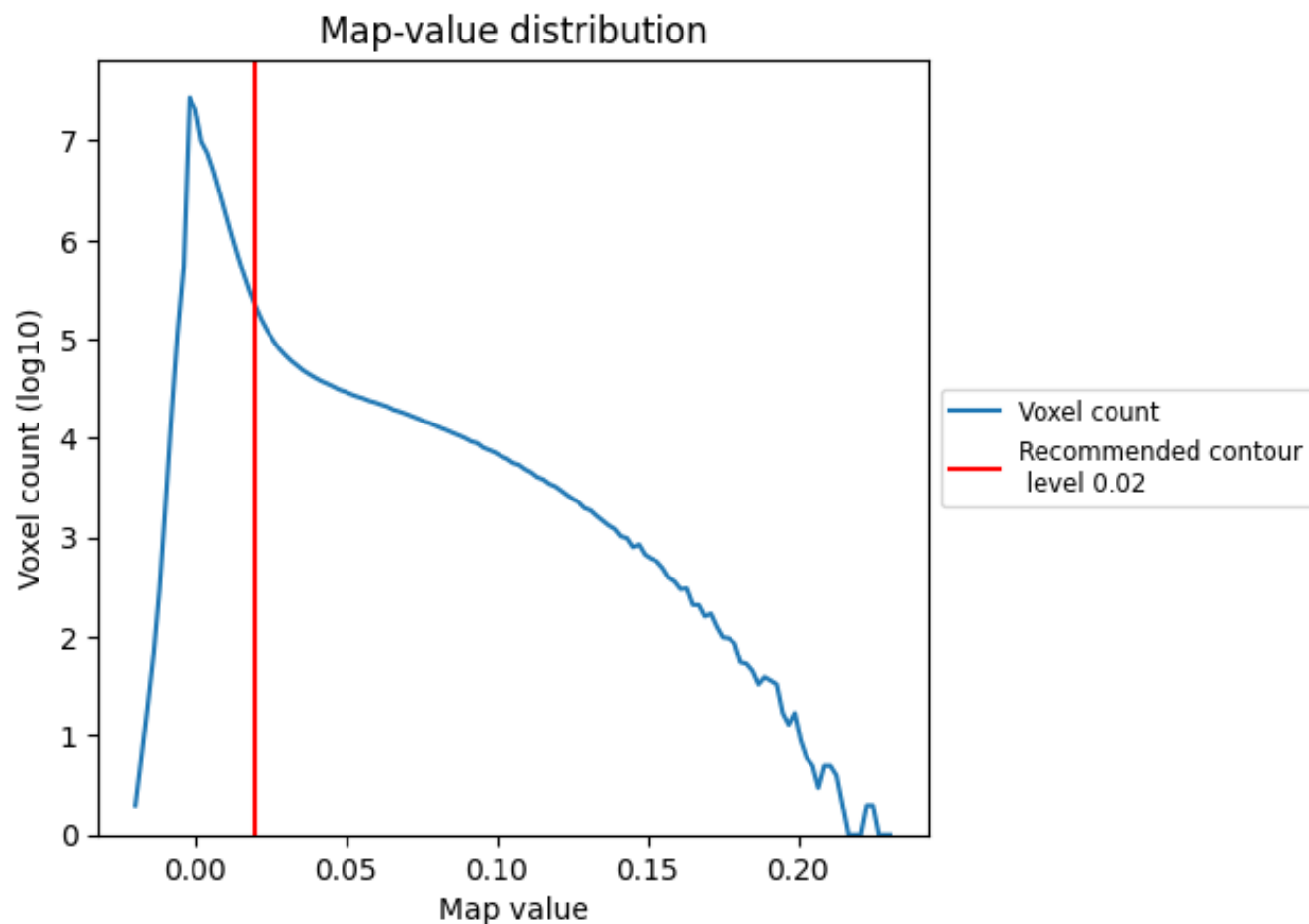
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

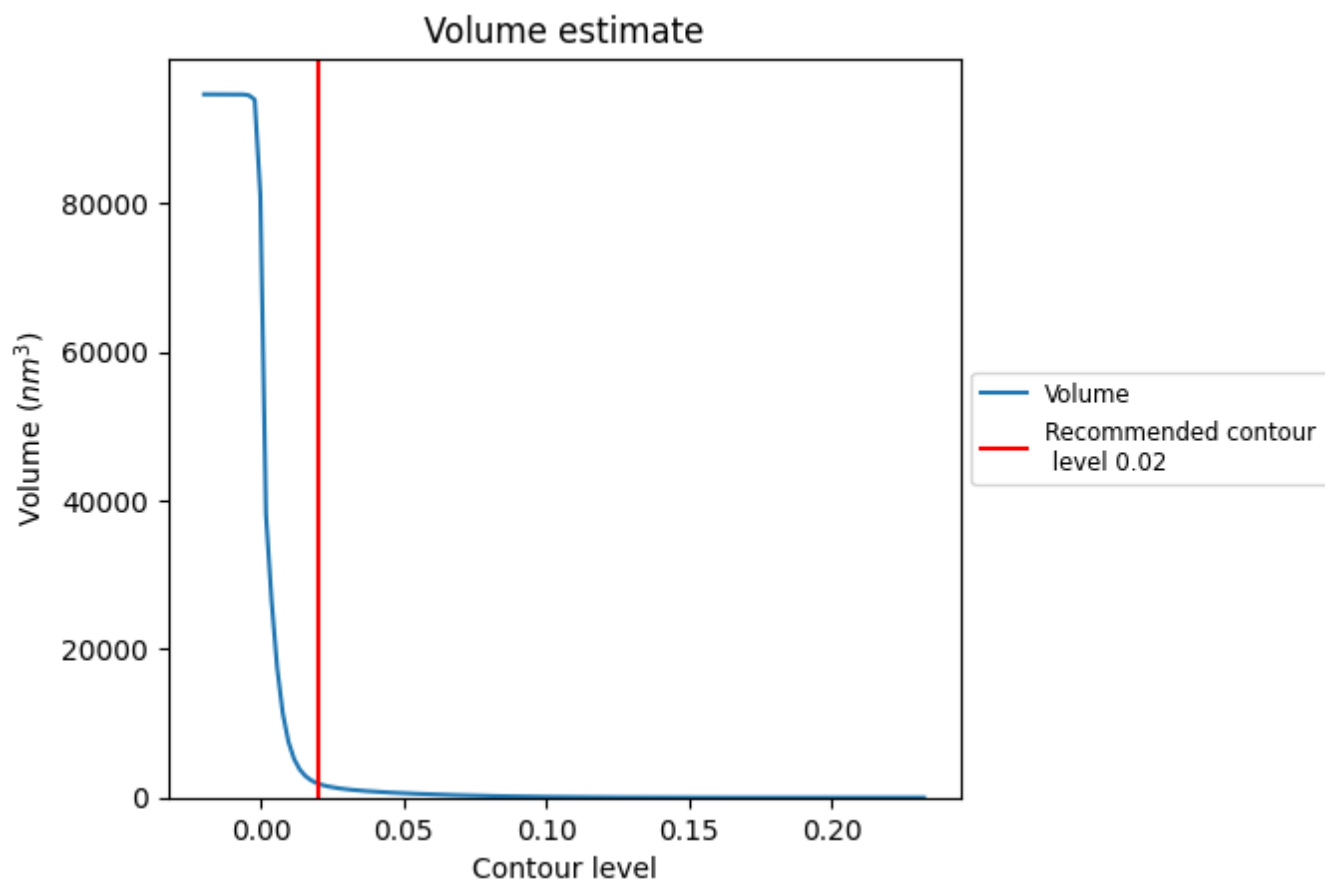
This section contains the results of statistical analysis of the map.

### 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](#)

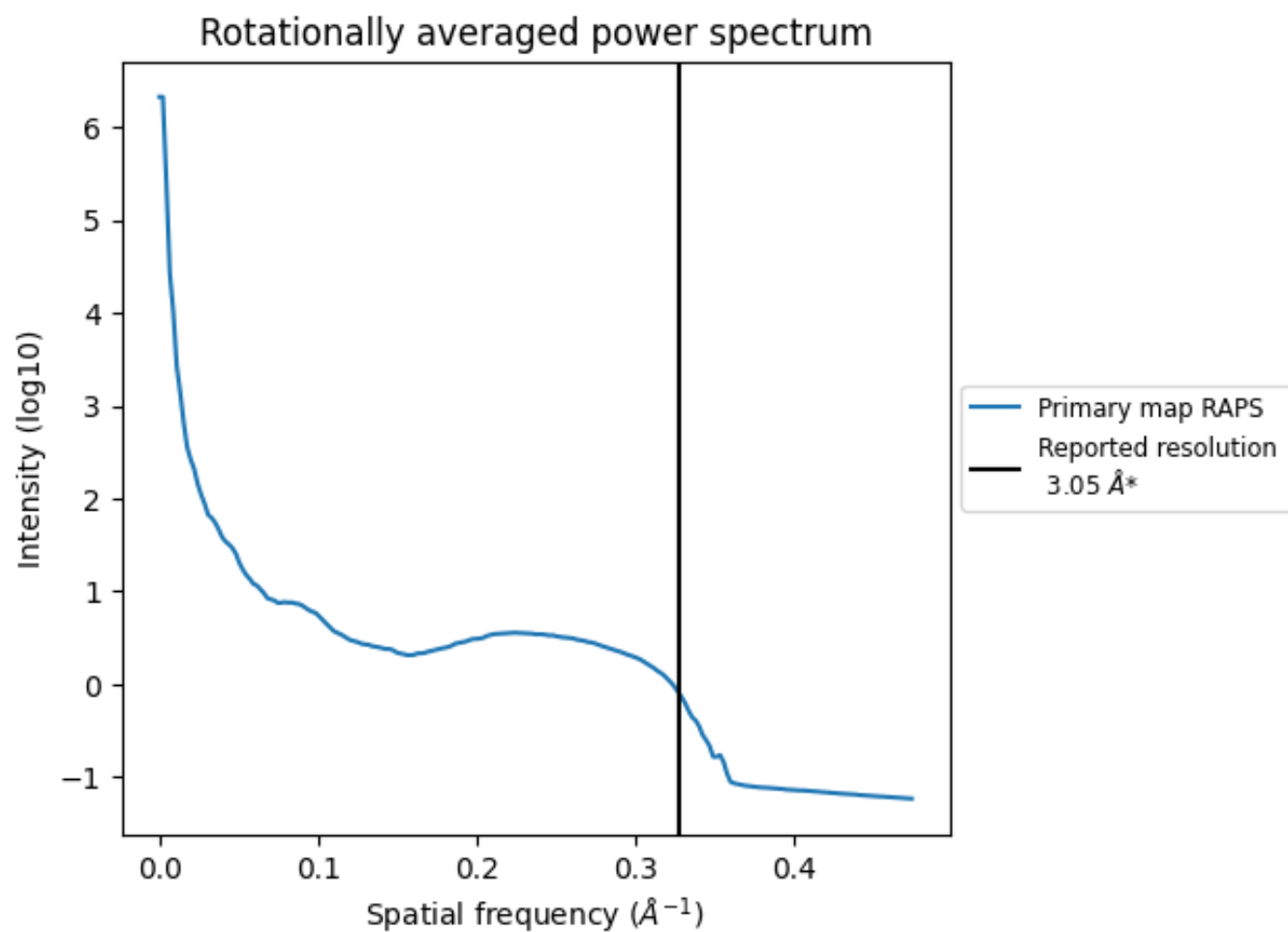


The volume at the recommended contour level is 1915  $\text{nm}^3$ ; this corresponds to an approximate mass of 1730 kDa.

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 0.328 Å<sup>-1</sup>

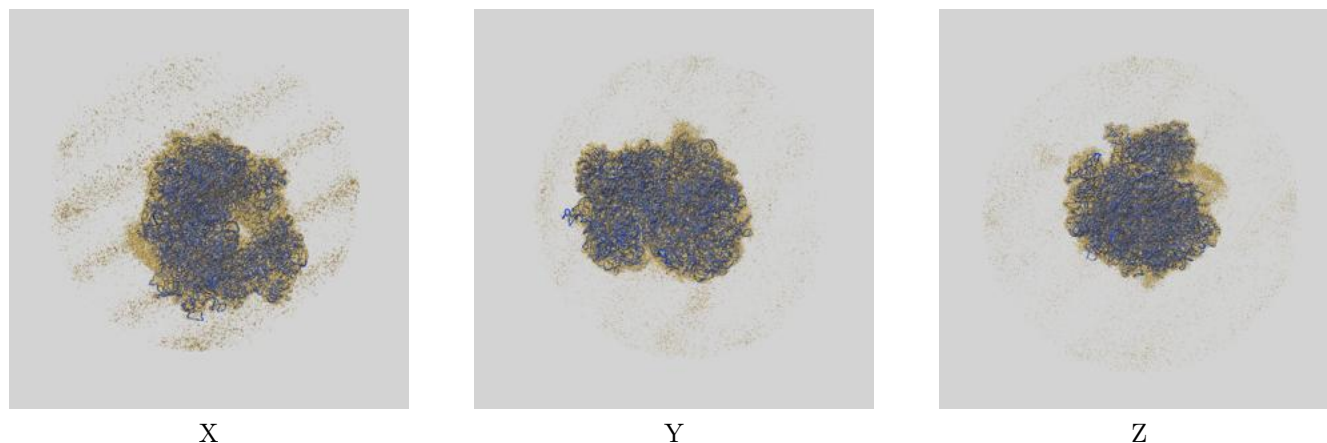
## 8 Fourier-Shell correlation

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

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

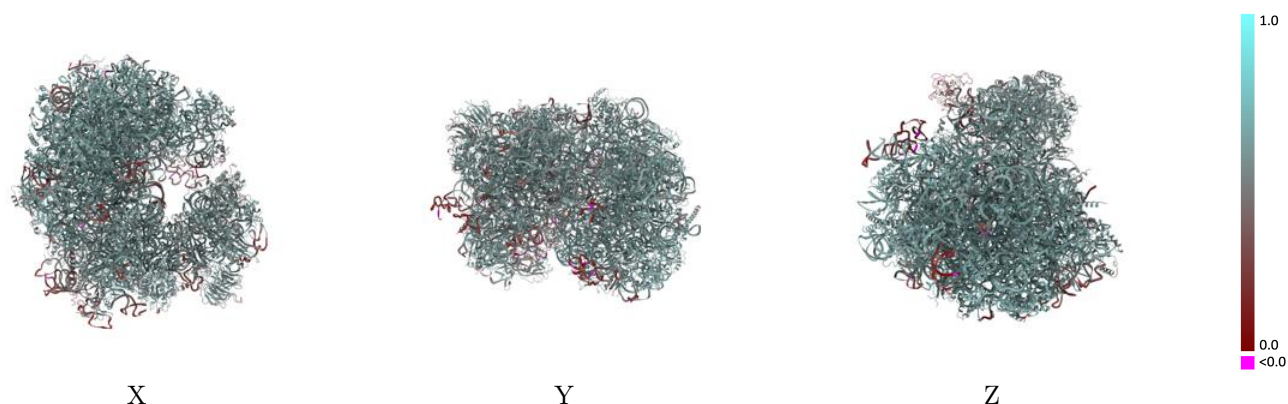
This section contains information regarding the fit between EMDB map EMD-24235 and PDB model 7N8B. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

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



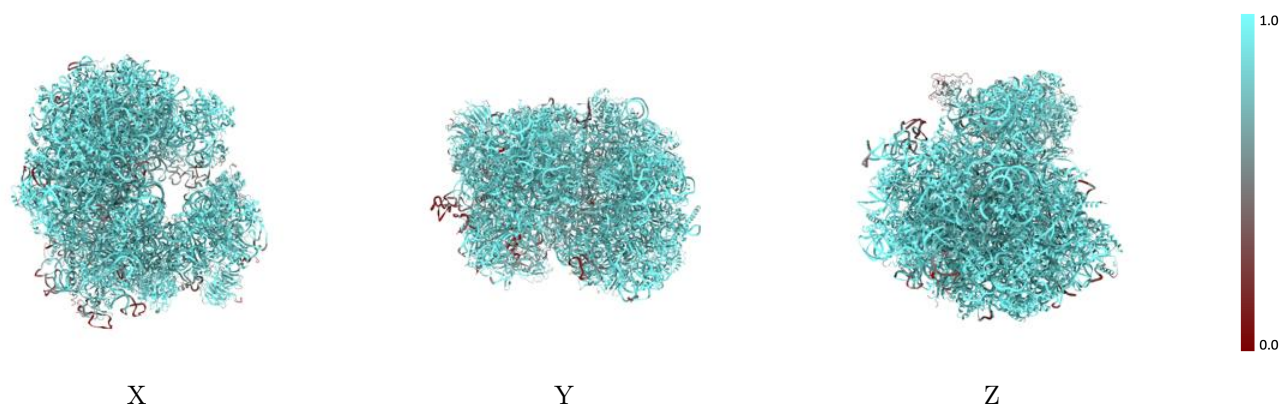
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



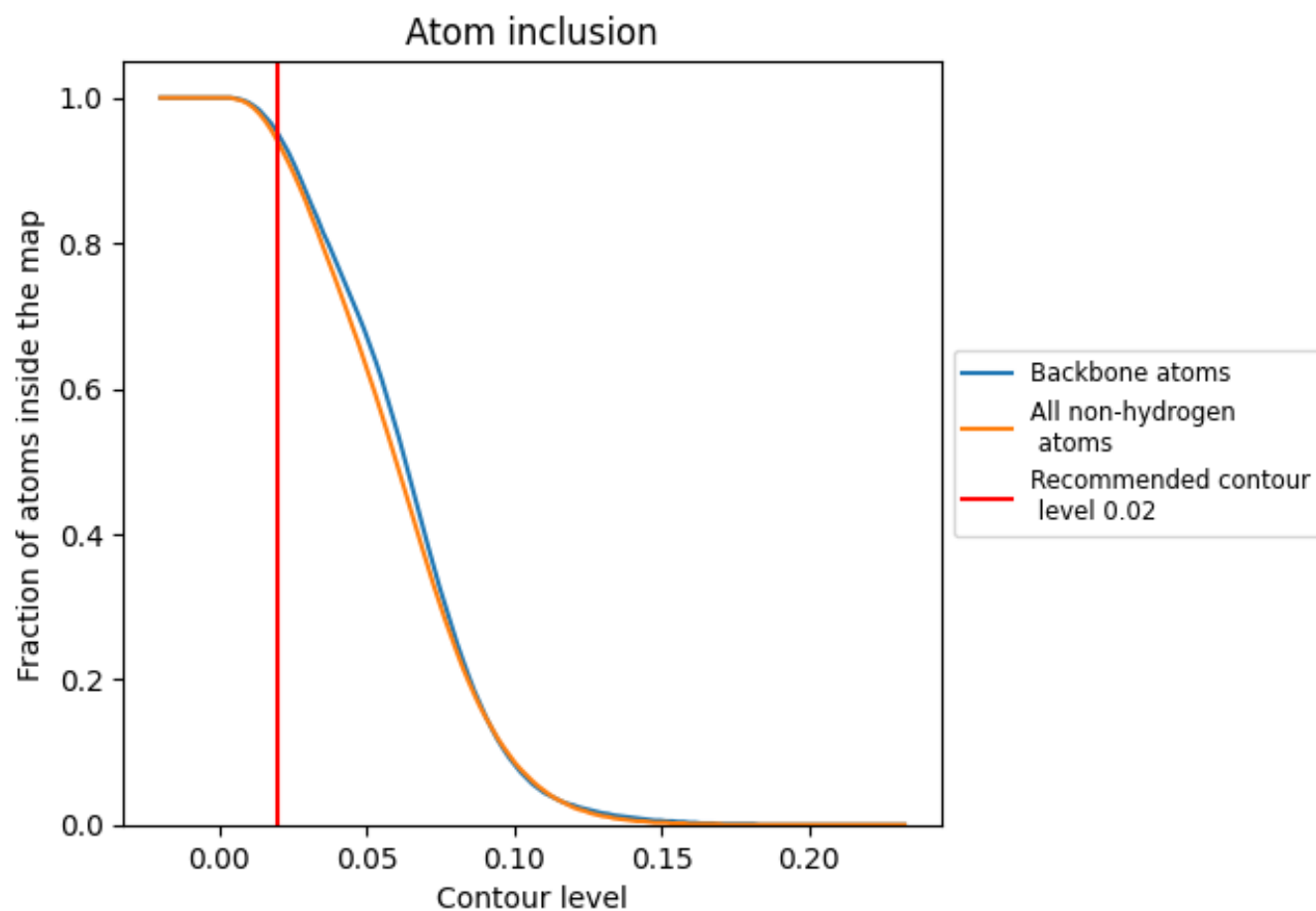
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9400   |  0.5700   |
| A1    |  0.9630   |  0.5830   |
| A3    |  0.9940   |  0.5940   |
| A4    |  0.9880   |  0.6100   |
| AA    |  0.9820   |  0.6150   |
| AB    |  0.9800   |  0.6200   |
| AC    |  0.9750   |  0.6080   |
| AD    |  0.9270   |  0.5640   |
| AE    |  0.9600   |  0.6000   |
| AF    |  0.9690   |  0.6050   |
| AG    |  0.9430   |  0.5870   |
| AH    |  0.9600   |  0.5970   |
| AI    |  0.9480   |  0.5810   |
| AJ    |  0.8730   |  0.5080   |
| AL    |  0.9540  |  0.6060  |
| AM    |  0.9710 |  0.6100 |
| AN    |  0.9900 |  0.6270 |
| AO    |  0.9770 |  0.6120 |
| AP    |  0.9750 |  0.6210 |
| AQ    |  0.9830 |  0.6200 |
| AR    |  0.8830 |  0.5390 |
| AS    |  0.9730 |  0.6120 |
| AT    |  0.9690 |  0.5970 |
| AU    |  0.9450 |  0.5640 |
| AV    |  0.9740 |  0.6090 |
| AW    |  0.9960 |  0.6260 |
| AX    |  0.9680 |  0.6080 |
| AY    |  0.9650 |  0.6120 |
| AZ    |  0.9640 |  0.5910 |
| Aa    |  0.9640 |  0.6110 |
| Ab    |  0.9470 |  0.5820 |
| Ac    |  0.9550 |  0.5880 |
| Ad    |  0.9290 |  0.6100 |
| Ae    |  0.9800 |  0.6220 |
| Af    |  0.9940 |  0.6330 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Ag    |  0.9580   |  0.5980   |
| Ah    |  0.9740   |  0.6150   |
| Ai    |  0.9330   |  0.5620   |
| Aj    |  0.9800   |  0.6190   |
| Ak    |  0.9300   |  0.5730   |
| Al    |  0.9810   |  0.6250   |
| Am    |  0.9400   |  0.5890   |
| An    |  0.8870   |  0.4910   |
| Ao    |  0.9470   |  0.5910   |
| Ap    |  0.9690   |  0.5960   |
| B5    |  0.9190   |  0.5340   |
| BA    |  0.9460   |  0.5750   |
| BB    |  0.9170   |  0.5570   |
| BC    |  0.9600   |  0.5870   |
| BD    |  0.9040   |  0.5250   |
| BE    |  0.9540   |  0.5950   |
| BF    |  0.9150   |  0.5450   |
| BG    |  0.9210   |  0.5630   |
| BH    |  0.8100   |  0.5110   |
| BI    |  0.9430  |  0.5740  |
| BJ    |  0.9280 |  0.5730 |
| BK    |  0.8260 |  0.4820 |
| BL    |  0.8710 |  0.5500 |
| BM    |  0.3920 |  0.2640 |
| BN    |  0.9490 |  0.5790 |
| BO    |  0.9220 |  0.5500 |
| BP    |  0.8380 |  0.5160 |
| BQ    |  0.9480 |  0.5790 |
| BR    |  0.8430 |  0.5110 |
| BS    |  0.8920 |  0.5350 |
| BT    |  0.9320 |  0.5630 |
| BU    |  0.8130 |  0.5050 |
| BV    |  0.9430 |  0.5860 |
| BW    |  0.9730 |  0.6070 |
| BX    |  0.9690 |  0.5950 |
| BY    |  0.9130 |  0.5750 |
| BZ    |  0.8780 |  0.5410 |
| Ba    |  0.9380 |  0.5700 |
| Bb    |  0.9190 |  0.5710 |
| Bc    |  0.8660 |  0.5190 |
| Bd    |  0.9790 |  0.5790 |
| Be    |  0.9080 |  0.5480 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Bf    |  0.4530 |  0.2350 |
| Bg    |  0.8660 |  0.5390 |
| Bh    |  0.5370 |  0.3250 |