



## Full wwPDB EM Validation Report ⓘ

Aug 25, 2026 – 05:05 PM EDT

PDB ID : 11HG / pdb\_000011hg  
EMDB ID : EMD-75689  
Title : Rabbit 80S with eEF2,CCDC124,and LARP1,40S-head-swiveled  
Authors : Seraj, Z.; Zottig, X.; Huang, C.H.; Loveland, A.B.; Diggs, S.; Sholi, E.; Grigorieff, N.; Korostelev, A.A.  
Deposited on : 2026-02-24  
Resolution : 2.90 Å(reported)  
Based on initial models : ., 7TOR

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:

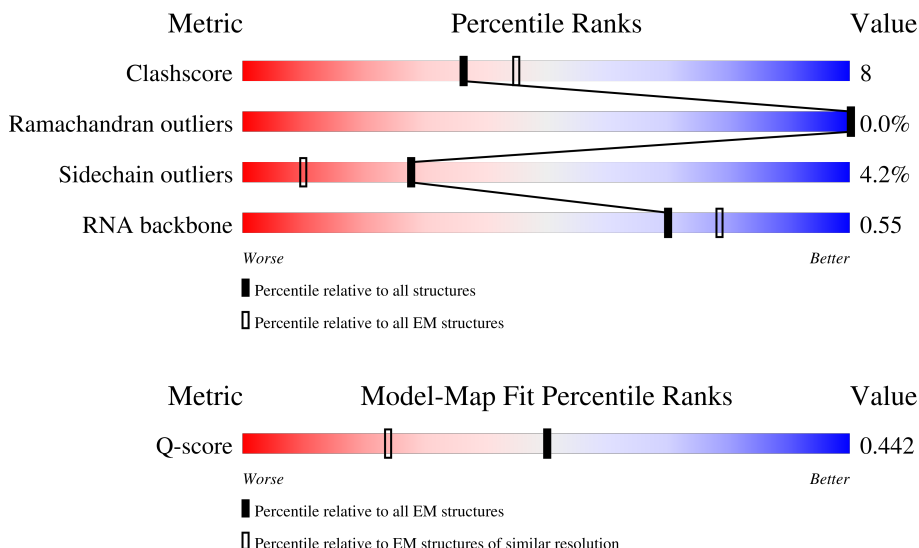
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

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

| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | BB    | 217    | <div> <div>50%</div> <div>76%</div> <div>24%</div> </div> |
| 2   | S2    | 221    | <div> <div>39%</div> <div>79%</div> <div>20%</div> </div> |
| 3   | PP    | 83     | <div> <div>59%</div> <div>84%</div> <div>14%</div> </div> |

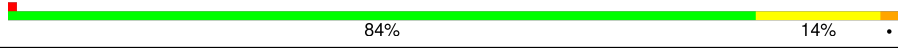
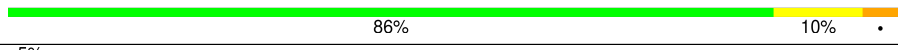
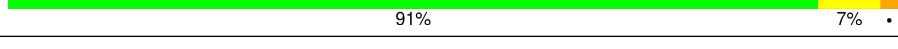
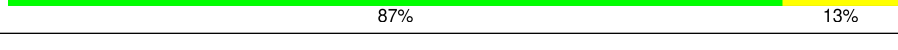
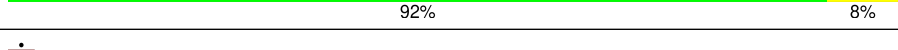
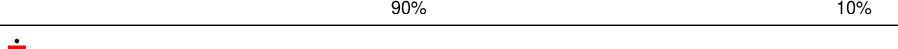
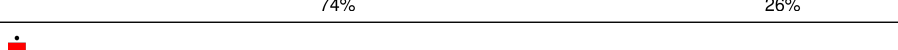
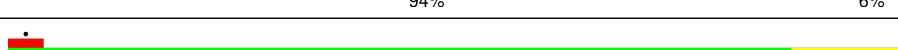
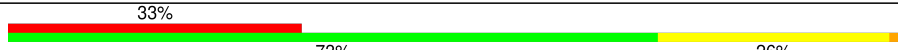
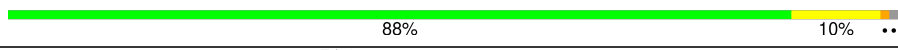
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | DD    | 151    |                  |
| 5   | 58    | 156    |                  |
| 6   | 6     | 120    |                  |
| 7   | L8    | 248    |                  |
| 8   | L3    | 394    |                  |
| 9   | L4    | 362    |                  |
| 10  | L5    | 293    |                  |
| 11  | L6    | 251    |                  |
| 12  | L7    | 225    |                  |
| 13  | aa    | 240    |                  |
| 14  | 10    | 213    |                  |
| 15  | 13    | 211    |                  |
| 16  | 14    | 138    |                  |
| 17  | 15    | 203    |                  |
| 18  | bb    | 199    |                  |
| 19  | 17    | 153    |                  |
| 20  | 19    | 180    |                  |
| 21  | 20    | 176    |                  |
| 22  | 21    | 159    |                  |
| 23  | 22    | 99     |                  |
| 24  | cc    | 118    |                  |
| 25  | 26    | 134    |                  |
| 26  | 27    | 135    |                  |
| 27  | dd    | 147    |                  |
| 28  | 29    | 245    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | 30    | 98     |    |
| 30  | 31    | 107    |    |
| 31  | 32    | 128    |    |
| 32  | ee    | 109    |    |
| 33  | 34    | 114    |    |
| 34  | 35    | 122    |    |
| 35  | 36    | 102    |    |
| 36  | 37    | 86     |    |
| 37  | 38    | 69     |    |
| 38  | 39    | 50     |    |
| 39  | 40    | 52     |    |
| 40  | 41    | 25     |  |
| 41  | 42    | 104    |  |
| 42  | ff    | 91     |  |
| 43  | gg    | 124    |  |
| 44  | AS    | 213    |  |
| 45  | FF    | 149    |  |
| 46  | VV    | 83     |  |
| 47  | s     | 196    |  |
| 48  | t     | 153    |  |
| 49  | F     | 358    |  |
| 50  | Q     | 188    |  |
| 51  | ZZ    | 68     |  |
| 52  | EE    | 117    |  |
| 53  | TT    | 75     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | S5    | 191    |                  |
| 55  | WW    | 62     |                  |
| 56  | II    | 142    |                  |
| 57  | CC    | 96     |                  |
| 58  | AA    | 313    |                  |
| 59  | OO    | 100    |                  |
| 60  | MM    | 141    |                  |
| 61  | LL    | 144    |                  |
| 62  | XX    | 55     |                  |
| 63  | RR    | 143    |                  |
| 64  | SS    | 124    |                  |
| 65  | S6    | 237    |                  |
| 66  | S4    | 262    |                  |
| 67  | S9    | 185    |                  |
| 68  | S7    | 189    |                  |
| 69  | YY    | 55     |                  |
| 70  | S3    | 214    |                  |
| 71  | RS    | 132    |                  |
| 72  | WX    | 129    |                  |
| 73  | S8    | 206    |                  |
| 74  | W     | 121    |                  |
| 75  | GG    | 136    |                  |
| 76  | UU    | 101    |                  |
| 77  | 11    | 170    |                  |
| 78  | L9    | 190    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 79  | 18    | 1688   |                  |
| 80  | v     | 857    |                  |
| 81  | LA    | 1096   |                  |
| 82  | CE    | 223    |                  |
| 83  | A     | 121    |                  |
| 84  | ES    | 5070   |                  |
| 85  | 28    | 4808   |                  |
| 86  | 23    | 140    |                  |

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 221973 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S\_SA\_C domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | BB    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1710  | 1086 | 300 | 316 | 8 |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | S2    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1716  | 1111 | 295 | 301 | 9 |         |       |

- Molecule 3 is a protein called eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | PP    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 4 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | DD    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1175  | 749 | 222 | 198 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5   | 58    | 151      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3208  | 1432 | 564 | 1062 | 150 |         |       |

- Molecule 6 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 6   | 6     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | L8    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | L3    | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3172  | 2020 | 597 | 542 | 13 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | L4    | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2883  | 1812 | 577 | 480 | 14 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | L5    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2391  | 1512 | 438 | 427 | 14 |         |       |

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | L6    | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1729  | 1115 | 329 | 282 | 3 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | L7    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1875  | 1205 | 358 | 303 | 9 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein eL8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | aa    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1879  | 1199 | 361 | 315 | 4 |         |       |

- Molecule 14 is a protein called Ribosomal protein L10.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | 10    | 205      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1664  | 1056 | 321 | 274 | 13 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | 13    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1702  | 1065 | 354 | 279 | 4 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | 14    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1137  | 727 | 221 | 182 | 7 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | 15    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | bb    | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1630  | 1051 | 319 | 255 | 5 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | 17    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 777 | 241 | 215 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | 19    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 933 | 328 | 238 | 9 |         |       |

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | 20    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1462  | 930 | 285 | 236 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 21    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | 22    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 809   | 519 | 141 | 147 | 2 |         |       |

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | cc    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 618 | 181 | 167 | 1 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | 26    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | 27    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | dd    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 734 | 239 | 185 | 4 |         |       |

- Molecule 28 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | 29    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 527 | 189 | 129 | 3 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | 30    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 761   | 481 | 134 | 140 | 6 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | 31    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 31 is a protein called Large ribosomal subunit protein eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | 32    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | ee    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 143 | 4 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | 34    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | 35    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 640 | 204 | 168 | 1 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | 36    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 520 | 176 | 129 | 5 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | 37    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein eL38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 37  | 38    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | 39    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 447   | 286 | 96 | 64 | 1 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | 40    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 40 is a protein called eL41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | 41    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 41 is a protein called eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | 42    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 851   | 533 | 174 | 138 | 6 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | ff    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | gg    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 990   | 615 | 202 | 167 | 6 |         |       |

- Molecule 44 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | AS    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1729  | 1098 | 309 | 308 | 14 |         |       |

- Molecule 45 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | FF    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1202  | 770 | 228 | 203 | 1 |         |       |

- Molecule 46 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | VV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | s     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1507  | 959 | 263 | 276 | 9 |         |       |

- Molecule 48 is a protein called uL11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | t     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1160  | 722 | 218 | 217 | 3 |         |       |

- Molecule 49 is a protein called Proliferation-associated protein 2G4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | F     | 358      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2798  | 1762 | 482 | 537 | 17 |         |       |

- Molecule 50 is a protein called Large ribosomal subunit protein eL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | Q     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1514  | 946 | 315 | 249 | 4 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51  | ZZ    | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 555   | 351 | 103 | 94 | 7 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | EE    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 908   | 570 | 161 | 169 | 8 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | TT    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 54 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | S5    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1471  | 921 | 277 | 266 | 7 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | WW    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 488   | 297 | 97 | 92 | 2 |         |       |

- Molecule 56 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | II    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 717 | 213 | 195 | 3 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | CC    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 530 | 143 | 131 | 6 |         |       |

- Molecule 58 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | AA    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | OO    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 795   | 498 | 152 | 141 | 4 |         |       |

- Molecule 60 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | MM    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1097  | 688 | 211 | 195 | 3 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | LL    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1190  | 746 | 241 | 202 | 1 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 62  | XX    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 63 is a protein called uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | RR    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | SS    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 640 | 198 | 168 | 5 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | S6    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 66  | S4    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | S9    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 68 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | S7    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1488  | 952 | 271 | 264 | 1 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 69  | YY    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 443   | 274 | 97 | 71 | 1 |         |       |

- Molecule 70 is a protein called Small ribosomal subunit protein uS3.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 70  | S3    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1662  | 1060 | 302 | 292 | 8 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | RS    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1068  | 670 | 199 | 195 | 4 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | WX    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 73  | S8    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

- Molecule 74 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | W     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 860   | 538 | 174 | 144 | 4 |         |       |

- Molecule 75 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | GG    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1007  | 615 | 198 | 188 | 6 |         |       |

- Molecule 76 is a protein called eS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | UU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 814   | 507 | 170 | 132 | 5 |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | 11    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1362  | 861 | 254 | 241 | 6 |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | L9    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 954 | 284 | 272 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 79  | 18    | 1688     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36043 | 16088 | 6476 | 11792 | 1687 |         |       |

- Molecule 80 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 80  | v     | 829      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6470  | 4114 | 1108 | 1205 | 43 |         |       |

- Molecule 81 is a protein called La-related protein 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 81  | LA    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 421   | 264 | 74 | 82 | 1 |         |       |

- Molecule 82 is a protein called Coiled-coil domain-containing protein 124.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | CE    | 73       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 613   | 369 | 122 | 121 | 1 |         |       |

- Molecule 83 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | A     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 983   | 622 | 184 | 170 | 7 |         |       |

- Molecule 84 is a RNA chain called ES27L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 84  | ES    | 35       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 756   | 335 | 142 | 244 | 35 |         |       |

- Molecule 85 is a RNA chain called 28s rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 85  | 28    | 3502     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 75105 | 33448 | 13761 | 24394 | 3502 |         |       |

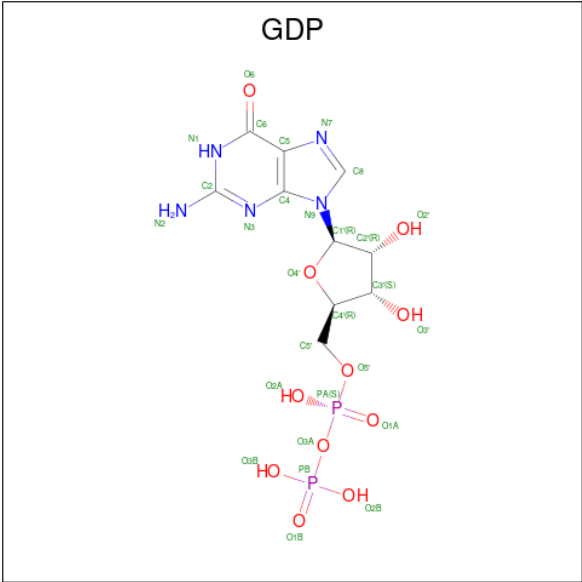
- Molecule 86 is a protein called Ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 86  | 23    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 648 | 199 | 182 | 5 |         |       |

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 87  | 34    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | 37    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | ff    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | UU    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

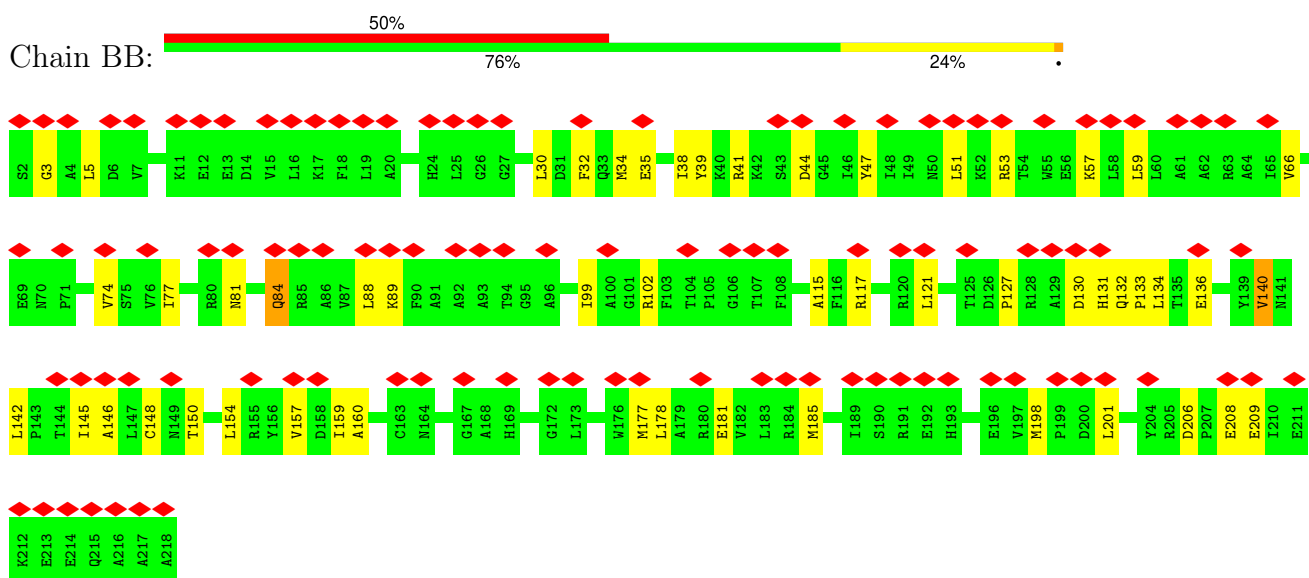


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 88  | v     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

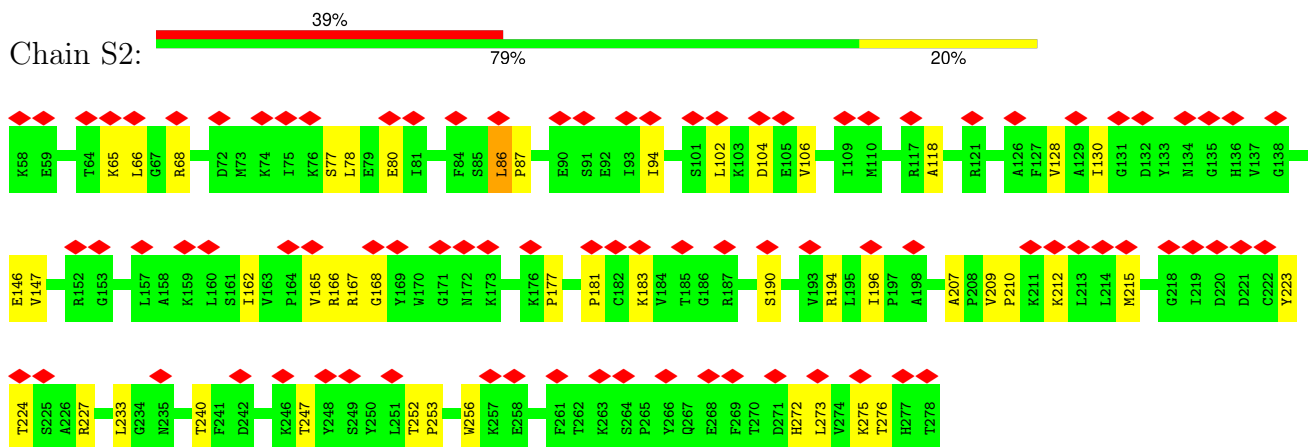
### 3 Residue-property plots

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

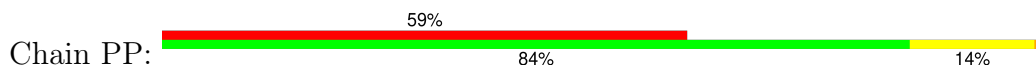
- Molecule 1: 40S\_SA\_C domain-containing protein

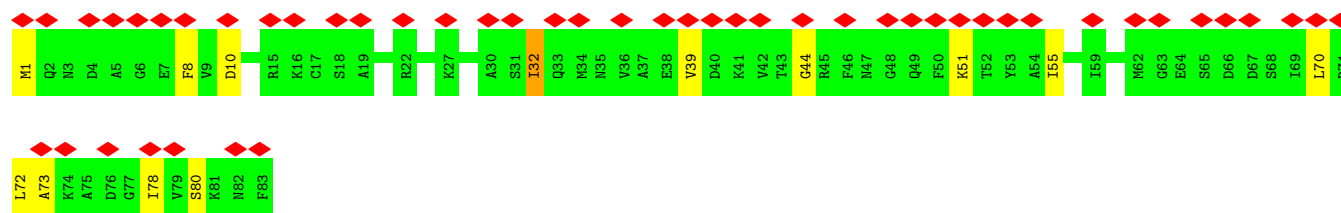


- Molecule 2: 40S ribosomal protein S2

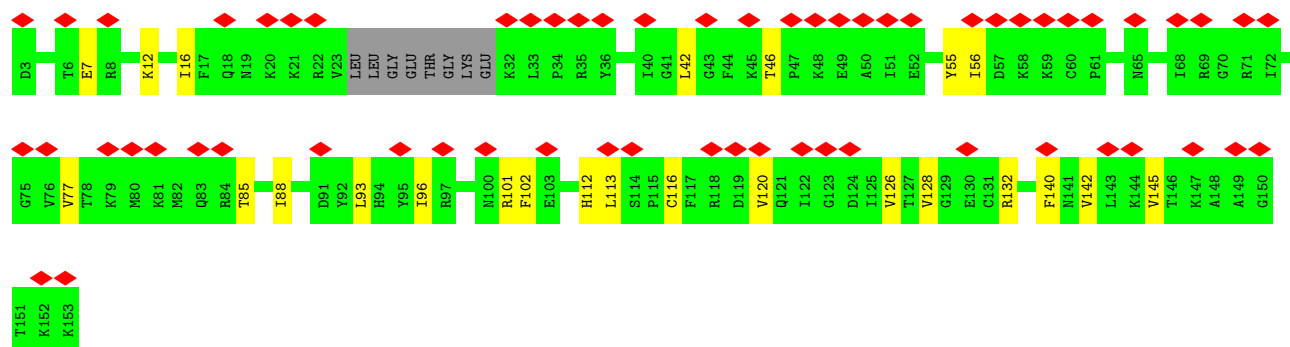
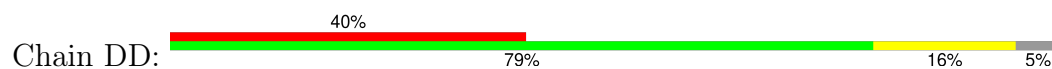


- Molecule 3: eS21

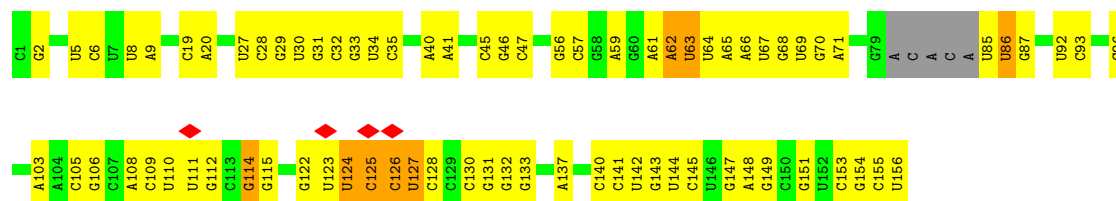




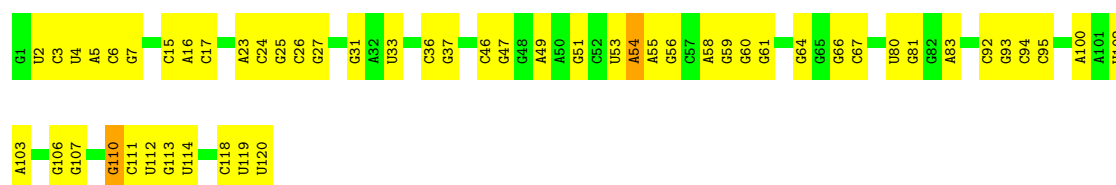
• Molecule 4: Small ribosomal subunit protein uS17



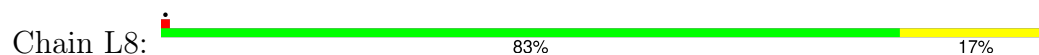
• Molecule 5: 5.8S rRNA

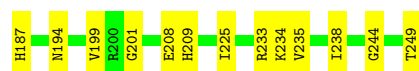


• Molecule 6: 5S rRNA



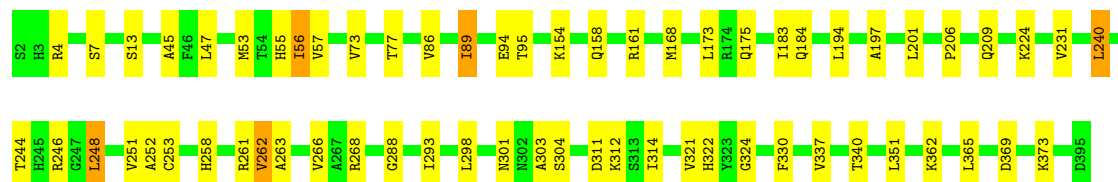
• Molecule 7: 60S ribosomal protein L8





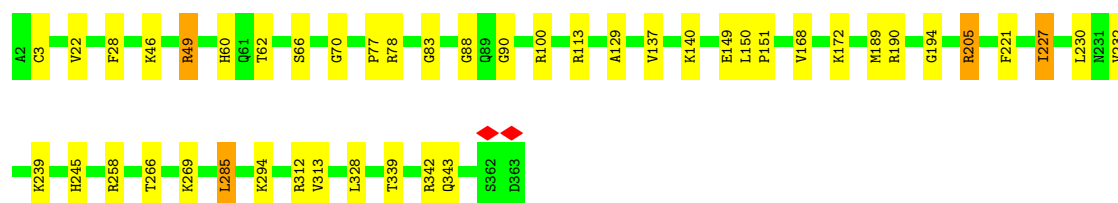
• Molecule 8: 60S ribosomal protein L3

Chain L3: 84% 15%



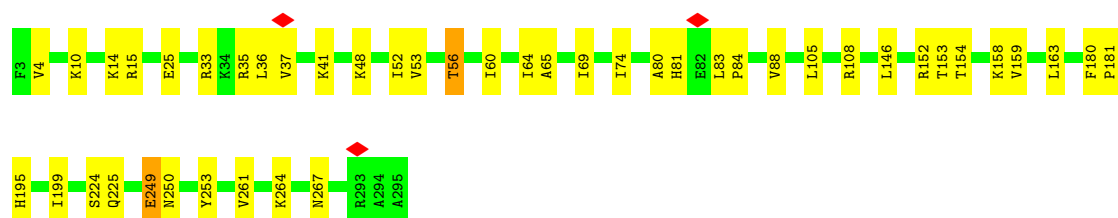
• Molecule 9: 60S ribosomal protein L4

Chain L4: 88% 11%



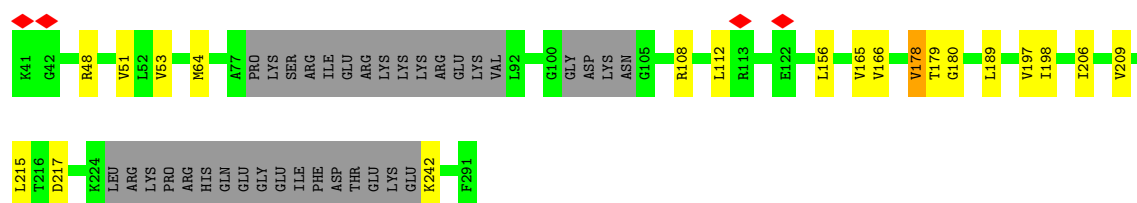
• Molecule 10: 60S ribosomal protein L5

Chain L5: 85% 15%



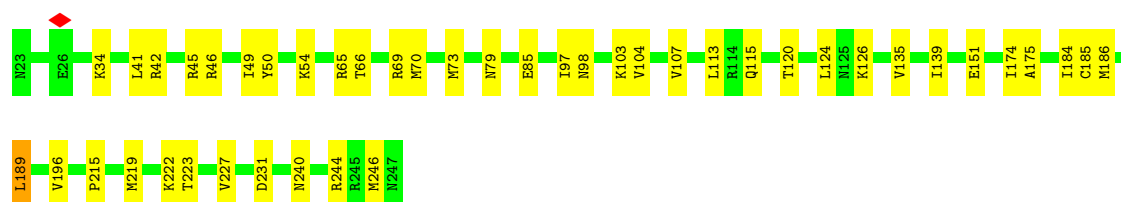
• Molecule 11: Large ribosomal subunit protein eL6

Chain L6: 78% 8% 14%

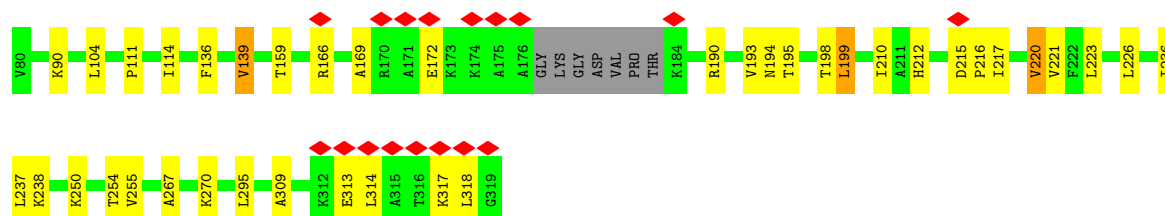
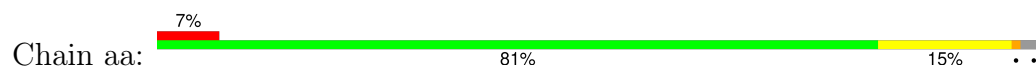


• Molecule 12: 60S ribosomal protein L7

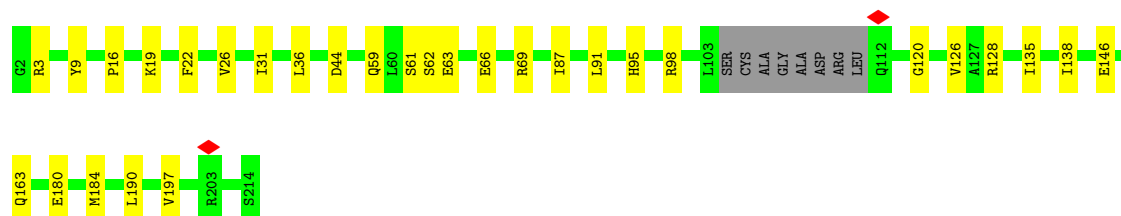
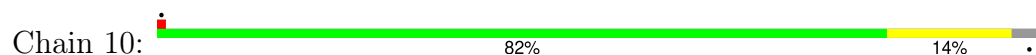
Chain L7: 80% 19%



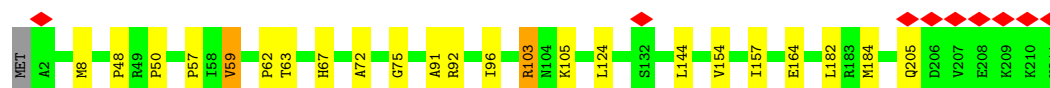
- Molecule 13: Large ribosomal subunit protein eL8



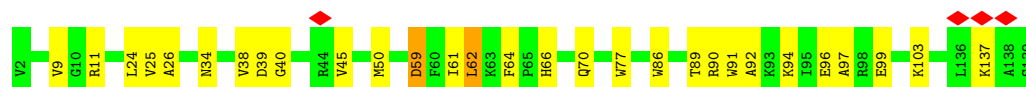
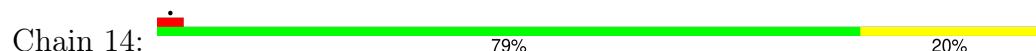
- Molecule 14: Ribosomal protein L10



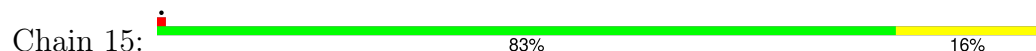
- Molecule 15: 60S ribosomal protein L13



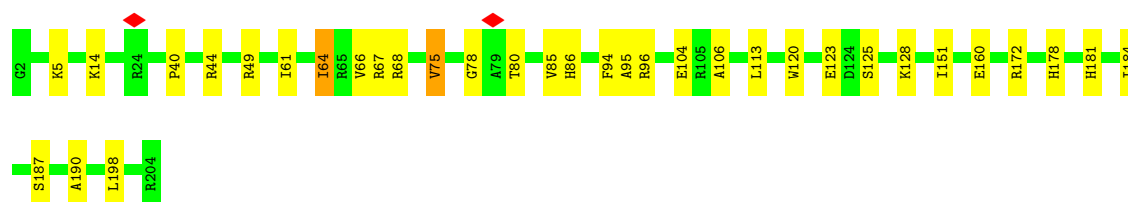
- Molecule 16: 60S ribosomal protein L14



- Molecule 17: 60S ribosomal protein L15







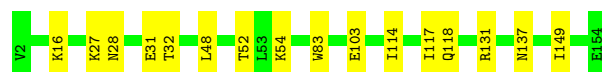
- Molecule 18: Large ribosomal subunit protein uL13

Chain bb: 79% 20% .



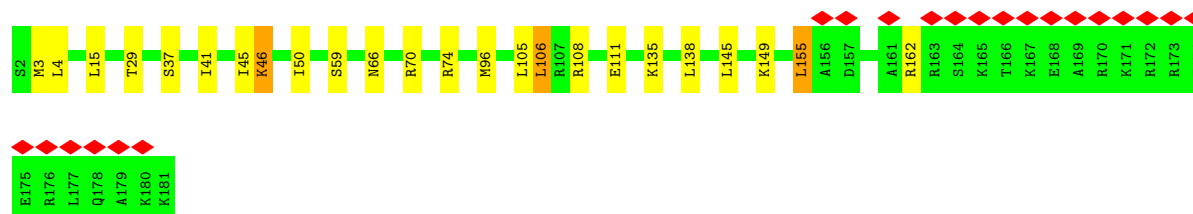
- Molecule 19: 60S ribosomal protein L17

Chain 17: 90% 10% .



- Molecule 20: 60S ribosomal protein L19

Chain 19: 12% 87% 12% .



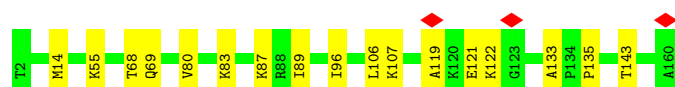
- Molecule 21: Large ribosomal subunit protein eL20

Chain 20: 85% 14% .



- Molecule 22: 60S ribosomal protein L21

Chain 21: 89% 11% .



- [illegible]

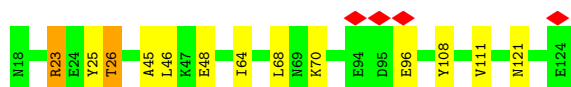
- Molecule 29: 60S ribosomal protein L30

Chain 30:  87% 12%



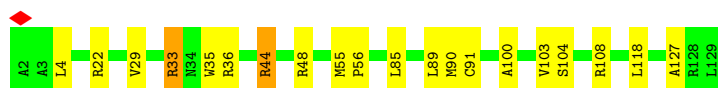
- Molecule 30: 60S ribosomal protein L31

Chain 31:  88% 10%



- Molecule 31: Large ribosomal subunit protein eL32

Chain 32:  84% 14%



- Molecule 32: Large ribosomal subunit protein eL33

Chain ee:  86% 10%

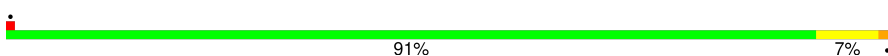


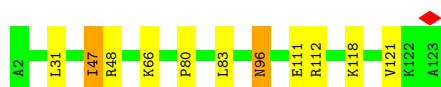
- Molecule 33: 60S ribosomal protein L34

Chain 34:  5% 90% 9%



- Molecule 34: 60S ribosomal protein L35

Chain 35:  91% 7%



- Molecule 35: 60S ribosomal protein L36

Chain 36:  87% 13%



- Molecule 36: 60S ribosomal protein L37

Chain 37: 92% 8%



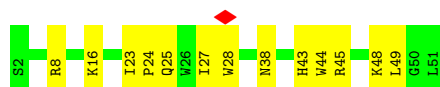
- Molecule 37: Large ribosomal subunit protein eL38

Chain 38: 90% 10%



- Molecule 38: 60S ribosomal protein L39

Chain 39: 74% 26%



- Molecule 39: Large ribosomal subunit protein eL40

Chain 40: 94% 6%



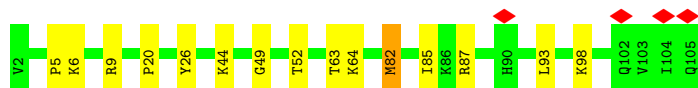
- Molecule 40: eL41

Chain 41: 88% 12%



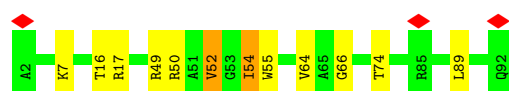
- Molecule 41: eL42

Chain 42: 86% 13%



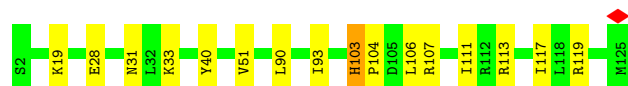
- Molecule 42: 60S ribosomal protein L37a

Chain ff:  87% 11% .



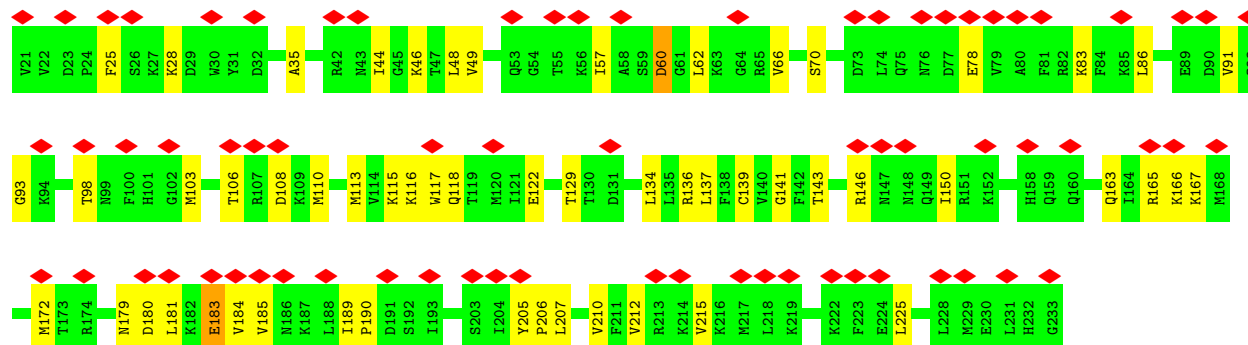
- Molecule 43: 60S ribosomal protein L28

Chain gg:  87% 12% .



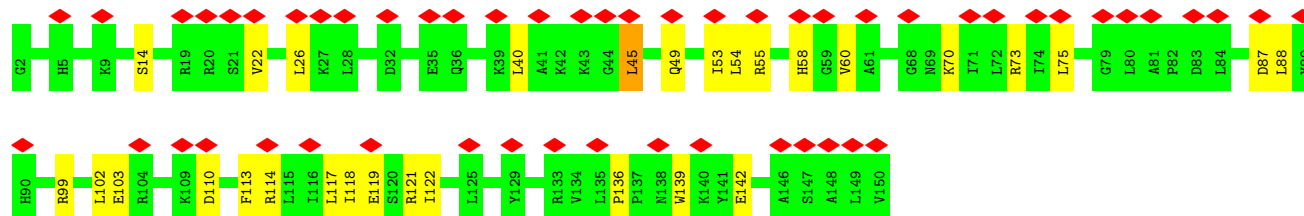
- Molecule 44: 40S ribosomal protein S3a

Chain AS:  33% 73% 26% .

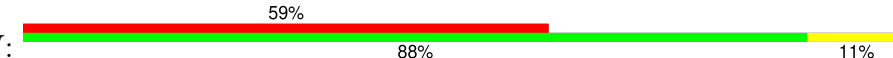


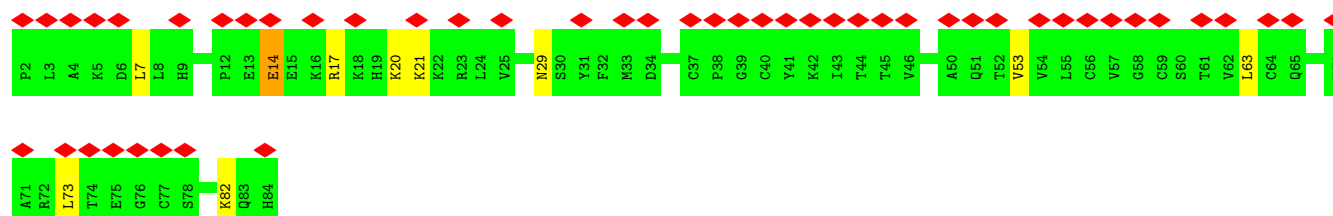
- Molecule 45: 40S ribosomal protein S13

Chain FF:  36% 80% 19% .

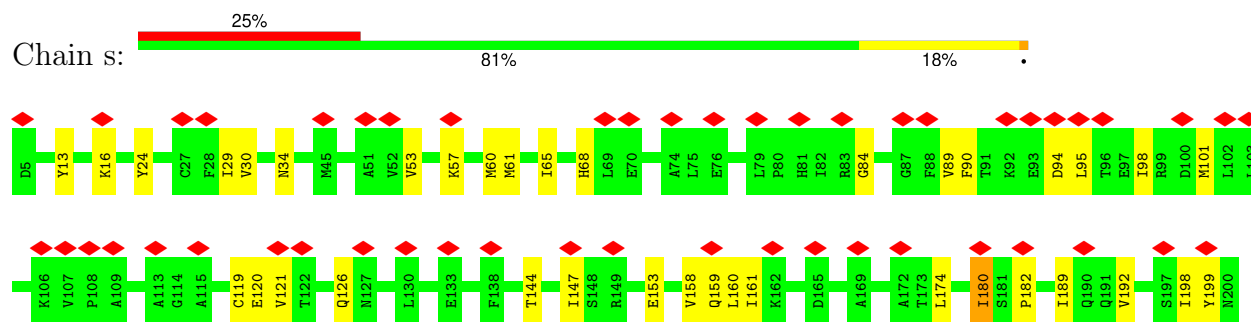


- Molecule 46: 40S ribosomal protein S27

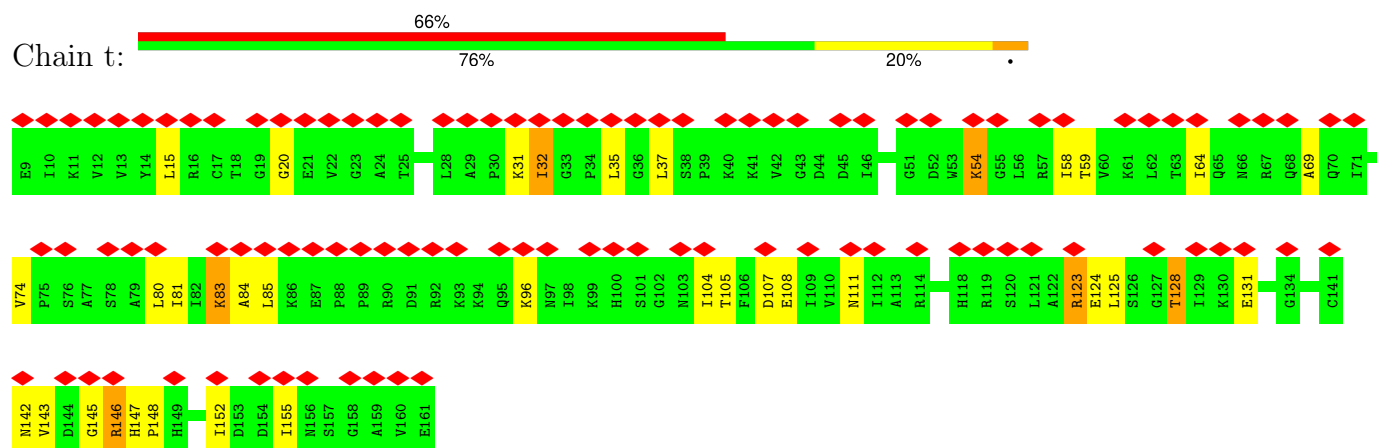
Chain VV:  59% 88% 11% .



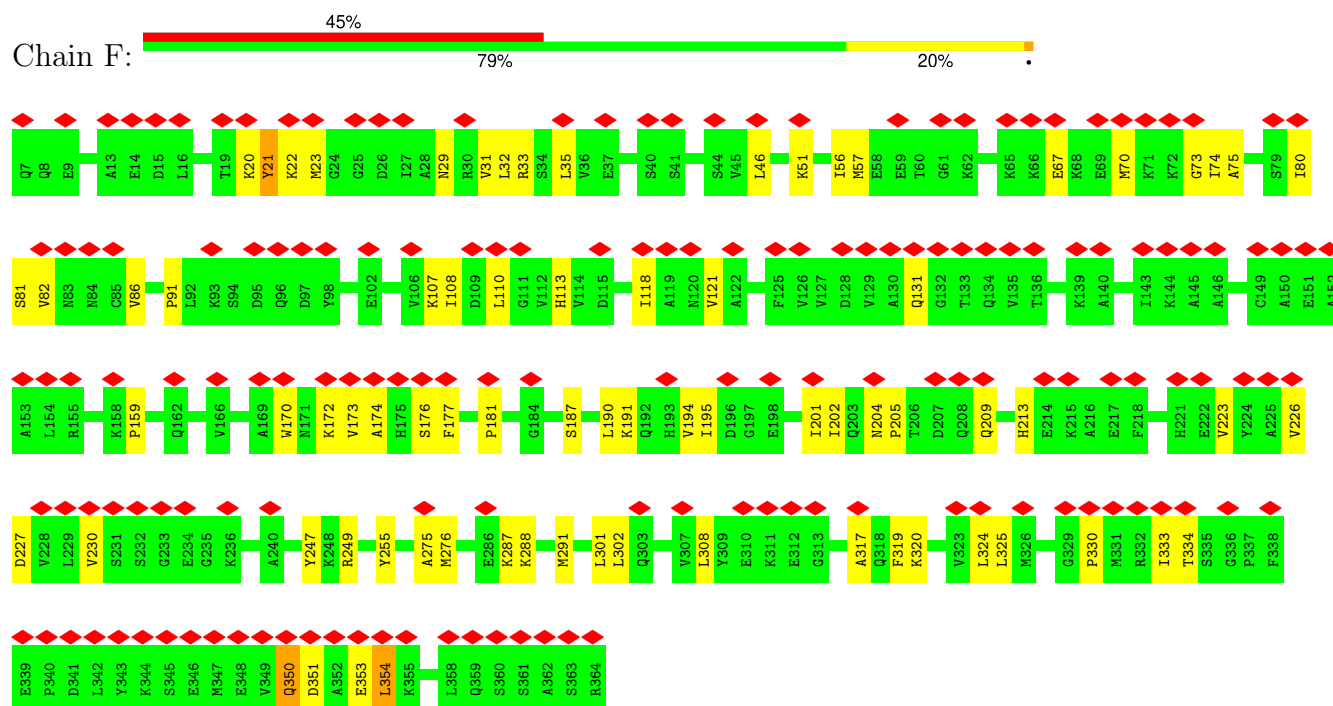
- Molecule 47: 60S acidic ribosomal protein P0



- Molecule 48: uL11



- Molecule 49: Proliferation-associated protein 2G4



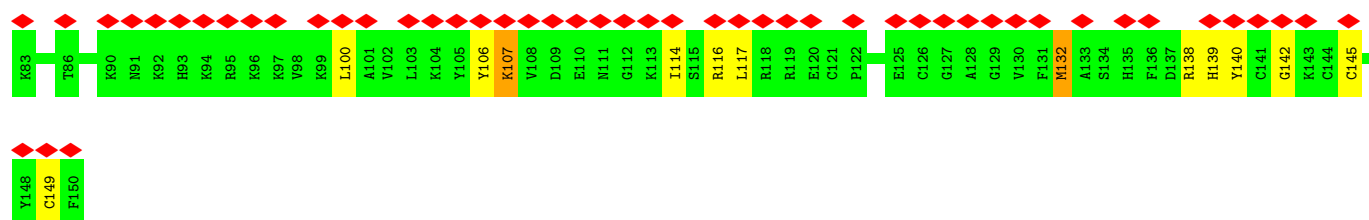
- Molecule 50: Large ribosomal subunit protein eL18

Chain Q:  88% 10% ..



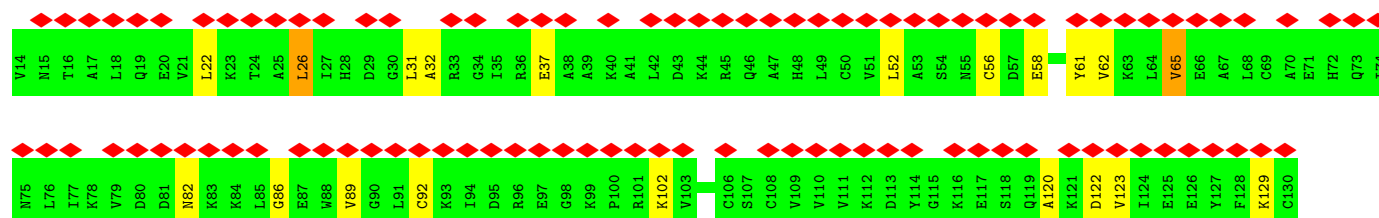
- Molecule 51: 40S ribosomal protein S27a

Chain ZZ:  74% 81% 16% .



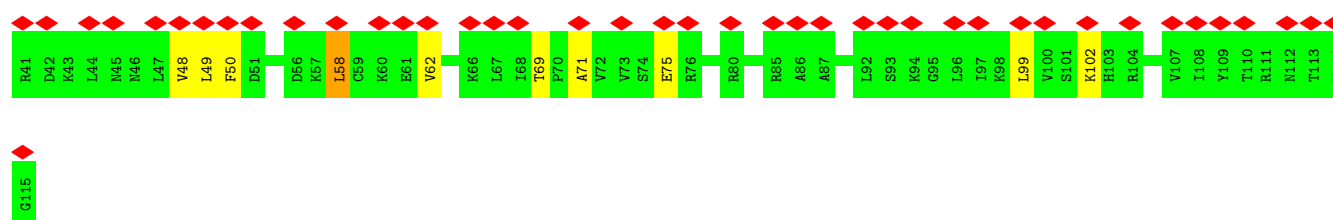
- Molecule 52: 40S ribosomal protein S12

Chain EE:  84% 83% 15% .



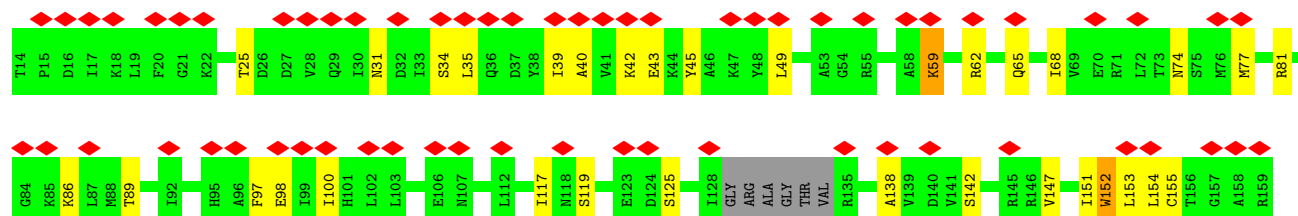
- Molecule 53: 40S ribosomal protein S25

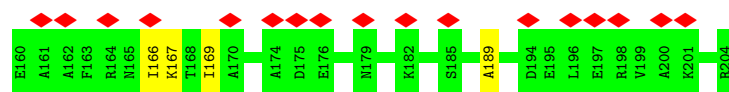
Chain TT:  56% 87% 12% .



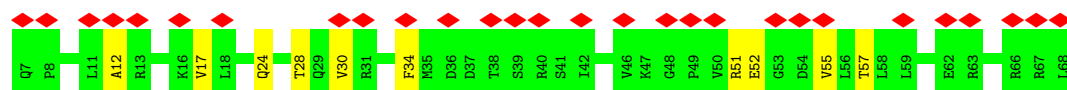
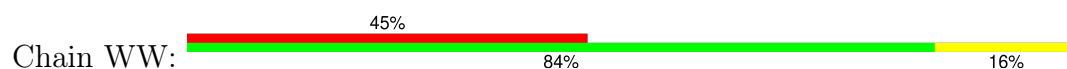
- Molecule 54: Small ribosomal subunit protein uS7

Chain S5:  41% 77% 18% ..

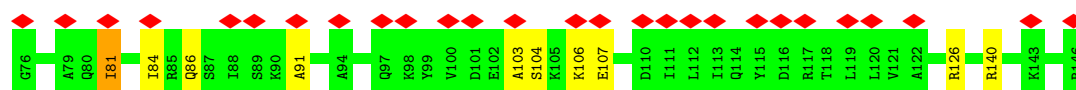
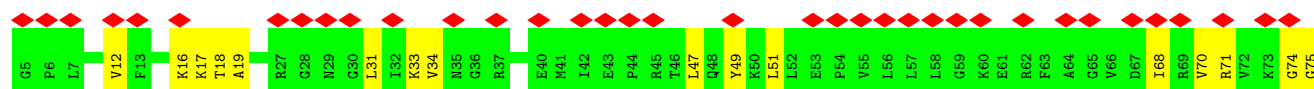
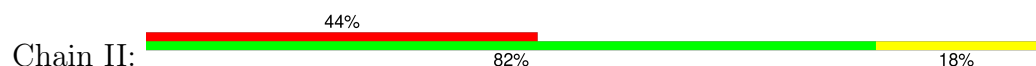




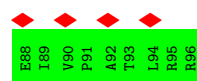
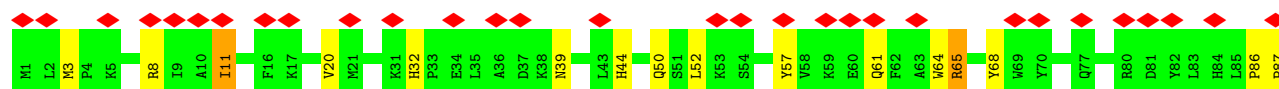
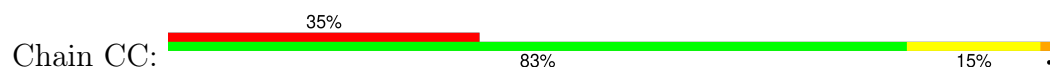
- Molecule 55: 40S ribosomal protein S28



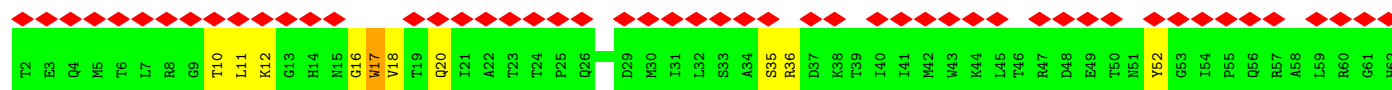
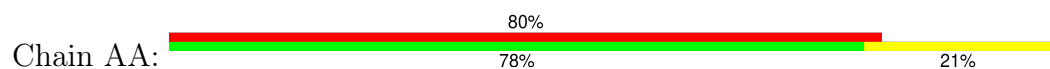
- Molecule 56: Small ribosomal subunit protein uS9



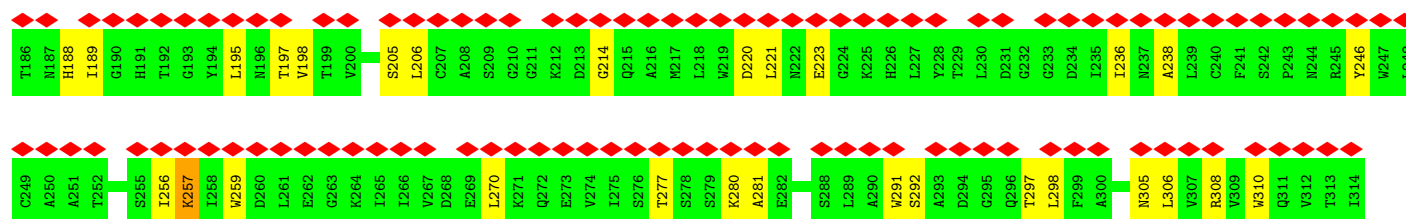
- Molecule 57: 40S ribosomal protein S10



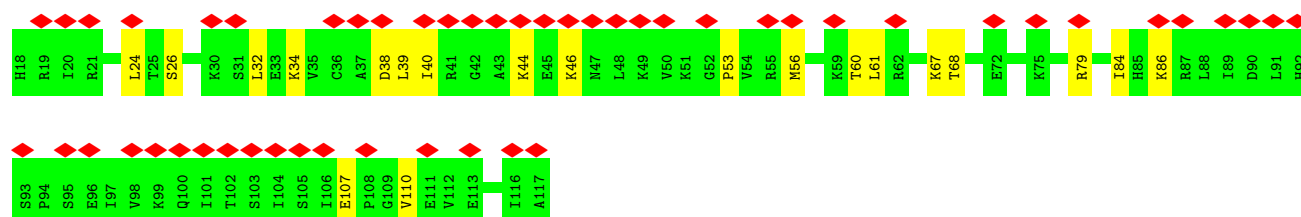
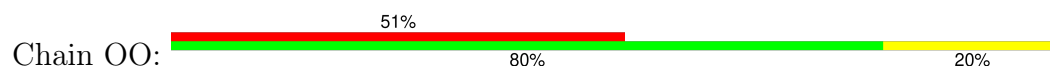
- Molecule 58: Receptor of activated protein C kinase 1



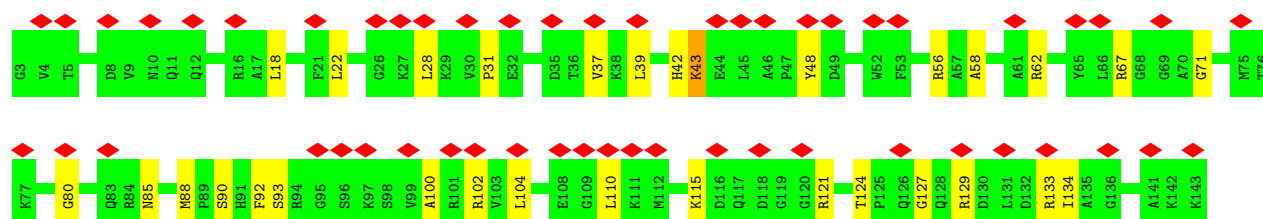
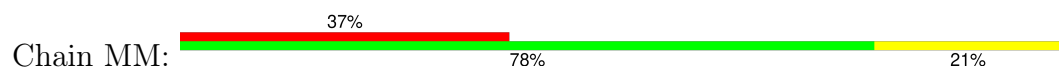




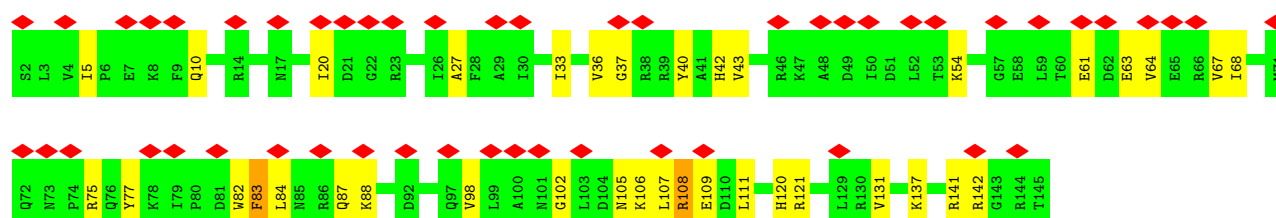
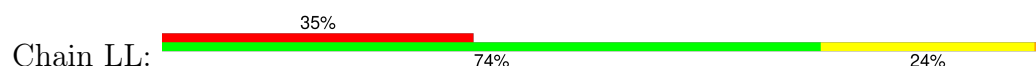
• Molecule 59: 40S ribosomal protein S20



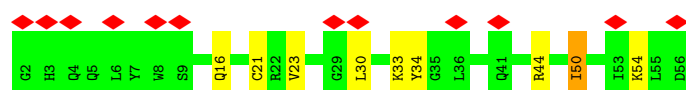
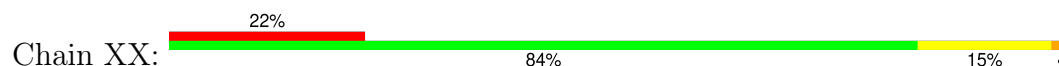
• Molecule 60: Small ribosomal subunit protein eS19



• Molecule 61: 40S ribosomal protein S18

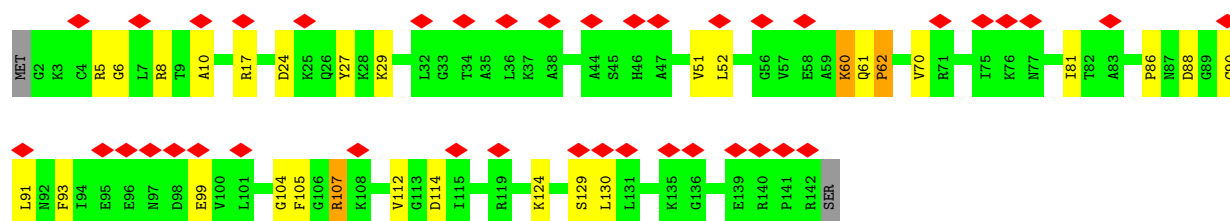


• Molecule 62: 40S ribosomal protein S29



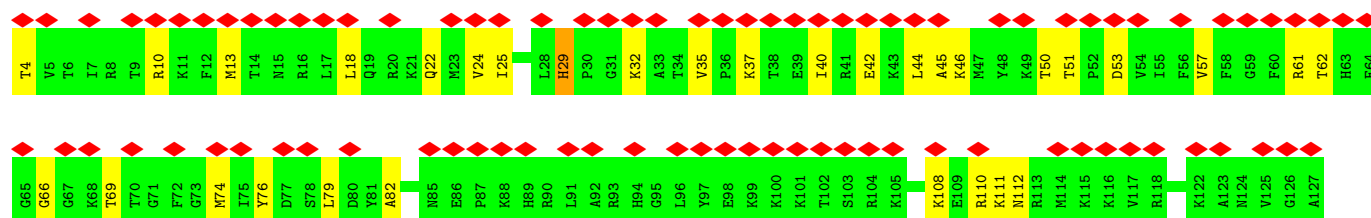
• Molecule 63: uS12

Chain RR: 



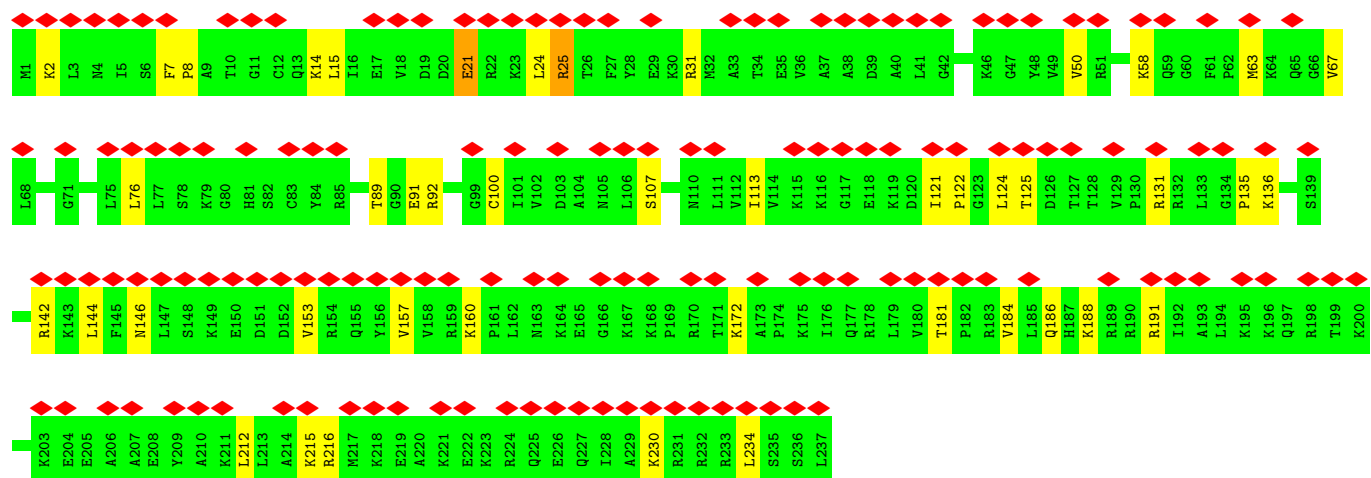
• Molecule 64: 40S ribosomal protein S24

Chain SS: 



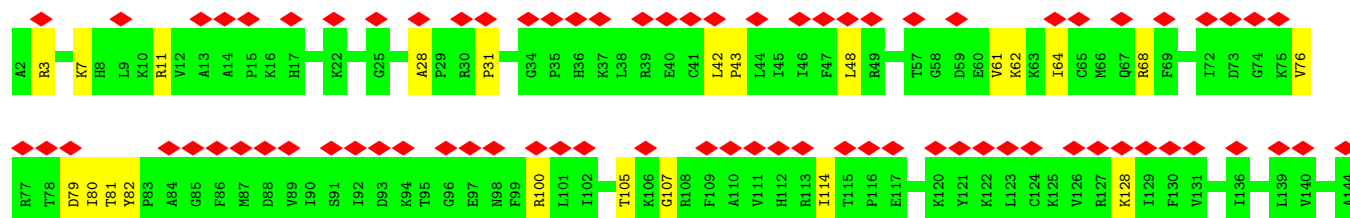
• Molecule 65: 40S ribosomal protein S6

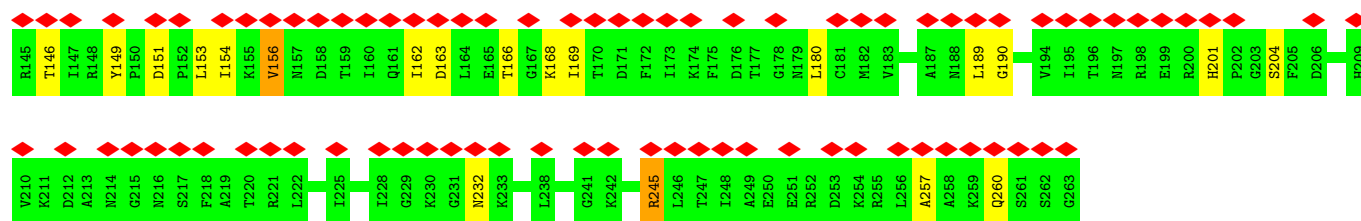
Chain S6: 



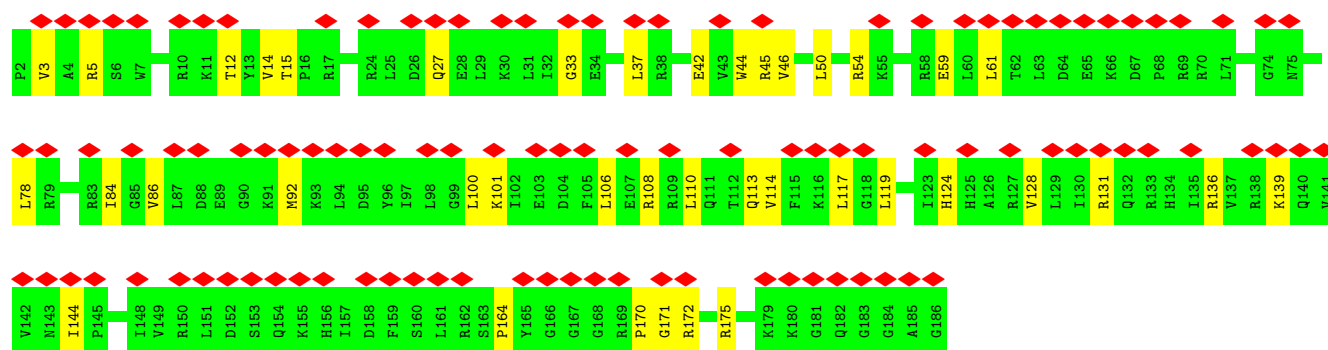
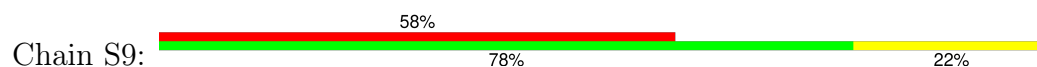
• Molecule 66: 40S ribosomal protein S4

Chain S4: 

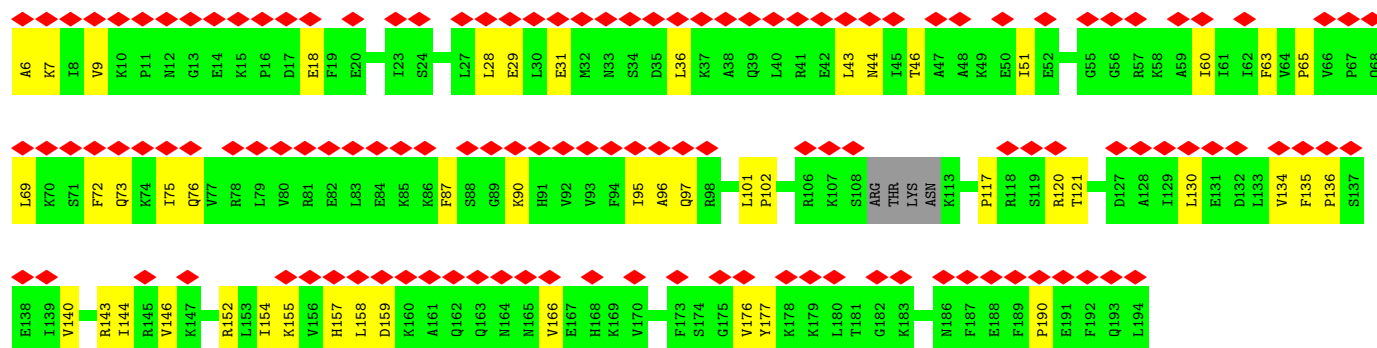




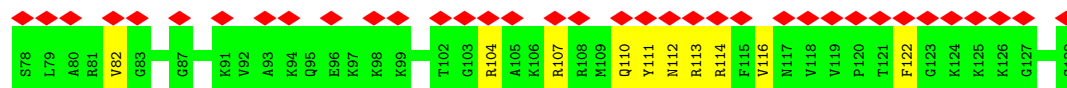
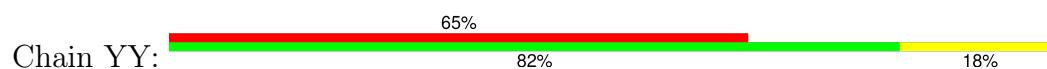
• Molecule 67: 40S ribosomal protein S9



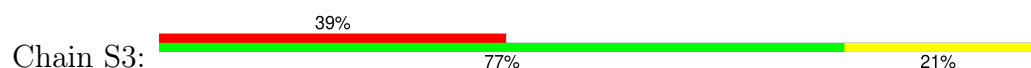
• Molecule 68: Small ribosomal subunit protein eS7

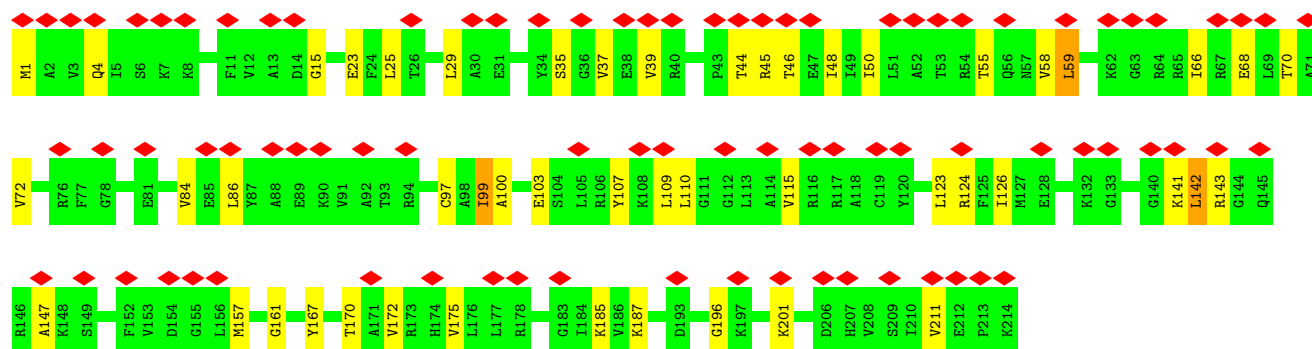


• Molecule 69: 40S ribosomal protein S30

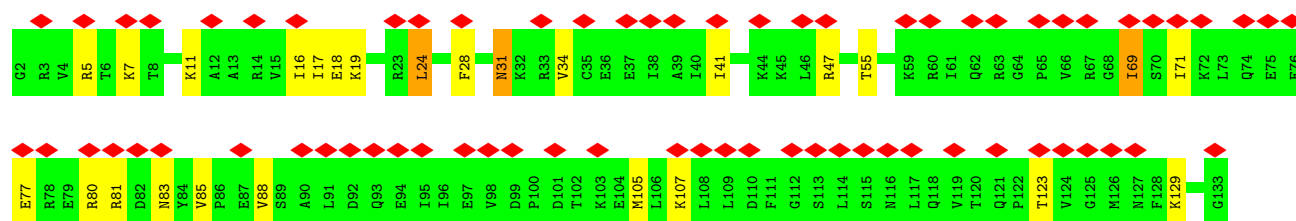
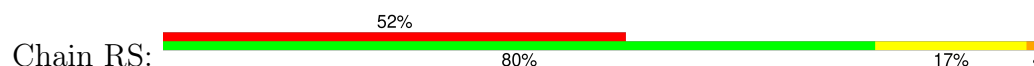


• Molecule 70: Small ribosomal subunit protein uS3

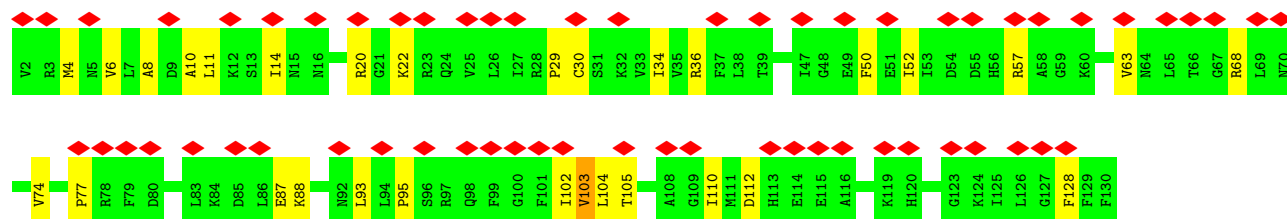
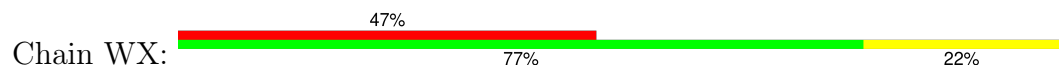




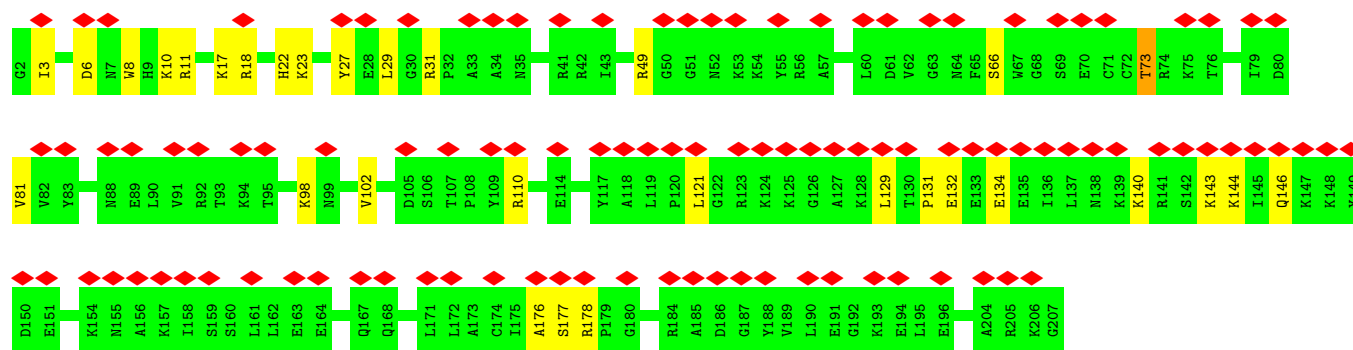
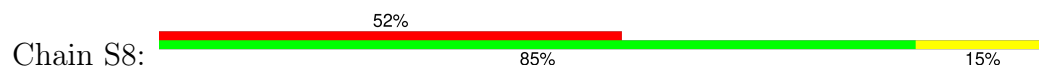
• Molecule 71: 40S ribosomal protein S17



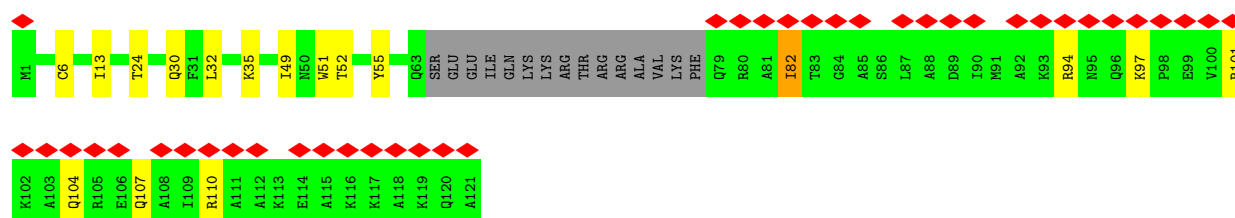
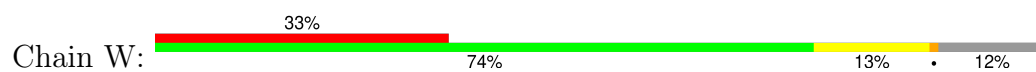
• Molecule 72: 40S ribosomal protein S15a



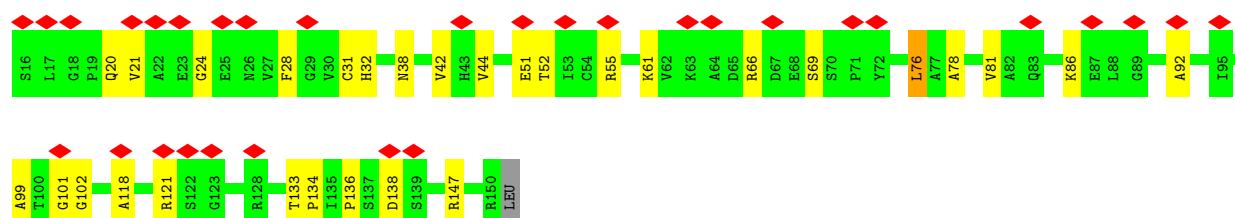
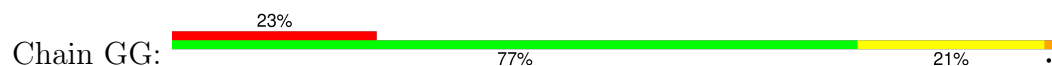
• Molecule 73: 40S ribosomal protein S8



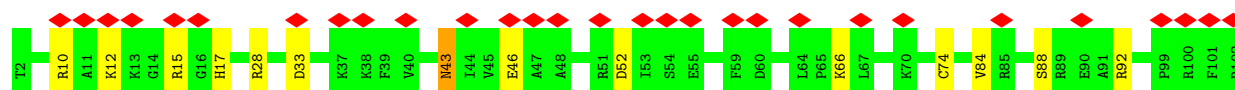
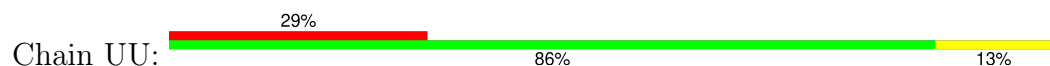
• Molecule 74: Ribosomal protein L24



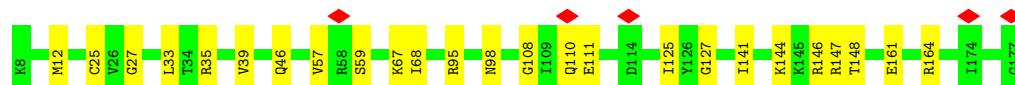
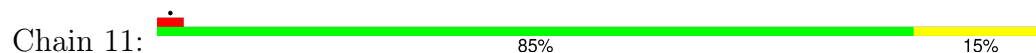
- Molecule 75: Small ribosomal subunit protein uS11



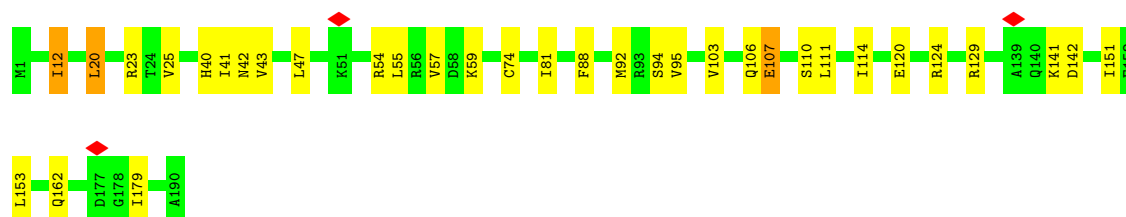
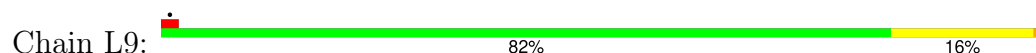
- Molecule 76: eS26



- Molecule 77: 60S ribosomal protein L11

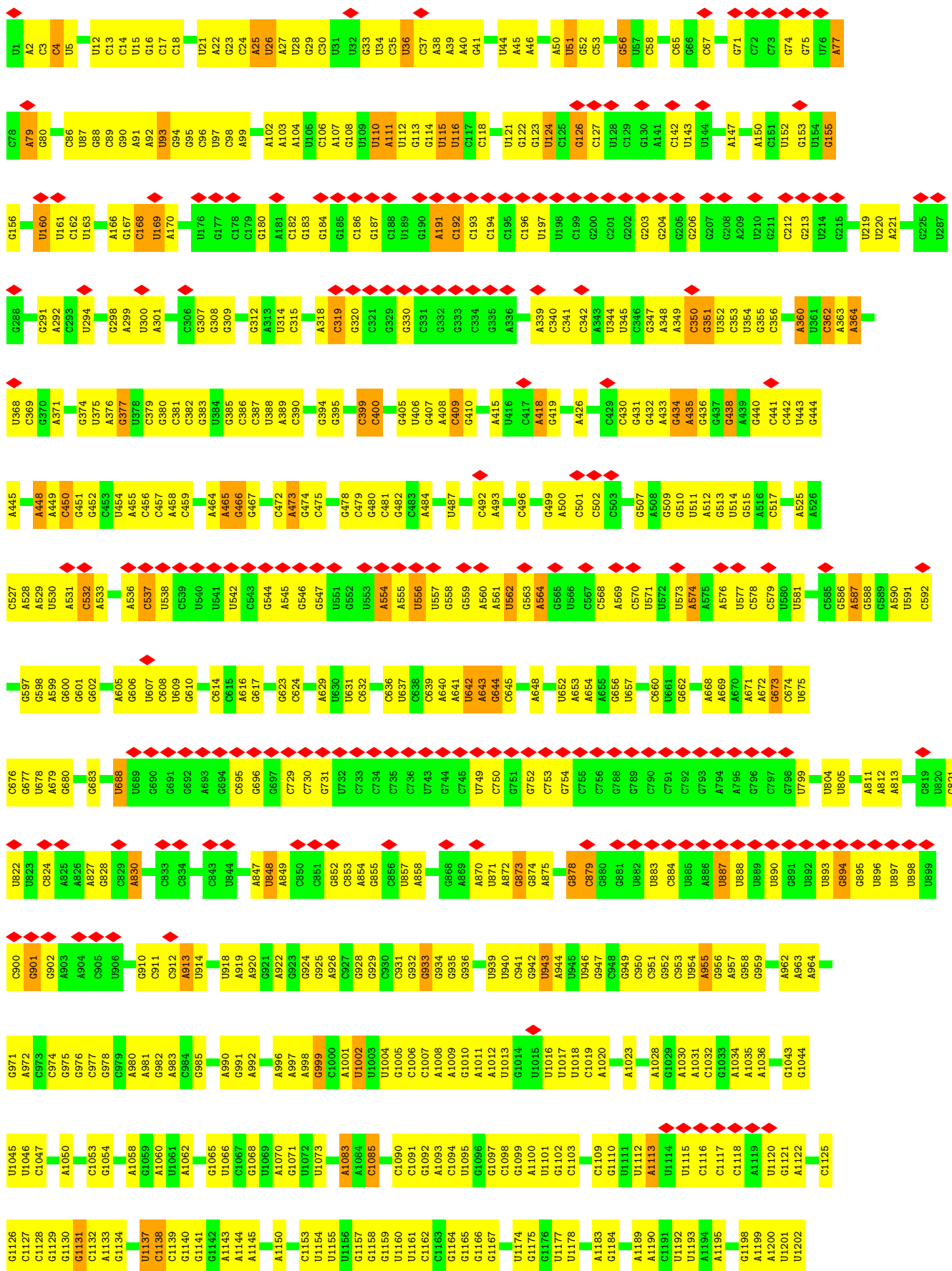


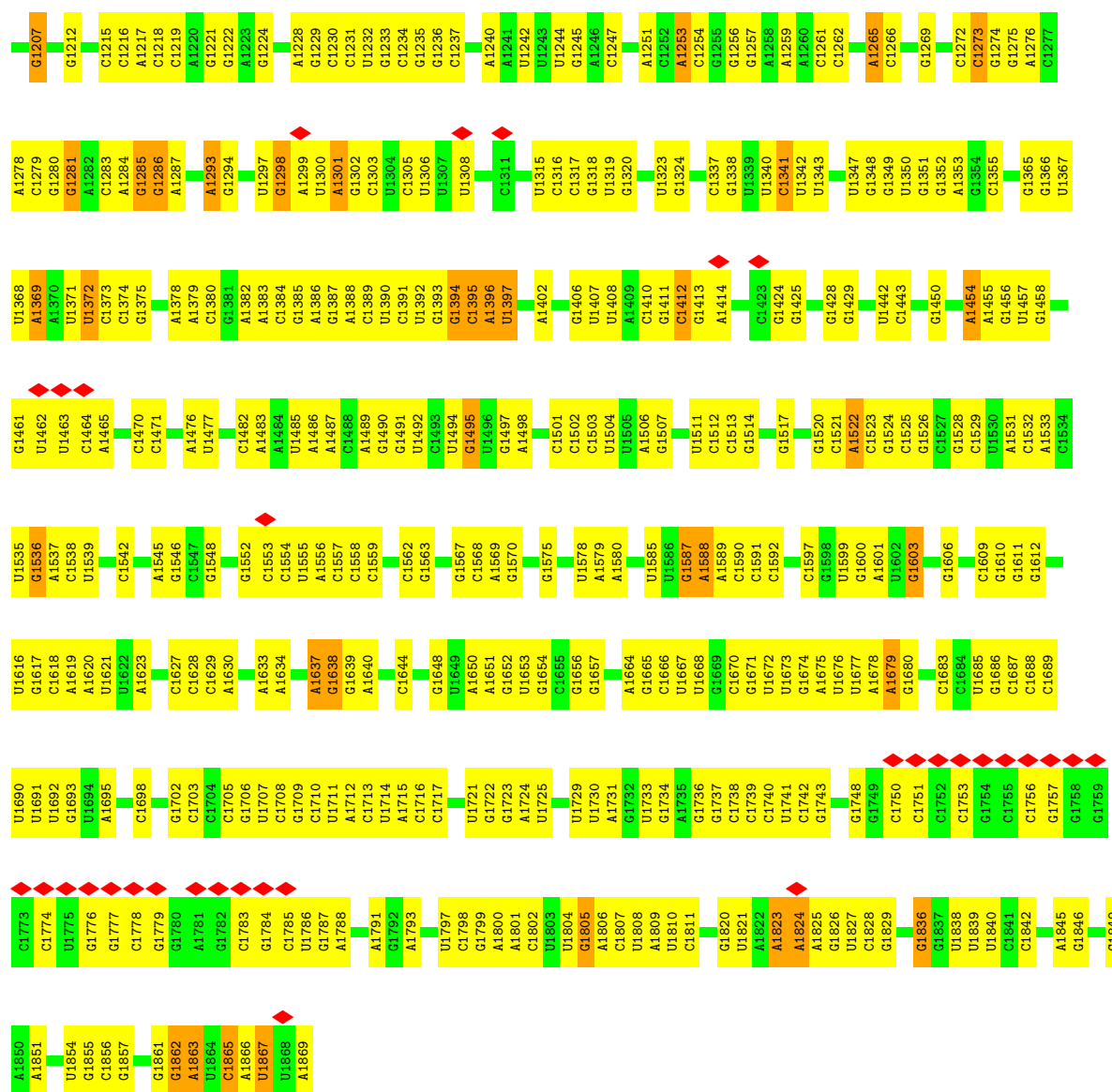
- Molecule 78: 60S ribosomal protein L9



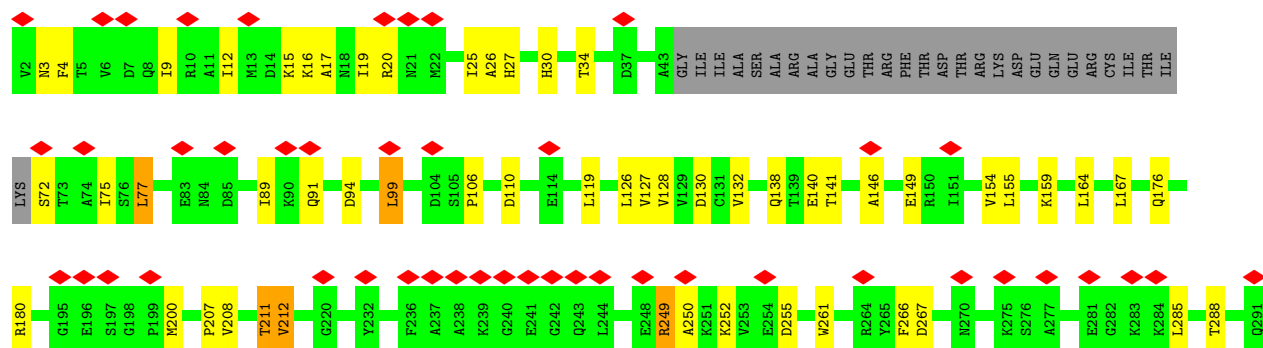
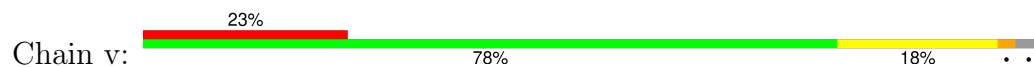
- Molecule 79: 18S rRNA

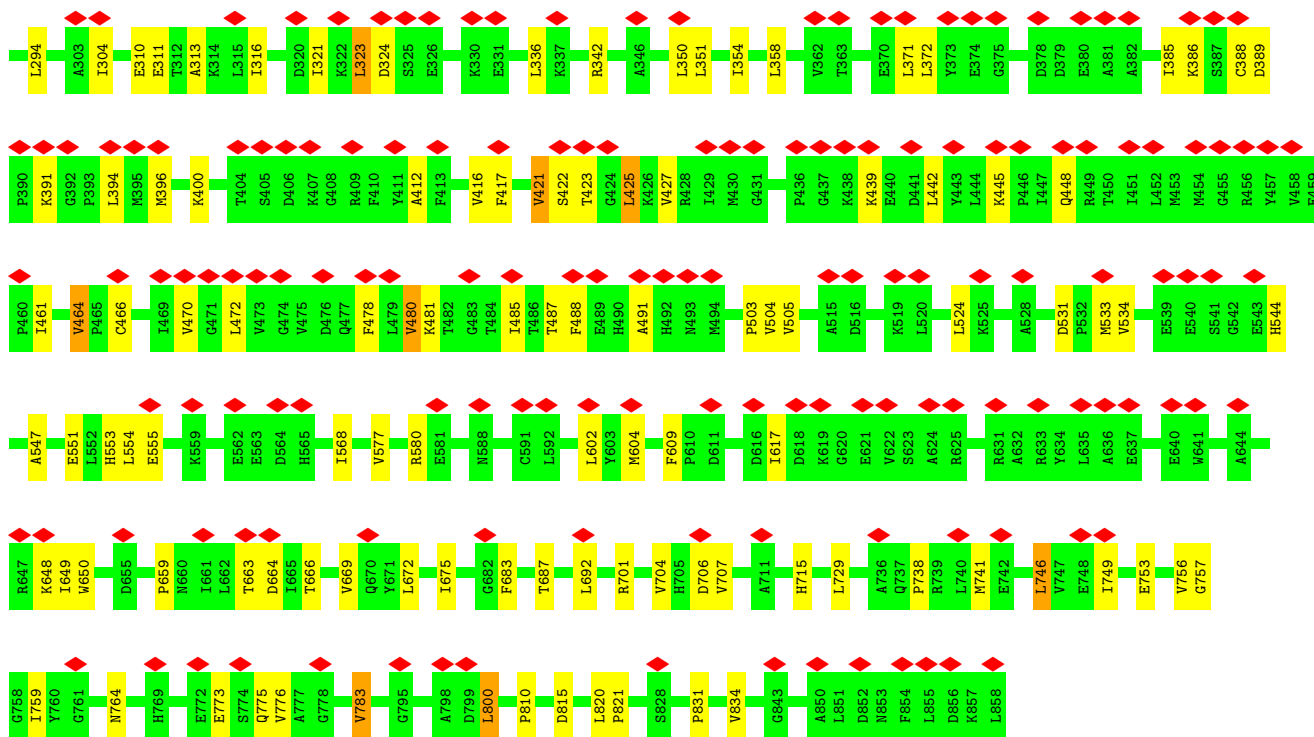




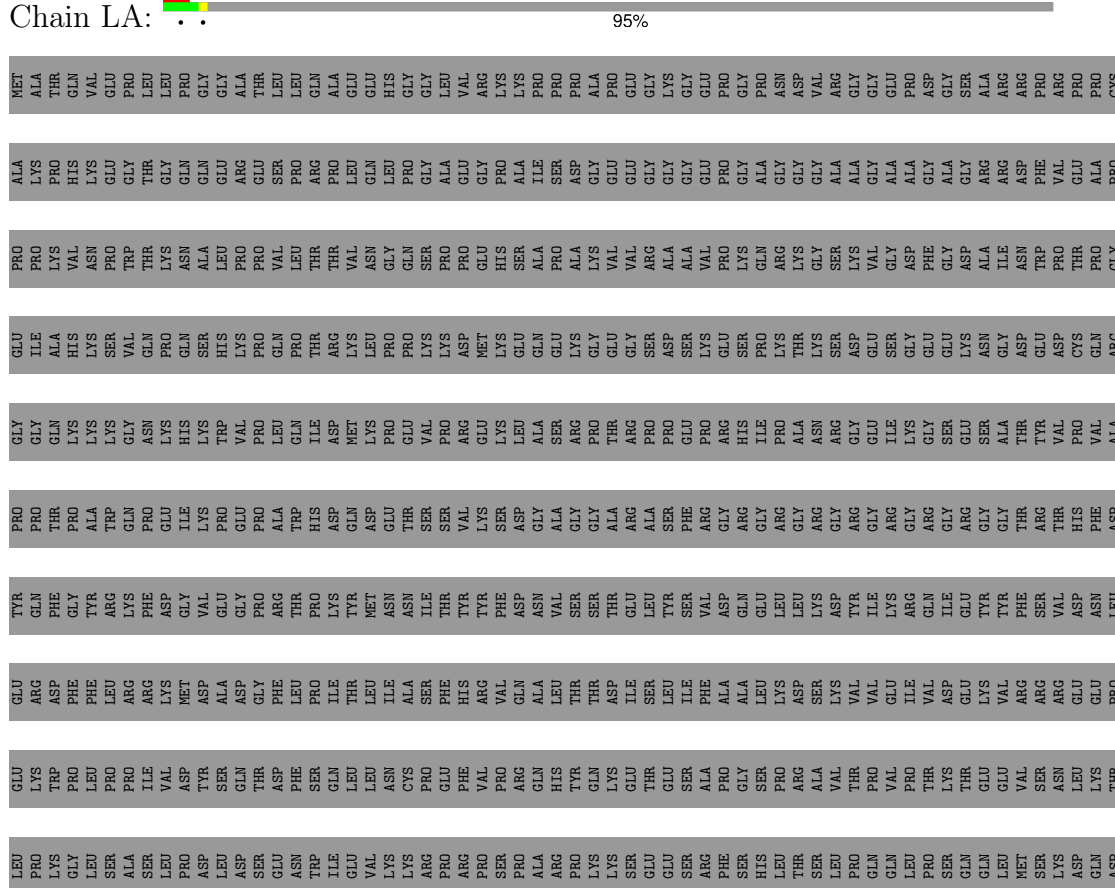


• Molecule 80: Elongation factor 2





- Molecule 81: La-related protein 1

Chain LA: 





Chain ES: ■

99%

| Amino Acid | Percentage |
|------------|------------|
| Ala        | 10%        |
| Gly        | 10%        |
| Ser        | 10%        |
| Val        | 10%        |
| Leu        | 10%        |
| Ile        | 10%        |
| Pro        | 10%        |
| Thr        | 10%        |
| Met        | 10%        |
| Asp        | 10%        |
| Asn        | 10%        |
| Glu        | 10%        |
| Gln        | 10%        |
| Arg        | 10%        |
| Lys        | 10%        |
| His        | 10%        |
| Phe        | 10%        |
| Tyr        | 10%        |
| Trp        | 10%        |
| Cys        | 10%        |
| Protein    | 10%        |

02940



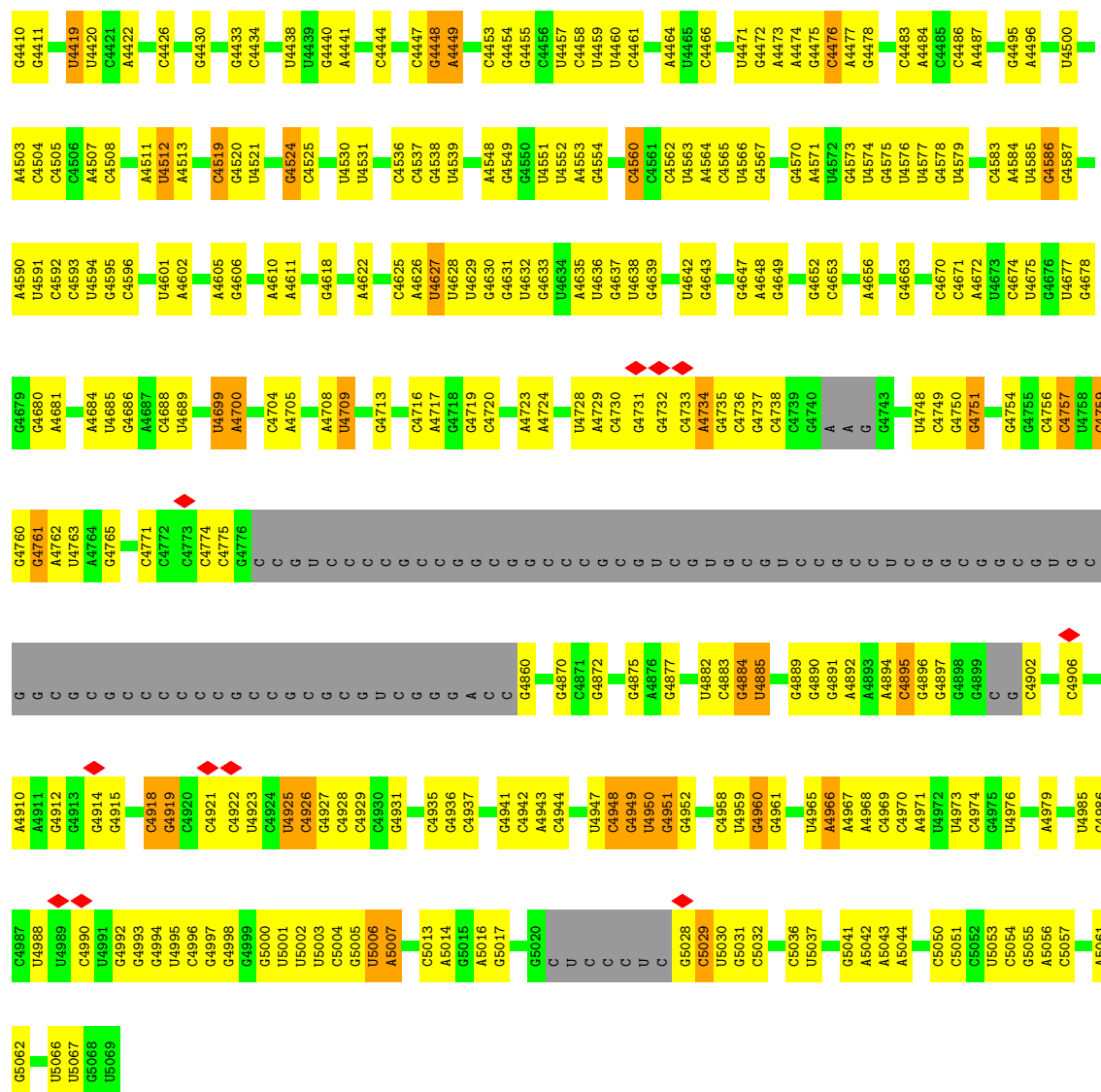




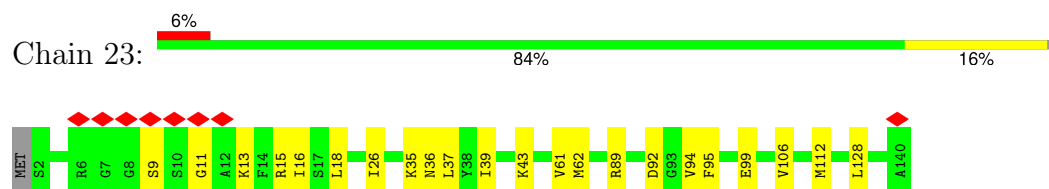
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2896 | A2787 | C2704 | G2624 | G2522 | C2441 | G2348 | G     | A2103 | C2011 | A1941 | A1825 | A1742 | G1654 |
| G2897 | U2788 | G2705 | G2625 | G2523 | C2446 | G2349 | C     | A2104 | A2012 | A1942 | C1828 | A1743 | G1655 |
| C2898 | U2789 | U2706 | U2626 | A2524 | U2447 | C2351 | G2261 | G2105 | U2015 | A1943 | C1829 | U1744 | C1661 |
| U2900 | U2790 | U2707 | C2627 | U2530 | U2448 | G2357 | A2263 | A2106 | C2016 | G1948 | G1830 | A1746 | C1662 |
| G     | G2796 | U2708 | U2630 | C2533 | A2449 | G2358 | C2264 | G2108 | A2017 | U1949 | C1831 | U1664 | C1663 |
| G     | C2710 | C2709 | G     | G     | A2449 | U2359 | G2265 | A2109 | G     | U1950 | C1832 | U1749 | U1664 |
| C     | C2711 | U2710 | U2633 | A2537 | U2454 | A2360 | U2267 | G2110 | U2020 | G1951 | G1836 | U1750 | C1665 |
| C     | G2712 | U2711 | C2634 | U2538 | U2455 | A2361 | A2268 | G     | G2021 | G1955 | A1837 | U1751 | G     |
| C     | C2713 | C2712 | U2635 | U2539 | G2456 | C2373 | G2273 | G     | A2025 | A1956 | G1842 | U1752 | A1669 |
| C     | G2714 | U2713 | U2636 | U2540 | G2457 | A2374 | C2274 | A     | A2026 | U1957 | G     | U1753 | U1672 |
| C     | U2715 | G2714 | U2637 | C2541 | C2458 | A2375 | G2275 | G     | A2033 | A1958 | G     | U1754 | U1673 |
| C     | C2716 | U2715 | U2638 | G2542 | C2459 | A2376 | G2276 | C     | G2034 | U1959 | G     | C1674 | C1674 |
| C     | G     | U2716 | U2639 | U2543 | C2460 | C2377 | A2277 | G     | C2035 | A1960 | G     | U1757 | C1675 |
| C     | G     | U2717 | U2640 | A2544 | G2466 | G     | G2278 | C     | G     | G1961 | G     | C1676 | C1676 |
| C     | G     | U2718 | A2641 | U2545 | G2467 | G2380 | G2279 | C     | G2046 | A1962 | G     | U1758 | U1677 |
| C     | G     | U2719 | A2642 | U2546 | C2470 | G     | G2280 | C     | A2047 | C1963 | G     | U1759 | G     |
| C     | G     | U2720 | A2643 | G2547 | G2471 | U2385 | U2281 | C     | U2048 | A1964 | G     | U1760 | U1681 |
| C     | G     | U2721 | C2644 | C2548 | G2472 | U2386 | A2282 | C     | G     | G1965 | G     | U1761 | U1682 |
| C     | G     | U2722 | C2645 | A2553 | G2473 | G2387 | G2283 | G     | C2051 | C1966 | G     | C1762 | A1684 |
| C     | G     | U2723 | C2646 | U2554 | G2474 | U2388 | G2284 | C     | G2052 | A1967 | G     | C1763 | G1685 |
| C     | G     | U2724 | C2647 | G2555 | G2475 | A2389 | G2285 | C     | G2053 | G1968 | G     | U1764 | C1686 |
| C     | G     | U2725 | A2648 | U2556 | A2476 | A2390 | G2286 | C     | G2054 | U1969 | G     | U1765 | U1687 |
| C     | G     | U2726 | C2649 | G2557 | A2477 | A2391 | G2287 | C     | G2055 | A1970 | G     | U1766 | G1688 |
| C     | G     | U2727 | C2650 | C2558 | G2478 | A2392 | G2288 | C     | G2056 | U1971 | G     | A1766 | C1689 |
| C     | G     | U2728 | C2651 | C2559 | G2479 | A2393 | G2289 | C     | A2057 | U1972 | G     | U1767 | G1690 |
| C     | G     | U2729 | C2652 | C2560 | G2480 | A2394 | G2290 | C     | G2058 | U1973 | G     | C1768 | C1691 |
| C     | G     | U2730 | C2653 | C2561 | G2481 | U2395 | G2291 | C     | C2059 | A1974 | G     | U1769 | G1692 |
| C     | G     | U2731 | C2654 | C2562 | G2482 | G2400 | G2292 | C     | G2060 | U1975 | G     | U1770 | U1693 |
| C     | G     | U2732 | C2655 | C2563 | G2483 | G2401 | G2293 | C     | U2061 | G1976 | G     | C1771 | C1694 |
| C     | G     | U2733 | C2656 | G2564 | G2484 | G2402 | G2294 | C     | A2069 | A1977 | G     | U1772 | G1695 |
| C     | G     | U2734 | C2657 | C2565 | G2485 | G2403 | G2295 | C     | U2070 | U1978 | G     | C1773 | G     |
| C     | G     | U2735 | C2658 | C2566 | G2486 | A2404 | G2296 | C     | G2075 | A1984 | G     | U1774 | A     |
| C     | G     | U2736 | C2659 | C2567 | G2487 | G2405 | G2297 | C     | G2076 | G1985 | G     | A1776 | A     |
| C     | G     | U2737 | C2660 | C2568 | G2488 | G2406 | G2298 | C     | G2077 | U1986 | G     | C1777 | C     |
| C     | G     | U2738 | C2661 | C2569 | G2489 | G2407 | G2299 | C     | C2078 | C1987 | G     | U1778 | C     |
| C     | G     | U2739 | C2662 | C2570 | G2490 | C2411 | G2300 | C     | U2079 | G1988 | G     | U1779 | C     |
| C     | G     | U2740 | C2663 | C2571 | G2491 | G2412 | G2301 | C     | U2080 | G1989 | G     | A1780 | C     |
| C     | G     | U2741 | C2664 | C2572 | G2492 | U2413 | G2302 | C     | C2081 | A1990 | G     | C1720 | G1721 |
| C     | G     | U2742 | C2665 | C2573 | G2493 | U2414 | G2303 | C     | G2082 | U1991 | G     | U1781 | G     |
| C     | G     | U2743 | C2666 | C2574 | G2494 | U2415 | G2304 | C     | G2083 | A1992 | G     | U1782 | G     |
| C     | G     | U2744 | C2667 | C2575 | G2495 | G2416 | G2305 | C     | U2084 | U1993 | G     | U1783 | G     |
| C     | G     | U2745 | C2668 | C2576 | G2496 | A2417 | G2306 | C     | G     | C1994 | G     | A1787 | U1726 |
| C     | G     | U2746 | C2669 | C2577 | G2497 | A2418 | G2307 | C     | G     | C1995 | G     | U1727 | U1727 |
| C     | G     | U2747 | C2670 | C2578 | G2498 | G2419 | G2308 | C     | U2089 | G1996 | G     | U1728 | U1728 |
| C     | G     | U2748 | C2671 | C2579 | G2499 | G2420 | G2309 | C     | U2090 | C1997 | G     | A1729 | G1729 |
| C     | G     | U2749 | C2672 | C2580 | G2500 | G2421 | G2310 | C     | C2091 | U1997 | G     | U1730 | U1730 |
| C     | G     | U2750 | C2673 | C2581 | G2501 | G2422 | G2311 | C     | G2092 | G     | G     | C1731 | C1731 |
| C     | G     | U2751 | C2674 | C2582 | G2502 | G2423 | G2312 | C     | G2093 | G     | G     | C1732 | C1732 |
| C     | G     | U2752 | C2675 | C2583 | G2503 | U2424 | G2313 | C     | G2094 | G     | G     | U1733 | U1733 |
| C     | G     | U2753 | C2676 | C2584 | G2504 | U2425 | G2314 | C     | C2095 | G     | G     | U1734 | U1734 |
| C     | G     | U2754 | C2677 | C2585 | G2505 | U2426 | G2315 | C     | A2096 | G     | G     | U1735 | U1735 |
| C     | G     | U2755 | C2678 | C2586 | G2506 | G2427 | G2316 | C     | G2097 | G     | G     | A1736 | A1736 |
| C     | G     | U2756 | C2679 | C2587 | G2507 | A2428 | G2317 | C     | C2098 | G     | G     | A1737 | A1737 |
| C     | G     | U2757 | C2680 | C2588 | G2508 | A2429 | G2318 | C     | G2099 | G     | G     | A1804 | A1804 |
| C     | G     | U2758 | C2681 | C2589 | G2509 | G2430 | G2319 | C     | C2100 | G     | G     | A1805 | A1805 |
| C     | G     | U2759 | C2682 | C2590 | G2510 | G2431 | G2320 | C     | A2101 | G     | G     | G1806 | G1806 |
| C     | G     | U2760 | C2683 | C2591 | G2511 | G2432 | G2321 | C     | G2102 | G     | G     | C1807 | C1807 |
| C     | G     | U2761 | C2684 | C2592 | G2512 | G2433 | G2322 | C     | G     | G     | G     | C1808 | C1808 |
| C     | G     | U2762 | C2685 | C2593 | G2513 | G2434 | G2323 | C     | G     | G     | G     | G1821 | G1821 |
| C     | G     | U2763 | C2686 | C2594 | G2514 | U2435 | G2324 | C     | G     | G     | G     | U1822 | U1822 |
| C     | G     | U2764 | C2687 | C2595 | G2515 | U2436 | G2325 | C     | G     | G     | G     | G1823 | G1823 |
| C     | G     | U2765 | C2688 | C2596 | G2516 | U2437 | G2326 | C     | G     | G     | G     | G1824 | G1824 |
| C     | G     | U2766 | C2689 | C2597 | G2517 | U2438 | G2327 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2767 | C2690 | C2598 | G2518 | U2439 | G2328 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2768 | C2691 | C2599 | G2519 | U2440 | G2329 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2769 | C2692 | C2600 | G2520 | U2441 | G2330 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2770 | C2693 | C2601 | G2521 | U2442 | G2331 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2771 | C2694 | C2602 | G2522 | U2443 | G2332 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2772 | C2695 | C2603 | G2523 | U2444 | G2333 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2773 | C2696 | C2604 | G2524 | U2445 | G2334 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2774 | C2697 | C2605 | G2525 | U2446 | G2335 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2775 | C2698 | C2606 | G2526 | U2447 | G2336 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2776 | C2699 | C2607 | G2527 | U2448 | G2337 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2777 | C2700 | C2608 | G2528 | U2449 | G2338 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2778 | C2701 | C2609 | G2529 | U2450 | G2339 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2779 | C2702 | C2610 | G2530 | U2451 | G2340 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2780 | C2703 | C2611 | G2531 | U2452 | G2341 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2781 | C2704 | C2612 | G2532 | U2453 | G2342 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2782 | C2705 | C2613 | G2533 | U2454 | G2343 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2783 | C2706 | C2614 | G2534 | U2455 | G2344 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2784 | C2707 | C2615 | G2535 | U2456 | G2345 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2785 | C2708 | C2616 | G2536 | U2457 | G2346 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2786 | C2709 | C2617 | G2537 | U2458 | G2347 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2787 | C2710 | C2618 | G2538 | U2459 | G2348 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2788 | C2711 | C2619 | G2539 | U2460 | G2349 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2789 | C2712 | C2620 | G2540 | U2461 | G2350 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2790 | C2713 | C2621 | G2541 | U2462 | G2351 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2791 | C2714 | C2622 | G2542 | U2463 | G2352 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2792 | C2715 | C2623 | G2543 | U2464 | G2353 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2793 | C2716 | C2624 | G2544 | U2465 | G2354 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2794 | C2717 | C2625 | G2545 | U2466 | G2355 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2795 | C2718 | C2626 | G2546 | U2467 | G2356 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2796 | C2719 | C2627 | G2547 | U2468 | G2357 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2797 | C2720 | C2628 | G2548 | U2469 | G2358 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2798 | C2721 | C2629 | G2549 | U2470 | G2359 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2799 | C2722 | C2630 | G2550 | U2471 | G2360 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2800 | C2723 | C2631 | G2551 | U2472 | G2361 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2801 | C2724 | C2632 | G2552 | U2473 | G2362 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2802 | C2725 | C2633 | G2553 | U2474 | G2363 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2803 | C2726 | C2634 | G2554 | U2475 | G2364 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2804 | C2727 | C2635 | G2555 | U2476 | G2365 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2805 | C2728 | C2636 | G2556 | U2477 | G2366 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2806 | C2729 | C2637 | G2557 | U2478 | G2367 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2807 | C2730 | C2638 | G2558 | U2479 | G2368 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2808 | C2731 | C2639 | G2559 | U2480 | G2369 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2809 | C2732 | C2640 | G2560 | U2481 | G2370 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2810 | C2733 | C2641 | G2561 | U2482 | G2371 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2811 | C2734 | C2642 | G2562 | U2483 | G2372 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2812 | C2735 | C2643 | G2563 | U2484 | G2373 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2813 | C2736 | C2644 | G2564 | U2485 | G2374 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2814 | C2737 | C2645 | G2565 | U2486 | G2375 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2815 | C2738 | C2646 | G2566 | U2487 | G2376 | C     | G     | G     | G     | G     | G     |
| C     | G     | U2816 | C2739 | C2647 | G2567 | U248  |       |       |       |       |       |       |       |

|       |       |       |   |       |   |       |       |       |       |   |   |
|-------|-------|-------|---|-------|---|-------|-------|-------|-------|---|---|
| U4321 | C4335 | U4232 | C | C4088 | C | C3893 | C3810 | A3719 | G3619 | C | G |
| G4322 | U4340 | A4233 | C | G4089 | G | A3894 | G3811 | G3720 | G     | G | G |
| A4323 | C4341 | G4234 | G | U4090 | A | G3895 | G3812 | U3721 | C     | C | C |
| G4328 | U4342 | C4235 | C | G4091 | C | G3896 | U3813 | G3722 | C     | C | C |
| G4329 | U4343 | U4236 | C | U4092 | U | G3897 | G3814 | A3723 | C     | C | C |
| G4330 | U4344 | G4237 | C | G4093 | C | G3900 | G3815 | G3726 | C     | C | C |
| G4331 | U4345 | U4238 | G | U4094 | U | G3901 | A3816 | A3727 | C     | C | C |
| A4332 | A4239 | A4239 | C | G4095 | G | G3904 | A3817 | G3728 | G     | A | C |
| C4335 | G4147 | G4147 | G | C     | G | G3906 | G3818 | U3729 | C     | C | C |
| U4340 | C4148 | C4148 | G | C     | G | A3905 | G3819 | G     | G     | C | C |
| C4341 | G4152 | G4152 | C | C     | G | G3907 | G3820 | A3732 | C     | C | C |
| G4342 | C4153 | C4153 | C | C     | G | A3908 | U3821 | A3733 | G     | C | C |
| U4343 | C4158 | C4158 | G | A     | C | G3909 | U3822 | U3734 | C     | C | C |
| C4344 | C4159 | C4159 | C | C     | C | C3910 | U3823 | G3735 | G     | G | G |
| U4345 | C4162 | C4162 | C | G     | C | G3911 | C3833 | A3736 | G     | G | G |
| A4253 | U4163 | U4163 | C | U4108 | U | C3912 | C3834 | A3737 | C     | C | C |
| G4254 | C4164 | C4164 | G | G4109 | G | U3915 | C3835 | G3738 | C     | C | C |
| C4258 | A4170 | A4170 | C | U4110 | C | G3916 | A3836 | C3739 | C     | C | C |
| U4259 | G4173 | G4173 | C | U4111 | C | G3917 | G3839 | G3740 | C     | C | C |
| C4261 | U4174 | U4174 | A | C     | G | A3918 | U3840 | A3746 | C     | C | C |
| G4262 | G4175 | G4175 | C | U4112 | C | C3919 | U3841 | A3747 | C     | C | C |
| C4263 | C4176 | C4176 | C | C4116 | C | U3920 | A3842 | A3748 | C     | C | C |
| U4264 | C4177 | C4177 | A | C     | C | G3921 | A3843 | G3751 | G     | G | G |
| U4265 | G4178 | G4178 | C | C4119 | C | G3922 | A3844 | C3752 | C     | C | C |
| G4266 | C4179 | C4179 | C | U4120 | C | A3923 | U3845 | G3753 | C     | C | C |
| G4267 | C4183 | C4183 | U | G4121 | C | C3924 | U3846 | G3754 | C     | C | C |
| A4268 | G4184 | G4184 | A | C4122 | C | U3927 | C3850 | A3760 | C     | C | C |
| A4273 | U4188 | U4188 | C | C4123 | C | A3928 | U3851 | C3761 | U     | U | U |
| C4275 | U4189 | U4189 | U | C     | C | G3929 | A3852 | U3762 | C     | C | C |
| A4281 | U4190 | U4190 | U | U4127 | U | U3930 | C3853 | A3763 | C     | C | C |
| C4291 | G4191 | G4191 | C | C4130 | C | C3931 | G3854 | G3681 | C     | C | C |
| U4292 | U4194 | U4194 | C | G4131 | A | U3932 | G3855 | A3682 | C     | C | C |
| U4293 | G4197 | G4197 | G | C4132 | U | G3933 | G3856 | G3683 | C     | C | C |
| C4294 | C4198 | C4198 | U | U4133 | C | G3934 | G3857 | G3684 | C     | C | C |
| G4297 | G4200 | G4200 | C | C4134 | C | C     | G3858 | U3770 | C     | C | C |
| U4300 | U4201 | U4201 | C | U4135 | C | U3937 | G3859 | C3771 | C     | C | C |
| U4301 | A4202 | A4202 | U | G4136 | C | G3938 | A3860 | U3772 | G     | G | G |
| G4305 | C4203 | C4203 | C | C4137 | C | C     | A3861 | U3773 | C     | C | C |
| U4306 | U4208 | U4208 | G | C     | U | G3944 | A3862 | A3774 | C     | C | C |
| A4307 | G4209 | G4209 | C | U4068 | U | A     | A3865 | A3775 | G     | G | G |
| C4308 | A4212 | A4212 | U | U4069 | G | G3944 | G3866 | G3776 | C     | C | C |
| C4314 | C4215 | C4215 | C | U4070 | C | A     | A3867 | G3777 | C     | C | C |
| A4317 | G4216 | G4216 | C | U4071 | C | G     | G3868 | G3778 | C     | C | C |
| C4318 | C4219 | C4219 | C | C4072 | C | G     | C3869 | A3784 | C     | C | C |
| G4406 | G4407 | G4407 | C | U4073 | C | U     | A3870 | A3785 | C     | C | C |
| G4408 | C4319 | C4319 | C | G4076 | C | G     | A3871 | U3786 | C     | C | C |
| C4409 | U4228 | U4228 | C | C4080 | C | G     | A3872 | G3787 | C     | C | C |
|       | G4229 | G4229 | C | G4081 | C | A     | G3873 | C3788 | U3707 | C | C |
|       |       |       | C | U4082 | C | G     | G3874 | C3789 | C3708 | C | C |
|       |       |       | C | U4083 | C | G     | C3875 | G3794 | A3711 | C | C |
|       |       |       | C | G4084 | C | U     | A3876 | A3795 | A3712 | C | C |
|       |       |       | C | U4085 | C | U     | A3877 | U3796 | U3713 | C | C |
|       |       |       | C | G4086 | C | U     | C3878 | C3797 | G3714 | C | C |
|       |       |       | C | G4087 | C | A     | G3879 | A3803 | G3717 | C | C |
|       |       |       | C |       | C |       | A3890 | G3804 | A3718 | C | C |





• Molecule 86: Ribosomal protein L23



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 8501                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 39                                      | Depositor |
| Minimum defocus (nm)                 | 700                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | OTHER                                   | Depositor |
| Maximum map value                    | 26.920                                  | Depositor |
| Minimum map value                    | -14.119                                 | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 1.115                                   | Depositor |
| Recommended contour level            | 3.3                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 664.0, 664.0, 664.0                     | wwPDB     |
| Map dimensions                       | 800, 800, 800                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.83, 0.83, 0.83                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DDE, GDP, ZN

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   | BB    | 0.13         | 0/1747      | 0.34        | 0/2374      |
| 2   | S2    | 0.13         | 0/1753      | 0.31        | 0/2369      |
| 3   | PP    | 0.12         | 0/643       | 0.28        | 0/860       |
| 4   | DD    | 0.12         | 0/1195      | 0.32        | 0/1597      |
| 5   | 58    | 0.13         | 0/3581      | 0.29        | 0/5577      |
| 6   | 6     | 0.13         | 0/2858      | 0.26        | 0/4455      |
| 7   | L8    | 0.13         | 0/1936      | 0.32        | 0/2596      |
| 8   | L3    | 0.13         | 0/3240      | 0.33        | 0/4339      |
| 9   | L4    | 0.12         | 0/2937      | 0.31        | 0/3946      |
| 10  | L5    | 0.13         | 0/2437      | 0.32        | 0/3264      |
| 11  | L6    | 0.13         | 0/1762      | 0.32        | 0/2362      |
| 12  | L7    | 0.12         | 0/1911      | 0.28        | 0/2549      |
| 13  | aa    | 0.14         | 0/1910      | 0.33        | 0/2569      |
| 14  | 10    | 0.12         | 0/1702      | 0.29        | 0/2272      |
| 15  | 13    | 0.12         | 0/1733      | 0.30        | 0/2316      |
| 16  | 14    | 0.14         | 0/1158      | 0.33        | 0/1547      |
| 17  | 15    | 0.13         | 0/1746      | 0.32        | 0/2338      |
| 18  | bb    | 0.13         | 0/1662      | 0.31        | 0/2222      |
| 19  | 17    | 0.13         | 0/1268      | 0.33        | 0/1700      |
| 20  | 19    | 0.13         | 0/1524      | 0.29        | 0/2013      |
| 21  | 20    | 0.13         | 0/1501      | 0.28        | 0/2012      |
| 22  | 21    | 0.11         | 0/1326      | 0.27        | 0/1770      |
| 23  | 22    | 0.13         | 0/823       | 0.35        | 0/1104      |
| 24  | cc    | 0.12         | 0/984       | 0.30        | 0/1323      |
| 25  | 26    | 0.12         | 0/1132      | 0.31        | 0/1504      |
| 26  | 27    | 0.12         | 0/1130      | 0.30        | 0/1507      |
| 27  | dd    | 0.13         | 0/1191      | 0.33        | 0/1590      |
| 28  | 29    | 0.12         | 0/861       | 0.29        | 0/1138      |
| 29  | 30    | 0.12         | 0/771       | 0.27        | 0/1034      |
| 30  | 31    | 0.14         | 0/903       | 0.33        | 0/1216      |
| 31  | 32    | 0.12         | 0/1071      | 0.32        | 0/1429      |
| 32  | ee    | 0.13         | 0/895       | 0.33        | 0/1198      |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 33  | 34    | 0.13         | 0/916         | 0.33        | 0/1220        |
| 34  | 35    | 0.12         | 0/1021        | 0.31        | 0/1348        |
| 35  | 36    | 0.12         | 0/841         | 0.29        | 0/1112        |
| 36  | 37    | 0.12         | 0/720         | 0.34        | 0/952         |
| 37  | 38    | 0.11         | 0/575         | 0.28        | 0/761         |
| 38  | 39    | 0.13         | 0/459         | 0.29        | 0/608         |
| 39  | 40    | 0.12         | 0/435         | 0.28        | 0/575         |
| 40  | 41    | 0.13         | 0/240         | 0.26        | 0/305         |
| 41  | 42    | 0.13         | 0/864         | 0.30        | 0/1140        |
| 42  | ff    | 0.12         | 0/718         | 0.34        | 0/953         |
| 43  | gg    | 0.12         | 0/1006        | 0.29        | 0/1349        |
| 44  | AS    | 0.14         | 0/1756        | 0.34        | 0/2350        |
| 45  | FF    | 0.15         | 0/1226        | 0.36        | 0/1649        |
| 46  | VV    | 0.13         | 0/665         | 0.30        | 0/891         |
| 47  | s     | 0.14         | 0/1530        | 0.37        | 0/2064        |
| 48  | t     | 0.16         | 0/1174        | 0.43        | 0/1582        |
| 49  | F     | 0.25         | 1/2845 (0.0%) | 0.33        | 0/3828        |
| 50  | Q     | 0.12         | 0/1538        | 0.36        | 0/2054        |
| 51  | ZZ    | 0.13         | 0/567         | 0.35        | 0/753         |
| 52  | EE    | 0.15         | 0/918         | 0.36        | 0/1233        |
| 53  | TT    | 0.29         | 1/604 (0.2%)  | 0.39        | 0/810         |
| 54  | S5    | 0.14         | 0/1492        | 0.36        | 0/2005        |
| 55  | WW    | 0.11         | 0/490         | 0.29        | 0/656         |
| 56  | II    | 0.14         | 0/1146        | 0.35        | 0/1534        |
| 57  | CC    | 0.16         | 0/834         | 0.41        | 0/1125        |
| 58  | AA    | 0.13         | 0/2493        | 0.33        | 0/3394        |
| 59  | OO    | 0.13         | 0/805         | 0.33        | 0/1081        |
| 60  | MM    | 0.13         | 0/1115        | 0.33        | 0/1493        |
| 61  | LL    | 0.14         | 0/1208        | 0.39        | 0/1618        |
| 62  | XX    | 0.12         | 0/470         | 0.33        | 0/623         |
| 63  | RR    | 0.13         | 0/1116        | 0.35        | 0/1490        |
| 64  | SS    | 0.13         | 0/1028        | 0.31        | 0/1366        |
| 65  | S6    | 0.13         | 0/1946        | 0.35        | 1/2590 (0.0%) |
| 66  | S4    | 0.27         | 1/2118 (0.0%) | 0.35        | 0/2849        |
| 67  | S9    | 0.13         | 0/1550        | 0.32        | 0/2069        |
| 68  | S7    | 0.13         | 0/1510        | 0.34        | 0/2022        |
| 69  | YY    | 0.13         | 0/447         | 0.34        | 0/587         |
| 70  | S3    | 0.14         | 0/1688        | 0.34        | 0/2269        |
| 71  | RS    | 0.13         | 0/1082        | 0.35        | 0/1452        |
| 72  | WX    | 0.14         | 0/1051        | 0.34        | 0/1406        |
| 73  | S8    | 0.13         | 0/1715        | 0.32        | 0/2287        |
| 74  | W     | 0.13         | 0/873         | 0.31        | 0/1158        |
| 75  | GG    | 0.13         | 0/1020        | 0.35        | 0/1369        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 76  | UU    | 0.12         | 0/828           | 0.30        | 0/1109          |
| 77  | 11    | 0.12         | 0/1385          | 0.31        | 0/1852          |
| 78  | L9    | 0.13         | 0/1535          | 0.33        | 0/2063          |
| 79  | 18    | 0.13         | 0/40302         | 0.31        | 0/62804         |
| 80  | v     | 0.14         | 0/6577          | 0.33        | 0/8883          |
| 81  | LA    | 0.12         | 0/426           | 0.31        | 0/568           |
| 82  | CE    | 0.16         | 0/616           | 0.30        | 0/812           |
| 83  | A     | 0.14         | 0/1001          | 0.35        | 0/1339          |
| 84  | ES    | 0.16         | 0/844           | 0.40        | 0/1314          |
| 85  | 28    | 0.14         | 0/84014         | 0.31        | 0/131028        |
| 86  | 23    | 0.13         | 0/1048          | 0.32        | 0/1402          |
| All | All   | 0.14         | 3/237682 (0.0%) | 0.32        | 1/347244 (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 |
|-----|-------|---------------------|---------------------|
| 47  | s     | 0                   | 1                   |
| 63  | RR    | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 49  | F     | 204 | ASN  | C-O   | 10.96 | 1.29        | 1.23     |
| 66  | S4    | 149 | TYR  | C-O   | -9.98 | 1.19        | 1.23     |
| 53  | TT    | 62  | VAL  | CA-CB | 6.34  | 1.57        | 1.54     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 65  | S6    | 67  | VAL  | N-CA-C | -6.02 | 107.99      | 113.71   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 63  | RR    | 60  | LYS  | Peptide |
| 47  | s     | 119 | CYS  | 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   | BB    | 1710  | 0        | 1708     | 27      | 0            |
| 2   | S2    | 1716  | 0        | 1806     | 29      | 0            |
| 3   | PP    | 636   | 0        | 637      | 6       | 0            |
| 4   | DD    | 1175  | 0        | 1249     | 13      | 0            |
| 5   | 58    | 3208  | 0        | 1629     | 60      | 0            |
| 6   | 6     | 2558  | 0        | 1296     | 38      | 0            |
| 7   | L8    | 1898  | 0        | 1993     | 28      | 0            |
| 8   | L3    | 3172  | 0        | 3310     | 36      | 0            |
| 9   | L4    | 2883  | 0        | 3053     | 27      | 0            |
| 10  | L5    | 2391  | 0        | 2424     | 31      | 0            |
| 11  | L6    | 1729  | 0        | 1887     | 12      | 0            |
| 12  | L7    | 1875  | 0        | 1995     | 29      | 0            |
| 13  | aa    | 1879  | 0        | 2027     | 23      | 0            |
| 14  | 10    | 1664  | 0        | 1712     | 17      | 0            |
| 15  | 13    | 1702  | 0        | 1820     | 14      | 0            |
| 16  | 14    | 1137  | 0        | 1211     | 14      | 0            |
| 17  | 15    | 1701  | 0        | 1749     | 21      | 0            |
| 18  | bb    | 1630  | 0        | 1778     | 23      | 0            |
| 19  | 17    | 1242  | 0        | 1274     | 10      | 0            |
| 20  | 19    | 1508  | 0        | 1664     | 14      | 0            |
| 21  | 20    | 1462  | 0        | 1508     | 15      | 0            |
| 22  | 21    | 1298  | 0        | 1366     | 11      | 0            |
| 23  | 22    | 809   | 0        | 833      | 6       | 0            |
| 24  | cc    | 967   | 0        | 1040     | 12      | 0            |
| 25  | 26    | 1115  | 0        | 1205     | 10      | 0            |
| 26  | 27    | 1107  | 0        | 1182     | 13      | 0            |
| 27  | dd    | 1162  | 0        | 1209     | 16      | 0            |
| 28  | 29    | 848   | 0        | 920      | 6       | 0            |
| 29  | 30    | 761   | 0        | 794      | 8       | 0            |
| 30  | 31    | 888   | 0        | 930      | 7       | 0            |
| 31  | 32    | 1053  | 0        | 1147     | 13      | 0            |
| 32  | ee    | 876   | 0        | 912      | 11      | 0            |
| 33  | 34    | 906   | 0        | 1000     | 8       | 0            |
| 34  | 35    | 1013  | 0        | 1147     | 8       | 0            |
| 35  | 36    | 830   | 0        | 916      | 6       | 0            |
| 36  | 37    | 705   | 0        | 738      | 4       | 0            |
| 37  | 38    | 569   | 0        | 637      | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | 39    | 447   | 0        | 480      | 11      | 0            |
| 39  | 40    | 429   | 0        | 469      | 3       | 0            |
| 40  | 41    | 239   | 0        | 289      | 3       | 0            |
| 41  | 42    | 851   | 0        | 924      | 9       | 0            |
| 42  | ff    | 708   | 0        | 758      | 8       | 0            |
| 43  | gg    | 990   | 0        | 1044     | 9       | 0            |
| 44  | AS    | 1729  | 0        | 1803     | 35      | 0            |
| 45  | FF    | 1202  | 0        | 1289     | 16      | 0            |
| 46  | VV    | 651   | 0        | 672      | 3       | 0            |
| 47  | s     | 1507  | 0        | 1564     | 15      | 0            |
| 48  | t     | 1160  | 0        | 1218     | 24      | 0            |
| 49  | F     | 2798  | 0        | 2809     | 41      | 0            |
| 50  | Q     | 1514  | 0        | 1634     | 15      | 0            |
| 51  | ZZ    | 555   | 0        | 567      | 8       | 0            |
| 52  | EE    | 908   | 0        | 939      | 11      | 0            |
| 53  | TT    | 598   | 0        | 656      | 5       | 0            |
| 54  | S5    | 1471  | 0        | 1522     | 21      | 0            |
| 55  | WW    | 488   | 0        | 514      | 4       | 0            |
| 56  | II    | 1128  | 0        | 1195     | 16      | 0            |
| 57  | CC    | 810   | 0        | 836      | 12      | 0            |
| 58  | AA    | 2436  | 0        | 2393     | 36      | 0            |
| 59  | OO    | 795   | 0        | 862      | 11      | 0            |
| 60  | MM    | 1097  | 0        | 1132     | 18      | 0            |
| 61  | LL    | 1190  | 0        | 1249     | 23      | 0            |
| 62  | XX    | 459   | 0        | 452      | 9       | 0            |
| 63  | RR    | 1098  | 0        | 1167     | 19      | 0            |
| 64  | SS    | 1011  | 0        | 1083     | 18      | 0            |
| 65  | S6    | 1923  | 0        | 2089     | 27      | 0            |
| 66  | S4    | 2076  | 0        | 2177     | 23      | 0            |
| 67  | S9    | 1525  | 0        | 1640     | 23      | 0            |
| 68  | S7    | 1488  | 0        | 1582     | 24      | 0            |
| 69  | YY    | 443   | 0        | 492      | 6       | 0            |
| 70  | S3    | 1662  | 0        | 1760     | 27      | 0            |
| 71  | RS    | 1068  | 0        | 1121     | 15      | 0            |
| 72  | WX    | 1034  | 0        | 1080     | 20      | 0            |
| 73  | S8    | 1686  | 0        | 1772     | 20      | 0            |
| 74  | W     | 860   | 0        | 903      | 10      | 0            |
| 75  | GG    | 1007  | 0        | 1028     | 20      | 0            |
| 76  | UU    | 814   | 0        | 865      | 12      | 0            |
| 77  | 11    | 1362  | 0        | 1399     | 14      | 0            |
| 78  | L9    | 1516  | 0        | 1597     | 16      | 0            |
| 79  | 18    | 36043 | 0        | 18202    | 676     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 80  | v     | 6470   | 0        | 6548     | 75      | 0            |
| 81  | LA    | 421    | 0        | 405      | 2       | 0            |
| 82  | CE    | 613    | 0        | 625      | 2       | 0            |
| 83  | A     | 983    | 0        | 1030     | 11      | 0            |
| 84  | ES    | 756    | 0        | 384      | 21      | 0            |
| 85  | 28    | 75105  | 0        | 37942    | 1216    | 0            |
| 86  | 23    | 1034   | 0        | 1097     | 12      | 0            |
| 87  | 34    | 1      | 0        | 0        | 0       | 0            |
| 87  | 37    | 1      | 0        | 0        | 0       | 0            |
| 87  | UU    | 1      | 0        | 0        | 0       | 0            |
| 87  | ff    | 1      | 0        | 0        | 0       | 0            |
| 88  | v     | 28     | 0        | 12       | 1       | 0            |
| All | All   | 221973 | 0        | 168976   | 3002    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3002) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:18:639:C:H2'   | 79:18:640:A:H8    | 1.33                     | 0.91              |
| 85:28:2492:C:H2'  | 85:28:2493:G:H8   | 1.36                     | 0.91              |
| 79:18:730:C:H2'   | 79:18:731:G:C8    | 2.07                     | 0.88              |
| 79:18:677:G:H21   | 79:18:1028:A:H62  | 1.21                     | 0.87              |
| 85:28:2478:C:H2'  | 85:28:2479:G:H8   | 1.38                     | 0.86              |
| 61:LL:37:GLY:H    | 79:18:1630:A:H5'' | 1.41                     | 0.85              |
| 85:28:4949:G:H4'  | 85:28:4950:U:H5'  | 1.57                     | 0.84              |
| 79:18:1410:C:H2'  | 79:18:1411:G:H8   | 1.42                     | 0.84              |
| 85:28:3717:A:H2'  | 85:28:3718:A:H8   | 1.40                     | 0.83              |
| 85:28:3751:G:H21  | 85:28:3775:A:H8   | 1.22                     | 0.83              |
| 85:28:2457:G:H21  | 85:28:3672:G:H21  | 1.26                     | 0.83              |
| 79:18:957:A:H3'   | 79:18:958:G:H21   | 1.42                     | 0.82              |
| 85:28:2492:C:H2'  | 85:28:2493:G:C8   | 2.14                     | 0.82              |
| 85:28:2486:G:H2'  | 85:28:2487:G:C8   | 2.14                     | 0.82              |
| 57:CC:64:TRP:HB3  | 62:XX:23:VAL:HA   | 1.62                     | 0.81              |
| 79:18:639:C:H2'   | 79:18:640:A:C8    | 2.15                     | 0.81              |
| 85:28:4992:G:H2'  | 85:28:4993:G:C8   | 2.15                     | 0.81              |
| 85:28:2411:C:H2'  | 85:28:2412:A:H8   | 1.46                     | 0.80              |
| 85:28:4618:G:H5'' | 86:23:15:ARG:HB3  | 1.62                     | 0.80              |
| 85:28:1538:U:H2'  | 85:28:1539:G:H8   | 1.45                     | 0.80              |
| 5:58:85:U:H5''    | 5:58:86:U:H3'     | 1.65                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:18:1536:G:H2'  | 79:18:1537:A:H8   | 1.48                     | 0.79              |
| 79:18:1004:U:H2'  | 79:18:1005:G:H8   | 1.48                     | 0.79              |
| 79:18:1776:G:H2'  | 79:18:1777:G:H8   | 1.47                     | 0.79              |
| 85:28:1970:A:H5'' | 85:28:1971:U:H5'  | 1.65                     | 0.79              |
| 51:ZZ:132:MET:HG3 | 51:ZZ:139:HIS:HB3 | 1.64                     | 0.79              |
| 78:L9:43:VAL:HG12 | 78:L9:59:LYS:HD3  | 1.66                     | 0.78              |
| 85:28:2745:A:H2'  | 85:28:2746:A:H8   | 1.48                     | 0.78              |
| 79:18:1486:A:H2'  | 79:18:1487:A:H8   | 1.45                     | 0.78              |
| 85:28:2335:C:H2'  | 85:28:2336:G:H8   | 1.48                     | 0.78              |
| 85:28:3717:A:H2'  | 85:28:3718:A:C8   | 2.19                     | 0.78              |
| 85:28:1198:G:H2'  | 85:28:1199:G:C8   | 2.19                     | 0.78              |
| 85:28:2478:C:H2'  | 85:28:2479:G:C8   | 2.19                     | 0.77              |
| 79:18:530:U:H2'   | 79:18:531:A:H8    | 1.49                     | 0.77              |
| 85:28:1327:C:H2'  | 85:28:1328:G:H8   | 1.50                     | 0.77              |
| 79:18:116:U:H3    | 79:18:347:G:H1    | 1.30                     | 0.77              |
| 52:EE:32:ALA:HB1  | 52:EE:37:GLU:HB3  | 1.66                     | 0.77              |
| 79:18:730:C:H2'   | 79:18:731:G:H8    | 1.50                     | 0.76              |
| 79:18:1221:G:H2'  | 79:18:1222:G:H8   | 1.50                     | 0.76              |
| 79:18:1711:U:H2'  | 79:18:1712:A:H8   | 1.50                     | 0.76              |
| 85:28:4967:A:H2'  | 85:28:4968:A:H8   | 1.47                     | 0.76              |
| 17:15:125:SER:HB3 | 85:28:3937:C:H1'  | 1.66                     | 0.76              |
| 85:28:1857:C:H2'  | 85:28:1858:A:H8   | 1.49                     | 0.76              |
| 85:28:2744:A:H2'  | 85:28:2745:A:C8   | 2.19                     | 0.76              |
| 79:18:1101:U:H2'  | 79:18:1102:G:H8   | 1.51                     | 0.76              |
| 79:18:1670:C:H2'  | 79:18:1671:G:C8   | 2.20                     | 0.76              |
| 85:28:2477:A:H2'  | 85:28:2478:C:C6   | 2.21                     | 0.76              |
| 80:v:17:ALA:HB3   | 80:v:94:ASP:HB2   | 1.66                     | 0.76              |
| 1:BB:66:VAL:HG21  | 1:BB:185:MET:HB3  | 1.66                     | 0.75              |
| 85:28:1332:C:H2'  | 85:28:1333:A:H8   | 1.47                     | 0.75              |
| 33:34:60:ARG:HG3  | 33:34:61:PRO:HD2  | 1.69                     | 0.75              |
| 79:18:941:C:H2'   | 79:18:942:G:C8    | 2.22                     | 0.75              |
| 85:28:1769:G:H2'  | 85:28:1770:A:C8   | 2.21                     | 0.75              |
| 80:v:354:ILE:HG23 | 80:v:358:LEU:HD12 | 1.69                     | 0.75              |
| 79:18:1098:C:H2'  | 79:18:1099:G:C8   | 2.22                     | 0.74              |
| 85:28:1169:G:H2'  | 85:28:1170:G:H8   | 1.50                     | 0.74              |
| 67:S9:5:ARG:HD3   | 79:18:38:A:H5''   | 1.69                     | 0.74              |
| 79:18:511:U:H2'   | 79:18:512:A:H8    | 1.51                     | 0.74              |
| 80:v:604:MET:HE3  | 80:v:704:VAL:HG12 | 1.68                     | 0.73              |
| 66:S4:201:HIS:HB3 | 66:S4:204:SER:HB3 | 1.69                     | 0.73              |
| 85:28:1461:C:H2'  | 85:28:1462:A:H8   | 1.52                     | 0.73              |
| 79:18:1711:U:H2'  | 79:18:1712:A:C8   | 2.23                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:894:G:H2'    | 79:18:895:G:H8     | 1.54                     | 0.73              |
| 58:AA:87:LEU:HB2   | 58:AA:101:PHE:HB2  | 1.69                     | 0.73              |
| 85:28:4537:C:H2'   | 85:28:4538:G:H8    | 1.54                     | 0.73              |
| 68:S7:134:VAL:HG13 | 68:S7:166:VAL:HG21 | 1.71                     | 0.72              |
| 79:18:1144:A:H5'   | 79:18:1355:C:H41   | 1.54                     | 0.72              |
| 79:18:1244:U:H2'   | 79:18:1245:G:H8    | 1.54                     | 0.72              |
| 79:18:640:A:H2'    | 79:18:641:A:C8     | 2.23                     | 0.72              |
| 79:18:1007:C:H2'   | 79:18:1008:A:C8    | 2.24                     | 0.72              |
| 85:28:3868:G:H22   | 85:28:3900:G:H1'   | 1.54                     | 0.72              |
| 85:28:4319:C:H2'   | 85:28:4320:G:H8    | 1.53                     | 0.72              |
| 21:20:147:ASP:HB3  | 21:20:150:ILE:HB   | 1.69                     | 0.72              |
| 65:S6:58:LYS:HA    | 65:S6:107:SER:HB2  | 1.72                     | 0.72              |
| 79:18:1776:G:H2'   | 79:18:1777:G:C8    | 2.25                     | 0.72              |
| 80:v:267:ASP:HA    | 80:v:285:LEU:HD11  | 1.72                     | 0.72              |
| 79:18:24:C:H2'     | 79:18:25:A:C8      | 2.25                     | 0.72              |
| 85:28:2480:G:H2'   | 85:28:2481:G:C8    | 2.24                     | 0.72              |
| 74:W:101:ARG:HA    | 74:W:104:GLN:HG2   | 1.71                     | 0.72              |
| 79:18:1410:C:H2'   | 79:18:1411:G:C8    | 2.24                     | 0.72              |
| 80:v:77:LEU:HD21   | 80:v:351:LEU:HD21  | 1.72                     | 0.72              |
| 85:28:2448:G:H2'   | 85:28:2449:A:C8    | 2.25                     | 0.71              |
| 85:28:1306:C:H2'   | 85:28:1307:A:H8    | 1.53                     | 0.71              |
| 80:v:531:ASP:HB3   | 80:v:534:VAL:HG22  | 1.72                     | 0.71              |
| 84:ES:3238:C:H2'   | 84:ES:3239:G:H8    | 1.55                     | 0.71              |
| 85:28:4967:A:H2'   | 85:28:4968:A:C8    | 2.25                     | 0.71              |
| 66:S4:107:GLY:HA2  | 66:S4:189:LEU:HD23 | 1.71                     | 0.71              |
| 85:28:1414:C:H2'   | 85:28:1415:G:C8    | 2.24                     | 0.71              |
| 46:VV:14:GLU:HA    | 46:VV:17:ARG:HD3   | 1.72                     | 0.71              |
| 75:GG:21:VAL:HG22  | 75:GG:24:GLY:H     | 1.55                     | 0.71              |
| 85:28:963:G:HO2'   | 85:28:964:A:H8     | 1.38                     | 0.71              |
| 85:28:4274:A:H2'   | 85:28:4275:G:H8    | 1.56                     | 0.71              |
| 50:Q:67:ILE:HD12   | 50:Q:96:PRO:HD2    | 1.73                     | 0.71              |
| 70:S3:196:GLY:HA3  | 70:S3:201:LYS:HE3  | 1.72                     | 0.71              |
| 79:18:1486:A:H2'   | 79:18:1487:A:C8    | 2.26                     | 0.70              |
| 79:18:1536:G:H2'   | 79:18:1537:A:C8    | 2.27                     | 0.70              |
| 85:28:1942:A:H2'   | 85:28:1943:A:C8    | 2.25                     | 0.70              |
| 13:aa:111:PRO:HD2  | 13:aa:114:ILE:HD12 | 1.73                     | 0.70              |
| 85:28:2707:U:H3'   | 85:28:2708:U:H5''  | 1.73                     | 0.70              |
| 85:28:4134:C:H2'   | 85:28:4135:G:H8    | 1.56                     | 0.70              |
| 85:28:4321:U:H2'   | 85:28:4322:G:C8    | 2.26                     | 0.70              |
| 63:RR:61:GLN:HB3   | 63:RR:62:PRO:HD3   | 1.74                     | 0.70              |
| 66:S4:163:ASP:HB3  | 66:S4:166:THR:HG22 | 1.71                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:28:2520:C:H2'   | 85:28:2521:G:H8   | 1.55                     | 0.70              |
| 66:S4:11:ARG:HA    | 66:S4:28:ALA:HB2  | 1.73                     | 0.70              |
| 19:17:118:GLN:HE22 | 85:28:423:G:H21   | 1.36                     | 0.70              |
| 79:18:58:C:H5''    | 79:18:499:G:H21   | 1.55                     | 0.70              |
| 79:18:1010:G:H2'   | 79:18:1011:A:C8   | 2.27                     | 0.70              |
| 24:cc:93:ASN:HB3   | 24:cc:95:THR:HG23 | 1.74                     | 0.70              |
| 49:F:190:LEU:HB2   | 49:F:223:VAL:HG23 | 1.74                     | 0.70              |
| 79:18:300:U:H2'    | 79:18:301:A:C8    | 2.27                     | 0.70              |
| 85:28:4896:G:H2'   | 85:28:4897:G:H8   | 1.56                     | 0.70              |
| 85:28:1086:C:H2'   | 85:28:1087:A:H8   | 1.57                     | 0.70              |
| 85:28:1344:C:H2'   | 85:28:1345:A:H8   | 1.54                     | 0.69              |
| 66:S4:146:THR:HB   | 79:18:123:G:H1'   | 1.74                     | 0.69              |
| 80:v:464:VAL:HG11  | 80:v:470:VAL:HG11 | 1.74                     | 0.69              |
| 7:L8:234:LYS:HG2   | 7:L8:238:ILE:HD12 | 1.72                     | 0.69              |
| 79:18:126:G:H21    | 79:18:180:G:H21   | 1.40                     | 0.69              |
| 79:18:640:A:H2'    | 79:18:641:A:H8    | 1.55                     | 0.69              |
| 84:ES:3239:G:H2'   | 84:ES:3240:A:H8   | 1.57                     | 0.69              |
| 85:28:1327:C:H2'   | 85:28:1328:G:C8   | 2.27                     | 0.69              |
| 85:28:2607:C:H2'   | 85:28:2608:G:H8   | 1.56                     | 0.69              |
| 84:ES:2946:G:H2'   | 84:ES:2947:G:C8   | 2.28                     | 0.69              |
| 85:28:4761:G:H2'   | 85:28:4762:A:H8   | 1.56                     | 0.69              |
| 57:CC:61:GLN:HB3   | 57:CC:68:TYR:HB2  | 1.75                     | 0.69              |
| 49:F:159:PRO:HD3   | 49:F:325:LEU:HD11 | 1.75                     | 0.69              |
| 79:18:941:C:H2'    | 79:18:942:G:H8    | 1.58                     | 0.69              |
| 85:28:1193:C:H2'   | 85:28:1194:G:C8   | 2.28                     | 0.69              |
| 20:19:162:ARG:HB3  | 79:18:873:G:H5'   | 1.74                     | 0.68              |
| 49:F:57:MET:HE3    | 49:F:74:ILE:HG13  | 1.74                     | 0.68              |
| 80:v:488:PHE:HB3   | 80:v:491:ALA:HB2  | 1.74                     | 0.68              |
| 79:18:75:G:H21     | 79:18:77:A:H5''   | 1.59                     | 0.68              |
| 79:18:122:G:H2'    | 79:18:123:G:H8    | 1.58                     | 0.68              |
| 85:28:710:G:H2'    | 85:28:711:A:H8    | 1.57                     | 0.68              |
| 79:18:1101:U:H2'   | 79:18:1102:G:C8   | 2.28                     | 0.68              |
| 66:S4:31:PRO:HG3   | 66:S4:43:PRO:HG3  | 1.75                     | 0.68              |
| 79:18:389:A:H2'    | 79:18:390:C:C6    | 2.28                     | 0.68              |
| 49:F:57:MET:HE1    | 49:F:73:GLY:HA2   | 1.74                     | 0.68              |
| 79:18:1424:G:H2'   | 79:18:1425:G:H8   | 1.58                     | 0.68              |
| 85:28:1198:G:H2'   | 85:28:1199:G:H8   | 1.57                     | 0.68              |
| 79:18:1010:G:H2'   | 79:18:1011:A:H8   | 1.59                     | 0.68              |
| 64:SS:108:LYS:HD3  | 79:18:53:C:H4'    | 1.75                     | 0.68              |
| 85:28:1197:C:H2'   | 85:28:1198:G:C8   | 2.29                     | 0.68              |
| 47:s:13:TYR:HA     | 47:s:16:LYS:HG2   | 1.75                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:981:A:H2'    | 79:18:982:G:C8     | 2.28                     | 0.67              |
| 85:28:2486:G:H2'   | 85:28:2487:G:H8    | 1.59                     | 0.67              |
| 31:32:90:MET:HG3   | 43:gg:33:LYS:HA    | 1.76                     | 0.67              |
| 45:FF:136:PRO:HG2  | 45:FF:139:TRP:HB2  | 1.76                     | 0.67              |
| 78:L9:12:ILE:HG22  | 78:L9:81:ILE:HD11  | 1.76                     | 0.67              |
| 85:28:2411:C:H2'   | 85:28:2412:A:C8    | 2.30                     | 0.67              |
| 85:28:2485:U:H2'   | 85:28:2486:G:C8    | 2.29                     | 0.67              |
| 85:28:4992:G:H2'   | 85:28:4993:G:H8    | 1.59                     | 0.67              |
| 57:CC:64:TRP:HE1   | 70:S3:23:GLU:HG2   | 1.60                     | 0.67              |
| 79:18:110:U:H2'    | 79:18:111:A:C8     | 2.28                     | 0.67              |
| 85:28:3848:U:H2'   | 85:28:3849:A:H8    | 1.59                     | 0.67              |
| 10:L5:4:VAL:HG11   | 85:28:4247:G:H5''  | 1.76                     | 0.67              |
| 49:F:29:ASN:HD21   | 49:F:334:THR:HA    | 1.59                     | 0.67              |
| 49:F:176:SER:HB3   | 49:F:350:GLN:H     | 1.60                     | 0.67              |
| 85:28:4274:A:H2'   | 85:28:4275:G:C8    | 2.28                     | 0.67              |
| 26:27:103:ASP:HB3  | 26:27:106:LEU:HB2  | 1.75                     | 0.67              |
| 69:YY:113:ARG:HG3  | 69:YY:114:ARG:HG3  | 1.77                     | 0.67              |
| 70:S3:37:VAL:HG12  | 70:S3:50:ILE:HA    | 1.75                     | 0.67              |
| 10:L5:83:LEU:HB3   | 10:L5:88:VAL:HB    | 1.77                     | 0.67              |
| 79:18:874:G:H2'    | 79:18:875:A:H8     | 1.60                     | 0.67              |
| 85:28:1669:A:H4'   | 85:28:1685:G:N2    | 2.09                     | 0.67              |
| 85:28:1683:U:H2'   | 85:28:1684:A:C8    | 2.30                     | 0.67              |
| 85:28:4239:A:H2'   | 85:28:4240:G:C8    | 2.30                     | 0.67              |
| 79:18:1221:G:H2'   | 79:18:1222:G:C8    | 2.28                     | 0.67              |
| 85:28:2015:U:H2'   | 85:28:2016:C:H6    | 1.60                     | 0.67              |
| 11:L6:165:VAL:HG13 | 11:L6:180:GLY:N    | 2.09                     | 0.66              |
| 14:10:87:ILE:HG12  | 14:10:138:ILE:HG12 | 1.78                     | 0.66              |
| 49:F:255:TYR:HB3   | 49:F:301:LEU:HD21  | 1.75                     | 0.66              |
| 79:18:14:C:H2'     | 79:18:15:U:C6      | 2.30                     | 0.66              |
| 85:28:1503:A:H1'   | 85:28:1504:G:C8    | 2.30                     | 0.66              |
| 79:18:1692:U:H2'   | 79:18:1693:G:C8    | 2.30                     | 0.66              |
| 5:58:67:U:H2'      | 5:58:68:G:H8       | 1.59                     | 0.66              |
| 26:27:59:LYS:HA    | 26:27:62:ILE:HB    | 1.77                     | 0.66              |
| 85:28:1512:G:H2'   | 85:28:1513:U:H6    | 1.61                     | 0.66              |
| 85:28:3684:G:H2'   | 85:28:3685:C:C6    | 2.30                     | 0.66              |
| 60:MM:124:THR:HG23 | 60:MM:127:GLY:H    | 1.60                     | 0.66              |
| 85:28:1190:C:H2'   | 85:28:1191:C:C6    | 2.31                     | 0.66              |
| 44:AS:110:MET:HA   | 44:AS:113:MET:HE2  | 1.78                     | 0.66              |
| 75:GG:61:LYS:HB3   | 75:GG:76:LEU:HD12  | 1.76                     | 0.66              |
| 79:18:1705:C:H2'   | 79:18:1706:G:C8    | 2.31                     | 0.66              |
| 85:28:3610:A:H2'   | 85:28:3611:A:H8    | 1.61                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:175:C:H2'    | 85:28:176:G:H8     | 1.61                     | 0.66              |
| 85:28:1414:C:H2'   | 85:28:1415:G:H8    | 1.60                     | 0.66              |
| 85:28:1683:U:H2'   | 85:28:1684:A:H8    | 1.61                     | 0.66              |
| 85:28:1769:G:H2'   | 85:28:1770:A:H8    | 1.60                     | 0.66              |
| 42:ff:17:ARG:HH22  | 85:28:1578:U:H5''  | 1.60                     | 0.66              |
| 58:AA:17:TRP:HA    | 58:AA:305:ASN:HA   | 1.76                     | 0.66              |
| 7:L8:137:ILE:HD11  | 7:L8:149:LYS:HB3   | 1.78                     | 0.65              |
| 50:Q:78:LYS:HG2    | 50:Q:137:VAL:HG23  | 1.78                     | 0.65              |
| 79:18:28:U:H2'     | 79:18:29:G:H8      | 1.60                     | 0.65              |
| 85:28:4239:A:H2'   | 85:28:4240:G:H8    | 1.61                     | 0.65              |
| 53:TT:48:VAL:HG23  | 53:TT:49:LEU:HG    | 1.78                     | 0.65              |
| 80:v:746:LEU:HB2   | 80:v:815:ASP:HB2   | 1.78                     | 0.65              |
| 79:18:1125:C:H2'   | 79:18:1126:G:H8    | 1.61                     | 0.65              |
| 79:18:1198:G:H2'   | 79:18:1199:A:C8    | 2.32                     | 0.65              |
| 85:28:2413:U:H2'   | 85:28:2414:G:H8    | 1.61                     | 0.65              |
| 85:28:2845:A:H61   | 85:28:3843:C:H42   | 1.42                     | 0.65              |
| 85:28:3893:C:H2'   | 85:28:3894:A:H8    | 1.62                     | 0.65              |
| 31:32:104:SER:HB2  | 85:28:2303:C:H5''  | 1.77                     | 0.65              |
| 85:28:1344:C:H2'   | 85:28:1345:A:C8    | 2.32                     | 0.65              |
| 11:L6:165:VAL:HG11 | 11:L6:178:VAL:HG13 | 1.79                     | 0.65              |
| 85:28:1093:C:H2'   | 85:28:1094:G:H8    | 1.62                     | 0.65              |
| 63:RR:24:ASP:HB3   | 63:RR:27:TYR:HB3   | 1.79                     | 0.65              |
| 68:S7:144:ILE:HB   | 72:WX:52:ILE:HB    | 1.79                     | 0.65              |
| 85:28:1332:C:H2'   | 85:28:1333:A:C8    | 2.30                     | 0.65              |
| 85:28:3721:U:H2'   | 85:28:3722:G:H8    | 1.62                     | 0.65              |
| 17:15:14:LYS:HE2   | 85:28:280:G:H5''   | 1.79                     | 0.64              |
| 36:37:33:THR:HG22  | 36:37:40:PRO:HG2   | 1.79                     | 0.64              |
| 84:ES:2943:C:H2'   | 84:ES:2944:G:H8    | 1.62                     | 0.64              |
| 85:28:4260:U:H2'   | 85:28:4261:C:C6    | 2.32                     | 0.64              |
| 85:28:3893:C:H2'   | 85:28:3894:A:C8    | 2.32                     | 0.64              |
| 16:14:40:GLY:HA3   | 16:14:45:VAL:HB    | 1.79                     | 0.64              |
| 85:28:983:U:H2'    | 85:28:984:C:C6     | 2.33                     | 0.64              |
| 24:cc:83:THR:HG21  | 85:28:2434:G:H4'   | 1.79                     | 0.64              |
| 50:Q:178:ARG:HA    | 50:Q:184:ARG:HB3   | 1.78                     | 0.64              |
| 79:18:152:U:H2'    | 79:18:153:G:C8     | 2.32                     | 0.64              |
| 85:28:3598:C:H2'   | 85:28:3599:A:C8    | 2.33                     | 0.64              |
| 79:18:894:G:H2'    | 79:18:895:G:C8     | 2.31                     | 0.64              |
| 79:18:1125:C:H2'   | 79:18:1126:G:C8    | 2.33                     | 0.64              |
| 79:18:1854:U:H2'   | 79:18:1855:G:H8    | 1.62                     | 0.64              |
| 85:28:3911:C:H2'   | 85:28:3912:U:H6    | 1.63                     | 0.64              |
| 5:58:19:C:H2'      | 5:58:20:A:C8       | 2.33                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:15:67:ARG:HD2  | 85:28:2458:C:H5'' | 1.80                     | 0.64              |
| 79:18:121:U:H2'   | 79:18:122:G:C8    | 2.33                     | 0.64              |
| 85:28:3598:C:H2'  | 85:28:3599:A:H8   | 1.63                     | 0.64              |
| 49:F:333:ILE:HG23 | 49:F:334:THR:HG23 | 1.80                     | 0.64              |
| 67:S9:136:ARG:HE  | 67:S9:139:LYS:HA  | 1.63                     | 0.64              |
| 79:18:374:G:H2'   | 79:18:375:U:C6    | 2.33                     | 0.64              |
| 85:28:1358:G:N2   | 85:28:1381:U:O4   | 2.31                     | 0.64              |
| 79:18:389:A:H2'   | 79:18:390:C:H6    | 1.62                     | 0.63              |
| 79:18:1217:A:H2'  | 79:18:1218:C:C6   | 2.33                     | 0.63              |
| 79:18:1845:A:H2'  | 79:18:1846:G:C8   | 2.32                     | 0.63              |
| 85:28:1942:A:H2'  | 85:28:1943:A:H8   | 1.63                     | 0.63              |
| 1:BB:34:MET:HE3   | 1:BB:154:LEU:HD11 | 1.79                     | 0.63              |
| 5:58:19:C:H2'     | 5:58:20:A:H8      | 1.63                     | 0.63              |
| 78:L9:94:SER:HB3  | 78:L9:142:ASP:HB3 | 1.80                     | 0.63              |
| 8:L3:13:SER:HB2   | 85:28:4622:A:H4'  | 1.80                     | 0.63              |
| 68:S7:143:ARG:HB2 | 68:S7:155:LYS:HB2 | 1.79                     | 0.63              |
| 79:18:928:G:H1    | 79:18:1013:U:H3   | 1.46                     | 0.63              |
| 85:28:2480:G:H2'  | 85:28:2481:G:H8   | 1.63                     | 0.63              |
| 85:28:3619:G:H22  | 85:28:3624:A:H1'  | 1.63                     | 0.63              |
| 85:28:3917:A:H2'  | 85:28:3918:G:H8   | 1.63                     | 0.63              |
| 27:dd:36:GLY:HA2  | 27:dd:39:HIS:HB2  | 1.79                     | 0.63              |
| 84:ES:2945:C:H2'  | 84:ES:2946:G:H8   | 1.63                     | 0.63              |
| 49:F:118:ILE:HG13 | 49:F:195:ILE:HG22 | 1.81                     | 0.63              |
| 85:28:1402:C:H2'  | 85:28:1403:G:C8   | 2.34                     | 0.63              |
| 2:S2:167:ARG:HB2  | 2:S2:177:PRO:HB2  | 1.81                     | 0.63              |
| 23:22:28:PRO:HB2  | 23:22:34:MET:HG2  | 1.79                     | 0.63              |
| 70:S3:35:SER:HA   | 70:S3:99:ILE:HG13 | 1.81                     | 0.63              |
| 79:18:454:U:H2'   | 79:18:455:A:H8    | 1.64                     | 0.63              |
| 79:18:804:U:H2'   | 79:18:805:U:C6    | 2.33                     | 0.63              |
| 85:28:4504:C:H2'  | 85:28:4505:C:C6   | 2.33                     | 0.63              |
| 72:WX:6:VAL:HG12  | 72:WX:34:ILE:HD11 | 1.81                     | 0.63              |
| 85:28:4774:C:H2'  | 85:28:4775:C:C6   | 2.34                     | 0.63              |
| 79:18:677:G:N2    | 79:18:1028:A:H62  | 1.96                     | 0.63              |
| 80:v:119:LEU:HD21 | 80:v:146:ALA:HA   | 1.79                     | 0.63              |
| 84:ES:2943:C:H2'  | 84:ES:2944:G:C8   | 2.34                     | 0.63              |
| 79:18:106:C:H2'   | 79:18:107:A:H8    | 1.62                     | 0.62              |
| 79:18:729:C:H2'   | 79:18:730:C:C6    | 2.34                     | 0.62              |
| 79:18:940:U:H3    | 79:18:1002:U:H3   | 1.45                     | 0.62              |
| 85:28:1503:A:H4'  | 85:28:1504:G:H5'  | 1.81                     | 0.62              |
| 85:28:4095:G:H22  | 85:28:4113:U:H3   | 1.47                     | 0.62              |
| 85:28:517:C:H2'   | 85:28:518:G:H8    | 1.63                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:13:62:PRO:HG3   | 85:28:74:G:H1'    | 1.81                     | 0.62              |
| 70:S3:70:THR:HG22  | 70:S3:86:LEU:HD13 | 1.80                     | 0.62              |
| 85:28:3736:A:H2'   | 85:28:3737:A:H8   | 1.63                     | 0.62              |
| 49:F:187:SER:HB3   | 49:F:201:ILE:HB   | 1.81                     | 0.62              |
| 4:DD:126:VAL:HG22  | 4:DD:145:VAL:HG22 | 1.81                     | 0.62              |
| 79:18:878:G:C2     | 79:18:879:C:H1'   | 2.35                     | 0.62              |
| 85:28:3736:A:H2'   | 85:28:3737:A:C8   | 2.34                     | 0.62              |
| 85:28:4680:G:H2'   | 85:28:4681:A:C8   | 2.35                     | 0.62              |
| 79:18:1714:U:H2'   | 79:18:1715:A:C8   | 2.34                     | 0.62              |
| 15:13:8:MET:HG3    | 50:Q:166:TYR:HB3  | 1.82                     | 0.62              |
| 17:15:104:GLU:HA   | 17:15:160:GLU:HG3 | 1.82                     | 0.62              |
| 68:S7:46:THR:HG23  | 68:S7:65:PRO:HG3  | 1.82                     | 0.62              |
| 85:28:1382:G:H2'   | 85:28:1383:G:H8   | 1.65                     | 0.62              |
| 85:28:1984:A:H2'   | 85:28:2011:C:H5'  | 1.80                     | 0.62              |
| 85:28:3910:C:H2'   | 85:28:3911:C:H6   | 1.65                     | 0.62              |
| 2:S2:102:LEU:HD21  | 2:S2:130:ILE:HD11 | 1.81                     | 0.62              |
| 9:L4:60:HIS:HE1    | 9:L4:100:ARG:HD3  | 1.64                     | 0.62              |
| 55:WW:12:ALA:HA    | 55:WW:34:PHE:HA   | 1.81                     | 0.62              |
| 75:GG:101:GLY:HA3  | 75:GG:134:PRO:HG2 | 1.82                     | 0.62              |
| 85:28:233:U:H2'    | 85:28:234:G:C8    | 2.35                     | 0.62              |
| 85:28:1307:A:H2'   | 85:28:1308:C:H6   | 1.65                     | 0.62              |
| 12:L7:46:ARG:NH1   | 85:28:976:C:H5''  | 2.15                     | 0.61              |
| 63:RR:91:LEU:HB3   | 69:YY:82:VAL:HG21 | 1.82                     | 0.61              |
| 79:18:1128:C:H2'   | 79:18:1129:G:H8   | 1.63                     | 0.61              |
| 85:28:2745:A:H2'   | 85:28:2746:A:C8   | 2.34                     | 0.61              |
| 85:28:5030:U:H2'   | 85:28:5031:G:H8   | 1.65                     | 0.61              |
| 44:AS:86:LEU:HB3   | 44:AS:98:THR:HB   | 1.81                     | 0.61              |
| 79:18:1845:A:H2'   | 79:18:1846:G:H8   | 1.65                     | 0.61              |
| 84:ES:3244:U:H2'   | 84:ES:3245:G:H8   | 1.63                     | 0.61              |
| 85:28:1093:C:H2'   | 85:28:1094:G:C8   | 2.35                     | 0.61              |
| 85:28:1073:G:H1    | 85:28:1238:A:H2   | 1.47                     | 0.61              |
| 85:28:1326:A:H2'   | 85:28:1327:C:C6   | 2.36                     | 0.61              |
| 80:v:72:SER:HB3    | 80:v:106:PRO:HD3  | 1.82                     | 0.61              |
| 85:28:469:C:H2'    | 85:28:470:A:H8    | 1.65                     | 0.61              |
| 85:28:1341:U:H2'   | 85:28:1342:A:H8   | 1.64                     | 0.61              |
| 58:AA:197:THR:HG21 | 58:AA:238:ALA:HA  | 1.82                     | 0.61              |
| 59:OO:40:ILE:HD11  | 59:OO:53:PRO:HG3  | 1.83                     | 0.61              |
| 79:18:441:C:H41    | 79:18:448:A:H1'   | 1.66                     | 0.61              |
| 85:28:651:C:H2'    | 85:28:652:G:H8    | 1.64                     | 0.61              |
| 85:28:1857:C:H2'   | 85:28:1858:A:C8   | 2.33                     | 0.61              |
| 85:28:3664:G:H2'   | 85:28:3665:G:H8   | 1.66                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:28:3848:U:H2'   | 85:28:3849:A:C8   | 2.35                     | 0.61              |
| 25:26:30:MET:HB3   | 25:26:101:PRO:HG2 | 1.83                     | 0.61              |
| 79:18:874:G:H2'    | 79:18:875:A:C8    | 2.36                     | 0.61              |
| 83:A:34:MET:HB3    | 83:A:42:ARG:HG3   | 1.81                     | 0.61              |
| 85:28:93:G:H2'     | 85:28:94:A:C8     | 2.36                     | 0.61              |
| 85:28:4993:G:H2'   | 85:28:4994:G:H8   | 1.66                     | 0.61              |
| 85:28:440:U:H2'    | 85:28:441:G:H8    | 1.65                     | 0.61              |
| 85:28:2607:C:H2'   | 85:28:2608:G:C8   | 2.35                     | 0.61              |
| 28:29:3:LYS:HD3    | 85:28:4194:U:H3'  | 1.83                     | 0.61              |
| 85:28:1964:A:C8    | 85:28:1965:G:C8   | 2.89                     | 0.61              |
| 85:28:3861:A:H2'   | 85:28:3862:A:H8   | 1.64                     | 0.61              |
| 74:W:24:THR:HG23   | 86:23:99:GLU:HB3  | 1.82                     | 0.61              |
| 79:18:418:A:H3'    | 79:18:419:G:H8    | 1.64                     | 0.61              |
| 85:28:1358:G:C2    | 85:28:1381:U:O4   | 2.53                     | 0.61              |
| 85:28:1749:A:H2'   | 85:28:1750:G:H8   | 1.66                     | 0.61              |
| 85:28:4448:G:H5''  | 85:28:4449:A:H5'' | 1.83                     | 0.61              |
| 54:S5:39:ILE:HG23  | 54:S5:68:ILE:HG21 | 1.83                     | 0.61              |
| 68:S7:157:HIS:HB3  | 68:S7:190:PRO:HG3 | 1.83                     | 0.60              |
| 79:18:382:C:H2'    | 79:18:383:G:H8    | 1.65                     | 0.60              |
| 79:18:952:G:H2'    | 79:18:953:C:C6    | 2.35                     | 0.60              |
| 85:28:3910:C:H2'   | 85:28:3911:C:C6   | 2.36                     | 0.60              |
| 79:18:1797:U:H2'   | 79:18:1798:C:C6   | 2.37                     | 0.60              |
| 79:18:556:U:H2'    | 79:18:557:U:H6    | 1.66                     | 0.60              |
| 80:v:666:THR:HG22  | 80:v:706:ASP:HA   | 1.83                     | 0.60              |
| 85:28:1338:G:H4'   | 85:28:1339:U:H6   | 1.66                     | 0.60              |
| 85:28:4637:G:H2'   | 85:28:4638:U:C6   | 2.37                     | 0.60              |
| 48:t:80:LEU:HA     | 48:t:83:LYS:HG2   | 1.82                     | 0.60              |
| 57:CC:64:TRP:NE1   | 70:S3:23:GLU:HG2  | 2.15                     | 0.60              |
| 73:S8:110:ARG:HG3  | 73:S8:121:LEU:HB3 | 1.83                     | 0.60              |
| 27:dd:21:ARG:HG3   | 85:28:2282:A:H4'  | 1.82                     | 0.60              |
| 61:LL:84:LEU:HB2   | 61:LL:87:GLN:HG2  | 1.84                     | 0.60              |
| 85:28:1307:A:H2'   | 85:28:1308:C:C6   | 2.35                     | 0.60              |
| 29:30:105:ILE:HD12 | 29:30:106:ARG:HG3 | 1.82                     | 0.60              |
| 44:AS:189:ILE:HB   | 44:AS:190:PRO:HD3 | 1.82                     | 0.60              |
| 79:18:1004:U:H2'   | 79:18:1005:G:C8   | 2.34                     | 0.60              |
| 4:DD:77:VAL:HA     | 4:DD:88:ILE:HG22  | 1.84                     | 0.60              |
| 19:17:114:ILE:HD11 | 19:17:117:ILE:HB  | 1.84                     | 0.60              |
| 79:18:381:C:H2'    | 79:18:382:C:C6    | 2.37                     | 0.60              |
| 84:ES:3238:C:H2'   | 84:ES:3239:G:C8   | 2.36                     | 0.60              |
| 85:28:1169:G:H2'   | 85:28:1170:G:C8   | 2.36                     | 0.60              |
| 85:28:1436:C:H42   | 85:28:1448:G:H1   | 1.49                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:S2:190:SER:HB2   | 79:18:1143:A:H5'   | 1.83                     | 0.60              |
| 44:AS:141:GLY:HA2  | 44:AS:210:VAL:HG22 | 1.84                     | 0.60              |
| 76:UU:12:LYS:HG3   | 76:UU:15:ARG:HB2   | 1.82                     | 0.60              |
| 85:28:4970:C:C2    | 85:28:4971:A:C8    | 2.89                     | 0.60              |
| 5:58:148:A:H2'     | 5:58:149:G:C8      | 2.36                     | 0.60              |
| 8:L3:240:LEU:HB3   | 8:L3:244:THR:HG21  | 1.84                     | 0.60              |
| 65:S6:14:LYS:HB2   | 65:S6:124:LEU:HD11 | 1.84                     | 0.60              |
| 67:S9:164:PRO:HG3  | 79:18:561:A:H5''   | 1.83                     | 0.60              |
| 79:18:318:A:H3'    | 79:18:319:C:H5''   | 1.84                     | 0.60              |
| 85:28:1461:C:H2'   | 85:28:1462:A:C8    | 2.34                     | 0.60              |
| 85:28:1204:C:H2'   | 85:28:1205:G:H8    | 1.66                     | 0.60              |
| 13:aa:139:VAL:HG11 | 13:aa:238:LYS:HD2  | 1.84                     | 0.59              |
| 27:dd:38:MET:HA    | 27:dd:42:ARG:HE    | 1.67                     | 0.59              |
| 79:18:115:U:H2'    | 79:18:116:U:C6     | 2.37                     | 0.59              |
| 14:10:61:SER:HA    | 14:10:126:VAL:HG23 | 1.83                     | 0.59              |
| 16:14:96:GLU:HA    | 16:14:99:GLU:HG2   | 1.85                     | 0.59              |
| 44:AS:91:VAL:HG12  | 44:AS:93:GLY:H     | 1.67                     | 0.59              |
| 79:18:912:C:H3'    | 79:18:913:A:H5''   | 1.83                     | 0.59              |
| 85:28:1512:G:H2'   | 85:28:1513:U:C6    | 2.37                     | 0.59              |
| 5:58:65:A:H2'      | 5:58:66:A:H8       | 1.67                     | 0.59              |
| 8:L3:56:ILE:O      | 8:L3:73:VAL:HA     | 2.02                     | 0.59              |
| 17:15:75:VAL:HG23  | 17:15:78:GLY:HA2   | 1.85                     | 0.59              |
| 79:18:107:A:H2'    | 79:18:108:G:C8     | 2.37                     | 0.59              |
| 85:28:2640:G:H2'   | 85:28:2641:A:H8    | 1.66                     | 0.59              |
| 19:17:118:GLN:NE2  | 85:28:423:G:H21    | 2.00                     | 0.59              |
| 79:18:1736:G:H2'   | 79:18:1737:G:C8    | 2.38                     | 0.59              |
| 3:PP:32:ILE:HD12   | 3:PP:55:ILE:HB     | 1.83                     | 0.59              |
| 53:TT:71:ALA:HB1   | 54:S5:167:LYS:HA   | 1.84                     | 0.59              |
| 78:L9:107:GLU:HG3  | 78:L9:110:SER:HB2  | 1.83                     | 0.59              |
| 65:S6:50:VAL:HG12  | 65:S6:113:ILE:HD13 | 1.85                     | 0.59              |
| 66:S4:162:ILE:HG22 | 66:S4:169:ILE:HA   | 1.85                     | 0.59              |
| 79:18:16:G:H2'     | 79:18:17:C:C6      | 2.38                     | 0.59              |
| 79:18:556:U:H2'    | 79:18:557:U:C6     | 2.37                     | 0.59              |
| 83:A:22:LEU:HA     | 83:A:25:LEU:HD23   | 1.85                     | 0.59              |
| 85:28:1317:U:H2'   | 85:28:1318:C:C6    | 2.37                     | 0.59              |
| 85:28:4344:U:H2'   | 85:28:4345:C:C6    | 2.38                     | 0.59              |
| 74:W:104:GLN:O     | 74:W:107:GLN:HG3   | 2.02                     | 0.59              |
| 79:18:1007:C:H2'   | 79:18:1008:A:H8    | 1.68                     | 0.59              |
| 79:18:1008:A:H2'   | 79:18:1009:A:C8    | 2.38                     | 0.59              |
| 85:28:4091:G:H2'   | 85:28:4092:G:H8    | 1.67                     | 0.59              |
| 26:27:54:THR:H     | 26:27:57:MET:HE2   | 1.67                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:1714:U:H2'   | 79:18:1715:A:H8    | 1.68                     | 0.59              |
| 8:L3:224:LYS:HG2   | 8:L3:340:THR:HB    | 1.85                     | 0.59              |
| 12:L7:227:VAL:HA   | 21:20:39:VAL:HG12  | 1.85                     | 0.59              |
| 71:RS:28:PHE:HA    | 71:RS:55:THR:HG21  | 1.85                     | 0.59              |
| 79:18:1008:A:H2'   | 79:18:1009:A:H8    | 1.67                     | 0.59              |
| 80:v:266:PHE:HB2   | 80:v:288:THR:HG22  | 1.83                     | 0.59              |
| 85:28:2409:U:H4'   | 85:28:2428:A:H4'   | 1.85                     | 0.59              |
| 85:28:4458:C:H2'   | 85:28:4459:U:C6    | 2.38                     | 0.59              |
| 79:18:1513:C:H2'   | 79:18:1514:G:H8    | 1.68                     | 0.59              |
| 85:28:1298:C:H2'   | 85:28:1299:G:H8    | 1.67                     | 0.59              |
| 85:28:1524:A:H61   | 85:28:1651:G:H22   | 1.51                     | 0.59              |
| 60:MM:71:GLY:HA3   | 79:18:1562:C:H5''  | 1.84                     | 0.58              |
| 85:28:1088:C:H2'   | 85:28:1089:G:H8    | 1.67                     | 0.58              |
| 85:28:4319:C:H2'   | 85:28:4320:G:C8    | 2.37                     | 0.58              |
| 73:S8:29:LEU:HD13  | 79:18:448:A:H62    | 1.67                     | 0.58              |
| 78:L9:120:GLU:HG2  | 85:28:4611:A:H2    | 1.69                     | 0.58              |
| 79:18:112:U:H2'    | 79:18:115:U:H5     | 1.68                     | 0.58              |
| 80:v:692:LEU:HD11  | 80:v:738:PRO:HB2   | 1.84                     | 0.58              |
| 85:28:2413:U:H2'   | 85:28:2414:G:C8    | 2.38                     | 0.58              |
| 85:28:4080:C:H2'   | 85:28:4081:G:H8    | 1.69                     | 0.58              |
| 8:L3:56:ILE:HD12   | 8:L3:365:LEU:HD22  | 1.86                     | 0.58              |
| 15:13:59:VAL:HG22  | 85:28:74:G:H5'     | 1.86                     | 0.58              |
| 79:18:121:U:H2'    | 79:18:122:G:H8     | 1.68                     | 0.58              |
| 79:18:1545:A:H2'   | 79:18:1546:G:C8    | 2.37                     | 0.58              |
| 85:28:300:A:H2'    | 85:28:301:G:H8     | 1.68                     | 0.58              |
| 85:28:713:C:H2'    | 85:28:714:G:H8     | 1.68                     | 0.58              |
| 85:28:907:C:H2'    | 85:28:908:G:H8     | 1.68                     | 0.58              |
| 85:28:1893:C:H1'   | 85:28:1937:C:O2    | 2.03                     | 0.58              |
| 85:28:2870:A:H2'   | 85:28:2871:A:H8    | 1.68                     | 0.58              |
| 79:18:1382:A:H2'   | 79:18:1383:A:C8    | 2.37                     | 0.58              |
| 85:28:2528:G:H4'   | 85:28:2783:A:H4'   | 1.86                     | 0.58              |
| 50:Q:59:PRO:HG3    | 50:Q:143:ARG:HA    | 1.85                     | 0.58              |
| 84:ES:2945:C:H2'   | 84:ES:2946:G:C8    | 2.37                     | 0.58              |
| 4:DD:93:LEU:HB3    | 4:DD:102:PHE:HB3   | 1.86                     | 0.58              |
| 10:L5:64:ILE:HG13  | 10:L5:105:LEU:HD21 | 1.85                     | 0.58              |
| 11:L6:156:LEU:HD11 | 11:L6:198:ILE:HG13 | 1.85                     | 0.58              |
| 18:bb:185:VAL:HG22 | 18:bb:188:LYS:HB3  | 1.85                     | 0.58              |
| 49:F:80:ILE:HG12   | 49:F:108:ILE:HG12  | 1.85                     | 0.58              |
| 79:18:314:U:H2'    | 79:18:315:C:C6     | 2.39                     | 0.58              |
| 13:aa:136:PHE:HB3  | 13:aa:212:HIS:HB2  | 1.85                     | 0.58              |
| 79:18:514:U:H2'    | 79:18:515:G:O4'    | 2.03                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:1280:G:H2'   | 79:18:1281:G:C8    | 2.39                     | 0.58              |
| 85:28:679:C:H2'    | 85:28:680:G:H8     | 1.69                     | 0.58              |
| 76:UU:43:ASN:HA    | 76:UU:66:LYS:HA    | 1.84                     | 0.58              |
| 79:18:93:U:H2'     | 79:18:94:G:O4'     | 2.04                     | 0.58              |
| 85:28:667:A:H5''   | 85:28:668:C:H5     | 1.69                     | 0.58              |
| 85:28:3911:C:H2'   | 85:28:3912:U:C6    | 2.38                     | 0.58              |
| 85:28:3916:G:H2'   | 85:28:3917:A:C8    | 2.38                     | 0.58              |
| 67:S9:172:ARG:HH12 | 79:18:586:G:H3'    | 1.69                     | 0.58              |
| 79:18:418:A:H3'    | 79:18:419:G:C8     | 2.39                     | 0.58              |
| 79:18:1777:G:H2'   | 79:18:1778:C:H6    | 1.68                     | 0.58              |
| 72:WX:88:LYS:HE2   | 79:18:419:G:H4'    | 1.86                     | 0.58              |
| 79:18:1201:U:H2'   | 79:18:1202:U:C6    | 2.39                     | 0.58              |
| 84:ES:3244:U:H2'   | 84:ES:3245:G:C8    | 2.39                     | 0.58              |
| 85:28:3796:U:H2'   | 85:28:3797:C:C6    | 2.38                     | 0.58              |
| 85:28:4537:C:H2'   | 85:28:4538:G:C8    | 2.37                     | 0.58              |
| 85:28:4736:C:H2'   | 85:28:4737:G:H8    | 1.69                     | 0.58              |
| 86:23:9:SER:HB2    | 86:23:128:LEU:HD12 | 1.86                     | 0.58              |
| 56:II:12:VAL:HG21  | 56:II:91:ALA:HA    | 1.86                     | 0.57              |
| 65:S6:2:LYS:HB3    | 65:S6:15:LEU:HD11  | 1.86                     | 0.57              |
| 67:S9:108:ARG:HA   | 67:S9:113:GLN:HE21 | 1.69                     | 0.57              |
| 79:18:79:A:H3'     | 79:18:80:G:H8      | 1.69                     | 0.57              |
| 85:28:2521:G:H2'   | 85:28:2522:G:H8    | 1.68                     | 0.57              |
| 85:28:3684:G:H2'   | 85:28:3685:C:H6    | 1.68                     | 0.57              |
| 2:S2:78:LEU:HD23   | 2:S2:78:LEU:H      | 1.69                     | 0.57              |
| 25:26:11:ARG:HG3   | 85:28:229:G:H5''   | 1.85                     | 0.57              |
| 58:AA:128:THR:HG22 | 58:AA:143:GLN:HA   | 1.86                     | 0.57              |
| 68:S7:51:ILE:HD11  | 68:S7:176:VAL:HG22 | 1.85                     | 0.57              |
| 79:18:1494:U:H4'   | 79:18:1495:G:H5''  | 1.86                     | 0.57              |
| 79:18:1801:A:H2'   | 79:18:1802:C:H6    | 1.67                     | 0.57              |
| 85:28:4577:U:H2'   | 85:28:4578:G:H8    | 1.69                     | 0.57              |
| 49:F:202:ILE:HG12  | 49:F:205:PRO:HB3   | 1.86                     | 0.57              |
| 49:F:351:ASP:HB3   | 49:F:354:LEU:HD21  | 1.86                     | 0.57              |
| 58:AA:10:THR:HB    | 58:AA:306:LEU:HD11 | 1.85                     | 0.57              |
| 80:v:649:ILE:HG22  | 80:v:663:THR:HG22  | 1.86                     | 0.57              |
| 85:28:2566:G:H2'   | 85:28:2567:G:C8    | 2.39                     | 0.57              |
| 85:28:4232:U:H4'   | 85:28:4233:A:O5'   | 2.04                     | 0.57              |
| 85:28:5006:U:H4'   | 85:28:5007:A:H5'   | 1.86                     | 0.57              |
| 5:58:153:C:H2'     | 5:58:154:G:H8      | 1.70                     | 0.57              |
| 29:30:38:ILE:HG21  | 29:30:63:TYR:HB3   | 1.85                     | 0.57              |
| 79:18:1130:G:C8    | 79:18:1131:G:C8    | 2.93                     | 0.57              |
| 79:18:1382:A:H2'   | 79:18:1383:A:H8    | 1.69                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:28:3932:U:H2'   | 85:28:3933:G:H8   | 1.69                     | 0.57              |
| 85:28:4260:U:H2'   | 85:28:4261:C:H6   | 1.68                     | 0.57              |
| 47:s:180:ILE:HG12  | 47:s:182:PRO:HD3  | 1.85                     | 0.57              |
| 79:18:643:A:H4'    | 79:18:644:G:H5'   | 1.86                     | 0.57              |
| 85:28:2373:C:H2'   | 85:28:2374:A:H8   | 1.68                     | 0.57              |
| 85:28:2706:G:H2'   | 85:28:2708:U:H5'  | 1.85                     | 0.57              |
| 9:L4:343:GLN:HG2   | 85:28:724:C:H1'   | 1.85                     | 0.57              |
| 26:27:46:ILE:HD11  | 26:27:49:TYR:HA   | 1.86                     | 0.57              |
| 73:S8:129:LEU:HG   | 73:S8:131:PRO:HD2 | 1.86                     | 0.57              |
| 79:18:1737:G:H1    | 79:18:1797:U:H3   | 1.53                     | 0.57              |
| 79:18:1801:A:H2'   | 79:18:1802:C:C6   | 2.40                     | 0.57              |
| 80:v:820:LEU:HD12  | 80:v:821:PRO:HD2  | 1.86                     | 0.57              |
| 85:28:673:C:H2'    | 85:28:674:G:H8    | 1.69                     | 0.57              |
| 85:28:1505:C:H2'   | 85:28:1506:G:H8   | 1.69                     | 0.57              |
| 2:S2:166:ARG:HB3   | 2:S2:247:THR:HB   | 1.86                     | 0.57              |
| 9:L4:190:ARG:HD2   | 9:L4:194:GLY:HA3  | 1.87                     | 0.57              |
| 32:ee:54:LYS:HE2   | 85:28:4748:U:H5'' | 1.87                     | 0.57              |
| 44:AS:25:PHE:HA    | 44:AS:28:LYS:HG2  | 1.87                     | 0.57              |
| 79:18:1637:A:H4'   | 79:18:1638:G:O5'  | 2.04                     | 0.57              |
| 85:28:2493:G:H2'   | 85:28:2494:U:H6   | 1.69                     | 0.57              |
| 85:28:4577:U:H2'   | 85:28:4578:G:C8   | 2.39                     | 0.57              |
| 18:bb:60:LYS:HE2   | 85:28:2046:G:H5'  | 1.87                     | 0.57              |
| 79:18:931:C:H2'    | 79:18:932:G:C8    | 2.39                     | 0.57              |
| 85:28:2568:C:H2'   | 85:28:2569:G:C8   | 2.40                     | 0.57              |
| 85:28:2568:C:H2'   | 85:28:2569:G:H8   | 1.69                     | 0.57              |
| 60:MM:42:HIS:HB3   | 60:MM:93:SER:HB3  | 1.85                     | 0.57              |
| 75:GG:31:CYS:HB3   | 75:GG:44:VAL:HG22 | 1.87                     | 0.57              |
| 79:18:942:G:H2'    | 79:18:943:U:C6    | 2.40                     | 0.57              |
| 85:28:163:A:H2'    | 85:28:164:G:H8    | 1.68                     | 0.57              |
| 85:28:922:C:H2'    | 85:28:922(A):G:H8 | 1.70                     | 0.57              |
| 85:28:4173:G:H2'   | 85:28:4174:U:C6   | 2.40                     | 0.57              |
| 15:13:62:PRO:O     | 85:28:71:C:H1'    | 2.05                     | 0.57              |
| 48:t:146:ARG:HB3   | 48:t:148:PRO:HD2  | 1.86                     | 0.57              |
| 65:S6:121:ILE:HD12 | 65:S6:122:PRO:HD2 | 1.85                     | 0.57              |
| 68:S7:87:PHE:HB3   | 68:S7:90:LYS:HD3  | 1.86                     | 0.57              |
| 79:18:528:A:H2'    | 79:18:529:A:H8    | 1.69                     | 0.57              |
| 79:18:1337:C:H2'   | 79:18:1338:G:H8   | 1.69                     | 0.57              |
| 79:18:1347:U:H2'   | 79:18:1348:G:N3   | 2.19                     | 0.57              |
| 79:18:1633:A:H2'   | 79:18:1634:A:C8   | 2.40                     | 0.57              |
| 85:28:134:G:H4'    | 85:28:135:G:O5'   | 2.05                     | 0.57              |
| 85:28:3845:A:H2'   | 85:28:3846:C:H6   | 1.70                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:4471:U:H2'   | 85:28:4472:G:H8    | 1.70                     | 0.57              |
| 9:L4:78:ARG:HB3    | 9:L4:88:GLY:HA2    | 1.85                     | 0.56              |
| 11:L6:108:ARG:HD2  | 85:28:470:A:H1'    | 1.87                     | 0.56              |
| 85:28:3648:A:H1'   | 85:28:3785:A:N6    | 2.20                     | 0.56              |
| 85:28:4174:U:H2'   | 85:28:4175:G:H8    | 1.70                     | 0.56              |
| 38:39:24:PRO:HG2   | 38:39:27:ILE:HG12  | 1.87                     | 0.56              |
| 63:RR:51:VAL:HG22  | 63:RR:70:VAL:HG11  | 1.87                     | 0.56              |
| 78:L9:114:ILE:HB   | 78:L9:124:ARG:HG3  | 1.86                     | 0.56              |
| 79:18:219:U:H2'    | 79:18:220:U:C6     | 2.40                     | 0.56              |
| 85:28:423:G:H2'    | 85:28:424:U:C6     | 2.40                     | 0.56              |
| 85:28:1329:G:C2    | 85:28:3865:A:H1'   | 2.39                     | 0.56              |
| 85:28:1341:U:H2'   | 85:28:1342:A:C8    | 2.41                     | 0.56              |
| 12:L7:104:VAL:HG13 | 12:L7:135:VAL:HG12 | 1.87                     | 0.56              |
| 68:S7:144:ILE:HG12 | 68:S7:154:ILE:HG13 | 1.87                     | 0.56              |
| 74:W:52:THR:HG23   | 74:W:55:TYR:H      | 1.70                     | 0.56              |
| 79:18:1854:U:H2'   | 79:18:1855:G:C8    | 2.41                     | 0.56              |
| 85:28:2521:G:H5'   | 85:28:2640:G:H1'   | 1.88                     | 0.56              |
| 85:28:3727:A:H2'   | 85:28:3728:A:C8    | 2.40                     | 0.56              |
| 85:28:4344:U:H2'   | 85:28:4345:C:H6    | 1.70                     | 0.56              |
| 6:6:49:A:H5''      | 10:L5:224:SER:HB3  | 1.88                     | 0.56              |
| 6:6:110:G:H2'      | 6:6:111:C:C6       | 2.40                     | 0.56              |
| 54:S5:153:LEU:HB3  | 54:S5:189:ALA:HA   | 1.87                     | 0.56              |
| 79:18:963:A:H2'    | 79:18:964:A:C8     | 2.39                     | 0.56              |
| 85:28:710:G:H2'    | 85:28:711:A:C8     | 2.38                     | 0.56              |
| 85:28:2496:G:H2'   | 85:28:2497:C:C6    | 2.41                     | 0.56              |
| 2:S2:86:LEU:HD13   | 2:S2:87:PRO:HD2    | 1.87                     | 0.56              |
| 5:58:106:G:H4'     | 5:58:137:A:H5'     | 1.87                     | 0.56              |
| 32:ee:7:CYS:HB2    | 32:ee:103:VAL:HG23 | 1.86                     | 0.56              |
| 53:TT:49:LEU:HB3   | 61:LL:5:ILE:HG12   | 1.87                     | 0.56              |
| 85:28:478:G:H2'    | 85:28:479:G:H8     | 1.71                     | 0.56              |
| 85:28:1538:U:H2'   | 85:28:1539:G:C8    | 2.35                     | 0.56              |
| 85:28:4635:A:H2    | 85:28:4663:G:H21   | 1.52                     | 0.56              |
| 21:20:13:VAL:HG23  | 21:20:62:VAL:HB    | 1.87                     | 0.56              |
| 48:t:85:LEU:HD21   | 48:t:104:ILE:HB    | 1.86                     | 0.56              |
| 56:II:103:ALA:O    | 56:II:106:LYS:HG3  | 2.06                     | 0.56              |
| 58:AA:172:LYS:HA   | 58:AA:195:LEU:HG   | 1.88                     | 0.56              |
| 79:18:1692:U:H2'   | 79:18:1693:G:H8    | 1.68                     | 0.56              |
| 85:28:265:C:H4'    | 85:28:266:C:OP2    | 2.05                     | 0.56              |
| 85:28:1504:G:H2'   | 85:28:1505:C:C6    | 2.40                     | 0.56              |
| 85:28:1749:A:H2'   | 85:28:1750:G:C8    | 2.40                     | 0.56              |
| 85:28:2844:A:O2'   | 85:28:4631:G:H4'   | 2.05                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:28:3606:U:H2'  | 85:28:3607:U:C6    | 2.40                     | 0.56              |
| 85:28:3870:C:H2'  | 85:28:3871:A:H8    | 1.71                     | 0.56              |
| 18:bb:5:GLN:HG2   | 18:bb:6:VAL:HG23   | 1.87                     | 0.56              |
| 37:38:26:LYS:HE3  | 37:38:28:ASN:HB3   | 1.87                     | 0.56              |
| 49:F:31:VAL:HG21  | 49:F:56:ILE:HG22   | 1.86                     | 0.56              |
| 79:18:545:A:H2'   | 79:18:546:G:C8     | 2.40                     | 0.56              |
| 79:18:1121:G:C2   | 79:18:1122:A:C8    | 2.94                     | 0.56              |
| 79:18:1228:A:H2'  | 79:18:1229:G:C8    | 2.40                     | 0.56              |
| 79:18:1228:A:H2'  | 79:18:1229:G:H8    | 1.71                     | 0.56              |
| 79:18:1457:U:H2'  | 79:18:1458:G:H8    | 1.71                     | 0.56              |
| 85:28:448:G:H3'   | 85:28:449:C:H5''   | 1.86                     | 0.56              |
| 18:bb:125:LYS:HG3 | 18:bb:129:LEU:HD12 | 1.86                     | 0.56              |
| 80:v:602:LEU:HB3  | 80:v:604:MET:HE1   | 1.88                     | 0.56              |
| 85:28:4563:U:H2'  | 85:28:4564:A:H8    | 1.71                     | 0.56              |
| 85:28:4594:U:H2'  | 85:28:4595:G:H8    | 1.71                     | 0.56              |
| 85:28:4629:U:C2   | 85:28:4630:G:C8    | 2.94                     | 0.56              |
| 85:28:4884:G:H2'  | 85:28:4885:U:O4'   | 2.06                     | 0.56              |
| 34:35:31:LEU:HB3  | 34:35:47:ILE:HG22  | 1.87                     | 0.56              |
| 79:18:1633:A:H2'  | 79:18:1634:A:H8    | 1.71                     | 0.56              |
| 85:28:268:G:H2'   | 85:28:269:G:H8     | 1.71                     | 0.56              |
| 85:28:1760:G:O6   | 85:28:1773:U:O2    | 2.23                     | 0.56              |
| 85:28:4699:U:H1'  | 85:28:4700:A:H5''  | 1.87                     | 0.56              |
| 1:BB:198:MET:HB3  | 71:RS:85:VAL:HG11  | 1.87                     | 0.56              |
| 58:AA:205:SER:HA  | 58:AA:221:LEU:HB2  | 1.87                     | 0.56              |
| 79:18:382:C:H2'   | 79:18:383:G:C8     | 2.41                     | 0.56              |
| 79:18:974:C:H2'   | 79:18:975:G:H8     | 1.70                     | 0.56              |
| 85:28:462:G:H2'   | 85:28:463:A:C8     | 2.41                     | 0.56              |
| 85:28:2080:U:H2'  | 85:28:2081:C:C6    | 2.41                     | 0.56              |
| 85:28:2412:A:H2'  | 85:28:2413:U:C6    | 2.41                     | 0.56              |
| 85:28:2457:G:H21  | 85:28:3672:G:N2    | 2.01                     | 0.56              |
| 85:28:2540:C:H2'  | 85:28:2541:G:H8    | 1.71                     | 0.56              |
| 85:28:3606:U:H2'  | 85:28:3607:U:H6    | 1.71                     | 0.56              |
| 85:28:4948:C:H2'  | 85:28:4949:G:N2    | 2.21                     | 0.56              |
| 4:DD:101:ARG:HB2  | 63:RR:10:ALA:HB2   | 1.89                     | 0.55              |
| 71:RS:41:ILE:HG21 | 71:RS:47:ARG:HB2   | 1.88                     | 0.55              |
| 79:18:1279:C:H2'  | 79:18:1280:G:H8    | 1.71                     | 0.55              |
| 79:18:1616:U:H2'  | 79:18:1617:G:C8    | 2.41                     | 0.55              |
| 80:v:617:ILE:HD12 | 80:v:659:PRO:HA    | 1.88                     | 0.55              |
| 85:28:418:A:H4'   | 85:28:2311:C:H5'   | 1.88                     | 0.55              |
| 85:28:1770:A:H2'  | 85:28:1771:U:C6    | 2.40                     | 0.55              |
| 11:L6:48:ARG:HB2  | 11:L6:64:MET:HE1   | 1.87                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:18:1035:A:H2'  | 79:18:1036:A:H8    | 1.71                     | 0.55              |
| 79:18:1413:G:H2'  | 79:18:1414:A:H8    | 1.71                     | 0.55              |
| 84:ES:2953:C:H2'  | 84:ES:2954:G:C8    | 2.41                     | 0.55              |
| 12:L7:126:LYS:HB2 | 22:21:133:ALA:HB3  | 1.88                     | 0.55              |
| 51:ZZ:140:TYR:CE1 | 51:ZZ:145:CYS:HA   | 2.41                     | 0.55              |
| 53:TT:99:LEU:HD21 | 53:TT:102:LYS:HB2  | 1.87                     | 0.55              |
| 75:GG:78:ALA:HB3  | 75:GG:118:ALA:HB3  | 1.87                     | 0.55              |
| 79:18:1424:G:H2'  | 79:18:1425:G:C8    | 2.41                     | 0.55              |
| 85:28:922:C:H2'   | 85:28:922(A):G:C8  | 2.41                     | 0.55              |
| 85:28:3720:G:H22  | 85:28:3733:A:H2    | 1.53                     | 0.55              |
| 85:28:3721:U:H2'  | 85:28:3722:G:C8    | 2.41                     | 0.55              |
| 85:28:3933:G:H2'  | 85:28:3934:G:H8    | 1.70                     | 0.55              |
| 85:28:4070:U:H2'  | 85:28:4071:U:C6    | 2.41                     | 0.55              |
| 85:28:4601:U:H2'  | 85:28:4602:A:H8    | 1.71                     | 0.55              |
| 4:DD:132:ARG:HD3  | 79:18:114:G:H5'    | 1.88                     | 0.55              |
| 49:F:227:ASP:HB3  | 49:F:320:LYS:HD3   | 1.89                     | 0.55              |
| 85:28:1669:A:H4'  | 85:28:1685:G:H22   | 1.69                     | 0.55              |
| 6:6:66:G:H5'      | 10:L5:10:LYS:HG3   | 1.88                     | 0.55              |
| 38:39:45:ARG:NH2  | 85:28:2796:G:H5'   | 2.22                     | 0.55              |
| 43:gg:19:LYS:HG3  | 85:28:2337:C:H4'   | 1.89                     | 0.55              |
| 54:S5:34:SER:HA   | 55:WW:55:VAL:HB    | 1.88                     | 0.55              |
| 79:18:479:C:C2    | 79:18:480:G:C8     | 2.95                     | 0.55              |
| 79:18:1511:U:H2'  | 79:18:1512:C:C6    | 2.41                     | 0.55              |
| 85:28:426:A:H2'   | 85:28:427:A:H8     | 1.71                     | 0.55              |
| 5:58:8:U:H2'      | 5:58:9:A:H8        | 1.71                     | 0.55              |
| 41:42:98:LYS:HE3  | 85:28:4233:A:H4'   | 1.89                     | 0.55              |
| 56:II:74:GLY:HA2  | 79:18:1545:A:H4'   | 1.88                     | 0.55              |
| 64:SS:108:LYS:HB3 | 79:18:53:C:H5''    | 1.87                     | 0.55              |
| 73:S8:81:VAL:HG22 | 73:S8:102:VAL:HG12 | 1.89                     | 0.55              |
| 79:18:96:C:H2'    | 79:18:97:U:C6      | 2.41                     | 0.55              |
| 79:18:1183:A:H2'  | 79:18:1184:G:H8    | 1.71                     | 0.55              |
| 79:18:1470:C:H2'  | 79:18:1471:C:H6    | 1.71                     | 0.55              |
| 80:v:580:ARG:HB2  | 80:v:741:MET:HB2   | 1.89                     | 0.55              |
| 85:28:1338:G:H4'  | 85:28:1339:U:C6    | 2.41                     | 0.55              |
| 85:28:4238:G:H2'  | 85:28:4239:A:H8    | 1.71                     | 0.55              |
| 17:15:187:SER:H   | 17:15:190:ALA:HB3  | 1.70                     | 0.55              |
| 44:AS:179:ASN:HB3 | 44:AS:183:GLU:HB2  | 1.89                     | 0.55              |
| 79:18:1301:A:H2'  | 79:18:1303:C:O2    | 2.07                     | 0.55              |
| 85:28:233:U:H2'   | 85:28:234:G:H8     | 1.70                     | 0.55              |
| 85:28:2078:C:H2'  | 85:28:2079:G:C8    | 2.42                     | 0.55              |
| 85:28:3739:C:C2   | 85:28:3740:G:C8    | 2.95                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:28:4591:U:H2'  | 85:28:4592:C:C6    | 2.42                     | 0.55              |
| 5:58:67:U:H2'     | 5:58:68:G:C8       | 2.40                     | 0.55              |
| 18:bb:157:GLU:HA  | 18:bb:160:ARG:HG2  | 1.89                     | 0.55              |
| 20:19:41:ILE:O    | 20:19:45:ILE:HG12  | 2.07                     | 0.55              |
| 26:27:11:VAL:HG11 | 26:27:80:LEU:HB3   | 1.88                     | 0.55              |
| 79:18:35:C:H2'    | 79:18:36:U:C6      | 2.40                     | 0.55              |
| 79:18:1159:G:H2'  | 79:18:1160:U:H6    | 1.72                     | 0.55              |
| 85:28:4642:U:H2'  | 85:28:4643:G:H8    | 1.70                     | 0.55              |
| 45:FF:99:ARG:O    | 45:FF:103:GLU:HG2  | 2.07                     | 0.55              |
| 61:LL:121:ARG:HG3 | 61:LL:131:VAL:HG21 | 1.89                     | 0.55              |
| 85:28:2521:G:H2'  | 85:28:2522:G:C8    | 2.42                     | 0.55              |
| 85:28:2683:C:H2'  | 85:28:2684:C:C6    | 2.41                     | 0.55              |
| 85:28:3845:A:H2'  | 85:28:3846:C:C6    | 2.42                     | 0.55              |
| 85:28:4563:U:C2   | 85:28:4564:A:C8    | 2.95                     | 0.55              |
| 85:28:5028:G:H2'  | 85:28:5029:C:O4'   | 2.07                     | 0.55              |
| 15:13:50:PRO:HG3  | 34:35:121:VAL:HG22 | 1.88                     | 0.55              |
| 21:20:13:VAL:HG22 | 21:20:63:TYR:HB3   | 1.89                     | 0.55              |
| 24:cc:93:ASN:ND2  | 85:28:2533:C:H5'   | 2.21                     | 0.55              |
| 79:18:1828:C:H2'  | 79:18:1829:G:C8    | 2.42                     | 0.55              |
| 85:28:1340:C:H2'  | 85:28:1341:U:C6    | 2.42                     | 0.55              |
| 85:28:1727:U:H2'  | 85:28:1728:U:C6    | 2.42                     | 0.55              |
| 85:28:4398:C:H2'  | 85:28:4399:U:H6    | 1.71                     | 0.55              |
| 85:28:4578:G:H2'  | 85:28:4579:U:C6    | 2.42                     | 0.55              |
| 85:28:4716:C:H2'  | 85:28:4717:A:H8    | 1.72                     | 0.55              |
| 20:19:46:LYS:HE3  | 85:28:2710:C:H41   | 1.71                     | 0.54              |
| 79:18:122:G:H2'   | 79:18:123:G:C8     | 2.41                     | 0.54              |
| 85:28:1867:A:H2'  | 85:28:1868:A:C8    | 2.43                     | 0.54              |
| 85:28:2539:C:H2'  | 85:28:2540:C:C6    | 2.42                     | 0.54              |
| 48:t:142:ASN:HA   | 48:t:146:ARG:HH11  | 1.73                     | 0.54              |
| 79:18:387:C:H2'   | 79:18:388:U:C6     | 2.42                     | 0.54              |
| 79:18:432:G:H2'   | 79:18:433:A:H8     | 1.72                     | 0.54              |
| 5:58:8:U:H2'      | 5:58:9:A:C8        | 2.43                     | 0.54              |
| 9:L4:140:LYS:HE3  | 9:L4:245:HIS:HB2   | 1.87                     | 0.54              |
| 79:18:857:U:H2'   | 79:18:858:A:C8     | 2.42                     | 0.54              |
| 79:18:957:A:H3'   | 79:18:958:G:N2     | 2.18                     | 0.54              |
| 80:v:30:HIS:CE1   | 80:v:130:ASP:H     | 2.26                     | 0.54              |
| 85:28:4458:C:H2'  | 85:28:4459:U:H6    | 1.73                     | 0.54              |
| 2:S2:207:ALA:HB2  | 79:18:4:C:H4'      | 1.89                     | 0.54              |
| 13:aa:317:LYS:HG2 | 44:AS:225:LEU:HB3  | 1.88                     | 0.54              |
| 17:15:40:PRO:HG3  | 85:28:8:U:H5''     | 1.88                     | 0.54              |
| 47:s:121:VAL:HG13 | 47:s:182:PRO:HG2   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:s:160:LEU:HG   | 47:s:161:ILE:HG23  | 1.89                     | 0.54              |
| 71:RS:17:ILE:HD13 | 71:RS:24:LEU:HD23  | 1.90                     | 0.54              |
| 73:S8:66:SER:HA   | 73:S8:73:THR:HB    | 1.90                     | 0.54              |
| 85:28:1504:G:H2'  | 85:28:1505:C:H6    | 1.72                     | 0.54              |
| 85:28:2608:G:H2'  | 85:28:2609:G:H8    | 1.72                     | 0.54              |
| 85:28:2689:C:H2'  | 85:28:2690:C:H6    | 1.71                     | 0.54              |
| 5:58:70:G:H22     | 5:58:87:G:H1'      | 1.71                     | 0.54              |
| 5:58:147:G:H2'    | 5:58:148:A:H8      | 1.72                     | 0.54              |
| 14:10:16:PRO:HA   | 14:10:95:HIS:CD2   | 2.42                     | 0.54              |
| 48:t:108:GLU:HA   | 48:t:111:ASN:ND2   | 2.22                     | 0.54              |
| 66:S4:62:LYS:HE2  | 79:18:502:C:H4'    | 1.88                     | 0.54              |
| 79:18:29:G:H2'    | 79:18:30:C:C6      | 2.42                     | 0.54              |
| 58:AA:162:ASN:HB3 | 58:AA:164:ILE:HD12 | 1.88                     | 0.54              |
| 67:S9:50:LEU:O    | 67:S9:54:ARG:HG3   | 2.07                     | 0.54              |
| 79:18:674:C:H2'   | 79:18:675:U:C6     | 2.43                     | 0.54              |
| 79:18:1365:G:H2'  | 79:18:1366:G:H8    | 1.72                     | 0.54              |
| 85:28:1593:A:H5'' | 85:28:2839:U:H5''  | 1.89                     | 0.54              |
| 85:28:2555:G:H2'  | 85:28:2556:G:H8    | 1.72                     | 0.54              |
| 85:28:2858:A:H2'  | 85:28:2859:G:H8    | 1.70                     | 0.54              |
| 85:28:2890:C:H2'  | 85:28:2891:U:C6    | 2.43                     | 0.54              |
| 85:28:3861:A:H2'  | 85:28:3862:A:C8    | 2.42                     | 0.54              |
| 85:28:4092:G:H2'  | 85:28:4093:G:H8    | 1.72                     | 0.54              |
| 85:28:4188:U:H2'  | 85:28:4189:U:C6    | 2.42                     | 0.54              |
| 85:28:4704:C:H2'  | 85:28:4705:A:H8    | 1.73                     | 0.54              |
| 4:DD:113:LEU:HD21 | 4:DD:120:VAL:HG21  | 1.90                     | 0.54              |
| 31:32:100:ALA:HB3 | 31:32:103:VAL:HG23 | 1.90                     | 0.54              |
| 65:S6:131:ARG:HG3 | 74:W:82:ILE:HG22   | 1.90                     | 0.54              |
| 66:S4:48:LEU:HD23 | 66:S4:61:VAL:HG22  | 1.90                     | 0.54              |
| 79:18:126:G:H21   | 79:18:180:G:N2     | 2.04                     | 0.54              |
| 79:18:354:U:H2'   | 79:18:355:G:C8     | 2.43                     | 0.54              |
| 79:18:509:G:H2'   | 79:18:510:G:H8     | 1.72                     | 0.54              |
| 79:18:935:G:H2'   | 79:18:936:G:H8     | 1.73                     | 0.54              |
| 85:28:1348:U:H2'  | 85:28:1349:G:H8    | 1.72                     | 0.54              |
| 5:58:144:U:H2'    | 5:58:145:C:C6      | 2.43                     | 0.54              |
| 12:L7:42:ARG:O    | 12:L7:46:ARG:HG2   | 2.08                     | 0.54              |
| 73:S8:177:SER:HB3 | 79:18:220:U:H5'    | 1.89                     | 0.54              |
| 79:18:479:C:H2'   | 79:18:480:G:H8     | 1.72                     | 0.54              |
| 79:18:1058:A:C8   | 82:CE:12:SER:HB3   | 2.43                     | 0.54              |
| 85:28:676:C:H2'   | 85:28:677:G:H8     | 1.73                     | 0.54              |
| 85:28:4996:C:C2   | 85:28:4997:G:C8    | 2.96                     | 0.54              |
| 52:EE:56:CYS:SG   | 52:EE:82:ASN:HB2   | 2.48                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:CC:8:ARG:O      | 57:CC:11:ILE:HG12  | 2.08                     | 0.54              |
| 79:18:530:U:H3     | 79:18:554:A:H61    | 1.55                     | 0.54              |
| 79:18:1395:C:H4'   | 79:18:1396:A:OP1   | 2.08                     | 0.54              |
| 85:28:517:C:H2'    | 85:28:518:G:C8     | 2.43                     | 0.54              |
| 85:28:1450:C:H2'   | 85:28:1451:G:C8    | 2.42                     | 0.54              |
| 85:28:2292:C:H2'   | 85:28:2293:U:C6    | 2.43                     | 0.54              |
| 85:28:2292:C:H2'   | 85:28:2293:U:H6    | 1.73                     | 0.54              |
| 85:28:3610:A:H2'   | 85:28:3611:A:C8    | 2.42                     | 0.54              |
| 85:28:4948:C:H2'   | 85:28:4949:G:H21   | 1.73                     | 0.54              |
| 4:DD:85:THR:HG22   | 4:DD:112:HIS:HA    | 1.89                     | 0.53              |
| 15:13:91:ALA:HB1   | 15:13:96:ILE:HB    | 1.89                     | 0.53              |
| 43:gg:28:GLU:HB2   | 43:gg:31:ASN:HB2   | 1.90                     | 0.53              |
| 58:AA:270:LEU:HB3  | 58:AA:310:TRP:CZ2  | 2.43                     | 0.53              |
| 59:OO:24:LEU:HB3   | 59:OO:32:LEU:HD11  | 1.90                     | 0.53              |
| 75:GG:121:ARG:HD3  | 76:UU:52:ASP:HB2   | 1.90                     | 0.53              |
| 79:18:848:U:H2'    | 79:18:849:A:H8     | 1.73                     | 0.53              |
| 79:18:1232:U:H2'   | 79:18:1233:G:H8    | 1.73                     | 0.53              |
| 85:28:4163:U:H5'   | 85:28:4164:C:H5''  | 1.90                     | 0.53              |
| 7:L8:90:CYS:HB3    | 7:L8:101:VAL:HG13  | 1.89                     | 0.53              |
| 9:L4:78:ARG:HA     | 9:L4:90:GLY:HA2    | 1.90                     | 0.53              |
| 66:S4:166:THR:HG23 | 66:S4:168:LYS:H    | 1.73                     | 0.53              |
| 73:S8:27:TYR:HB2   | 79:18:381:C:H41    | 1.73                     | 0.53              |
| 79:18:89:C:H2'     | 79:18:90:G:C8      | 2.42                     | 0.53              |
| 79:18:186:C:H2'    | 79:18:187:G:H8     | 1.73                     | 0.53              |
| 80:v:412:ALA:HB3   | 80:v:472:LEU:H     | 1.73                     | 0.53              |
| 85:28:1340:C:H2'   | 85:28:1341:U:H6    | 1.73                     | 0.53              |
| 85:28:2566:G:H2'   | 85:28:2567:G:H8    | 1.72                     | 0.53              |
| 85:28:2684:C:H2'   | 85:28:2685:C:C6    | 2.43                     | 0.53              |
| 85:28:4238:G:H2'   | 85:28:4239:A:C8    | 2.43                     | 0.53              |
| 85:28:4704:C:H2'   | 85:28:4705:A:C8    | 2.44                     | 0.53              |
| 9:L4:339:THR:HG22  | 9:L4:342:ARG:NH2   | 2.23                     | 0.53              |
| 14:10:98:ARG:HB3   | 14:10:120:GLY:HA3  | 1.90                     | 0.53              |
| 24:cc:77:ILE:HD12  | 24:cc:116:LEU:HD12 | 1.88                     | 0.53              |
| 58:AA:79:LEU:HB2   | 58:AA:113:PHE:CZ   | 2.42                     | 0.53              |
| 59:OO:26:SER:HB3   | 59:OO:32:LEU:HB2   | 1.90                     | 0.53              |
| 74:W:13:ILE:HD11   | 74:W:32:LEU:HB2    | 1.90                     | 0.53              |
| 79:18:107:A:H2'    | 79:18:108:G:H8     | 1.73                     | 0.53              |
| 79:18:949:G:H2'    | 79:18:950:C:C6     | 2.42                     | 0.53              |
| 79:18:982:G:H2'    | 79:18:983:A:H8     | 1.73                     | 0.53              |
| 79:18:1017:U:H2'   | 79:18:1018:U:H6    | 1.73                     | 0.53              |
| 79:18:1590:C:H3'   | 79:18:1591:C:H6    | 1.72                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:1088:C:H2'   | 85:28:1089:G:C8    | 2.43                     | 0.53              |
| 85:28:1468:C:H2'   | 85:28:1469:C:H6    | 1.73                     | 0.53              |
| 85:28:1558:A:H2'   | 85:28:1559:G:H8    | 1.73                     | 0.53              |
| 85:28:3732:A:H2'   | 85:28:3733:A:H8    | 1.73                     | 0.53              |
| 85:28:4993:G:H2'   | 85:28:4994:G:C8    | 2.42                     | 0.53              |
| 27:dd:72:THR:HG22  | 27:dd:110:LYS:HB3  | 1.90                     | 0.53              |
| 27:dd:100:ILE:HG13 | 27:dd:123:ILE:HB   | 1.90                     | 0.53              |
| 61:LL:63:GLU:O     | 61:LL:67:VAL:HG23  | 2.09                     | 0.53              |
| 79:18:17:C:H2'     | 79:18:18:C:H6      | 1.74                     | 0.53              |
| 79:18:1337:C:H2'   | 79:18:1338:G:C8    | 2.43                     | 0.53              |
| 79:18:1690:U:H2'   | 79:18:1691:U:H6    | 1.74                     | 0.53              |
| 80:v:252:LYS:HA    | 80:v:255:ASP:OD2   | 2.08                     | 0.53              |
| 80:v:323:LEU:HD13  | 80:v:324:ASP:H     | 1.73                     | 0.53              |
| 85:28:1346:C:H2'   | 85:28:1347:G:H8    | 1.74                     | 0.53              |
| 85:28:1420:A:H4'   | 85:28:1421:G:H5'   | 1.91                     | 0.53              |
| 85:28:2634:C:H2'   | 85:28:2635:U:H6    | 1.73                     | 0.53              |
| 45:FF:14:SER:HB2   | 79:18:1016:U:H5''  | 1.90                     | 0.53              |
| 73:S8:49:ARG:HD3   | 79:18:381:C:C5     | 2.43                     | 0.53              |
| 79:18:1283:C:H4'   | 79:18:1287:A:H5'   | 1.90                     | 0.53              |
| 85:28:287:U:H2'    | 85:28:288:G:C8     | 2.44                     | 0.53              |
| 85:28:674:G:H2'    | 85:28:675:C:H6     | 1.73                     | 0.53              |
| 85:28:2414:G:H2'   | 85:28:2415:U:H6    | 1.74                     | 0.53              |
| 85:28:2895:A:H2'   | 85:28:2896:G:C8    | 2.43                     | 0.53              |
| 85:28:3871:A:H2'   | 85:28:3872:A:C8    | 2.44                     | 0.53              |
| 85:28:3873:G:H2'   | 85:28:3874:G:C8    | 2.43                     | 0.53              |
| 8:L3:263:ALA:HB3   | 8:L3:266:VAL:HG23  | 1.91                     | 0.53              |
| 59:OO:26:SER:HB2   | 59:OO:110:VAL:HG13 | 1.91                     | 0.53              |
| 79:18:925:G:H1     | 79:18:1017:U:H3    | 1.55                     | 0.53              |
| 79:18:996:A:H2'    | 79:18:997:A:C8     | 2.43                     | 0.53              |
| 79:18:1102:G:H2'   | 79:18:1103:C:C6    | 2.43                     | 0.53              |
| 79:18:1318:G:H2'   | 79:18:1319:U:C6    | 2.44                     | 0.53              |
| 80:v:503:PRO:HD3   | 80:v:533:MET:HE2   | 1.91                     | 0.53              |
| 83:A:77:LYS:HE2    | 83:A:79:HIS:CE1    | 2.43                     | 0.53              |
| 85:28:440:U:H2'    | 85:28:441:G:C8     | 2.43                     | 0.53              |
| 85:28:2373:C:H2'   | 85:28:2374:A:C8    | 2.44                     | 0.53              |
| 9:L4:168:VAL:O     | 9:L4:172:LYS:HG2   | 2.08                     | 0.53              |
| 24:cc:76:ILE:HA    | 24:cc:101:ASP:HB2  | 1.90                     | 0.53              |
| 41:42:63:THR:HG21  | 41:42:87:ARG:HB3   | 1.91                     | 0.53              |
| 49:F:107:LYS:HD3   | 49:F:317:ALA:HA    | 1.90                     | 0.53              |
| 50:Q:181:ARG:HB2   | 50:Q:184:ARG:HB2   | 1.89                     | 0.53              |
| 79:18:430:C:C2     | 79:18:431:G:C8     | 2.97                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:18:949:G:H2'    | 79:18:950:C:H6    | 1.74                     | 0.53              |
| 85:28:1204:C:H2'   | 85:28:1205:G:C8   | 2.43                     | 0.53              |
| 85:28:1494:U:H2'   | 85:28:1495:G:H8   | 1.74                     | 0.53              |
| 85:28:2633:U:H2'   | 85:28:2634:C:H6   | 1.74                     | 0.53              |
| 85:28:2676:A:C4    | 85:28:2677:G:C8   | 2.97                     | 0.53              |
| 85:28:3697:U:H5''  | 85:28:3698:G:H5'  | 1.91                     | 0.53              |
| 8:L3:53:MET:HG2    | 8:L3:77:THR:HG22  | 1.91                     | 0.53              |
| 16:14:26:ALA:HB2   | 16:14:77:TRP:HZ3  | 1.74                     | 0.53              |
| 20:19:66:ASN:O     | 20:19:70:ARG:HG2  | 2.09                     | 0.53              |
| 41:42:5:PRO:HD3    | 85:28:4232:U:C2   | 2.43                     | 0.53              |
| 79:18:1035:A:C4    | 79:18:1036:A:C8   | 2.97                     | 0.53              |
| 79:18:1140:G:H2'   | 79:18:1141:G:H8   | 1.72                     | 0.53              |
| 79:18:1708:C:H2'   | 79:18:1709:G:H8   | 1.73                     | 0.53              |
| 85:28:2483:G:H1    | 85:28:2495:U:H3   | 1.55                     | 0.53              |
| 85:28:3732:A:H2'   | 85:28:3733:A:C8   | 2.44                     | 0.53              |
| 85:28:4894:A:H5''  | 85:28:4895:C:H2'  | 1.90                     | 0.53              |
| 7:L8:21:LYS:HG2    | 85:28:1541:C:H5'' | 1.90                     | 0.53              |
| 9:L4:77:PRO:O      | 9:L4:90:GLY:HA2   | 2.09                     | 0.53              |
| 79:18:26:U:H2'     | 79:18:27:A:H8     | 1.73                     | 0.53              |
| 79:18:1323:U:H2'   | 79:18:1324:G:C8   | 2.44                     | 0.53              |
| 79:18:1558:C:H2'   | 79:18:1559:C:C6   | 2.44                     | 0.53              |
| 85:28:496:G:H2'    | 85:28:497:G:H5'   | 1.90                     | 0.53              |
| 85:28:4399:U:C2    | 85:28:4400:G:C8   | 2.97                     | 0.53              |
| 5:58:64:U:C2       | 5:58:65:A:C8      | 2.97                     | 0.53              |
| 11:L6:165:VAL:HG13 | 11:L6:180:GLY:H   | 1.72                     | 0.53              |
| 12:L7:175:ALA:HB1  | 85:28:2102:G:C8   | 2.44                     | 0.53              |
| 58:AA:11:LEU:HD21  | 58:AA:52:TYR:HB3  | 1.90                     | 0.53              |
| 64:SS:66:GLY:HA2   | 79:18:581:U:H4'   | 1.90                     | 0.53              |
| 79:18:1687:C:H2'   | 79:18:1688:C:H6   | 1.74                     | 0.53              |
| 85:28:245:C:H4'    | 85:28:246:G:O5'   | 2.09                     | 0.53              |
| 85:28:677:G:H2'    | 85:28:678:C:H6    | 1.72                     | 0.53              |
| 85:28:2078:C:H2'   | 85:28:2079:G:H8   | 1.74                     | 0.53              |
| 85:28:4756:C:H5'   | 85:28:4757:C:OP1  | 2.09                     | 0.53              |
| 7:L8:194:ASN:HB2   | 85:28:1539:G:H4'  | 1.90                     | 0.52              |
| 52:EE:52:LEU:HD13  | 52:EE:65:VAL:HG11 | 1.91                     | 0.52              |
| 52:EE:86:GLY:O     | 52:EE:89:VAL:HG12 | 2.09                     | 0.52              |
| 79:18:1189:A:H2'   | 79:18:1190:A:H8   | 1.75                     | 0.52              |
| 79:18:1537:A:H2'   | 79:18:1538:C:C6   | 2.44                     | 0.52              |
| 85:28:460:C:H2'    | 85:28:461:G:H8    | 1.73                     | 0.52              |
| 5:58:130:C:H2'     | 5:58:131:G:H8     | 1.73                     | 0.52              |
| 10:L5:37:VAL:HG23  | 10:L5:48:LYS:O    | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L5:65:ALA:HB2   | 10:L5:74:ILE:HD13  | 1.92                     | 0.52              |
| 48:t:123:ARG:NH1   | 48:t:123:ARG:HA    | 2.24                     | 0.52              |
| 56:II:140:ARG:HB2  | 79:18:1644:C:H4'   | 1.90                     | 0.52              |
| 79:18:5:U:O2'      | 79:18:602:G:H4'    | 2.08                     | 0.52              |
| 79:18:89:C:H2'     | 79:18:90:G:H8      | 1.74                     | 0.52              |
| 79:18:110:U:H2'    | 79:18:111:A:H8     | 1.71                     | 0.52              |
| 79:18:925:G:C2     | 79:18:926:A:C8     | 2.97                     | 0.52              |
| 85:28:33:A:H3'     | 85:28:47:A:H61     | 1.73                     | 0.52              |
| 85:28:423:G:H2'    | 85:28:424:U:H6     | 1.73                     | 0.52              |
| 85:28:1195:G:H2'   | 85:28:1196:G:H8    | 1.72                     | 0.52              |
| 85:28:1591:U:OP1   | 85:28:1592:G:H5'   | 2.08                     | 0.52              |
| 85:28:2093:G:H22   | 85:28:2262:G:H1    | 1.57                     | 0.52              |
| 85:28:2478:C:C2    | 85:28:2479:G:N7    | 2.78                     | 0.52              |
| 85:28:2539:C:H2'   | 85:28:2540:C:H6    | 1.74                     | 0.52              |
| 85:28:2699:C:H2'   | 85:28:2700:G:H8    | 1.74                     | 0.52              |
| 2:S2:65:LYS:HD3    | 2:S2:273:LEU:HD13  | 1.90                     | 0.52              |
| 12:L7:85:GLU:HB2   | 22:21:135:PRO:HB3  | 1.90                     | 0.52              |
| 17:15:49:ARG:HH12  | 85:28:152:U:P      | 2.32                     | 0.52              |
| 18:bb:168:TYR:CE2  | 18:bb:172:LYS:HD2  | 2.44                     | 0.52              |
| 49:F:46:LEU:HB3    | 49:F:91:PRO:HG2    | 1.91                     | 0.52              |
| 79:18:1823:A:C5    | 79:18:1824:A:H1'   | 2.44                     | 0.52              |
| 85:28:456:C:H2'    | 85:28:457:G:H8     | 1.74                     | 0.52              |
| 85:28:1333:A:H2'   | 85:28:1334:A:C8    | 2.44                     | 0.52              |
| 85:28:4091:G:H2'   | 85:28:4092:G:C8    | 2.44                     | 0.52              |
| 85:28:4343:U:H2'   | 85:28:4344:U:C6    | 2.44                     | 0.52              |
| 1:BB:132:GLN:HB3   | 1:BB:133:PRO:HD3   | 1.91                     | 0.52              |
| 5:58:70:G:N2       | 5:58:87:G:H1'      | 2.24                     | 0.52              |
| 26:27:59:LYS:HE2   | 85:28:4148:C:H5''  | 1.91                     | 0.52              |
| 40:41:2:ARG:HD3    | 40:41:5:TRP:CD1    | 2.44                     | 0.52              |
| 54:S5:169:ILE:HG12 | 79:18:1535:U:C5    | 2.44                     | 0.52              |
| 79:18:729:C:H2'    | 79:18:730:C:H6     | 1.73                     | 0.52              |
| 79:18:1798:C:H2'   | 79:18:1799:G:O4'   | 2.09                     | 0.52              |
| 85:28:2465:C:H2'   | 85:28:2466:G:O4'   | 2.09                     | 0.52              |
| 85:28:2704:C:H2'   | 85:28:2705:G:O4'   | 2.09                     | 0.52              |
| 85:28:3607:U:H2'   | 85:28:3608:A:H8    | 1.75                     | 0.52              |
| 27:dd:98:ALA:HB2   | 27:dd:121:PRO:HB2  | 1.92                     | 0.52              |
| 54:S5:97:PHE:HA    | 54:S5:100:ILE:HD12 | 1.90                     | 0.52              |
| 79:18:573:U:H2'    | 79:18:574:A:H5''   | 1.90                     | 0.52              |
| 79:18:1670:C:H2'   | 79:18:1671:G:H8    | 1.72                     | 0.52              |
| 85:28:1339:U:H2'   | 85:28:1340:C:C6    | 2.45                     | 0.52              |
| 6:6:2:U:H2'        | 6:6:3:C:H6         | 1.75                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:6:26:C:H5''     | 10:L5:56:THR:HG21  | 1.91                     | 0.52              |
| 37:38:2:PRO:HB2   | 85:28:2692:U:O2    | 2.10                     | 0.52              |
| 79:18:544:G:C2    | 79:18:545:A:C5     | 2.97                     | 0.52              |
| 80:v:159:LYS:HG2  | 88:v:900:GDP:C6    | 2.44                     | 0.52              |
| 84:ES:2946:G:H2'  | 84:ES:2947:G:H8    | 1.72                     | 0.52              |
| 85:28:1236:C:H2'  | 85:28:1238:A:C8    | 2.44                     | 0.52              |
| 65:S6:142:ARG:HG2 | 65:S6:153:VAL:HG11 | 1.90                     | 0.52              |
| 79:18:1144:A:H2'  | 79:18:1145:A:C8    | 2.44                     | 0.52              |
| 79:18:1240:A:C4   | 83:A:100:LYS:HD2   | 2.44                     | 0.52              |
| 79:18:1523:C:H2'  | 79:18:1524:G:H8    | 1.74                     | 0.52              |
| 79:18:1748:G:H1   | 79:18:1786:U:H3    | 1.57                     | 0.52              |
| 85:28:162:A:H2'   | 85:28:163:A:C8     | 2.45                     | 0.52              |
| 6:6:6:C:H4'       | 10:L5:52:ILE:HD13  | 1.91                     | 0.52              |
| 9:L4:312:ARG:HB3  | 85:28:2274:C:H5'   | 1.90                     | 0.52              |
| 27:dd:29:PRO:HA   | 85:28:1654:G:H5''  | 1.91                     | 0.52              |
| 44:AS:103:MET:HE3 | 44:AS:215:VAL:HG23 | 1.92                     | 0.52              |
| 69:YY:112:ASN:HA  | 69:YY:116:VAL:HG12 | 1.91                     | 0.52              |
| 79:18:528:A:H2'   | 79:18:529:A:C8     | 2.44                     | 0.52              |
| 79:18:910:G:H2'   | 79:18:911:C:C6     | 2.45                     | 0.52              |
| 79:18:1350:U:C2   | 79:18:1351:G:C8    | 2.98                     | 0.52              |
| 79:18:1501:C:H2'  | 79:18:1502:C:H6    | 1.74                     | 0.52              |
| 79:18:1627:C:H2'  | 79:18:1628:C:C6    | 2.45                     | 0.52              |
| 85:28:247:G:H2'   | 85:28:248:C:H6     | 1.74                     | 0.52              |
| 85:28:1958:A:H4'  | 85:28:1962:A:H1'   | 1.90                     | 0.52              |
| 85:28:3719:A:C4   | 85:28:3720:G:C8    | 2.97                     | 0.52              |
| 85:28:4459:U:H2'  | 85:28:4460:U:C6    | 2.44                     | 0.52              |
| 2:S2:196:ILE:HB   | 2:S2:223:TYR:HB2   | 1.92                     | 0.52              |
| 79:18:21:U:H2'    | 79:18:22:A:C8      | 2.45                     | 0.52              |
| 85:28:175:C:H2'   | 85:28:176:G:C8     | 2.43                     | 0.52              |
| 85:28:270:U:H2'   | 85:28:271:C:H6     | 1.75                     | 0.52              |
| 85:28:2544:G:H5'' | 85:28:2545:U:H5    | 1.75                     | 0.52              |
| 85:28:2743:A:H2'  | 85:28:2744:A:C8    | 2.44                     | 0.52              |
| 14:10:16:PRO:HA   | 14:10:95:HIS:HD2   | 1.75                     | 0.52              |
| 79:18:409:C:H2'   | 79:18:410:G:H8     | 1.75                     | 0.52              |
| 79:18:1092:G:H2'  | 79:18:1093:A:H8    | 1.75                     | 0.52              |
| 80:v:138:GLN:HA   | 80:v:141:THR:HG22  | 1.91                     | 0.52              |
| 85:28:714:G:H2'   | 85:28:715:G:H8     | 1.75                     | 0.52              |
| 85:28:1345:A:H2'  | 85:28:1346:C:C6    | 2.45                     | 0.52              |
| 85:28:1933:G:H2'  | 85:28:1934:A:C8    | 2.45                     | 0.52              |
| 85:28:2560:C:H42  | 85:28:2567:G:H1    | 1.57                     | 0.52              |
| 85:28:4652:G:H2'  | 85:28:4653:C:H6    | 1.75                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:28:4716:C:H2'  | 85:28:4717:A:C8    | 2.45                     | 0.52              |
| 85:28:4889:G:H2'  | 85:28:4890:G:H8    | 1.74                     | 0.52              |
| 57:CC:20:VAL:HG21 | 70:S3:72:VAL:HG22  | 1.90                     | 0.51              |
| 58:AA:174:VAL:HB  | 58:AA:188:HIS:HB2  | 1.91                     | 0.51              |
| 64:SS:35:VAL:HG21 | 64:SS:40:ILE:HD11  | 1.93                     | 0.51              |
| 66:S4:79:ASP:HB3  | 66:S4:82:TYR:HB2   | 1.92                     | 0.51              |
| 79:18:677:G:H21   | 79:18:1028:A:N6    | 2.00                     | 0.51              |
| 85:28:1505:C:H2'  | 85:28:1506:G:C8    | 2.44                     | 0.51              |
| 85:28:1527:A:H2'  | 85:28:1528:U:C6    | 2.45                     | 0.51              |
| 85:28:2556:G:H2'  | 85:28:2557:G:H8    | 1.75                     | 0.51              |
| 85:28:4320:G:H2'  | 85:28:4321:U:C6    | 2.45                     | 0.51              |
| 85:28:4357:G:H2'  | 85:28:4358:U:H6    | 1.76                     | 0.51              |
| 5:58:70:G:H5''    | 25:26:27:ARG:CZ    | 2.40                     | 0.51              |
| 18:bb:54:TYR:CD1  | 18:bb:145:VAL:HG21 | 2.46                     | 0.51              |
| 41:42:6:LYS:HG2   | 41:42:93:LEU:HB3   | 1.92                     | 0.51              |
| 77:11:108:GLY:HA3 | 85:28:4251:A:H5''  | 1.91                     | 0.51              |
| 79:18:102:A:H4'   | 79:18:104:A:C8     | 2.45                     | 0.51              |
| 79:18:481:C:H2'   | 79:18:482:G:C8     | 2.44                     | 0.51              |
| 79:18:511:U:H2'   | 79:18:512:A:C8     | 2.37                     | 0.51              |
| 85:28:674:G:H2'   | 85:28:675:C:C6     | 2.46                     | 0.51              |
| 85:28:734:G:C2    | 85:28:735:G:C8     | 2.98                     | 0.51              |
| 85:28:3726:A:H2'  | 85:28:3727:A:C8    | 2.45                     | 0.51              |
| 7:L8:14:SER:H     | 7:L8:17:ARG:HG3    | 1.76                     | 0.51              |
| 7:L8:183:GLY:HA2  | 85:28:1613:A:H5''  | 1.92                     | 0.51              |
| 7:L8:233:ARG:HB2  | 85:28:4184:G:H5'   | 1.93                     | 0.51              |
| 26:27:38:TYR:HB3  | 85:28:2656:U:H5''  | 1.91                     | 0.51              |
| 44:AS:46:LYS:HE3  | 75:GG:20:GLN:HB2   | 1.92                     | 0.51              |
| 44:AS:48:LEU:HD23 | 44:AS:48:LEU:H     | 1.75                     | 0.51              |
| 60:MM:37:VAL:HG23 | 79:18:1567:G:H4'   | 1.91                     | 0.51              |
| 79:18:440:G:H2'   | 79:18:441:C:O4'    | 2.10                     | 0.51              |
| 79:18:1609:C:H2'  | 79:18:1610:G:H8    | 1.75                     | 0.51              |
| 79:18:1808:U:H2'  | 79:18:1809:A:H8    | 1.75                     | 0.51              |
| 85:28:158:A:H5''  | 85:28:159:C:H2'    | 1.92                     | 0.51              |
| 85:28:2277:C:H2'  | 85:28:2278:G:C8    | 2.45                     | 0.51              |
| 85:28:2726:G:H2'  | 85:28:2727:C:C6    | 2.45                     | 0.51              |
| 85:28:4578:G:H2'  | 85:28:4579:U:H6    | 1.74                     | 0.51              |
| 85:28:4685:U:H2'  | 85:28:4686:G:C8    | 2.45                     | 0.51              |
| 16:14:25:VAL:HG11 | 16:14:50:MET:HE1   | 1.91                     | 0.51              |
| 58:AA:12:LYS:HB3  | 58:AA:306:LEU:HD13 | 1.93                     | 0.51              |
| 79:18:344:U:H2'   | 79:18:345:U:C6     | 2.46                     | 0.51              |
| 79:18:509:G:H2'   | 79:18:510:G:C8     | 2.46                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:v:524:LEU:HD21 | 80:v:544:HIS:HB3   | 1.93                     | 0.51              |
| 85:28:3719:A:H2'  | 85:28:3720:G:H8    | 1.75                     | 0.51              |
| 5:58:65:A:H2'     | 5:58:66:A:C8       | 2.46                     | 0.51              |
| 11:L6:53:VAL:HG11 | 85:28:947:C:H5''   | 1.93                     | 0.51              |
| 30:31:26:THR:HG23 | 85:28:4996:C:H4'   | 1.91                     | 0.51              |
| 32:ee:45:LYS:HD2  | 32:ee:105:LEU:HA   | 1.92                     | 0.51              |
| 60:MM:100:ALA:O   | 60:MM:104:LEU:HG   | 2.11                     | 0.51              |
| 79:18:28:U:H2'    | 79:18:29:G:C8      | 2.45                     | 0.51              |
| 79:18:656:G:H5'   | 79:18:662:G:N2     | 2.25                     | 0.51              |
| 79:18:1131:G:H2'  | 79:18:1132:C:C6    | 2.46                     | 0.51              |
| 79:18:1511:U:H2'  | 79:18:1512:C:H6    | 1.74                     | 0.51              |
| 79:18:1823:A:N7   | 79:18:1824:A:H1'   | 2.26                     | 0.51              |
| 85:28:1329:G:H2'  | 85:28:3865:A:H5'   | 1.91                     | 0.51              |
| 85:28:2859:G:H2'  | 85:28:2860:C:H6    | 1.74                     | 0.51              |
| 85:28:4208:U:H2'  | 85:28:4209:G:H8    | 1.75                     | 0.51              |
| 5:58:47:C:H1'     | 5:58:61:A:H2'      | 1.93                     | 0.51              |
| 45:FF:26:LEU:HD21 | 45:FF:60:VAL:HG12  | 1.92                     | 0.51              |
| 72:WX:105:THR:HB  | 72:WX:110:ILE:HG12 | 1.92                     | 0.51              |
| 76:UU:17:HIS:HB3  | 79:18:999:G:C8     | 2.45                     | 0.51              |
| 79:18:192:C:H2'   | 79:18:193:C:H6     | 1.74                     | 0.51              |
| 85:28:164:G:H2'   | 85:28:165:A:H8     | 1.76                     | 0.51              |
| 5:58:144:U:H2'    | 5:58:145:C:H6      | 1.76                     | 0.51              |
| 13:aa:250:LYS:HB3 | 85:28:6:C:H5''     | 1.92                     | 0.51              |
| 23:22:84:LYS:HG3  | 23:22:102:VAL:HG11 | 1.92                     | 0.51              |
| 79:18:192:C:H2'   | 79:18:193:C:C6     | 2.46                     | 0.51              |
| 79:18:1174:U:H2'  | 79:18:1175:G:H8    | 1.75                     | 0.51              |
| 79:18:1244:U:H2'  | 79:18:1245:G:C8    | 2.40                     | 0.51              |
| 85:28:50:C:C2     | 85:28:51:A:C8      | 2.99                     | 0.51              |
| 85:28:956:A:H1'   | 85:28:2076:G:H5''  | 1.93                     | 0.51              |
| 85:28:2079:G:H2'  | 85:28:2080:U:C6    | 2.46                     | 0.51              |
| 85:28:2858:A:H2'  | 85:28:2859:G:C8    | 2.45                     | 0.51              |
| 85:28:4173:G:H2'  | 85:28:4174:U:H6    | 1.76                     | 0.51              |
| 85:28:5004:C:H2'  | 85:28:5005:G:O4'   | 2.10                     | 0.51              |
| 2:S2:168:GLY:HA2  | 3:PP:1:MET:HE1     | 1.93                     | 0.51              |
| 19:17:16:LYS:HG2  | 19:17:149:ILE:HG12 | 1.92                     | 0.51              |
| 33:34:66:ARG:HD3  | 85:28:2539:C:H5''  | 1.93                     | 0.51              |
| 44:AS:129:THR:HB  | 44:AS:180:ASP:HA   | 1.93                     | 0.51              |
| 67:S9:86:VAL:HG12 | 67:S9:100:LEU:HD11 | 1.92                     | 0.51              |
| 70:S3:99:ILE:H    | 70:S3:99:ILE:HD13  | 1.75                     | 0.51              |
| 79:18:431:G:C2    | 79:18:432:G:C8     | 2.99                     | 0.51              |
| 79:18:1839:U:H2'  | 79:18:1840:U:C6    | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:v:110:ASP:HB3   | 80:v:553:HIS:HB2   | 1.93                     | 0.51              |
| 80:v:154:VAL:HG12  | 80:v:211:THR:HG22  | 1.93                     | 0.51              |
| 80:v:445:LYS:HG3   | 80:v:478:PHE:CZ    | 2.46                     | 0.51              |
| 85:28:734:G:H1     | 85:28:929:A:H62    | 1.59                     | 0.51              |
| 85:28:3769:C:H2'   | 85:28:3770:U:C6    | 2.46                     | 0.51              |
| 10:L5:60:ILE:HB    | 10:L5:80:ALA:HB2   | 1.93                     | 0.51              |
| 22:21:87:LYS:NZ    | 85:28:4305:G:H22   | 2.09                     | 0.51              |
| 25:26:89:LYS:HG2   | 25:26:90:ALA:H     | 1.76                     | 0.51              |
| 66:S4:80:ILE:HG23  | 66:S4:81:THR:HG23  | 1.92                     | 0.51              |
| 79:18:126:G:N2     | 79:18:180:G:H21    | 2.07                     | 0.51              |
| 85:28:424:U:H2'    | 85:28:425:U:H6     | 1.76                     | 0.51              |
| 85:28:1645:C:H2'   | 85:28:1646:A:C8    | 2.45                     | 0.51              |
| 85:28:2376:A:H2'   | 85:28:2377:C:C6    | 2.46                     | 0.51              |
| 85:28:3707:U:H2'   | 85:28:3708:C:C6    | 2.46                     | 0.51              |
| 85:28:3917:A:H2'   | 85:28:3918:G:C8    | 2.44                     | 0.51              |
| 85:28:4273:A:H2'   | 85:28:4274:A:C8    | 2.46                     | 0.51              |
| 85:28:4356:G:C2    | 85:28:4357:G:C8    | 2.99                     | 0.51              |
| 1:BB:32:PHE:HA     | 1:BB:35:GLU:HG3    | 1.93                     | 0.51              |
| 18:bb:54:TYR:HD1   | 18:bb:145:VAL:HG21 | 1.76                     | 0.51              |
| 77:11:141:ILE:HG23 | 77:11:144:LYS:HE2  | 1.93                     | 0.51              |
| 79:18:152:U:H2'    | 79:18:153:G:H8     | 1.76                     | 0.51              |
| 79:18:454:U:H2'    | 79:18:455:A:C8     | 2.46                     | 0.51              |
| 79:18:1006:C:H2'   | 79:18:1007:C:C6    | 2.45                     | 0.51              |
| 79:18:1030:A:H2'   | 79:18:1031:A:H8    | 1.76                     | 0.51              |
| 79:18:1031:A:H2'   | 79:18:1032:C:C6    | 2.46                     | 0.51              |
| 79:18:1207:G:P     | 79:18:1207:G:H8    | 2.34                     | 0.51              |
| 85:28:1684:A:C4    | 85:28:1685:G:C8    | 2.99                     | 0.51              |
| 85:28:2417:A:C4    | 85:28:2418:A:C8    | 2.98                     | 0.51              |
| 85:28:2591:A:H2'   | 85:28:2592:U:C6    | 2.45                     | 0.51              |
| 85:28:3722:G:H2'   | 85:28:3723:A:H8    | 1.75                     | 0.51              |
| 85:28:4507:A:H2'   | 85:28:4508:C:C6    | 2.46                     | 0.51              |
| 85:28:4563:U:H2'   | 85:28:4564:A:C8    | 2.45                     | 0.51              |
| 51:ZZ:138:ARG:HB2  | 51:ZZ:149:CYS:HA   | 1.93                     | 0.50              |
| 73:S8:98:LYS:HB3   | 79:18:377:G:H5'    | 1.93                     | 0.50              |
| 79:18:394:G:C2     | 79:18:395:G:C8     | 2.99                     | 0.50              |
| 80:v:89:ILE:HG13   | 80:v:91:GLN:H      | 1.76                     | 0.50              |
| 85:28:262:G:H2'    | 85:28:263:G:H8     | 1.76                     | 0.50              |
| 85:28:4178:A:H2'   | 85:28:4179:G:C8    | 2.46                     | 0.50              |
| 85:28:4383:U:H2'   | 85:28:4384:U:C6    | 2.46                     | 0.50              |
| 85:28:4538:G:H2'   | 85:28:4539:U:C6    | 2.47                     | 0.50              |
| 2:S2:66:LEU:HD12   | 2:S2:86:LEU:HD12   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:S3:115:VAL:HG11 | 70:S3:142:LEU:HD21 | 1.93                     | 0.50              |
| 70:S3:141:LYS:HA   | 70:S3:147:ALA:HA   | 1.92                     | 0.50              |
| 79:18:455:A:H2'    | 79:18:456:C:C6     | 2.46                     | 0.50              |
| 85:28:653:C:H2'    | 85:28:654:C:H6     | 1.76                     | 0.50              |
| 85:28:2293:U:H2'   | 85:28:2294:G:C8    | 2.46                     | 0.50              |
| 85:28:2412:A:H2'   | 85:28:2413:U:H6    | 1.76                     | 0.50              |
| 85:28:2640:G:H2'   | 85:28:2641:A:C8    | 2.45                     | 0.50              |
| 85:28:2682:G:H2'   | 85:28:2683:C:C6    | 2.46                     | 0.50              |
| 85:28:4925:U:H1'   | 85:28:4926:C:OP2   | 2.11                     | 0.50              |
| 2:S2:166:ARG:HG2   | 2:S2:181:PRO:HG3   | 1.94                     | 0.50              |
| 28:29:4:SER:HB2    | 85:28:1855:G:OP1   | 2.10                     | 0.50              |
| 54:S5:40:ALA:HB1   | 54:S5:45:TYR:CD2   | 2.46                     | 0.50              |
| 70:S3:107:TYR:HA   | 70:S3:110:LEU:HB2  | 1.92                     | 0.50              |
| 79:18:12:U:H2'     | 79:18:13:C:C6      | 2.46                     | 0.50              |
| 79:18:123:G:H3'    | 79:18:124:U:H5''   | 1.94                     | 0.50              |
| 79:18:441:C:H2'    | 79:18:442:C:H6     | 1.76                     | 0.50              |
| 79:18:1740:C:H2'   | 79:18:1741:U:C6    | 2.47                     | 0.50              |
| 84:ES:2947:G:H1    | 84:ES:3247:A:H2    | 1.54                     | 0.50              |
| 85:28:162:A:H2'    | 85:28:163:A:H8     | 1.75                     | 0.50              |
| 85:28:223:G:H4'    | 85:28:225:G:N7     | 2.25                     | 0.50              |
| 85:28:433:A:C2     | 85:28:3867:A:H4'   | 2.46                     | 0.50              |
| 85:28:2425:U:H5'   | 85:28:2426:U:H5    | 1.76                     | 0.50              |
| 10:L5:146:LEU:HD22 | 85:28:4323:A:H2    | 1.75                     | 0.50              |
| 14:10:22:PHE:CZ    | 85:28:1788:A:H2'   | 2.46                     | 0.50              |
| 24:cc:71:LEU:HG    | 24:cc:76:ILE:HG22  | 1.92                     | 0.50              |
| 45:FF:87:ASP:HB3   | 79:18:924:G:H21    | 1.75                     | 0.50              |
| 52:EE:26:LEU:HD12  | 52:EE:31:LEU:HD21  | 1.93                     | 0.50              |
| 53:TT:50:PHE:CZ    | 53:TT:58:LEU:HD13  | 2.46                     | 0.50              |
| 61:LL:102:GLY:HA2  | 61:LL:105:ASN:HB2  | 1.94                     | 0.50              |
| 79:18:409:C:H2'    | 79:18:410:G:C8     | 2.47                     | 0.50              |
| 79:18:749:U:H2'    | 79:18:750:C:C6     | 2.46                     | 0.50              |
| 85:28:1458:C:C2    | 85:28:1459:A:C8    | 2.99                     | 0.50              |
| 85:28:1846:G:H2'   | 85:28:1847:C:H6    | 1.76                     | 0.50              |
| 85:28:1973:G:OP2   | 85:28:1974:U:H3'   | 2.11                     | 0.50              |
| 85:28:2075:G:H2'   | 85:28:2076:G:H8    | 1.77                     | 0.50              |
| 85:28:4228:G:H5''  | 85:28:4229:U:O4'   | 2.12                     | 0.50              |
| 85:28:4503:A:H2'   | 85:28:4504:C:H6    | 1.77                     | 0.50              |
| 45:FF:110:ASP:O    | 45:FF:114:ARG:HG2  | 2.11                     | 0.50              |
| 48:t:143:VAL:C     | 48:t:145:GLY:H     | 2.19                     | 0.50              |
| 66:S4:257:ALA:HA   | 66:S4:260:GLN:HG3  | 1.94                     | 0.50              |
| 68:S7:146:VAL:HG22 | 68:S7:152:ARG:HG2  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:18:212:C:H2'   | 79:18:213:G:C8     | 2.46                     | 0.50              |
| 79:18:1232:U:H2'  | 79:18:1233:G:C8    | 2.46                     | 0.50              |
| 79:18:1656:G:C2   | 79:18:1657:G:C8    | 2.99                     | 0.50              |
| 85:28:1298:C:H2'  | 85:28:1299:G:C8    | 2.45                     | 0.50              |
| 85:28:2293:U:H2'  | 85:28:2294:G:H8    | 1.77                     | 0.50              |
| 85:28:4688:C:H2'  | 85:28:4689:U:C6    | 2.46                     | 0.50              |
| 50:Q:53:MET:HB3   | 50:Q:57:ASN:HB2    | 1.93                     | 0.50              |
| 56:II:104:SER:HA  | 56:II:107:GLU:HG3  | 1.93                     | 0.50              |
| 68:S7:73:GLN:HA   | 68:S7:76:GLN:HG2   | 1.93                     | 0.50              |
| 85:28:64:A:H1'    | 85:28:76:A:H1'     | 1.92                     | 0.50              |
| 85:28:2290:C:C2   | 85:28:2291:G:C8    | 2.99                     | 0.50              |
| 5:58:141:C:H2'    | 5:58:142:U:C6      | 2.47                     | 0.50              |
| 6:6:59:G:H4'      | 10:L5:267:ASN:HD21 | 1.76                     | 0.50              |
| 7:L8:24:LYS:HG3   | 7:L8:49:ILE:HD12   | 1.93                     | 0.50              |
| 56:II:51:LEU:HD21 | 56:II:81:ILE:HG13  | 1.94                     | 0.50              |
| 79:18:570:C:H2'   | 79:18:571:U:C6     | 2.47                     | 0.50              |
| 79:18:1305:C:H2'  | 79:18:1306:U:C6    | 2.47                     | 0.50              |
| 85:28:1199:G:H2'  | 85:28:1200:G:H8    | 1.76                     | 0.50              |
| 85:28:1333:A:H2'  | 85:28:1334:A:H8    | 1.75                     | 0.50              |
| 85:28:2845:A:H61  | 85:28:3843:C:N4    | 2.10                     | 0.50              |
| 85:28:3707:U:H2'  | 85:28:3708:C:H6    | 1.77                     | 0.50              |
| 10:L5:108:ARG:CZ  | 10:L5:253:TYR:HB2  | 2.42                     | 0.50              |
| 12:L7:103:LYS:O   | 12:L7:107:VAL:HG23 | 2.12                     | 0.50              |
| 20:19:108:ARG:HA  | 20:19:111:GLU:HG2  | 1.93                     | 0.50              |
| 25:26:100:HIS:CD2 | 85:28:231:U:H4'    | 2.46                     | 0.50              |
| 85:28:161:G:H2'   | 85:28:162:A:H8     | 1.76                     | 0.50              |
| 85:28:163:A:H2'   | 85:28:164:G:C8     | 2.47                     | 0.50              |
| 85:28:3832:U:H2'  | 85:28:3833:C:H6    | 1.77                     | 0.50              |
| 85:28:4258:C:H2'  | 85:28:4259:C:H6    | 1.77                     | 0.50              |
| 85:28:4586:G:C2   | 85:28:4587:G:C8    | 3.00                     | 0.50              |
| 85:28:4760:G:H2'  | 85:28:4761:G:O4'   | 2.12                     | 0.50              |
| 5:58:5:U:H2'      | 5:58:6:C:C6        | 2.46                     | 0.50              |
| 7:L8:125:LYS:HB3  | 85:28:3681:G:C6    | 2.47                     | 0.50              |
| 7:L8:209:HIS:CE1  | 7:L8:235:VAL:HG11  | 2.47                     | 0.50              |
| 12:L7:70:MET:HA   | 12:L7:73:MET:HE2   | 1.94                     | 0.50              |
| 60:MM:42:HIS:CD2  | 60:MM:43:LYS:HG2   | 2.47                     | 0.50              |
| 70:S3:59:LEU:HA   | 70:S3:66:ILE:HG13  | 1.93                     | 0.50              |
| 79:18:51:U:H2'    | 79:18:52:G:H8      | 1.77                     | 0.50              |
| 79:18:438:G:H8    | 79:18:1800:A:H4'   | 1.77                     | 0.50              |
| 79:18:1058:A:H8   | 82:CE:12:SER:HB3   | 1.75                     | 0.50              |
| 79:18:1065:G:H2'  | 79:18:1066:U:C6    | 2.46                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:1407:U:H2'   | 79:18:1408:U:H6    | 1.77                     | 0.50              |
| 79:18:1537:A:H2'   | 79:18:1538:C:H6    | 1.76                     | 0.50              |
| 79:18:1653:U:H2'   | 79:18:1654:G:C8    | 2.47                     | 0.50              |
| 84:ES:3239:G:H2'   | 84:ES:3240:A:C8    | 2.43                     | 0.50              |
| 85:28:222:C:H2'    | 85:28:223:G:O4'    | 2.12                     | 0.50              |
| 85:28:287:U:H2'    | 85:28:288:G:H8     | 1.77                     | 0.50              |
| 85:28:1090:G:H2'   | 85:28:1091:C:C6    | 2.47                     | 0.50              |
| 85:28:1463:C:H2'   | 85:28:1464:C:C6    | 2.47                     | 0.50              |
| 85:28:1528:U:H2'   | 85:28:1529:G:C8    | 2.47                     | 0.50              |
| 85:28:1804:A:H4'   | 85:28:1805:A:O5'   | 2.10                     | 0.50              |
| 85:28:1875:C:H2'   | 85:28:1876:U:C6    | 2.47                     | 0.50              |
| 85:28:4595:G:H2'   | 85:28:4596:C:C6    | 2.46                     | 0.50              |
| 2:S2:147:VAL:HB    | 81:LA:682:GLY:HA3  | 1.94                     | 0.49              |
| 5:58:124:U:H4'     | 5:58:125:C:O5'     | 2.10                     | 0.49              |
| 8:L3:303:ALA:HB3   | 8:L3:312:LYS:HG3   | 1.93                     | 0.49              |
| 23:22:62:SER:HB3   | 23:22:73:THR:HG23  | 1.94                     | 0.49              |
| 29:30:29:LEU:HD23  | 29:30:94:LEU:HD13  | 1.94                     | 0.49              |
| 63:RR:107:ARG:HB2  | 63:RR:112:VAL:HG22 | 1.94                     | 0.49              |
| 85:28:1072:C:C2    | 85:28:1073:G:C8    | 3.00                     | 0.49              |
| 85:28:1315:C:H2'   | 85:28:1316:G:H8    | 1.76                     | 0.49              |
| 85:28:1676:C:H41   | 85:28:4378:A:H5''  | 1.77                     | 0.49              |
| 85:28:2610:G:H2'   | 85:28:2611:A:H8    | 1.75                     | 0.49              |
| 85:28:3611:A:H2    | 85:28:5016:A:H8    | 1.60                     | 0.49              |
| 85:28:4346:U:H2'   | 85:28:4347:G:H8    | 1.76                     | 0.49              |
| 2:S2:65:LYS:HA     | 2:S2:68:ARG:HD2    | 1.94                     | 0.49              |
| 17:15:64:ILE:HG21  | 17:15:106:ALA:HB2  | 1.94                     | 0.49              |
| 41:42:64:LYS:HD2   | 85:28:4370:G:H5''  | 1.93                     | 0.49              |
| 54:S5:35:LEU:HD23  | 54:S5:35:LEU:H     | 1.77                     | 0.49              |
| 58:AA:173:LEU:HD22 | 58:AA:189:ILE:HG12 | 1.94                     | 0.49              |
| 71:RS:5:ARG:NH2    | 79:18:1454:A:H5'   | 2.27                     | 0.49              |
| 74:W:6:CYS:HB2     | 74:W:13:ILE:HD11   | 1.95                     | 0.49              |
| 79:18:991:G:C6     | 79:18:1134:G:H4'   | 2.47                     | 0.49              |
| 10:L5:152:ARG:HG3  | 10:L5:154:THR:HG23 | 1.94                     | 0.49              |
| 12:L7:49:ILE:HD12  | 12:L7:185:CYS:HB3  | 1.94                     | 0.49              |
| 12:L7:184:ILE:HG21 | 85:28:2102:G:C6    | 2.47                     | 0.49              |
| 17:15:172:ARG:HG2  | 85:28:29:G:H5''    | 1.94                     | 0.49              |
| 18:bb:26:GLN:HG3   | 21:20:167:PHE:HZ   | 1.77                     | 0.49              |
| 31:32:90:MET:HE2   | 31:32:90:MET:HA    | 1.94                     | 0.49              |
| 32:ee:47:CYS:HB3   | 32:ee:103:VAL:HG12 | 1.94                     | 0.49              |
| 44:AS:35:ALA:HB2   | 44:AS:44:ILE:HD11  | 1.93                     | 0.49              |
| 45:FF:55:ARG:HE    | 79:18:1017:U:H5'   | 1.77                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:F:191:LYS:HB2   | 49:F:194:VAL:HB    | 1.95                     | 0.49              |
| 54:S5:125:SER:HA   | 54:S5:138:ALA:HA   | 1.95                     | 0.49              |
| 67:S9:42:GLU:HA    | 67:S9:45:ARG:HB3   | 1.94                     | 0.49              |
| 79:18:350:C:C2     | 79:18:351:G:C8     | 3.00                     | 0.49              |
| 79:18:1128:C:H2'   | 79:18:1129:G:C8    | 2.47                     | 0.49              |
| 79:18:1627:C:H2'   | 79:18:1628:C:H6    | 1.76                     | 0.49              |
| 79:18:1750:C:H2'   | 79:18:1751:C:H6    | 1.77                     | 0.49              |
| 80:v:310:GLU:HG2   | 80:v:311:GLU:N     | 2.26                     | 0.49              |
| 85:28:1306:C:H2'   | 85:28:1307:A:C8    | 2.41                     | 0.49              |
| 85:28:2402:G:C2    | 85:28:2403:A:C8    | 3.00                     | 0.49              |
| 85:28:3607:U:H2'   | 85:28:3608:A:C8    | 2.47                     | 0.49              |
| 85:28:4495:G:C2    | 85:28:4496:A:N7    | 2.80                     | 0.49              |
| 5:58:5:U:H2'       | 5:58:6:C:H6        | 1.77                     | 0.49              |
| 13:aa:195:THR:O    | 13:aa:199:LEU:HG   | 2.11                     | 0.49              |
| 58:AA:292:SER:HB2  | 58:AA:297:THR:HB   | 1.93                     | 0.49              |
| 60:MM:22:LEU:HB3   | 60:MM:28:LEU:HD11  | 1.95                     | 0.49              |
| 68:S7:36:LEU:HD22  | 68:S7:75:ILE:HD11  | 1.93                     | 0.49              |
| 76:UU:17:HIS:HB3   | 79:18:999:G:N7     | 2.26                     | 0.49              |
| 79:18:166:A:C6     | 79:18:167:G:N7     | 2.80                     | 0.49              |
| 79:18:1017:U:H2'   | 79:18:1018:U:C6    | 2.48                     | 0.49              |
| 85:28:673:C:C2     | 85:28:674:G:C8     | 3.01                     | 0.49              |
| 85:28:1094:G:H1    | 85:28:1202:C:H42   | 1.61                     | 0.49              |
| 85:28:4178:A:H2'   | 85:28:4179:G:H8    | 1.77                     | 0.49              |
| 85:28:5002:U:H2'   | 85:28:5003:U:H6    | 1.76                     | 0.49              |
| 13:aa:139:VAL:HG23 | 13:aa:236:ILE:HG22 | 1.95                     | 0.49              |
| 13:aa:317:LYS:HE3  | 44:AS:225:LEU:HB2  | 1.95                     | 0.49              |
| 19:17:54:LYS:HA    | 19:17:83:TRP:CD1   | 2.47                     | 0.49              |
| 63:RR:60:LYS:HB2   | 63:RR:114:ASP:OD1  | 2.12                     | 0.49              |
| 79:18:87:U:C2      | 79:18:88:G:C8      | 3.01                     | 0.49              |
| 79:18:1126:G:H2'   | 79:18:1127:C:C6    | 2.47                     | 0.49              |
| 85:28:125:C:H2'    | 85:28:126:C:H6     | 1.76                     | 0.49              |
| 85:28:325:U:H2'    | 85:28:326:C:C6     | 2.47                     | 0.49              |
| 85:28:4244:A:H2'   | 85:28:4245:G:O4'   | 2.12                     | 0.49              |
| 4:DD:96:ILE:HD12   | 63:RR:10:ALA:HB1   | 1.95                     | 0.49              |
| 8:L3:55:HIS:HB2    | 8:L3:369:ASP:HB2   | 1.95                     | 0.49              |
| 44:AS:146:ARG:HD3  | 44:AS:206:PRO:HG3  | 1.95                     | 0.49              |
| 47:s:98:ILE:HG13   | 47:s:101:MET:HE3   | 1.93                     | 0.49              |
| 67:S9:117:LEU:HD23 | 67:S9:119:LEU:HD11 | 1.95                     | 0.49              |
| 79:18:812:A:C5     | 79:18:813:A:C8     | 3.00                     | 0.49              |
| 79:18:1189:A:H2'   | 79:18:1190:A:C8    | 2.47                     | 0.49              |
| 79:18:1739:C:H2'   | 79:18:1740:C:C6    | 2.47                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:1824:G:H2'   | 85:28:1825:A:C8    | 2.47                     | 0.49              |
| 85:28:2308:A:H4'   | 85:28:2334:C:H4'   | 1.94                     | 0.49              |
| 85:28:2683:C:H2'   | 85:28:2684:C:H6    | 1.77                     | 0.49              |
| 85:28:3930:U:H2'   | 85:28:3931:C:C6    | 2.47                     | 0.49              |
| 26:27:51:ARG:HB2   | 26:27:65:ARG:HG3   | 1.93                     | 0.49              |
| 48:t:59:THR:HG23   | 48:t:74:VAL:HB     | 1.94                     | 0.49              |
| 79:18:441:C:H2'    | 79:18:442:C:C6     | 2.47                     | 0.49              |
| 79:18:600:G:C2     | 79:18:601:G:C8     | 3.00                     | 0.49              |
| 79:18:1457:U:H2'   | 79:18:1458:G:C8    | 2.48                     | 0.49              |
| 79:18:1712:A:H2'   | 79:18:1713:C:H6    | 1.78                     | 0.49              |
| 85:28:734:G:H1     | 85:28:929:A:N6     | 2.11                     | 0.49              |
| 5:58:65:A:C4       | 5:58:66:A:C8       | 3.01                     | 0.49              |
| 14:10:91:LEU:HD12  | 14:10:135:ILE:HG23 | 1.95                     | 0.49              |
| 79:18:17:C:H2'     | 79:18:18:C:C6      | 2.48                     | 0.49              |
| 79:18:354:U:H2'    | 79:18:355:G:H8     | 1.78                     | 0.49              |
| 79:18:1365:G:H2'   | 79:18:1366:G:C8    | 2.48                     | 0.49              |
| 85:28:58:G:H4'     | 85:28:59:A:H4'     | 1.95                     | 0.49              |
| 85:28:699:C:H2'    | 85:28:700:G:H8     | 1.77                     | 0.49              |
| 85:28:2404:A:H61   | 85:28:2787:A:H61   | 1.59                     | 0.49              |
| 85:28:3770:U:H2'   | 85:28:3771:C:C6    | 2.47                     | 0.49              |
| 85:28:4208:U:H2'   | 85:28:4209:G:C8    | 2.48                     | 0.49              |
| 85:28:4406:U:C2    | 85:28:4407:G:C8    | 3.00                     | 0.49              |
| 6:6:3:C:H2'        | 6:6:4:U:H6         | 1.76                     | 0.49              |
| 6:6:23:A:H2'       | 6:6:24:C:C6        | 2.48                     | 0.49              |
| 58:AA:154:VAL:HG12 | 58:AA:167:SER:HB2  | 1.95                     | 0.49              |
| 77:11:110:GLN:HG2  | 77:11:111:GLU:HG2  | 1.95                     | 0.49              |
| 79:18:15:U:H2'     | 79:18:16:G:O4'     | 2.13                     | 0.49              |
| 79:18:37:C:H2'     | 79:18:38:A:O4'     | 2.13                     | 0.49              |
| 79:18:1348:G:C8    | 79:18:1349:G:C8    | 3.01                     | 0.49              |
| 79:18:1482:C:H2'   | 79:18:1483:A:O4'   | 2.13                     | 0.49              |
| 79:18:1706:G:H2'   | 79:18:1707:U:H6    | 1.76                     | 0.49              |
| 84:ES:3242:U:H2'   | 84:ES:3243:C:C6    | 2.48                     | 0.49              |
| 85:28:271:C:H2'    | 85:28:272:U:H6     | 1.77                     | 0.49              |
| 85:28:1617:G:H1'   | 85:28:2513:A:N6    | 2.28                     | 0.49              |
| 85:28:1662:C:H2'   | 85:28:1663:C:C6    | 2.47                     | 0.49              |
| 85:28:2780:C:H2'   | 85:28:2781:G:H8    | 1.78                     | 0.49              |
| 85:28:4460:U:H2'   | 85:28:4461:C:H6    | 1.77                     | 0.49              |
| 85:28:5003:U:H2'   | 85:28:5004:C:C6    | 2.47                     | 0.49              |
| 6:6:36:C:H2'       | 6:6:37:G:C8        | 2.47                     | 0.49              |
| 8:L3:321:VAL:HG12  | 8:L3:322:HIS:HD1   | 1.78                     | 0.49              |
| 15:13:182:LEU:HD23 | 35:36:7:MET:HE3    | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:t:128:THR:HA   | 48:t:131:GLU:HG2   | 1.94                     | 0.49              |
| 50:Q:67:ILE:HD13  | 50:Q:98:LEU:HD11   | 1.95                     | 0.49              |
| 63:RR:86:PRO:HG2  | 63:RR:130:LEU:HD22 | 1.94                     | 0.49              |
| 79:18:356:C:O2    | 79:18:356:C:H2'    | 2.13                     | 0.49              |
| 79:18:1651:A:H2'  | 79:18:1652:G:H8    | 1.78                     | 0.49              |
| 85:28:1398:A:H61  | 85:28:1419:G:H2'   | 1.78                     | 0.49              |
| 85:28:2080:U:H2'  | 85:28:2081:C:H6    | 1.78                     | 0.49              |
| 85:28:2895:A:H2'  | 85:28:2896:G:H8    | 1.77                     | 0.49              |
| 1:BB:201:LEU:HD11 | 71:RS:83:ASN:HA    | 1.95                     | 0.48              |
| 8:L3:57:VAL:HG22  | 8:L3:73:VAL:HG12   | 1.95                     | 0.48              |
| 49:F:174:ALA:HB2  | 49:F:181:PRO:HD3   | 1.94                     | 0.48              |
| 60:MM:85:ASN:HB2  | 60:MM:88:MET:HB2   | 1.95                     | 0.48              |
| 61:LL:40:TYR:HA   | 61:LL:43:VAL:HG22  | 1.93                     | 0.48              |
| 79:18:1101:U:C2   | 79:18:1102:G:N7    | 2.81                     | 0.48              |
| 79:18:1159:G:H2'  | 79:18:1160:U:C6    | 2.48                     | 0.48              |
| 79:18:1199:A:H2'  | 79:18:1200:A:C8    | 2.48                     | 0.48              |
| 79:18:1688:C:H2'  | 79:18:1689:C:C6    | 2.48                     | 0.48              |
| 85:28:1565:A:C5   | 85:28:1566:C:H1'   | 2.48                     | 0.48              |
| 85:28:5042:A:C4   | 85:28:5043:A:C8    | 3.01                     | 0.48              |
| 2:S2:104:ASP:HB3  | 2:S2:130:ILE:HG13  | 1.95                     | 0.48              |
| 47:s:34:ASN:HA    | 85:28:1968:G:O2'   | 2.12                     | 0.48              |
| 78:L9:129:ARG:HG2 | 78:L9:153:LEU:HD22 | 1.95                     | 0.48              |
| 79:18:1673:U:H2'  | 79:18:1674:G:O4'   | 2.13                     | 0.48              |
| 80:v:208:VAL:HG12 | 80:v:261:TRP:HB3   | 1.95                     | 0.48              |
| 85:28:490:C:H2'   | 85:28:491:G:C8     | 2.48                     | 0.48              |
| 85:28:654:C:H2'   | 85:28:655:C:H6     | 1.78                     | 0.48              |
| 85:28:1564:A:H2'  | 85:28:1565:A:C8    | 2.48                     | 0.48              |
| 85:28:1804:A:H5'' | 85:28:1806:G:C8    | 2.49                     | 0.48              |
| 85:28:2870:A:H2'  | 85:28:2871:A:C8    | 2.48                     | 0.48              |
| 85:28:3855:C:H2'  | 85:28:3856:A:H8    | 1.78                     | 0.48              |
| 85:28:4552:U:H2'  | 85:28:4553:A:C8    | 2.49                     | 0.48              |
| 85:28:4593:C:H2'  | 85:28:4594:U:H6    | 1.76                     | 0.48              |
| 85:28:4973:U:H2'  | 85:28:4974:C:C6    | 2.48                     | 0.48              |
| 8:L3:261:ARG:HB2  | 18:bb:64:THR:HG21  | 1.94                     | 0.48              |
| 10:L5:33:ARG:HA   | 10:L5:36:LEU:HB2   | 1.95                     | 0.48              |
| 10:L5:53:VAL:HB   | 10:L5:159:VAL:HG13 | 1.95                     | 0.48              |
| 49:F:75:ALA:HB1   | 49:F:118:ILE:HG23  | 1.96                     | 0.48              |
| 56:II:31:LEU:HD21 | 56:II:33:LYS:HE3   | 1.95                     | 0.48              |
| 79:18:319:C:H4'   | 79:18:319:C:OP1    | 2.11                     | 0.48              |
| 79:18:1628:C:H2'  | 79:18:1629:C:H6    | 1.79                     | 0.48              |
| 85:28:684:G:H5'   | 85:28:685:C:OP2    | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:28:2602:G:H2'  | 85:28:2603:C:C6   | 2.48                     | 0.48              |
| 85:28:3870:C:H2'  | 85:28:3871:A:C8   | 2.49                     | 0.48              |
| 85:28:3920:U:H2'  | 85:28:3921:U:C6   | 2.48                     | 0.48              |
| 85:28:4400:G:C6   | 85:28:4401:G:N7   | 2.81                     | 0.48              |
| 85:28:5031:G:H2'  | 85:28:5032:C:C6   | 2.48                     | 0.48              |
| 2:S2:106:VAL:HG22 | 2:S2:128:VAL:HG22 | 1.95                     | 0.48              |
| 5:58:127:U:H2'    | 5:58:128:C:O4'    | 2.12                     | 0.48              |
| 8:L3:301:ASN:HB3  | 8:L3:311:ASP:HA   | 1.94                     | 0.48              |
| 9:L4:230:LEU:HD11 | 9:L4:239:LYS:HB2  | 1.95                     | 0.48              |
| 62:XX:21:CYS:HA   | 62:XX:30:LEU:HD11 | 1.95                     | 0.48              |
| 79:18:644:G:H2'   | 79:18:645:C:C6    | 2.47                     | 0.48              |
| 79:18:1712:A:H2'  | 79:18:1713:C:C6   | 2.48                     | 0.48              |
| 80:v:26:ALA:HB2   | 80:v:128:VAL:HB   | 1.96                     | 0.48              |
| 85:28:271:C:H2'   | 85:28:272:U:C6    | 2.49                     | 0.48              |
| 85:28:422:C:H2'   | 85:28:423:G:H8    | 1.79                     | 0.48              |
| 85:28:1192:C:H2'  | 85:28:1193:C:C6   | 2.48                     | 0.48              |
| 85:28:1308:C:H2'  | 85:28:1309:C:C6   | 2.48                     | 0.48              |
| 85:28:1739:G:H2'  | 85:28:1740:C:C6   | 2.47                     | 0.48              |
| 85:28:1802:A:H5'' | 85:28:1803:G:H5'  | 1.93                     | 0.48              |
| 85:28:2561:C:H42  | 85:28:2566:G:H1   | 1.61                     | 0.48              |
| 85:28:3654:G:H22  | 85:28:3817:A:H2   | 1.61                     | 0.48              |
| 85:28:3769:C:H2'  | 85:28:3770:U:H6   | 1.79                     | 0.48              |
| 30:31:64:ILE:HD11 | 85:28:2373:C:H4'  | 1.95                     | 0.48              |
| 41:42:9:ARG:HA    | 41:42:20:PRO:HA   | 1.94                     | 0.48              |
| 44:AS:48:LEU:HG   | 75:GG:51:GLU:HG2  | 1.95                     | 0.48              |
| 47:s:57:LYS:HB3   | 47:s:60:MET:HB3   | 1.94                     | 0.48              |
| 58:AA:18:VAL:HA   | 58:AA:35:SER:HA   | 1.94                     | 0.48              |
| 58:AA:277:THR:HB  | 58:AA:281:ALA:HB3 | 1.95                     | 0.48              |
| 79:18:574:A:H2'   | 79:18:574:A:N3    | 2.29                     | 0.48              |
| 79:18:1102:G:H2'  | 79:18:1103:C:H6   | 1.79                     | 0.48              |
| 79:18:1253:A:H4'  | 79:18:1254:C:H5'' | 1.96                     | 0.48              |
| 79:18:1667:U:H2'  | 79:18:1668:U:C6   | 2.49                     | 0.48              |
| 80:v:389:ASP:HB2  | 80:v:391:LYS:HE3  | 1.95                     | 0.48              |
| 80:v:683:PHE:O    | 80:v:687:THR:HG22 | 2.14                     | 0.48              |
| 85:28:1191:C:H2'  | 85:28:1192:C:H6   | 1.79                     | 0.48              |
| 85:28:1744:U:C2   | 85:28:1745:G:C8   | 3.01                     | 0.48              |
| 85:28:4584:A:H2'  | 85:28:4585:U:O4'  | 2.12                     | 0.48              |
| 85:28:4594:U:C2   | 85:28:4595:G:C8   | 3.01                     | 0.48              |
| 85:28:4708:A:N3   | 85:28:4709:U:H5'  | 2.29                     | 0.48              |
| 85:28:5043:A:H2'  | 85:28:5044:A:C8   | 2.49                     | 0.48              |
| 14:10:31:ILE:HG22 | 14:10:62:SER:HB2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:27:51:ARG:HD2  | 26:27:65:ARG:HD2  | 1.95                     | 0.48              |
| 31:32:35:TRP:CZ2  | 31:32:56:PRO:HD2  | 2.49                     | 0.48              |
| 42:ff:7:LYS:HE2   | 85:28:2875:C:H2'  | 1.95                     | 0.48              |
| 59:OO:67:LYS:HB3  | 79:18:1337:C:H4'  | 1.95                     | 0.48              |
| 66:S4:7:LYS:HB2   | 79:18:93:U:O2'    | 2.13                     | 0.48              |
| 79:18:26:U:H2'    | 79:18:27:A:C8     | 2.49                     | 0.48              |
| 79:18:348:A:H2'   | 79:18:349:A:C8    | 2.49                     | 0.48              |
| 79:18:673:G:H2'   | 79:18:674:C:C6    | 2.49                     | 0.48              |
| 79:18:677:G:H2'   | 79:18:678:U:C6    | 2.49                     | 0.48              |
| 79:18:1198:G:H2'  | 79:18:1199:A:H8   | 1.78                     | 0.48              |
| 85:28:478:G:H2'   | 85:28:479:G:C8    | 2.48                     | 0.48              |
| 85:28:711:A:H2'   | 85:28:712:C:C6    | 2.48                     | 0.48              |
| 85:28:1557:C:H2'  | 85:28:1558:A:C8   | 2.49                     | 0.48              |
| 85:28:2689:C:H2'  | 85:28:2690:C:C6   | 2.48                     | 0.48              |
| 85:28:4254:G:H2'  | 85:28:4254:G:N3   | 2.28                     | 0.48              |
| 2:S2:272:HIS:HA   | 2:S2:275:LYS:HG2  | 1.96                     | 0.48              |
| 6:6:83:A:H4'      | 12:L7:223:THR:HB  | 1.95                     | 0.48              |
| 10:L5:181:PRO:HG2 | 10:L5:195:HIS:HD2 | 1.79                     | 0.48              |
| 17:15:5:LYS:NZ    | 35:36:37:THR:HG22 | 2.28                     | 0.48              |
| 26:27:95:VAL:HG12 | 26:27:110:ALA:HA  | 1.95                     | 0.48              |
| 32:ee:106:TYR:CD1 | 32:ee:107:PRO:HD3 | 2.49                     | 0.48              |
| 61:LL:137:LYS:HE2 | 79:18:1234:C:N4   | 2.28                     | 0.48              |
| 79:18:379:C:H2'   | 79:18:380:G:C8    | 2.49                     | 0.48              |
| 79:18:958:G:H2'   | 79:18:959:G:O4'   | 2.13                     | 0.48              |
| 80:v:551:GLU:O    | 80:v:555:GLU:HG2  | 2.14                     | 0.48              |
| 85:28:648:G:H2'   | 85:28:649:A:H8    | 1.79                     | 0.48              |
| 85:28:2589:C:C2   | 85:28:2590:G:C8   | 3.02                     | 0.48              |
| 6:6:2:U:H2'       | 6:6:3:C:C6        | 2.49                     | 0.48              |
| 44:AS:57:ILE:HB   | 44:AS:60:ASP:HB3  | 1.95                     | 0.48              |
| 61:LL:108:ARG:NH1 | 61:LL:109:GLU:HA  | 2.29                     | 0.48              |
| 73:S8:22:HIS:HB3  | 79:18:433:A:H5''  | 1.95                     | 0.48              |
| 79:18:220:U:H2'   | 79:18:221:A:H8    | 1.78                     | 0.48              |
| 79:18:349:A:H2'   | 79:18:350:C:C6    | 2.49                     | 0.48              |
| 79:18:482:G:N2    | 79:18:484:A:H3'   | 2.28                     | 0.48              |
| 79:18:1092:G:C2   | 79:18:1093:A:N7   | 2.81                     | 0.48              |
| 79:18:1230:C:H2'  | 79:18:1231:C:C6   | 2.48                     | 0.48              |
| 79:18:1347:U:H3'  | 79:18:1348:G:H21  | 1.79                     | 0.48              |
| 85:28:469:C:H2'   | 85:28:470:A:C8    | 2.46                     | 0.48              |
| 85:28:4345:C:H2'  | 85:28:4346:U:H6   | 1.78                     | 0.48              |
| 85:28:4605:A:H2'  | 85:28:4606:G:O4'  | 2.14                     | 0.48              |
| 85:28:4737:G:H2'  | 85:28:4738:C:C6   | 2.49                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:28:4890:G:H2'  | 85:28:4891:G:H8    | 1.78                     | 0.48              |
| 7:L8:244:GLY:HA3  | 85:28:3746:A:H5''  | 1.96                     | 0.48              |
| 7:L8:249:THR:HG22 | 79:18:1044:G:C8    | 2.49                     | 0.48              |
| 19:17:28:ASN:O    | 19:17:32:THR:HG22  | 2.14                     | 0.48              |
| 38:39:8:ARG:H     | 38:39:8:ARG:HD2    | 1.79                     | 0.48              |
| 49:F:21:TYR:CD1   | 49:F:324:LEU:HD21  | 2.49                     | 0.48              |
| 49:F:121:VAL:HB   | 49:F:334:THR:HB    | 1.95                     | 0.48              |
| 52:EE:22:LEU:HD21 | 52:EE:89:VAL:HB    | 1.96                     | 0.48              |
| 70:S3:161:GLY:CA  | 79:18:1388:A:H61   | 2.27                     | 0.48              |
| 75:GG:99:ALA:N    | 75:GG:133:THR:HG22 | 2.29                     | 0.48              |
| 79:18:1031:A:H2'  | 79:18:1032:C:H6    | 1.79                     | 0.48              |
| 85:28:1846:G:H2'  | 85:28:1847:C:C6    | 2.49                     | 0.48              |
| 85:28:2079:G:H2'  | 85:28:2080:U:H6    | 1.78                     | 0.48              |
| 5:58:132:G:H2'    | 5:58:133:G:H8      | 1.79                     | 0.48              |
| 6:6:15:C:H2'      | 6:6:16:A:H8        | 1.79                     | 0.48              |
| 6:6:16:A:H2'      | 6:6:17:C:C6        | 2.49                     | 0.48              |
| 24:cc:87:MET:HG3  | 49:F:291:MET:HE1   | 1.95                     | 0.48              |
| 30:31:68:LEU:HA   | 30:31:108:TYR:HB2  | 1.96                     | 0.48              |
| 79:18:557:U:H2'   | 79:18:558:G:C8     | 2.49                     | 0.48              |
| 85:28:519:C:H2'   | 85:28:520:U:C6     | 2.49                     | 0.48              |
| 85:28:4400:G:C2   | 85:28:4401:G:C8    | 3.02                     | 0.48              |
| 6:6:112:U:H2'     | 6:6:113:G:H8       | 1.79                     | 0.47              |
| 9:L4:28:PHE:HA    | 9:L4:129:ALA:HA    | 1.96                     | 0.47              |
| 9:L4:221:PHE:HB3  | 9:L4:227:ILE:HG21  | 1.96                     | 0.47              |
| 44:AS:115:LYS:H   | 44:AS:118:GLN:NE2  | 2.11                     | 0.47              |
| 61:LL:120:HIS:HD2 | 83:A:121:ILE:HG22  | 1.79                     | 0.47              |
| 67:S9:164:PRO:HB3 | 67:S9:170:PRO:HA   | 1.96                     | 0.47              |
| 68:S7:69:LEU:HD13 | 68:S7:96:ALA:HB2   | 1.96                     | 0.47              |
| 79:18:1297:U:H2'  | 79:18:1298:G:H2'   | 1.96                     | 0.47              |
| 79:18:1568:C:H2'  | 79:18:1569:A:C8    | 2.48                     | 0.47              |
| 79:18:1628:C:H2'  | 79:18:1629:C:C6    | 2.48                     | 0.47              |
| 79:18:1839:U:H2'  | 79:18:1840:U:H6    | 1.79                     | 0.47              |
| 85:28:1447:C:H2'  | 85:28:1448:G:H8    | 1.79                     | 0.47              |
| 85:28:1463:C:H2'  | 85:28:1464:C:H6    | 1.78                     | 0.47              |
| 85:28:1831:G:H2'  | 85:28:1832:C:O4'   | 2.14                     | 0.47              |
| 85:28:4737:G:H2'  | 85:28:4738:C:H6    | 1.79                     | 0.47              |
| 85:28:4970:C:H2'  | 85:28:4971:A:H8    | 1.77                     | 0.47              |
| 85:28:5043:A:H2'  | 85:28:5044:A:H8    | 1.79                     | 0.47              |
| 2:S2:272:HIS:O    | 2:S2:276:THR:HG22  | 2.15                     | 0.47              |
| 4:DD:101:ARG:HD2  | 63:RR:6:GLY:O      | 2.14                     | 0.47              |
| 9:L4:339:THR:HA   | 9:L4:342:ARG:HB3   | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:L7:79:ASN:HA    | 22:21:143:THR:HG22 | 1.96                     | 0.47              |
| 66:S4:189:LEU:HD12 | 66:S4:190:GLY:H    | 1.79                     | 0.47              |
| 68:S7:63:PHE:HB3   | 68:S7:97:GLN:HB2   | 1.95                     | 0.47              |
| 79:18:160:U:H3'    | 79:18:161:U:H5''   | 1.96                     | 0.47              |
| 79:18:478:G:H2'    | 79:18:479:C:C6     | 2.50                     | 0.47              |
| 79:18:900:C:H2'    | 79:18:901:G:C8     | 2.50                     | 0.47              |
| 79:18:901:G:H2'    | 79:18:902:G:H8     | 1.78                     | 0.47              |
| 79:18:1384:C:C2    | 79:18:1385:G:C8    | 3.02                     | 0.47              |
| 85:28:2744:A:H2'   | 85:28:2745:A:H8    | 1.75                     | 0.47              |
| 85:28:4130:C:H2'   | 85:28:4131:G:H8    | 1.79                     | 0.47              |
| 85:28:4346:U:H2'   | 85:28:4347:G:C8    | 2.48                     | 0.47              |
| 8:L3:45:ALA:HB3    | 8:L3:183:ILE:HG23  | 1.96                     | 0.47              |
| 8:L3:161:ARG:HG2   | 8:L3:184:GLN:HA    | 1.97                     | 0.47              |
| 13:aa:215:ASP:HB2  | 13:aa:216:PRO:HD3  | 1.96                     | 0.47              |
| 16:14:89:THR:HG22  | 16:14:91:TRP:H     | 1.79                     | 0.47              |
| 49:F:32:LEU:HA     | 49:F:35:LEU:HG     | 1.97                     | 0.47              |
| 58:AA:64:HIS:HB3   | 58:AA:83:TRP:HB2   | 1.96                     | 0.47              |
| 60:MM:48:TYR:HB2   | 79:18:1539:U:H1'   | 1.95                     | 0.47              |
| 73:S8:129:LEU:HD23 | 73:S8:132:GLU:H    | 1.79                     | 0.47              |
| 79:18:939:U:H2'    | 79:18:940:U:C6     | 2.48                     | 0.47              |
| 83:A:38:SER:HB3    | 83:A:41:GLN:OE1    | 2.15                     | 0.47              |
| 85:28:1077:C:C4    | 85:28:1078:A:N7    | 2.83                     | 0.47              |
| 85:28:1447:C:H2'   | 85:28:1448:G:C8    | 2.49                     | 0.47              |
| 85:28:2051:C:H2'   | 85:28:2052:G:O4'   | 2.14                     | 0.47              |
| 85:28:3690:U:H2'   | 85:28:3691:G:O4'   | 2.13                     | 0.47              |
| 85:28:4235:G:C2    | 85:28:4236:G:C8    | 3.03                     | 0.47              |
| 1:BB:39:TYR:CE2    | 71:RS:105:MET:HB3  | 2.49                     | 0.47              |
| 27:dd:35:ALA:HB2   | 85:28:38:A:H5''    | 1.97                     | 0.47              |
| 46:VV:20:LYS:HG3   | 46:VV:21:LYS:HG2   | 1.96                     | 0.47              |
| 60:MM:18:LEU:HD13  | 60:MM:134:ILE:HD13 | 1.97                     | 0.47              |
| 60:MM:67:ARG:HD3   | 79:18:1587:G:N7    | 2.29                     | 0.47              |
| 61:LL:88:LYS:HG2   | 83:A:18:ARG:HD3    | 1.96                     | 0.47              |
| 68:S7:7:LYS:HB3    | 68:S7:44:ASN:HA    | 1.96                     | 0.47              |
| 79:18:569:A:H2'    | 79:18:570:C:C6     | 2.50                     | 0.47              |
| 80:v:669:VAL:HG21  | 80:v:707:VAL:HG22  | 1.96                     | 0.47              |
| 85:28:270:U:H2'    | 85:28:271:C:C6     | 2.48                     | 0.47              |
| 85:28:731:G:C6     | 85:28:932:A:C4     | 3.02                     | 0.47              |
| 85:28:2547:G:H2'   | 85:28:2548:C:C6    | 2.49                     | 0.47              |
| 85:28:4454:G:H2'   | 85:28:4455:G:H8    | 1.80                     | 0.47              |
| 24:cc:140:LEU:HD11 | 24:cc:149:VAL:HG21 | 1.96                     | 0.47              |
| 41:42:44:LYS:HE3   | 41:42:52:THR:HB    | 1.97                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 65:S6:131:ARG:HB3 | 79:18:168:C:O2'    | 2.15                     | 0.47              |
| 77:11:127:GLY:HA3 | 85:28:4251:A:C2    | 2.50                     | 0.47              |
| 79:18:527:C:H2'   | 79:18:528:A:H8     | 1.79                     | 0.47              |
| 79:18:1112:U:H2'  | 79:18:1113:A:C8    | 2.50                     | 0.47              |
| 79:18:1278:A:C6   | 79:18:1320:G:C6    | 3.02                     | 0.47              |
| 79:18:1531:A:H2'  | 79:18:1532:C:C6    | 2.49                     | 0.47              |
| 79:18:1687:C:H2'  | 79:18:1688:C:C6    | 2.49                     | 0.47              |
| 85:28:60:A:C4     | 85:28:61:A:C8      | 3.03                     | 0.47              |
| 85:28:490:C:H2'   | 85:28:491:G:H8     | 1.79                     | 0.47              |
| 85:28:2749:C:H2'  | 85:28:2750:G:C8    | 2.49                     | 0.47              |
| 85:28:4734:A:H1'  | 85:28:4735:G:C8    | 2.49                     | 0.47              |
| 17:15:120:TRP:HZ2 | 17:15:123:GLU:HG2  | 1.80                     | 0.47              |
| 34:35:112:ARG:HG2 | 85:28:173:C:H1'    | 1.96                     | 0.47              |
| 38:39:23:ILE:HG23 | 38:39:38:ASN:HB2   | 1.97                     | 0.47              |
| 38:39:43:HIS:HE2  | 85:28:2429:A:H5''  | 1.79                     | 0.47              |
| 65:S6:2:LYS:HD2   | 65:S6:15:LEU:HD21  | 1.96                     | 0.47              |
| 75:GG:78:ALA:O    | 75:GG:81:VAL:HG12  | 2.15                     | 0.47              |
| 78:L9:20:LEU:HB3  | 78:L9:25:VAL:HG12  | 1.96                     | 0.47              |
| 79:18:22:A:C2     | 79:18:23:G:C8      | 3.03                     | 0.47              |
| 79:18:928:G:H2'   | 79:18:929:G:C8     | 2.49                     | 0.47              |
| 79:18:1046:U:H2'  | 79:18:1047:C:C6    | 2.49                     | 0.47              |
| 80:v:503:PRO:HB2  | 80:v:547:ALA:HB1   | 1.96                     | 0.47              |
| 85:28:652:G:H2'   | 85:28:653:C:H6     | 1.79                     | 0.47              |
| 85:28:1346:C:H2'  | 85:28:1347:G:C8    | 2.49                     | 0.47              |
| 85:28:2633:U:H2'  | 85:28:2634:C:C6    | 2.50                     | 0.47              |
| 85:28:2635:U:C4   | 85:28:2636:U:C4    | 3.02                     | 0.47              |
| 85:28:3904:G:H1'  | 85:28:3905:A:OP1   | 2.13                     | 0.47              |
| 85:28:4197:G:C4   | 85:28:4198:G:C8    | 3.02                     | 0.47              |
| 85:28:4266:G:H2'  | 85:28:4266:G:N3    | 2.30                     | 0.47              |
| 85:28:5031:G:H2'  | 85:28:5032:C:H6    | 1.79                     | 0.47              |
| 86:23:13:LYS:HB2  | 86:23:128:LEU:HD21 | 1.95                     | 0.47              |
| 5:58:142:U:C2     | 5:58:143:G:C8      | 3.02                     | 0.47              |
| 6:6:51:G:H21      | 77:11:12:MET:HE3   | 1.80                     | 0.47              |
| 7:L8:116:LEU:HA   | 7:L8:164:ALA:HB2   | 1.97                     | 0.47              |
| 12:L7:222:LYS:HE3 | 85:28:1907:A:H4'   | 1.97                     | 0.47              |
| 16:14:9:VAL:HG11  | 16:14:66:HIS:HA    | 1.96                     | 0.47              |
| 17:15:86:HIS:CE1  | 85:28:33:A:H5'     | 2.49                     | 0.47              |
| 54:S5:31:ASN:HB2  | 54:S5:117:ILE:HD13 | 1.97                     | 0.47              |
| 58:AA:214:GLY:HA2 | 58:AA:236:ILE:HG12 | 1.96                     | 0.47              |
| 61:LL:43:VAL:HG11 | 61:LL:83:PHE:CZ    | 2.49                     | 0.47              |
| 79:18:14:C:H2'    | 79:18:15:U:H6      | 1.76                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:18:23:G:C4     | 79:18:24:C:C5     | 3.02                     | 0.47              |
| 79:18:319:C:H2'   | 79:18:320:G:H8    | 1.80                     | 0.47              |
| 79:18:399:C:H3'   | 79:18:400:C:H5'   | 1.95                     | 0.47              |
| 79:18:465:A:H5''  | 79:18:466:G:C4    | 2.49                     | 0.47              |
| 79:18:527:C:H2'   | 79:18:528:A:C8    | 2.50                     | 0.47              |
| 79:18:1174:U:H2'  | 79:18:1175:G:C8   | 2.50                     | 0.47              |
| 79:18:1236:G:H2'  | 79:18:1237:C:C6   | 2.49                     | 0.47              |
| 85:28:20:U:H3'    | 85:28:21:G:H8     | 1.79                     | 0.47              |
| 85:28:153:G:H2'   | 85:28:154:G:H8    | 1.79                     | 0.47              |
| 85:28:673:C:H2'   | 85:28:674:G:C8    | 2.48                     | 0.47              |
| 85:28:1170:G:H2'  | 85:28:1171:G:H8   | 1.79                     | 0.47              |
| 85:28:1201:U:H2'  | 85:28:1202:C:C6   | 2.50                     | 0.47              |
| 85:28:1662:C:H2'  | 85:28:1663:C:H6   | 1.79                     | 0.47              |
| 85:28:2106:G:C6   | 85:28:2108:G:N7   | 2.83                     | 0.47              |
| 85:28:2555:G:C2   | 85:28:2556:G:C5   | 3.02                     | 0.47              |
| 85:28:2708:U:O2'  | 85:28:2709:C:H5'  | 2.14                     | 0.47              |
| 85:28:2815:A:C4   | 85:28:2816:G:C8   | 3.02                     | 0.47              |
| 85:28:3685:C:C2   | 85:28:3686:G:C8   | 3.03                     | 0.47              |
| 85:28:3784:A:O2'  | 85:28:3785:A:H3'  | 2.15                     | 0.47              |
| 85:28:4134:C:H2'  | 85:28:4135:G:C8   | 2.45                     | 0.47              |
| 85:28:4189:U:H2'  | 85:28:4190:U:O4'  | 2.14                     | 0.47              |
| 85:28:4433:G:H2'  | 85:28:4434:C:H6   | 1.80                     | 0.47              |
| 85:28:4440:G:C4   | 85:28:4441:A:C8   | 3.02                     | 0.47              |
| 85:28:4508:C:N3   | 85:28:4512:U:H5   | 2.13                     | 0.47              |
| 85:28:4551:U:H2'  | 85:28:4552:U:C6   | 2.50                     | 0.47              |
| 6:6:80:U:C2       | 6:6:81:G:C8       | 3.03                     | 0.47              |
| 8:L3:324:GLY:HA2  | 85:28:5051:C:H4'  | 1.97                     | 0.47              |
| 16:14:86:TRP:CE2  | 16:14:92:ALA:HB2  | 2.49                     | 0.47              |
| 22:21:119:ALA:HA  | 22:21:122:LYS:HB2 | 1.97                     | 0.47              |
| 58:AA:16:GLY:HA3  | 58:AA:36:ARG:HB2  | 1.96                     | 0.47              |
| 67:S9:12:THR:O    | 67:S9:45:ARG:HA   | 2.14                     | 0.47              |
| 79:18:828:G:N2    | 79:18:830:A:H1'   | 2.30                     | 0.47              |
| 79:18:933:G:H1'   | 79:18:1001:A:H5'  | 1.96                     | 0.47              |
| 79:18:1591:C:H2'  | 79:18:1592:C:C6   | 2.49                     | 0.47              |
| 80:v:759:ILE:HG13 | 80:v:800:LEU:HD21 | 1.97                     | 0.47              |
| 85:28:733:A:C4    | 85:28:734:G:C8    | 3.03                     | 0.47              |
| 85:28:1957:U:O2'  | 85:28:1958:A:H5'  | 2.14                     | 0.47              |
| 85:28:2732:G:H2'  | 85:28:2733:C:C6   | 2.50                     | 0.47              |
| 85:28:3753:G:H2'  | 85:28:3754:G:H8   | 1.80                     | 0.47              |
| 85:28:3834:C:H2'  | 85:28:3835:C:H6   | 1.80                     | 0.47              |
| 85:28:4996:C:H2'  | 85:28:4997:G:H8   | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:PP:39:VAL:HG22   | 3:PP:44:GLY:HA2    | 1.97                     | 0.47              |
| 5:58:27:U:H2'      | 5:58:28:C:H6       | 1.80                     | 0.47              |
| 5:58:32:C:H2'      | 5:58:33:G:O4'      | 2.15                     | 0.47              |
| 5:58:40:A:H2'      | 5:58:41:A:H8       | 1.80                     | 0.47              |
| 11:L6:165:VAL:HG12 | 11:L6:178:VAL:HG22 | 1.96                     | 0.47              |
| 12:L7:215:PRO:HD3  | 12:L7:246:MET:HE2  | 1.97                     | 0.47              |
| 19:17:83:TRP:O     | 85:28:3856:A:H5''  | 2.15                     | 0.47              |
| 66:S4:180:LEU:HG   | 66:S4:232:ASN:HA   | 1.97                     | 0.47              |
| 67:S9:33:GLY:HA3   | 69:YY:111:TYR:CD1  | 2.49                     | 0.47              |
| 79:18:1034:A:C4    | 79:18:1035:A:C8    | 3.02                     | 0.47              |
| 79:18:1166:G:H2'   | 79:18:1167:G:H8    | 1.80                     | 0.47              |
| 79:18:1372:U:H2'   | 79:18:1373:C:O4'   | 2.15                     | 0.47              |
| 79:18:1491:G:H2'   | 79:18:1492:U:C6    | 2.50                     | 0.47              |
| 79:18:1528:G:H2'   | 79:18:1529:C:C6    | 2.49                     | 0.47              |
| 84:ES:3245:G:H2'   | 84:ES:3246:G:H8    | 1.80                     | 0.47              |
| 85:28:652:G:H2'    | 85:28:653:C:C6     | 2.50                     | 0.47              |
| 85:28:2477:A:H2'   | 85:28:2478:C:C5    | 2.49                     | 0.47              |
| 85:28:2502:A:H4'   | 85:28:2503:G:OP2   | 2.15                     | 0.47              |
| 85:28:2538:U:H2'   | 85:28:2539:C:C6    | 2.50                     | 0.47              |
| 85:28:3762:U:H2'   | 85:28:3763:A:O4'   | 2.14                     | 0.47              |
| 85:28:3829:G:C2    | 85:28:3830:A:C8    | 3.02                     | 0.47              |
| 85:28:4092:G:H2'   | 85:28:4093:G:C8    | 2.49                     | 0.47              |
| 85:28:4625:C:O2'   | 85:28:4626:A:H5'   | 2.15                     | 0.47              |
| 85:28:4652:G:H2'   | 85:28:4653:C:C6    | 2.50                     | 0.47              |
| 5:58:140:C:H2'     | 5:58:141:C:H6      | 1.79                     | 0.47              |
| 5:58:147:G:H2'     | 5:58:148:A:C8      | 2.49                     | 0.47              |
| 8:L3:301:ASN:HB2   | 8:L3:304:SER:HB2   | 1.96                     | 0.47              |
| 18:bb:62:MET:HG2   | 18:bb:65:ASN:H     | 1.80                     | 0.47              |
| 38:39:16:LYS:HG3   | 38:39:49:LEU:HD11  | 1.97                     | 0.47              |
| 45:FF:70:LYS:HG2   | 45:FF:73:ARG:HD2   | 1.96                     | 0.47              |
| 51:ZZ:140:TYR:CE2  | 51:ZZ:142:GLY:HA2  | 2.50                     | 0.47              |
| 58:AA:10:THR:HG22  | 58:AA:308:ARG:HB3  | 1.98                     | 0.47              |
| 62:XX:33:LYS:HE2   | 62:XX:34:TYR:CZ    | 2.50                     | 0.47              |
| 79:18:112:U:H2'    | 79:18:115:U:C5     | 2.49                     | 0.47              |
| 79:18:168:C:H2'    | 79:18:169:U:H5'    | 1.96                     | 0.47              |
| 79:18:432:G:H2'    | 79:18:433:A:C8     | 2.50                     | 0.47              |
| 79:18:475:C:H1'    | 79:18:507:G:HO2'   | 1.80                     | 0.47              |
| 80:v:648:LYS:HB3   | 80:v:664:ASP:HB3   | 1.96                     | 0.47              |
| 85:28:178:C:H2'    | 85:28:179:G:C8     | 2.49                     | 0.47              |
| 85:28:299:C:H2'    | 85:28:300:A:C8     | 2.50                     | 0.47              |
| 85:28:951:G:H2'    | 85:28:952:G:H8     | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:970:G:H2'    | 85:28:971:U:O4'    | 2.15                     | 0.47              |
| 85:28:1750:G:C2    | 85:28:1751:A:C8    | 3.03                     | 0.47              |
| 85:28:2682:G:H2'   | 85:28:2683:C:H6    | 1.80                     | 0.47              |
| 85:28:4349:C:H3'   | 85:28:4350:C:H5'   | 1.97                     | 0.47              |
| 85:28:4419:U:C4    | 85:28:4420:U:C5    | 3.03                     | 0.47              |
| 85:28:5002:U:H2'   | 85:28:5003:U:C6    | 2.50                     | 0.47              |
| 5:58:67:U:C2       | 5:58:68:G:C8       | 3.03                     | 0.46              |
| 61:LL:64:VAL:O     | 61:LL:68:ILE:HG12  | 2.15                     | 0.46              |
| 68:S7:117:PRO:HG2  | 68:S7:120:ARG:HD3  | 1.97                     | 0.46              |
| 72:WX:11:LEU:HD12  | 72:WX:74:VAL:HB    | 1.98                     | 0.46              |
| 79:18:531:A:H3'    | 79:18:532:C:H5''   | 1.97                     | 0.46              |
| 79:18:577:U:H2'    | 79:18:578:C:H6     | 1.80                     | 0.46              |
| 79:18:976:G:H2'    | 79:18:977:C:O4'    | 2.16                     | 0.46              |
| 79:18:1126:G:H2'   | 79:18:1127:C:H6    | 1.80                     | 0.46              |
| 85:28:86:U:H2'     | 85:28:87:A:H8      | 1.80                     | 0.46              |
| 85:28:1566:C:H2'   | 85:28:1567:U:H6    | 1.80                     | 0.46              |
| 85:28:1965:G:H2'   | 85:28:1966:C:C6    | 2.50                     | 0.46              |
| 85:28:2034:G:H2'   | 85:28:2035:C:C6    | 2.50                     | 0.46              |
| 85:28:2894:A:H2'   | 85:28:2895:A:C8    | 2.50                     | 0.46              |
| 85:28:3932:U:H2'   | 85:28:3933:G:C8    | 2.49                     | 0.46              |
| 8:L3:231:VAL:HG21  | 8:L3:251:VAL:HG23  | 1.97                     | 0.46              |
| 13:aa:223:LEU:HD12 | 13:aa:254:THR:HG21 | 1.97                     | 0.46              |
| 39:40:56:LEU:HB3   | 78:L9:95:VAL:HG22  | 1.97                     | 0.46              |
| 44:AS:139:CYS:HB3  | 44:AS:172:MET:HE3  | 1.98                     | 0.46              |
| 51:ZZ:107:LYS:HG2  | 51:ZZ:117:LEU:HD11 | 1.96                     | 0.46              |
| 56:II:34:VAL:HG12  | 56:II:70:VAL:HB    | 1.96                     | 0.46              |
| 57:CC:50:GLN:HE22  | 79:18:1276:A:H4'   | 1.78                     | 0.46              |
| 60:MM:18:LEU:HB3   | 60:MM:58:ALA:HB1   | 1.96                     | 0.46              |
| 79:18:1352:G:H2'   | 79:18:1353:A:H8    | 1.79                     | 0.46              |
| 79:18:1597:C:H4'   | 79:18:1603:G:C6    | 2.51                     | 0.46              |
| 85:28:1582:U:C2    | 85:28:1583:A:C8    | 3.04                     | 0.46              |
| 85:28:1664:U:H2'   | 85:28:1665:C:C6    | 2.51                     | 0.46              |
| 85:28:3637:U:O4    | 85:28:3651:A:H2    | 1.98                     | 0.46              |
| 86:23:89:ARG:HB2   | 86:23:95:PHE:CE2   | 2.51                     | 0.46              |
| 5:58:30:U:H2'      | 5:58:31:G:H8       | 1.80                     | 0.46              |
| 7:L8:49:ILE:HD13   | 7:L8:60:LYS:HE3    | 1.95                     | 0.46              |
| 8:L3:262:VAL:HG21  | 8:L3:268:ARG:NH1   | 2.30                     | 0.46              |
| 14:10:3:ARG:NH2    | 85:28:4430:G:H5'   | 2.30                     | 0.46              |
| 15:13:72:ALA:HA    | 15:13:157:ILE:HD12 | 1.97                     | 0.46              |
| 21:20:83:ARG:HB3   | 21:20:125:GLN:HB2  | 1.98                     | 0.46              |
| 27:dd:89:ASN:HA    | 27:dd:92:LYS:HG2   | 1.97                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 65:S6:63:MET:HE3   | 65:S6:100:CYS:HA  | 1.98                     | 0.46              |
| 65:S6:136:LYS:HB2  | 79:18:65:C:N4     | 2.30                     | 0.46              |
| 71:RS:77:GLU:HA    | 71:RS:80:ARG:HG2  | 1.96                     | 0.46              |
| 76:UU:28:ARG:HD3   | 76:UU:74:CYS:SG   | 2.55                     | 0.46              |
| 79:18:155:G:C2     | 79:18:156:G:C8    | 3.03                     | 0.46              |
| 79:18:636:C:H2'    | 79:18:637:U:O4'   | 2.14                     | 0.46              |
| 79:18:1160:U:H2'   | 79:18:1161:U:H6   | 1.80                     | 0.46              |
| 79:18:1826:G:H2'   | 79:18:1827:U:C6   | 2.49                     | 0.46              |
| 85:28:164:G:H2'    | 85:28:165:A:C8    | 2.51                     | 0.46              |
| 85:28:424:U:H2'    | 85:28:425:U:C6    | 2.50                     | 0.46              |
| 85:28:950:G:H2'    | 85:28:951:G:H8    | 1.80                     | 0.46              |
| 85:28:1505:C:C2    | 85:28:1506:G:C8   | 3.03                     | 0.46              |
| 85:28:2479:G:C4    | 85:28:2480:G:C8   | 3.02                     | 0.46              |
| 85:28:2567:G:H2'   | 85:28:2568:C:H6   | 1.80                     | 0.46              |
| 85:28:2664:G:H4'   | 85:28:2677:G:H4'  | 1.97                     | 0.46              |
| 85:28:4968:A:H2'   | 85:28:4969:C:C6   | 2.50                     | 0.46              |
| 5:58:27:U:H2'      | 5:58:28:C:C6      | 2.51                     | 0.46              |
| 13:aa:104:LEU:HD11 | 85:28:4086:G:C4   | 2.51                     | 0.46              |
| 20:19:4:LEU:HD11   | 20:19:29:THR:HG23 | 1.96                     | 0.46              |
| 32:ee:46:ARG:HD2   | 32:ee:106:TYR:OH  | 2.15                     | 0.46              |
| 47:s:57:LYS:HD2    | 85:28:2020:U:H5'  | 1.98                     | 0.46              |
| 51:ZZ:106:TYR:CE2  | 51:ZZ:116:ARG:HG2 | 2.50                     | 0.46              |
| 58:AA:220:ASP:HB3  | 58:AA:223:GLU:O   | 2.15                     | 0.46              |
| 61:LL:27:ALA:HB1   | 61:LL:42:HIS:CE1  | 2.51                     | 0.46              |
| 77:11:146:ARG:HG2  | 77:11:147:ARG:HG2 | 1.97                     | 0.46              |
| 79:18:642:U:H4'    | 79:18:643:A:OP1   | 2.14                     | 0.46              |
| 79:18:1035:A:H2'   | 79:18:1036:A:C8   | 2.49                     | 0.46              |
| 79:18:1349:G:H2'   | 79:18:1350:U:C6   | 2.51                     | 0.46              |
| 79:18:1455:A:H2'   | 79:18:1456:G:H8   | 1.80                     | 0.46              |
| 85:28:713:C:H2'    | 85:28:714:G:C8    | 2.50                     | 0.46              |
| 85:28:726:G:H2'    | 85:28:727:C:C6    | 2.51                     | 0.46              |
| 85:28:1472:C:H2'   | 85:28:1473:U:C6   | 2.50                     | 0.46              |
| 85:28:2386:U:C2    | 85:28:2387:G:C8   | 3.03                     | 0.46              |
| 85:28:2634:C:C2    | 85:28:2635:U:C5   | 3.04                     | 0.46              |
| 85:28:3633:C:H2'   | 85:28:3634:G:C8   | 2.50                     | 0.46              |
| 85:28:3927:U:H2'   | 85:28:3928:A:H8   | 1.80                     | 0.46              |
| 85:28:4460:U:H2'   | 85:28:4461:C:C6   | 2.50                     | 0.46              |
| 8:L3:373:LYS:HE2   | 85:28:4627:U:H4'  | 1.97                     | 0.46              |
| 14:10:19:LYS:HB3   | 14:10:26:VAL:HG21 | 1.96                     | 0.46              |
| 19:17:131:ARG:HG3  | 19:17:137:ASN:ND2 | 2.31                     | 0.46              |
| 21:20:16:CYS:HB3   | 21:20:25:PRO:HG2  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:ee:23:GLU:H     | 32:ee:23:GLU:CD    | 2.24                     | 0.46              |
| 65:S6:230:LYS:O    | 65:S6:234:LEU:HG   | 2.15                     | 0.46              |
| 78:L9:88:PHE:CE2   | 78:L9:151:ILE:HB   | 2.50                     | 0.46              |
| 79:18:350:C:N3     | 79:18:351:G:C8     | 2.84                     | 0.46              |
| 79:18:848:U:O2     | 79:18:849:A:C8     | 2.68                     | 0.46              |
| 79:18:1006:C:H2'   | 79:18:1007:C:H6    | 1.80                     | 0.46              |
| 79:18:1177:U:H2'   | 79:18:1178:U:C6    | 2.51                     | 0.46              |
| 79:18:1375:G:H5'   | 79:18:1464:C:O2    | 2.15                     | 0.46              |
| 79:18:1412:C:C2    | 79:18:1413:G:C8    | 3.04                     | 0.46              |
| 79:18:1686:G:H2'   | 79:18:1687:C:C6    | 2.50                     | 0.46              |
| 85:28:311:G:H2'    | 85:28:312:G:H8     | 1.80                     | 0.46              |
| 85:28:317:A:C2     | 85:28:4361:U:H1'   | 2.50                     | 0.46              |
| 85:28:2771:G:H2'   | 85:28:2772:C:O4'   | 2.15                     | 0.46              |
| 85:28:2832:A:C4    | 85:28:2833:A:C8    | 3.04                     | 0.46              |
| 85:28:3890:A:N7    | 85:28:4571:A:H1'   | 2.31                     | 0.46              |
| 85:28:4089:G:H2'   | 85:28:4090:G:H8    | 1.80                     | 0.46              |
| 85:28:4968:A:H2'   | 85:28:4969:C:H6    | 1.81                     | 0.46              |
| 1:BB:59:LEU:HD22   | 1:BB:181:GLU:HG2   | 1.98                     | 0.46              |
| 4:DD:55:TYR:OH     | 4:DD:116:CYS:HB3   | 2.16                     | 0.46              |
| 5:58:141:C:H2'     | 5:58:142:U:H6      | 1.81                     | 0.46              |
| 13:aa:210:ILE:HA   | 13:aa:254:THR:HG22 | 1.97                     | 0.46              |
| 68:S7:101:LEU:HD13 | 68:S7:120:ARG:HG2  | 1.98                     | 0.46              |
| 79:18:443:U:H2'    | 79:18:444:G:C8     | 2.51                     | 0.46              |
| 79:18:1609:C:H2'   | 79:18:1610:G:C8    | 2.50                     | 0.46              |
| 80:v:9:ILE:HA      | 80:v:12:ILE:HG22   | 1.97                     | 0.46              |
| 80:v:126:LEU:HA    | 80:v:154:VAL:HG23  | 1.96                     | 0.46              |
| 85:28:1519:C:H2'   | 85:28:1520:C:C6    | 2.51                     | 0.46              |
| 85:28:1958:A:C4'   | 85:28:1962:A:H1'   | 2.46                     | 0.46              |
| 85:28:2556:G:C2    | 85:28:2557:G:N7    | 2.84                     | 0.46              |
| 85:28:3787:G:H1'   | 85:28:3789:C:N4    | 2.31                     | 0.46              |
| 85:28:4233:A:C8    | 85:28:4235:G:C8    | 3.03                     | 0.46              |
| 85:28:4503:A:H2'   | 85:28:4504:C:C6    | 2.50                     | 0.46              |
| 85:28:4637:G:H2'   | 85:28:4638:U:H6    | 1.78                     | 0.46              |
| 85:28:4951:G:C2    | 85:28:4952:G:C8    | 3.03                     | 0.46              |
| 1:BB:148:CYS:SG    | 1:BB:160:ALA:HB1   | 2.56                     | 0.46              |
| 10:L5:153:THR:HG21 | 85:28:4323:A:C6    | 2.50                     | 0.46              |
| 12:L7:240:ASN:O    | 12:L7:244:ARG:HG2  | 2.16                     | 0.46              |
| 38:39:25:GLN:HG3   | 38:39:28:TRP:CZ2   | 2.51                     | 0.46              |
| 47:s:24:TYR:CG     | 47:s:90:PHE:HB3    | 2.50                     | 0.46              |
| 49:F:32:LEU:HD12   | 49:F:110:LEU:HD21  | 1.96                     | 0.46              |
| 61:LL:82:TRP:CD1   | 61:LL:82:TRP:H     | 2.32                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:SS:62:THR:HA    | 64:SS:69:THR:HG22  | 1.97                     | 0.46              |
| 75:GG:28:PHE:HA    | 75:GG:92:ALA:HB3   | 1.98                     | 0.46              |
| 79:18:479:C:H2'    | 79:18:480:G:C8     | 2.50                     | 0.46              |
| 79:18:1588:A:H2'   | 79:18:1589:A:C8    | 2.51                     | 0.46              |
| 80:v:132:VAL:HG13  | 80:v:167:LEU:HD11  | 1.98                     | 0.46              |
| 80:v:480:VAL:HG13  | 80:v:481:LYS:H     | 1.81                     | 0.46              |
| 85:28:1348:U:H2'   | 85:28:1349:G:C8    | 2.51                     | 0.46              |
| 85:28:1382:G:N3    | 85:28:1383:G:C8    | 2.83                     | 0.46              |
| 85:28:1460:C:H2'   | 85:28:1461:C:H6    | 1.81                     | 0.46              |
| 85:28:1578:U:H2'   | 85:28:1579:C:C6    | 2.51                     | 0.46              |
| 85:28:1829:G:H2'   | 85:28:1830:G:C8    | 2.51                     | 0.46              |
| 85:28:2016:C:C2    | 85:28:2017:A:C8    | 3.03                     | 0.46              |
| 85:28:2542:G:H2'   | 85:28:2543:A:C8    | 2.50                     | 0.46              |
| 85:28:2557:G:H2'   | 85:28:2558:C:H6    | 1.79                     | 0.46              |
| 85:28:3768:U:H2'   | 85:28:3769:C:H6    | 1.81                     | 0.46              |
| 85:28:4524:G:H2'   | 85:28:4525:C:H6    | 1.81                     | 0.46              |
| 1:BB:131:HIS:HA    | 1:BB:134:LEU:HD12  | 1.97                     | 0.46              |
| 2:S2:256:TRP:CE2   | 72:WX:68:ARG:HB3   | 2.51                     | 0.46              |
| 7:L8:28:ARG:HD3    | 7:L8:123:ARG:HD3   | 1.98                     | 0.46              |
| 12:L7:50:TYR:CD1   | 85:28:1237:C:H2'   | 2.50                     | 0.46              |
| 20:19:105:LEU:HD22 | 20:19:135:LYS:HG3  | 1.98                     | 0.46              |
| 31:32:108:ARG:HD3  | 31:32:127:ALA:HB3  | 1.98                     | 0.46              |
| 44:AS:165:ARG:HD2  | 79:18:1004:U:OP1   | 2.15                     | 0.46              |
| 48:t:152:ILE:HD12  | 48:t:155:ILE:HD12  | 1.98                     | 0.46              |
| 58:AA:270:LEU:HD22 | 58:AA:310:TRP:CE3  | 2.50                     | 0.46              |
| 70:S3:66:ILE:O     | 70:S3:70:THR:HG23  | 2.15                     | 0.46              |
| 79:18:299:A:H2'    | 79:18:300:U:H6     | 1.81                     | 0.46              |
| 79:18:512:A:C2     | 79:18:513:G:C8     | 3.04                     | 0.46              |
| 79:18:953:C:H2'    | 79:18:954:U:O4'    | 2.16                     | 0.46              |
| 79:18:1367:U:H2'   | 79:18:1368:U:C6    | 2.51                     | 0.46              |
| 79:18:1501:C:H2'   | 79:18:1502:C:C6    | 2.51                     | 0.46              |
| 80:v:313:ALA:HA    | 80:v:316:ILE:HG12  | 1.98                     | 0.46              |
| 85:28:1359:G:H3'   | 85:28:1360:G:C8    | 2.51                     | 0.46              |
| 85:28:1590:C:H4'   | 85:28:2857:A:H5'   | 1.98                     | 0.46              |
| 85:28:2634:C:H2'   | 85:28:2635:U:C6    | 2.49                     | 0.46              |
| 85:28:4389:C:H2'   | 85:28:4390:A:H8    | 1.80                     | 0.46              |
| 86:23:11:GLY:H     | 86:23:128:LEU:HD13 | 1.81                     | 0.46              |
| 6:6:55:A:H2'       | 6:6:56:G:H8        | 1.80                     | 0.46              |
| 9:L4:189:MET:HE3   | 85:28:2333:G:N7    | 2.31                     | 0.46              |
| 49:F:181:PRO:HA    | 49:F:230:VAL:HA    | 1.97                     | 0.46              |
| 51:ZZ:100:LEU:HD11 | 79:18:1285:G:H1'   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:EE:52:LEU:HD11 | 52:EE:62:VAL:HG23  | 1.97                     | 0.46              |
| 65:S6:7:PHE:HD1   | 65:S6:8:PRO:HD2    | 1.80                     | 0.46              |
| 72:WX:8:ALA:HA    | 72:WX:74:VAL:HG11  | 1.97                     | 0.46              |
| 73:S8:8:TRP:HA    | 73:S8:18:ARG:HD2   | 1.98                     | 0.46              |
| 79:18:676:C:H2'   | 79:18:677:G:O4'    | 2.15                     | 0.46              |
| 79:18:1161:U:H2'  | 79:18:1162:C:C6    | 2.51                     | 0.46              |
| 79:18:1393:G:H2'  | 79:18:1394:G:C8    | 2.51                     | 0.46              |
| 79:18:1461:G:H1'  | 79:18:1465:A:N6    | 2.30                     | 0.46              |
| 85:28:221:C:H2'   | 85:28:222:C:C6     | 2.51                     | 0.46              |
| 85:28:1199:G:C2   | 85:28:1200:G:C5    | 3.04                     | 0.46              |
| 85:28:1291:G:H2'  | 85:28:1292:C:C6    | 2.51                     | 0.46              |
| 85:28:1421:G:C2   | 85:28:1422:G:C8    | 3.04                     | 0.46              |
| 85:28:1972:G:C4   | 85:28:1995:G:N2    | 2.84                     | 0.46              |
| 85:28:2499:C:H2'  | 85:28:2500:U:C6    | 2.51                     | 0.46              |
| 85:28:2885:A:H2'  | 85:28:2886:U:C6    | 2.51                     | 0.46              |
| 9:L4:149:GLU:HG2  | 9:L4:151:PRO:HD2   | 1.97                     | 0.46              |
| 16:14:39:ASP:OD2  | 16:14:70:GLN:HG2   | 2.16                     | 0.46              |
| 18:bb:188:LYS:HD3 | 85:28:4892:A:H5''  | 1.97                     | 0.46              |
| 24:cc:80:PRO:HA   | 24:cc:98:PHE:HA    | 1.98                     | 0.46              |
| 45:FF:113:PHE:CE2 | 45:FF:117:LEU:HD11 | 2.51                     | 0.46              |
| 76:UU:84:VAL:HB   | 79:18:1866:A:N6    | 2.30                     | 0.46              |
| 79:18:434:G:H2'   | 79:18:435:A:C8     | 2.51                     | 0.46              |
| 79:18:883:U:H2'   | 79:18:884:C:C6     | 2.51                     | 0.46              |
| 79:18:1413:G:H2'  | 79:18:1414:A:C8    | 2.51                     | 0.46              |
| 79:18:1610:G:H2'  | 79:18:1611:G:C8    | 2.51                     | 0.46              |
| 80:v:304:ILE:HD13 | 80:v:336:LEU:HA    | 1.97                     | 0.46              |
| 85:28:426:A:H2'   | 85:28:427:A:C8     | 2.51                     | 0.46              |
| 85:28:516:C:H2'   | 85:28:517:C:H6     | 1.81                     | 0.46              |
| 85:28:2421:G:OP2  | 85:28:2828:U:H1'   | 2.16                     | 0.46              |
| 85:28:2610:G:H2'  | 85:28:2611:A:C8    | 2.51                     | 0.46              |
| 85:28:3832:U:H2'  | 85:28:3833:C:C6    | 2.51                     | 0.46              |
| 85:28:3933:G:H2'  | 85:28:3934:G:C8    | 2.50                     | 0.46              |
| 85:28:4345:C:H2'  | 85:28:4346:U:C6    | 2.51                     | 0.46              |
| 85:28:4477:A:C4   | 85:28:4478:G:C8    | 3.04                     | 0.46              |
| 7:L8:83:HIS:HB3   | 42:ff:64:VAL:HG22  | 1.98                     | 0.45              |
| 61:LL:107:LEU:O   | 61:LL:111:LEU:HG   | 2.16                     | 0.45              |
| 73:S8:23:LYS:HD2  | 79:18:448:A:H3'    | 1.99                     | 0.45              |
| 79:18:98:C:H2'    | 79:18:426:A:H4'    | 1.97                     | 0.45              |
| 79:18:348:A:H2'   | 79:18:349:A:H8     | 1.79                     | 0.45              |
| 79:18:673:G:H2'   | 79:18:674:C:H6     | 1.82                     | 0.45              |
| 79:18:887:U:O2    | 79:18:887:U:H2'    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:18:1094:C:H2'  | 79:18:1095:U:C6   | 2.51                     | 0.45              |
| 79:18:1137:U:O2'  | 79:18:1138:C:H3'  | 2.16                     | 0.45              |
| 79:18:1688:C:H2'  | 79:18:1689:C:H6   | 1.81                     | 0.45              |
| 79:18:1733:U:H2'  | 79:18:1734:G:O4'  | 2.16                     | 0.45              |
| 79:18:1806:A:H2'  | 79:18:1807:C:C6   | 2.51                     | 0.45              |
| 85:28:263:G:H2'   | 85:28:264:C:C6    | 2.51                     | 0.45              |
| 85:28:1212:G:H2'  | 85:28:1213:G:C8   | 2.51                     | 0.45              |
| 85:28:1963:C:C2   | 85:28:1964:A:C2   | 3.04                     | 0.45              |
| 85:28:2000:G:H4'  | 85:28:2017:A:C2   | 2.52                     | 0.45              |
| 85:28:2281:U:C2   | 85:28:2282:A:C8   | 3.04                     | 0.45              |
| 85:28:2385:U:H2'  | 85:28:2386:U:H6   | 1.81                     | 0.45              |
| 85:28:2689:C:C2   | 85:28:2690:C:C5   | 3.03                     | 0.45              |
| 85:28:2893:U:H2'  | 85:28:2894:A:H8   | 1.80                     | 0.45              |
| 8:L3:154:LYS:HG3  | 8:L3:194:LEU:HD23 | 1.98                     | 0.45              |
| 18:bb:169:ARG:CZ  | 85:28:4860:G:H5'  | 2.46                     | 0.45              |
| 79:18:106:C:H2'   | 79:18:107:A:C8    | 2.49                     | 0.45              |
| 79:18:449:A:O2'   | 79:18:450:C:H4'   | 2.16                     | 0.45              |
| 79:18:501:C:H2'   | 79:18:502:C:H5''  | 1.99                     | 0.45              |
| 79:18:896:U:H2'   | 79:18:897:U:C6    | 2.52                     | 0.45              |
| 79:18:980:A:H2'   | 79:18:981:A:C8    | 2.51                     | 0.45              |
| 85:28:1687:U:H2'  | 85:28:1688:G:C8   | 2.51                     | 0.45              |
| 85:28:2358:G:H2'  | 85:28:2359:U:O4'  | 2.16                     | 0.45              |
| 85:28:2520:C:H2'  | 85:28:2521:G:C8   | 2.44                     | 0.45              |
| 85:28:2555:G:H2'  | 85:28:2556:G:C8   | 2.51                     | 0.45              |
| 85:28:2690:C:C4   | 85:28:2691:U:C4   | 3.05                     | 0.45              |
| 85:28:2815:A:H2'  | 85:28:2816:G:H8   | 1.80                     | 0.45              |
| 3:PP:8:PHE:CZ     | 3:PP:10:ASP:HB2   | 2.52                     | 0.45              |
| 6:6:55:A:C4       | 6:6:56:G:C8       | 3.05                     | 0.45              |
| 18:bb:26:GLN:HG3  | 21:20:167:PHE:CZ  | 2.52                     | 0.45              |
| 24:cc:72:ASP:O    | 24:cc:76:ILE:HG23 | 2.17                     | 0.45              |
| 67:S9:84:ILE:HG13 | 67:S9:86:VAL:HG23 | 1.97                     | 0.45              |
| 77:11:25:CYS:HB3  | 85:28:4252:C:H42  | 1.81                     | 0.45              |
| 79:18:89:C:O2'    | 79:18:499:G:H5''  | 2.16                     | 0.45              |
| 79:18:934:G:C2    | 79:18:935:G:C8    | 3.03                     | 0.45              |
| 84:ES:2953:C:H2'  | 84:ES:2954:G:H8   | 1.81                     | 0.45              |
| 85:28:233:U:C2'   | 85:28:234:G:C8    | 2.99                     | 0.45              |
| 85:28:275:C:H2'   | 85:28:276:C:C6    | 2.51                     | 0.45              |
| 85:28:1988:G:C2   | 85:28:1989:G:C8   | 3.04                     | 0.45              |
| 85:28:2295:C:H2'  | 85:28:2296:G:H8   | 1.81                     | 0.45              |
| 85:28:2587:A:H5'' | 85:28:2588:C:C5   | 2.51                     | 0.45              |
| 85:28:2623:A:H2'  | 85:28:2624:G:H8   | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:2858:A:H2'   | 85:28:2859:G:O4'   | 2.16                     | 0.45              |
| 12:L7:115:GLN:HG3  | 50:Q:3:VAL:HG12    | 1.97                     | 0.45              |
| 41:42:26:TYR:HB2   | 41:42:82:MET:HE1   | 1.98                     | 0.45              |
| 64:SS:53:ASP:HB3   | 64:SS:79:LEU:HD13  | 1.99                     | 0.45              |
| 65:S6:21:GLU:O     | 65:S6:25:ARG:HD3   | 2.16                     | 0.45              |
| 65:S6:135:PRO:HG2  | 65:S6:144:LEU:HD22 | 1.98                     | 0.45              |
| 71:RS:31:ASN:HA    | 71:RS:34:VAL:HB    | 1.97                     | 0.45              |
| 72:WX:103:VAL:HA   | 72:WX:112:ASP:HA   | 1.99                     | 0.45              |
| 73:S8:11:ARG:NH2   | 73:S8:17:LYS:HE3   | 2.31                     | 0.45              |
| 79:18:854:A:C2     | 79:18:855:G:C8     | 3.05                     | 0.45              |
| 79:18:950:C:H2'    | 79:18:951:C:H6     | 1.80                     | 0.45              |
| 79:18:1531:A:H2'   | 79:18:1532:C:H6    | 1.82                     | 0.45              |
| 79:18:1591:C:H2'   | 79:18:1592:C:H6    | 1.80                     | 0.45              |
| 85:28:1199:G:C2    | 85:28:1200:G:N7    | 2.85                     | 0.45              |
| 85:28:1315:C:H2'   | 85:28:1316:G:C8    | 2.51                     | 0.45              |
| 85:28:2264:C:H2'   | 85:28:2265:G:O4'   | 2.15                     | 0.45              |
| 85:28:2629:C:H2'   | 85:28:2630:U:O4'   | 2.15                     | 0.45              |
| 85:28:4638:U:H2'   | 85:28:4639:G:N3    | 2.30                     | 0.45              |
| 5:58:130:C:H2'     | 5:58:131:G:C8      | 2.51                     | 0.45              |
| 17:15:178:HIS:HA   | 17:15:181:HIS:NE2  | 2.31                     | 0.45              |
| 44:AS:163:GLN:O    | 44:AS:167:LYS:HG2  | 2.17                     | 0.45              |
| 67:S9:42:GLU:O     | 67:S9:46:VAL:HG23  | 2.16                     | 0.45              |
| 70:S3:211:VAL:HG12 | 81:LA:715:ILE:HG13 | 1.98                     | 0.45              |
| 79:18:1043:G:N2    | 79:18:1073:U:C4    | 2.85                     | 0.45              |
| 79:18:1351:G:H2'   | 79:18:1352:G:H8    | 1.81                     | 0.45              |
| 85:28:460:C:H2'    | 85:28:461:G:C8     | 2.51                     | 0.45              |
| 85:28:1479:G:H2'   | 85:28:1480:C:C6    | 2.51                     | 0.45              |
| 85:28:1664:U:H2'   | 85:28:1665:C:H6    | 1.82                     | 0.45              |
| 85:28:2413:U:C2    | 85:28:2414:G:C8    | 3.05                     | 0.45              |
| 85:28:2457:G:H2'   | 85:28:2458:C:C6    | 2.52                     | 0.45              |
| 85:28:3722:G:H2'   | 85:28:3723:A:C8    | 2.52                     | 0.45              |
| 49:F:113:HIS:CE1   | 49:F:276:MET:HG3   | 2.52                     | 0.45              |
| 63:RR:88:ASP:HB2   | 79:18:617:G:H4'    | 1.99                     | 0.45              |
| 79:18:458:A:H2'    | 79:18:459:C:C6     | 2.52                     | 0.45              |
| 79:18:493:A:C8     | 79:18:574:A:H8     | 2.34                     | 0.45              |
| 79:18:1090:C:H2'   | 79:18:1091:C:H6    | 1.82                     | 0.45              |
| 79:18:1272:C:O2'   | 79:18:1273:C:H5'   | 2.17                     | 0.45              |
| 79:18:1554:C:H2'   | 79:18:1555:U:C5    | 2.51                     | 0.45              |
| 85:28:1592:G:C2    | 85:28:1593:A:C8    | 3.05                     | 0.45              |
| 85:28:2588:C:H5''  | 85:28:2589:C:H5''  | 1.99                     | 0.45              |
| 85:28:2885:A:H2'   | 85:28:2886:U:H6    | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:3846:C:H2'   | 85:28:3847:C:H6    | 1.81                     | 0.45              |
| 1:BB:206:ASP:HB3   | 1:BB:209:GLU:HG3   | 1.98                     | 0.45              |
| 2:S2:210:PRO:HB3   | 2:S2:240:THR:HG21  | 1.99                     | 0.45              |
| 21:20:93:MET:HE1   | 21:20:117:HIS:CE1  | 2.52                     | 0.45              |
| 22:21:89:ILE:HG22  | 85:28:4300:U:H4'   | 1.99                     | 0.45              |
| 30:31:70:LYS:HE2   | 85:28:2389:A:H5'   | 1.99                     | 0.45              |
| 36:37:3:LYS:HB3    | 85:28:3642:A:C4    | 2.51                     | 0.45              |
| 47:s:84:GLY:C      | 85:28:2021:G:H4'   | 2.41                     | 0.45              |
| 48:t:105:THR:HG22  | 48:t:108:GLU:CD    | 2.41                     | 0.45              |
| 49:F:20:LYS:O      | 49:F:23:MET:HG2    | 2.16                     | 0.45              |
| 50:Q:63:LEU:O      | 50:Q:67:ILE:HG12   | 2.16                     | 0.45              |
| 59:OO:79:ARG:H     | 62:XX:54:LYS:HE3   | 1.81                     | 0.45              |
| 61:LL:108:ARG:HH11 | 61:LL:109:GLU:HA   | 1.82                     | 0.45              |
| 64:SS:37:LYS:HD2   | 64:SS:57:VAL:O     | 2.17                     | 0.45              |
| 79:18:456:C:H2'    | 79:18:457:C:H6     | 1.81                     | 0.45              |
| 79:18:609:U:H2'    | 79:18:610:G:H8     | 1.81                     | 0.45              |
| 79:18:1109:C:H2'   | 79:18:1110:G:O4'   | 2.17                     | 0.45              |
| 85:28:1206:C:H2'   | 85:28:1207:C:H6    | 1.82                     | 0.45              |
| 85:28:2404:A:H61   | 85:28:2787:A:N6    | 2.14                     | 0.45              |
| 85:28:2553:A:H2    | 85:28:2765:A:H62   | 1.62                     | 0.45              |
| 85:28:2556:G:N3    | 85:28:2557:G:C8    | 2.85                     | 0.45              |
| 85:28:5030:U:H2'   | 85:28:5031:G:C8    | 2.49                     | 0.45              |
| 6:6:102:U:C2       | 6:6:103:A:C8       | 3.05                     | 0.45              |
| 14:10:59:GLN:HG2   | 14:10:128:ARG:HB3  | 1.99                     | 0.45              |
| 27:dd:24:LYS:HE2   | 27:dd:24:LYS:HB2   | 1.74                     | 0.45              |
| 31:32:22:ARG:HG3   | 31:32:36:ARG:H     | 1.81                     | 0.45              |
| 33:34:5:LEU:HD21   | 33:34:30:ILE:HG22  | 1.98                     | 0.45              |
| 48:t:83:LYS:HG3    | 48:t:84:ALA:N      | 2.31                     | 0.45              |
| 50:Q:69:LYS:HD2    | 85:28:1458:C:H5''  | 1.97                     | 0.45              |
| 54:S5:39:ILE:HG23  | 54:S5:68:ILE:HD13  | 1.98                     | 0.45              |
| 57:CC:52:LEU:HB3   | 57:CC:57:TYR:HB2   | 1.98                     | 0.45              |
| 66:S4:128:LYS:HA   | 66:S4:156:VAL:HG13 | 1.99                     | 0.45              |
| 70:S3:39:VAL:HA    | 70:S3:48:ILE:HG22  | 1.98                     | 0.45              |
| 72:WX:36:ARG:HB2   | 72:WX:110:ILE:HD12 | 1.99                     | 0.45              |
| 79:18:946:U:H2'    | 79:18:947:G:C8     | 2.52                     | 0.45              |
| 79:18:1395:C:H2'   | 79:18:1396:A:C2    | 2.51                     | 0.45              |
| 79:18:1723:G:H2'   | 79:18:1724:A:H8    | 1.81                     | 0.45              |
| 80:v:609:PHE:CE1   | 80:v:701:ARG:HB2   | 2.51                     | 0.45              |
| 85:28:489:C:H2'    | 85:28:490:C:C6     | 2.51                     | 0.45              |
| 85:28:4174:U:H2'   | 85:28:4175:G:C8    | 2.51                     | 0.45              |
| 85:28:4307:A:H2'   | 85:28:4308:C:H6    | 1.80                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:28:4504:C:H2'   | 85:28:4505:C:H6   | 1.82                     | 0.45              |
| 85:28:5055:G:H2'   | 85:28:5056:A:H8   | 1.82                     | 0.45              |
| 2:S2:118:ALA:HB2   | 79:18:1486:A:H4'  | 1.99                     | 0.45              |
| 8:L3:253:CYS:SG    | 85:28:4521:U:H1'  | 2.57                     | 0.45              |
| 17:15:85:VAL:HA    | 41:42:49:GLY:HA2  | 1.99                     | 0.45              |
| 48:t:104:ILE:HG23  | 48:t:143:VAL:HG22 | 1.99                     | 0.45              |
| 65:S6:186:GLN:HE22 | 79:18:318:A:H61   | 1.65                     | 0.45              |
| 72:WX:50:PHE:HB3   | 72:WX:63:VAL:HG13 | 1.99                     | 0.45              |
| 79:18:563:G:C2     | 79:18:564:A:N7    | 2.85                     | 0.45              |
| 79:18:1090:C:H2'   | 79:18:1091:C:C6   | 2.52                     | 0.45              |
| 80:v:425:LEU:HD12  | 80:v:427:VAL:HG13 | 1.99                     | 0.45              |
| 83:A:95:GLY:HA2    | 83:A:104:GLN:HA   | 1.98                     | 0.45              |
| 85:28:272:U:H2'    | 85:28:273:U:C6    | 2.52                     | 0.45              |
| 85:28:679:C:C2     | 85:28:680:G:C8    | 3.05                     | 0.45              |
| 85:28:751:G:C4     | 85:28:752:G:C8    | 3.05                     | 0.45              |
| 85:28:1298:C:C2    | 85:28:1299:G:C8   | 3.05                     | 0.45              |
| 85:28:1569:U:H2'   | 85:28:1570:G:C8   | 2.52                     | 0.45              |
| 85:28:1732:C:O2'   | 85:28:1733:G:H5'  | 2.17                     | 0.45              |
| 85:28:4130:C:H2'   | 85:28:4131:G:C8   | 2.52                     | 0.45              |
| 85:28:4198:G:H2'   | 85:28:4199:C:H6   | 1.82                     | 0.45              |
| 85:28:4685:U:H2'   | 85:28:4686:G:H8   | 1.81                     | 0.45              |
| 7:L8:187:HIS:HB3   | 85:28:2740:U:O4'  | 2.17                     | 0.45              |
| 9:L4:113:ARG:HG3   | 85:28:1508:A:OP1  | 2.17                     | 0.45              |
| 68:S7:140:VAL:HG21 | 68:S7:159:ASP:HB3 | 1.99                     | 0.45              |
| 79:18:203:G:H2'    | 79:18:204:G:C8    | 2.51                     | 0.45              |
| 80:v:757:GLY:HA3   | 85:28:2009:A:H5'  | 1.99                     | 0.45              |
| 85:28:969:C:H42    | 85:28:2095:A:H61  | 1.64                     | 0.45              |
| 85:28:978:C:H2'    | 85:28:979:G:H8    | 1.82                     | 0.45              |
| 85:28:1195:G:N3    | 85:28:1196:G:C8   | 2.85                     | 0.45              |
| 85:28:1895:G:H2'   | 85:28:1896:A:O4'  | 2.17                     | 0.45              |
| 85:28:2479:G:H2'   | 85:28:2480:G:H8   | 1.82                     | 0.45              |
| 85:28:2540:C:H2'   | 85:28:2541:G:C8   | 2.51                     | 0.45              |
| 85:28:4152:G:H2'   | 85:28:4153:C:C6   | 2.52                     | 0.45              |
| 85:28:4407:G:H2'   | 85:28:4408:G:H8   | 1.82                     | 0.45              |
| 5:58:40:A:H2'      | 5:58:41:A:C8      | 2.51                     | 0.44              |
| 30:31:45:ALA:O     | 30:31:48:GLU:HG2  | 2.17                     | 0.44              |
| 32:ee:54:LYS:HB3   | 85:28:443:G:H5''  | 1.99                     | 0.44              |
| 36:37:12:ARG:HH11  | 85:28:2404:A:H1'  | 1.82                     | 0.44              |
| 48:t:146:ARG:HA    | 48:t:146:ARG:HD2  | 1.58                     | 0.44              |
| 58:AA:173:LEU:HB2  | 58:AA:175:LYS:HZ2 | 1.82                     | 0.44              |
| 60:MM:62:ARG:HD3   | 79:18:1542:C:OP1  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:RR:90:CYS:SG    | 63:RR:130:LEU:HD21 | 2.57                     | 0.44              |
| 79:18:431:G:N3     | 79:18:432:G:C8     | 2.85                     | 0.44              |
| 79:18:918:U:H2'    | 79:18:919:A:O4'    | 2.17                     | 0.44              |
| 79:18:1019:C:H2'   | 79:18:1020:A:O4'   | 2.17                     | 0.44              |
| 79:18:1671:G:H2'   | 79:18:1672:U:H6    | 1.82                     | 0.44              |
| 79:18:1730:U:C2    | 79:18:1731:A:C8    | 3.05                     | 0.44              |
| 84:ES:3245:G:H2'   | 84:ES:3246:G:C8    | 2.53                     | 0.44              |
| 85:28:1350:C:H2'   | 85:28:1351:G:C8    | 2.52                     | 0.44              |
| 85:28:1475:G:H2'   | 85:28:1476:C:C6    | 2.52                     | 0.44              |
| 85:28:4197:G:H2'   | 85:28:4198:G:H8    | 1.82                     | 0.44              |
| 85:28:4594:U:H2'   | 85:28:4595:G:C8    | 2.51                     | 0.44              |
| 85:28:4960:G:H2'   | 85:28:4961:G:C8    | 2.52                     | 0.44              |
| 85:28:5066:U:H2'   | 85:28:5067:U:C6    | 2.52                     | 0.44              |
| 9:L4:22:VAL:HG22   | 9:L4:258:ARG:NH1   | 2.32                     | 0.44              |
| 12:L7:174:ILE:HD13 | 12:L7:189:LEU:HD12 | 1.99                     | 0.44              |
| 18:bb:130:LYS:HB2  | 18:bb:133:ARG:HG2  | 2.00                     | 0.44              |
| 29:30:64:ALA:HB1   | 29:30:69:THR:O     | 2.16                     | 0.44              |
| 43:gg:104:PRO:O    | 43:gg:107:ARG:HG2  | 2.17                     | 0.44              |
| 45:FF:88:LEU:HD11  | 45:FF:122:ILE:HG23 | 1.99                     | 0.44              |
| 48:t:105:THR:HG23  | 48:t:107:ASP:H     | 1.82                     | 0.44              |
| 61:LL:20:ILE:HD11  | 61:LL:33:ILE:HD11  | 1.99                     | 0.44              |
| 63:RR:124:LYS:HA   | 63:RR:129:SER:HA   | 1.97                     | 0.44              |
| 79:18:219:U:H2'    | 79:18:220:U:H6     | 1.81                     | 0.44              |
| 79:18:943:U:C2     | 79:18:944:A:C8     | 3.06                     | 0.44              |
| 79:18:1217:A:H2'   | 79:18:1218:C:H6    | 1.79                     | 0.44              |
| 79:18:1340:U:H2'   | 79:18:1341:C:C5    | 2.53                     | 0.44              |
| 79:18:1689:C:H2'   | 79:18:1690:U:H6    | 1.82                     | 0.44              |
| 79:18:1862:G:H4'   | 79:18:1863:A:OP1   | 2.17                     | 0.44              |
| 85:28:25:A:C8      | 85:28:341:G:C8     | 3.05                     | 0.44              |
| 85:28:27:C:H2'     | 85:28:28:C:H6      | 1.81                     | 0.44              |
| 85:28:149:A:H5''   | 85:28:151:G:O4'    | 2.17                     | 0.44              |
| 85:28:1932:A:H2'   | 85:28:1933:G:C8    | 2.52                     | 0.44              |
| 85:28:1964:A:H2'   | 85:28:1965:G:O4'   | 2.16                     | 0.44              |
| 85:28:3896:C:H2'   | 85:28:3897:G:C4    | 2.52                     | 0.44              |
| 85:28:4069:U:H2'   | 85:28:4070:U:H6    | 1.82                     | 0.44              |
| 85:28:4263:C:H2'   | 85:28:4264:G:O4'   | 2.17                     | 0.44              |
| 1:BB:81:ASN:HA     | 1:BB:84:GLN:HE22   | 1.83                     | 0.44              |
| 5:58:28:C:H2'      | 5:58:29:G:H8       | 1.82                     | 0.44              |
| 5:58:96:C:H5''     | 34:35:66:LYS:HG2   | 1.99                     | 0.44              |
| 6:6:46:C:OP1       | 10:L5:158:LYS:HG3  | 2.18                     | 0.44              |
| 7:L8:47:ASP:HA     | 7:L8:84:THR:HG22   | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L3:86:VAL:HG12   | 8:L3:201:LEU:HD12  | 2.00                     | 0.44              |
| 34:35:80:PRO:HD2   | 34:35:83:LEU:HD12  | 2.00                     | 0.44              |
| 38:39:44:TRP:CZ3   | 38:39:45:ARG:HD3   | 2.53                     | 0.44              |
| 44:AS:49:VAL:HG21  | 44:AS:62:LEU:HD13  | 1.98                     | 0.44              |
| 48:t:20:GLY:H      | 48:t:54:LYS:HA     | 1.82                     | 0.44              |
| 59:OO:56:MET:SD    | 59:OO:86:LYS:HB3   | 2.58                     | 0.44              |
| 65:S6:7:PHE:CD1    | 65:S6:113:ILE:HB   | 2.52                     | 0.44              |
| 65:S6:181:THR:HG23 | 65:S6:184:VAL:H    | 1.82                     | 0.44              |
| 73:S8:10:LYS:HB2   | 79:18:371:A:OP2    | 2.18                     | 0.44              |
| 79:18:1743:G:H21   | 79:18:1791:A:H62   | 1.65                     | 0.44              |
| 85:28:677:G:H2'    | 85:28:678:C:C6     | 2.51                     | 0.44              |
| 85:28:963:G:N3     | 85:28:964:A:C8     | 2.85                     | 0.44              |
| 85:28:2478:C:C2    | 85:28:2479:G:C8    | 3.06                     | 0.44              |
| 85:28:2671:C:H2'   | 85:28:2672:C:C6    | 2.52                     | 0.44              |
| 85:28:2863:G:C4    | 85:28:2864:A:C8    | 3.05                     | 0.44              |
| 85:28:3702:A:C4    | 85:28:3703:G:C8    | 3.04                     | 0.44              |
| 85:28:4407:G:H1'   | 85:28:4438:U:C2    | 2.52                     | 0.44              |
| 12:L7:46:ARG:HH11  | 85:28:976:C:H5''   | 1.79                     | 0.44              |
| 29:30:105:ILE:H    | 29:30:105:ILE:HG13 | 1.53                     | 0.44              |
| 43:gg:51:VAL:HG12  | 43:gg:117:ILE:HD12 | 2.00                     | 0.44              |
| 51:ZZ:140:TYR:HE1  | 51:ZZ:145:CYS:HA   | 1.81                     | 0.44              |
| 58:AA:165:ILE:HD11 | 58:AA:177:TRP:HB2  | 1.99                     | 0.44              |
| 59:OO:34:LYS:O     | 59:OO:38:ASP:HB2   | 2.18                     | 0.44              |
| 67:S9:144:ILE:HG12 | 79:18:824:C:C2     | 2.52                     | 0.44              |
| 73:S8:31:ARG:HE    | 79:18:380:G:H5''   | 1.82                     | 0.44              |
| 79:18:464:A:H3'    | 79:18:465:A:H5'    | 1.99                     | 0.44              |
| 79:18:1261:C:C4    | 79:18:1262:C:C4    | 3.06                     | 0.44              |
| 79:18:1562:C:H2'   | 79:18:1563:G:H8    | 1.83                     | 0.44              |
| 79:18:1709:G:H2'   | 79:18:1710:C:H6    | 1.81                     | 0.44              |
| 79:18:1739:C:H2'   | 79:18:1740:C:H6    | 1.81                     | 0.44              |
| 79:18:1742:C:H2'   | 79:18:1743:G:O4'   | 2.18                     | 0.44              |
| 85:28:269:G:H2'    | 85:28:270:U:H6     | 1.81                     | 0.44              |
| 85:28:987:C:H2'    | 85:28:988:C:H6     | 1.82                     | 0.44              |
| 85:28:1557:C:H2'   | 85:28:1558:A:H8    | 1.82                     | 0.44              |
| 85:28:1558:A:H2'   | 85:28:1559:G:C8    | 2.52                     | 0.44              |
| 85:28:1730:U:H2'   | 85:28:1731:C:C6    | 2.53                     | 0.44              |
| 85:28:1792:U:H2'   | 85:28:1793:A:O4'   | 2.18                     | 0.44              |
| 85:28:1862:U:H4'   | 85:28:4212:A:OP2   | 2.18                     | 0.44              |
| 85:28:2479:G:N3    | 85:28:2480:G:C8    | 2.85                     | 0.44              |
| 85:28:3916:G:H2'   | 85:28:3917:A:H8    | 1.79                     | 0.44              |
| 85:28:4565:C:H2'   | 85:28:4566:U:H6    | 1.83                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:28:4678:G:N2   | 85:28:4713:G:H1'   | 2.33                     | 0.44              |
| 4:DD:102:PHE:H    | 63:RR:8:ARG:HA     | 1.82                     | 0.44              |
| 6:6:118:C:H2'     | 6:6:119:U:C6       | 2.52                     | 0.44              |
| 7:L8:3:ARG:HD3    | 85:28:1628:C:H42   | 1.82                     | 0.44              |
| 12:L7:65:ARG:CZ   | 85:28:1210:C:H41   | 2.31                     | 0.44              |
| 17:15:95:ALA:HB3  | 85:28:30:C:H5''    | 1.99                     | 0.44              |
| 20:19:70:ARG:HH22 | 85:28:2810:U:H5''  | 1.81                     | 0.44              |
| 25:26:59:ARG:HG3  | 25:26:103:LYS:HD2  | 1.98                     | 0.44              |
| 35:36:74:LYS:HA   | 35:36:83:ALA:HB2   | 1.99                     | 0.44              |
| 49:F:249:ARG:HB3  | 49:F:275:ALA:HA    | 1.99                     | 0.44              |
| 60:MM:39:LEU:HD23 | 60:MM:56:ARG:NH1   | 2.32                     | 0.44              |
| 68:S7:102:PRO:HA  | 79:18:688:U:C5     | 2.53                     | 0.44              |
| 72:WX:30:CYS:HA   | 72:WX:34:ILE:HD12  | 1.99                     | 0.44              |
| 80:v:249:ARG:HG3  | 80:v:250:ALA:N     | 2.32                     | 0.44              |
| 80:v:749:ILE:O    | 80:v:783:VAL:HA    | 2.17                     | 0.44              |
| 85:28:396:A:H2'   | 85:28:397:G:C8     | 2.53                     | 0.44              |
| 85:28:676:C:H2'   | 85:28:677:G:C8     | 2.51                     | 0.44              |
| 85:28:1690:C:H2'  | 85:28:1691:G:O4'   | 2.18                     | 0.44              |
| 85:28:2011:C:C2   | 85:28:2012:A:C8    | 3.06                     | 0.44              |
| 85:28:2329:U:H2'  | 85:28:2330:G:O4'   | 2.17                     | 0.44              |
| 85:28:2499:C:H2'  | 85:28:2500:U:H6    | 1.83                     | 0.44              |
| 85:28:3626:G:C6   | 85:28:3836:A:C2    | 3.06                     | 0.44              |
| 85:28:3664:G:C2   | 85:28:3665:G:N7    | 2.86                     | 0.44              |
| 1:BB:30:LEU:HD21  | 1:BB:35:GLU:HG2    | 1.98                     | 0.44              |
| 1:BB:127:PRO:HG3  | 1:BB:146:ALA:HB1   | 1.99                     | 0.44              |
| 5:58:153:C:H2'    | 5:58:154:G:C8      | 2.52                     | 0.44              |
| 9:L4:328:LEU:HB3  | 12:L7:186:MET:HG3  | 1.98                     | 0.44              |
| 14:10:190:LEU:HB3 | 14:10:197:VAL:HG21 | 1.99                     | 0.44              |
| 18:bb:80:PHE:HA   | 18:bb:83:THR:HG22  | 1.99                     | 0.44              |
| 21:20:35:PRO:HD2  | 21:20:39:VAL:HG21  | 1.99                     | 0.44              |
| 29:30:38:ILE:HD13 | 29:30:43:ALA:HB3   | 1.98                     | 0.44              |
| 44:AS:70:SER:HA   | 44:AS:83:LYS:HG2   | 1.99                     | 0.44              |
| 45:FF:54:LEU:HD23 | 45:FF:58:HIS:ND1   | 2.33                     | 0.44              |
| 55:WW:51:ARG:HG2  | 55:WW:52:GLU:H     | 1.81                     | 0.44              |
| 56:II:71:ARG:CZ   | 79:18:1407:U:H4'   | 2.48                     | 0.44              |
| 63:RR:90:CYS:HA   | 63:RR:93:PHE:CD1   | 2.52                     | 0.44              |
| 63:RR:105:PHE:HB3 | 63:RR:112:VAL:HG21 | 2.00                     | 0.44              |
| 74:W:49:ILE:O     | 74:W:52:THR:HG22   | 2.17                     | 0.44              |
| 79:18:23:G:C5     | 79:18:24:C:C4      | 3.06                     | 0.44              |
| 79:18:1676:U:C4   | 79:18:1677:U:C5    | 3.06                     | 0.44              |
| 80:v:421:VAL:HA   | 80:v:425:LEU:HG    | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:211:G:C2     | 85:28:212:A:C8     | 3.06                     | 0.44              |
| 85:28:221:C:H2'    | 85:28:222:C:H6     | 1.82                     | 0.44              |
| 85:28:470:A:C4     | 85:28:471:A:C8     | 3.05                     | 0.44              |
| 85:28:1808:C:H1'   | 85:28:1831:G:N2    | 2.32                     | 0.44              |
| 85:28:2804:C:H2'   | 85:28:2805:C:C6    | 2.53                     | 0.44              |
| 5:58:28:C:C2       | 5:58:29:G:C8       | 3.06                     | 0.44              |
| 5:58:92:U:H2'      | 5:58:93:C:O4'      | 2.17                     | 0.44              |
| 6:6:58:A:H2'       | 6:6:59:G:H8        | 1.81                     | 0.44              |
| 10:L5:15:ARG:CZ    | 85:28:1743:A:H1'   | 2.47                     | 0.44              |
| 13:aa:267:ALA:HA   | 13:aa:270:LYS:HG2  | 1.99                     | 0.44              |
| 14:10:9:TYR:HE1    | 85:28:1866:U:H5'   | 1.82                     | 0.44              |
| 16:14:24:LEU:HD11  | 16:14:86:TRP:CG    | 2.53                     | 0.44              |
| 20:19:3:MET:HG2    | 85:28:2385:U:H4'   | 2.00                     | 0.44              |
| 65:S6:216:ARG:NH1  | 66:S4:153:LEU:HD13 | 2.32                     | 0.44              |
| 75:GG:42:VAL:HG11  | 75:GG:81:VAL:HG11  | 1.99                     | 0.44              |
| 79:18:1266:C:C4    | 79:18:1517:G:N2    | 2.86                     | 0.44              |
| 79:18:1650:A:H2'   | 79:18:1651:A:O4'   | 2.17                     | 0.44              |
| 80:v:504:VAL:HG11  | 80:v:810:PRO:HG2   | 1.98                     | 0.44              |
| 85:28:1382:G:C2    | 85:28:1383:G:N7    | 2.86                     | 0.44              |
| 85:28:1545:G:H2'   | 85:28:1546:C:C6    | 2.53                     | 0.44              |
| 85:28:2089:G:H4'   | 85:28:2090:U:O5'   | 2.17                     | 0.44              |
| 1:BB:130:ASP:C     | 1:BB:133:PRO:HD2   | 2.43                     | 0.44              |
| 1:BB:140:VAL:HB    | 1:BB:142:LEU:HG    | 2.00                     | 0.44              |
| 6:6:60:G:C2        | 6:6:61:G:C8        | 3.06                     | 0.44              |
| 10:L5:146:LEU:HD22 | 85:28:4323:A:C2    | 2.52                     | 0.44              |
| 26:27:50:PRO:HD3   | 26:27:68:ILE:HD13  | 1.98                     | 0.44              |
| 44:AS:207:LEU:HD12 | 44:AS:210:VAL:HG21 | 1.99                     | 0.44              |
| 58:AA:12:LYS:H     | 58:AA:12:LYS:HD3   | 1.83                     | 0.44              |
| 64:SS:22:GLN:HB3   | 64:SS:74:MET:HG3   | 1.99                     | 0.44              |
| 69:YY:110:GLN:HA   | 69:YY:113:ARG:HG2  | 2.00                     | 0.44              |
| 79:18:186:C:H2'    | 79:18:187:G:C8     | 2.52                     | 0.44              |
| 79:18:537:C:H2'    | 79:18:538:U:C6     | 2.51                     | 0.44              |
| 79:18:1485:U:H2'   | 79:18:1486:A:O4'   | 2.18                     | 0.44              |
| 79:18:1666:C:H2'   | 79:18:1667:U:C6    | 2.53                     | 0.44              |
| 85:28:299:C:H2'    | 85:28:300:A:H8     | 1.83                     | 0.44              |
| 85:28:1095:A:H2'   | 85:28:1096:C:C6    | 2.53                     | 0.44              |
| 85:28:1514:U:H2'   | 85:28:1515:A:C8    | 2.53                     | 0.44              |
| 85:28:1519:C:H2'   | 85:28:1520:C:H6    | 1.83                     | 0.44              |
| 85:28:1951:G:C6    | 85:28:2033:A:C2    | 3.05                     | 0.44              |
| 5:58:140:C:H2'     | 5:58:141:C:C6      | 2.52                     | 0.44              |
| 7:L8:183:GLY:CA    | 85:28:1613:A:H5''  | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:bb:85:ARG:HG3   | 18:bb:99:LEU:HD11  | 1.99                     | 0.44              |
| 28:29:43:MET:HE2   | 28:29:43:MET:HB3   | 1.89                     | 0.44              |
| 31:32:35:TRP:HH2   | 31:32:55:MET:HG2   | 1.83                     | 0.44              |
| 60:MM:31:PRO:HG3   | 60:MM:102:ARG:HG2  | 1.99                     | 0.44              |
| 66:S4:151:ASP:HB3  | 66:S4:154:ILE:HG13 | 1.99                     | 0.44              |
| 77:11:27:GLY:HA2   | 77:11:68:ILE:HB    | 1.99                     | 0.44              |
| 77:11:111:GLU:HB2  | 77:11:125:ILE:HD11 | 1.99                     | 0.44              |
| 79:18:39:A:H2'     | 79:18:40:A:O4'     | 2.18                     | 0.44              |
| 85:28:1334:A:H2'   | 85:28:1335:G:H8    | 1.82                     | 0.44              |
| 85:28:1350:C:H2'   | 85:28:1351:G:H8    | 1.83                     | 0.44              |
| 85:28:1402:C:H2'   | 85:28:1403:G:H8    | 1.80                     | 0.44              |
| 85:28:1720:C:H2'   | 85:28:1721:G:O4'   | 2.18                     | 0.44              |
| 85:28:1797:G:H2'   | 85:28:1798:G:H8    | 1.83                     | 0.44              |
| 85:28:2380:G:N2    | 85:28:2424:G:H5''  | 2.33                     | 0.44              |
| 85:28:3768:U:H2'   | 85:28:3769:C:C6    | 2.53                     | 0.44              |
| 85:28:3851:U:H2'   | 85:28:3852:A:O4'   | 2.18                     | 0.44              |
| 85:28:4889:G:H2'   | 85:28:4890:G:C8    | 2.53                     | 0.44              |
| 4:DD:128:VAL:HB    | 4:DD:140:PHE:HB3   | 1.99                     | 0.43              |
| 6:6:51:G:H21       | 77:11:12:MET:CE    | 2.31                     | 0.43              |
| 8:L3:4:ARG:HD2     | 8:L3:7:SER:HA      | 1.99                     | 0.43              |
| 12:L7:45:ARG:O     | 12:L7:49:ILE:HG12  | 2.17                     | 0.43              |
| 13:aa:90:LYS:HG3   | 85:28:4127:A:C2    | 2.53                     | 0.43              |
| 27:dd:76:ASP:HB2   | 27:dd:115:GLY:HA3  | 1.99                     | 0.43              |
| 33:34:60:ARG:HB3   | 33:34:63:VAL:HG23  | 2.00                     | 0.43              |
| 34:35:47:ILE:HG13  | 34:35:48:ARG:N     | 2.31                     | 0.43              |
| 39:40:99:LYS:HG3   | 85:28:4474:A:H5'   | 2.00                     | 0.43              |
| 49:F:170:TRP:HA    | 49:F:173:VAL:HG22  | 2.00                     | 0.43              |
| 54:S5:59:LYS:HB3   | 54:S5:62:ARG:HB2   | 1.99                     | 0.43              |
| 56:II:12:VAL:HA    | 79:18:1397:U:O4    | 2.18                     | 0.43              |
| 58:AA:142:VAL:HG11 | 58:AA:145:GLU:HB3  | 1.99                     | 0.43              |
| 62:XX:50:ILE:HG13  | 70:S3:15:GLY:C     | 2.43                     | 0.43              |
| 64:SS:45:ALA:HB1   | 64:SS:50:THR:O     | 2.18                     | 0.43              |
| 67:S9:128:VAL:HG22 | 69:YY:104:ARG:HH22 | 1.83                     | 0.43              |
| 76:UU:92:ARG:HB3   | 79:18:1865:C:O2    | 2.17                     | 0.43              |
| 79:18:375:U:C2     | 79:18:376:A:C8     | 3.06                     | 0.43              |
| 79:18:537:C:H2'    | 79:18:538:U:C5     | 2.53                     | 0.43              |
| 79:18:1293:A:C5    | 79:18:1294:G:C8    | 3.06                     | 0.43              |
| 79:18:1716:C:H2'   | 79:18:1717:C:H6    | 1.83                     | 0.43              |
| 80:v:388:CYS:HB2   | 80:v:466:CYS:SG    | 2.58                     | 0.43              |
| 85:28:93:G:H2'     | 85:28:94:A:H8      | 1.82                     | 0.43              |
| 85:28:1077:C:C2    | 85:28:1078:A:C8    | 3.06                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:2688:G:H2'   | 85:28:2689:C:C6    | 2.53                     | 0.43              |
| 85:28:2893:U:H2'   | 85:28:2894:A:C8    | 2.53                     | 0.43              |
| 85:28:4638:U:C2    | 85:28:4639:G:C2    | 3.06                     | 0.43              |
| 86:23:43:LYS:HE2   | 86:23:62:MET:SD    | 2.57                     | 0.43              |
| 2:S2:183:LYS:HG3   | 72:WX:95:PRO:O     | 2.18                     | 0.43              |
| 8:L3:56:ILE:HA     | 8:L3:56:ILE:HD13   | 1.72                     | 0.43              |
| 13:aa:194:ASN:O    | 13:aa:198:THR:HG23 | 2.18                     | 0.43              |
| 22:21:107:LYS:HE3  | 22:21:107:LYS:HB3  | 1.88                     | 0.43              |
| 33:34:70:THR:HG21  | 85:28:2588:C:H41   | 1.82                     | 0.43              |
| 36:37:4:GLY:HA3    | 85:28:1601:A:OP2   | 2.18                     | 0.43              |
| 44:AS:150:ILE:HD13 | 71:RS:129:LYS:HB2  | 2.00                     | 0.43              |
| 49:F:29:ASN:O      | 49:F:33:ARG:HG2    | 2.18                     | 0.43              |
| 65:S6:91:GLU:HG2   | 65:S6:92:ARG:N     | 2.33                     | 0.43              |
| 66:S4:105:THR:HB   | 66:S4:245:ARG:HG2  | 2.00                     | 0.43              |
| 74:W:35:LYS:HD3    | 74:W:51:TRP:CZ2    | 2.53                     | 0.43              |
| 76:UU:84:VAL:HG12  | 79:18:1867:U:C4    | 2.53                     | 0.43              |
| 79:18:375:U:H2'    | 79:18:376:A:C8     | 2.54                     | 0.43              |
| 79:18:465:A:H4'    | 79:18:466:G:O5'    | 2.18                     | 0.43              |
| 79:18:493:A:H1'    | 79:18:574:A:O5'    | 2.18                     | 0.43              |
| 79:18:677:G:H2'    | 79:18:678:U:H6     | 1.83                     | 0.43              |
| 79:18:974:C:H2'    | 79:18:975:G:C8     | 2.53                     | 0.43              |
| 79:18:1369:A:H8    | 79:18:1369:A:OP1   | 2.01                     | 0.43              |
| 80:v:19:ILE:HD12   | 80:v:99:LEU:HB3    | 2.00                     | 0.43              |
| 85:28:12:A:H5'     | 85:28:13:U:OP2     | 2.18                     | 0.43              |
| 85:28:441:G:H2'    | 85:28:442:G:H8     | 1.82                     | 0.43              |
| 85:28:1753:G:N2    | 85:28:1778:C:C2    | 2.86                     | 0.43              |
| 85:28:2397:G:C8    | 85:28:2399:G:C8    | 3.06                     | 0.43              |
| 85:28:2662:G:H2'   | 85:28:2663:G:C8    | 2.53                     | 0.43              |
| 85:28:4251:A:H2'   | 85:28:4252:C:O4'   | 2.18                     | 0.43              |
| 85:28:4448:G:H4'   | 85:28:4449:A:OP2   | 2.18                     | 0.43              |
| 1:BB:102:ARG:HA    | 1:BB:102:ARG:HD2   | 1.65                     | 0.43              |
| 8:L3:175:GLN:HA    | 85:28:4986:G:H5'   | 2.00                     | 0.43              |
| 9:L4:83:GLY:H      | 85:28:368:C:H1'    | 1.83                     | 0.43              |
| 13:aa:309:ALA:O    | 13:aa:313:GLU:HG2  | 2.17                     | 0.43              |
| 65:S6:89:THR:HG22  | 79:18:91:A:H61     | 1.83                     | 0.43              |
| 65:S6:172:LYS:HE2  | 79:18:65:C:H4'     | 1.99                     | 0.43              |
| 67:S9:144:ILE:HG21 | 79:18:824:C:H1'    | 2.00                     | 0.43              |
| 79:18:298:G:C4     | 79:18:299:A:C8     | 3.06                     | 0.43              |
| 79:18:353:C:H2'    | 79:18:354:U:C6     | 2.53                     | 0.43              |
| 79:18:363:A:H4'    | 79:18:364:A:H4'    | 1.99                     | 0.43              |
| 80:v:764:ASN:HB3   | 85:28:4419:U:H1'   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:v:831:PRO:HA   | 80:v:834:VAL:HB    | 1.99                     | 0.43              |
| 85:28:962:C:C2    | 85:28:963:G:C8     | 3.05                     | 0.43              |
| 85:28:973:C:H2'   | 85:28:974:G:H8     | 1.83                     | 0.43              |
| 85:28:1464:C:C2   | 85:28:1465:G:C8    | 3.07                     | 0.43              |
| 85:28:1510:G:H2'  | 85:28:1511:U:C6    | 2.53                     | 0.43              |
| 85:28:2310:C:H2'  | 85:28:2311:C:C6    | 2.53                     | 0.43              |
| 85:28:2335:C:H2'  | 85:28:2336:G:C8    | 2.40                     | 0.43              |
| 85:28:2735:G:C2   | 85:28:2736:G:C8    | 3.07                     | 0.43              |
| 85:28:2864:A:H2'  | 85:28:2865:U:C6    | 2.53                     | 0.43              |
| 85:28:4357:G:H2'  | 85:28:4358:U:C6    | 2.54                     | 0.43              |
| 85:28:4647:G:C2   | 85:28:4648:A:C8    | 3.06                     | 0.43              |
| 85:28:4995:U:H2'  | 85:28:4996:C:C6    | 2.52                     | 0.43              |
| 3:PP:73:ALA:HB1   | 3:PP:78:ILE:HB     | 1.99                     | 0.43              |
| 6:6:3:C:H2'       | 6:6:4:U:C6         | 2.54                     | 0.43              |
| 14:10:66:GLU:CD   | 14:10:69:ARG:HH21  | 2.27                     | 0.43              |
| 16:14:90:ARG:O    | 16:14:94:LYS:HG2   | 2.17                     | 0.43              |
| 27:dd:55:LYS:HD3  | 85:28:92:C:C2      | 2.52                     | 0.43              |
| 33:34:26:PRO:HA   | 85:28:2639:U:H1'   | 2.00                     | 0.43              |
| 56:II:16:LYS:HG3  | 56:II:17:LYS:H     | 1.83                     | 0.43              |
| 64:SS:42:GLU:O    | 64:SS:46:LYS:HG3   | 2.18                     | 0.43              |
| 67:S9:110:LEU:O   | 67:S9:114:VAL:HG23 | 2.19                     | 0.43              |
| 77:11:57:VAL:HG12 | 77:11:59:SER:H     | 1.83                     | 0.43              |
| 79:18:609:U:H2'   | 79:18:610:G:C8     | 2.53                     | 0.43              |
| 79:18:1702:G:H2'  | 79:18:1703:C:O4'   | 2.19                     | 0.43              |
| 80:v:27:HIS:HB3   | 80:v:30:HIS:CE1    | 2.54                     | 0.43              |
| 85:28:385:A:H4'   | 85:28:386:A:OP1    | 2.18                     | 0.43              |
| 85:28:432:U:H4'   | 85:28:433:A:H5''   | 1.99                     | 0.43              |
| 85:28:1465:G:C2   | 85:28:1466:G:C8    | 3.06                     | 0.43              |
| 85:28:1490:G:H2'  | 85:28:1491:A:H8    | 1.83                     | 0.43              |
| 85:28:1633:G:H4'  | 85:28:1634:A:O5'   | 2.18                     | 0.43              |
| 85:28:1964:A:H2'  | 85:28:1965:G:H8    | 1.83                     | 0.43              |
| 85:28:2386:U:H2'  | 85:28:2387:G:H8    | 1.83                     | 0.43              |
| 85:28:2699:C:H2'  | 85:28:2700:G:C8    | 2.53                     | 0.43              |
| 6:6:4:U:H2'       | 6:6:5:A:H8         | 1.83                     | 0.43              |
| 6:6:106:G:C4      | 6:6:107:G:C8       | 3.06                     | 0.43              |
| 15:13:57:PRO:HG3  | 15:13:75:GLY:C     | 2.44                     | 0.43              |
| 18:bb:84:VAL:HG11 | 18:bb:102:LEU:HD22 | 2.00                     | 0.43              |
| 21:20:164:LYS:HB3 | 21:20:165:PRO:HD3  | 2.00                     | 0.43              |
| 30:31:70:LYS:HG3  | 85:28:2389:A:H4'   | 2.00                     | 0.43              |
| 44:AS:66:VAL:HA   | 44:AS:86:LEU:O     | 2.17                     | 0.43              |
| 56:II:18:THR:HB   | 56:II:75:GLY:HA2   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 58:AA:108:VAL:HA   | 58:AA:124:SER:HA  | 2.01                     | 0.43              |
| 64:SS:29:HIS:HB2   | 64:SS:32:LYS:HG3  | 2.01                     | 0.43              |
| 79:18:493:A:C8     | 79:18:574:A:C8    | 3.07                     | 0.43              |
| 79:18:1618:C:H2'   | 79:18:1619:A:C8   | 2.54                     | 0.43              |
| 79:18:1677:U:C2    | 79:18:1678:A:C8   | 3.06                     | 0.43              |
| 79:18:1686:G:H2'   | 79:18:1687:C:H6   | 1.83                     | 0.43              |
| 84:ES:2949:U:H2'   | 84:ES:2950:G:C8   | 2.53                     | 0.43              |
| 85:28:651:C:H2'    | 85:28:652:G:C8    | 2.50                     | 0.43              |
| 85:28:653:C:H2'    | 85:28:654:C:C6    | 2.54                     | 0.43              |
| 85:28:679:C:H2'    | 85:28:680:G:C8    | 2.49                     | 0.43              |
| 85:28:1594:C:O2'   | 85:28:1597:G:H1'  | 2.18                     | 0.43              |
| 85:28:1959:U:H1'   | 85:28:1961:G:N3   | 2.33                     | 0.43              |
| 85:28:1962:A:C2    | 85:28:1963:C:C6   | 3.06                     | 0.43              |
| 85:28:2357:G:C2    | 85:28:2358:G:C5   | 3.07                     | 0.43              |
| 85:28:5013:C:H4'   | 85:28:5014:A:H5'' | 2.00                     | 0.43              |
| 7:L8:199:VAL:HG21  | 85:28:1631:A:N7   | 2.34                     | 0.43              |
| 10:L5:249:GLU:HG3  | 10:L5:250:ASN:N   | 2.34                     | 0.43              |
| 31:32:29:VAL:HB    | 85:28:1332:C:H5'' | 2.00                     | 0.43              |
| 47:s:53:VAL:HA     | 47:s:89:VAL:HA    | 2.00                     | 0.43              |
| 49:F:288:LYS:HB2   | 49:F:288:LYS:HE3  | 1.68                     | 0.43              |
| 70:S3:68:GLU:O     | 70:S3:72:VAL:HG23 | 2.18                     | 0.43              |
| 75:GG:102:GLY:C    | 75:GG:136:PRO:HG3 | 2.44                     | 0.43              |
| 78:L9:47:LEU:HD13  | 78:L9:55:LEU:HD12 | 2.00                     | 0.43              |
| 79:18:150:A:H62    | 79:18:168:C:H42   | 1.66                     | 0.43              |
| 79:18:1650:A:H1'   | 79:18:1675:A:N6   | 2.33                     | 0.43              |
| 80:v:422:SER:H     | 80:v:425:LEU:HD23 | 1.84                     | 0.43              |
| 85:28:48:G:H1'     | 85:28:49:U:OP2    | 2.19                     | 0.43              |
| 85:28:1461:C:C2    | 85:28:1462:A:C8   | 3.07                     | 0.43              |
| 85:28:1490:G:H2'   | 85:28:1491:A:C8   | 2.54                     | 0.43              |
| 85:28:1884:C:H2'   | 85:28:1885:G:H8   | 1.83                     | 0.43              |
| 85:28:2492:C:C2    | 85:28:2493:G:N7   | 2.87                     | 0.43              |
| 85:28:4082:G:H2'   | 85:28:4083:U:C6   | 2.53                     | 0.43              |
| 1:BB:41:ARG:HB2    | 1:BB:47:TYR:CE1   | 2.54                     | 0.43              |
| 2:S2:253:PRO:HA    | 2:S2:256:TRP:CE2  | 2.54                     | 0.43              |
| 5:58:30:U:H2'      | 5:58:31:G:C8      | 2.53                     | 0.43              |
| 9:L4:137:VAL:HG21  | 9:L4:150:LEU:HD21 | 2.01                     | 0.43              |
| 12:L7:66:THR:O     | 12:L7:70:MET:HG2  | 2.19                     | 0.43              |
| 33:34:6:THR:HG22   | 85:28:2400:G:H21  | 1.84                     | 0.43              |
| 44:AS:106:THR:HG22 | 44:AS:108:ASP:H   | 1.84                     | 0.43              |
| 54:S5:152:TRP:CH2  | 79:18:1221:G:H4'  | 2.54                     | 0.43              |
| 79:18:1144:A:H5'   | 79:18:1355:C:N4   | 2.30                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:299:C:C2     | 85:28:300:A:C8     | 3.07                     | 0.43              |
| 85:28:1681:G:H2'   | 85:28:1682:A:C8    | 2.54                     | 0.43              |
| 85:28:2056:G:C8    | 85:28:2058:G:C8    | 3.06                     | 0.43              |
| 85:28:2897:G:H2'   | 85:28:2898:G:H8    | 1.83                     | 0.43              |
| 85:28:3794:C:H2'   | 85:28:3795:A:H8    | 1.84                     | 0.43              |
| 85:28:4985:U:H2'   | 85:28:4986:G:H8    | 1.83                     | 0.43              |
| 6:6:31:G:C6        | 6:6:47:G:C6        | 3.07                     | 0.43              |
| 8:L3:168:MET:HE3   | 8:L3:175:GLN:NE2   | 2.32                     | 0.43              |
| 14:10:36:LEU:HD23  | 14:10:69:ARG:HH11  | 1.83                     | 0.43              |
| 48:t:54:LYS:O      | 48:t:54:LYS:HG2    | 2.19                     | 0.43              |
| 48:t:146:ARG:HE    | 48:t:147:HIS:H     | 1.67                     | 0.43              |
| 50:Q:173:LYS:HE3   | 50:Q:173:LYS:HB2   | 1.89                     | 0.43              |
| 60:MM:129:ARG:O    | 60:MM:133:ARG:HG3  | 2.19                     | 0.43              |
| 65:S6:188:LYS:O    | 65:S6:191:ARG:HG2  | 2.19                     | 0.43              |
| 72:WX:93:LEU:HD21  | 72:WX:128:PHE:CD1  | 2.54                     | 0.43              |
| 79:18:1525:C:H2'   | 79:18:1526:G:H8    | 1.84                     | 0.43              |
| 79:18:1787:G:H2'   | 79:18:1788:A:H8    | 1.83                     | 0.43              |
| 80:v:394:LEU:HB3   | 80:v:487:THR:HG23  | 2.01                     | 0.43              |
| 85:28:283:G:H2'    | 85:28:284:G:H8     | 1.83                     | 0.43              |
| 85:28:324:A:H2'    | 85:28:325:U:H6     | 1.84                     | 0.43              |
| 85:28:1340:C:C2    | 85:28:1341:U:C5    | 3.07                     | 0.43              |
| 85:28:2505:C:H1'   | 85:28:2506:G:C8    | 2.54                     | 0.43              |
| 85:28:5001:U:H2'   | 85:28:5002:U:O4'   | 2.18                     | 0.43              |
| 86:23:92:ASP:OD1   | 86:23:94:VAL:HG22  | 2.19                     | 0.43              |
| 7:L8:201:GLY:HA3   | 7:L8:209:HIS:CE1   | 2.54                     | 0.43              |
| 11:L6:242:LYS:HB2  | 11:L6:242:LYS:HE2  | 1.80                     | 0.43              |
| 20:19:96:MET:SD    | 85:28:2607:C:H5''  | 2.59                     | 0.43              |
| 42:ff:49:ARG:HB2   | 42:ff:55:TRP:CZ3   | 2.54                     | 0.43              |
| 52:EE:120:ALA:HA   | 52:EE:123:VAL:HG12 | 1.99                     | 0.43              |
| 56:II:104:SER:HA   | 56:II:107:GLU:CG   | 2.48                     | 0.43              |
| 63:RR:5:ARG:O      | 72:WX:77:PRO:HD3   | 2.19                     | 0.43              |
| 70:S3:142:LEU:HD13 | 70:S3:143:ARG:HG3  | 2.00                     | 0.43              |
| 79:18:79:A:C8      | 79:18:80:G:C8      | 3.07                     | 0.43              |
| 79:18:1201:U:H2'   | 79:18:1202:U:H6    | 1.82                     | 0.43              |
| 79:18:1221:G:C2    | 79:18:1222:G:C5    | 3.07                     | 0.43              |
| 85:28:125:C:H2'    | 85:28:126:C:C6     | 2.53                     | 0.43              |
| 85:28:952:G:H2'    | 85:28:953:C:H6     | 1.84                     | 0.43              |
| 85:28:1577:G:O2'   | 85:28:1612:G:H4'   | 2.19                     | 0.43              |
| 85:28:1956:A:O2'   | 85:28:1957:U:H5'   | 2.19                     | 0.43              |
| 85:28:2015:U:H2'   | 85:28:2016:C:C6    | 2.46                     | 0.43              |
| 85:28:2078:C:C2    | 85:28:2079:G:C8    | 3.07                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:2317:C:H2'   | 85:28:2318:G:C8    | 2.54                     | 0.43              |
| 85:28:2446:C:H2'   | 85:28:2447:U:C6    | 2.54                     | 0.43              |
| 85:28:4378:A:O2'   | 85:28:4379:A:H2'   | 2.19                     | 0.43              |
| 85:28:4389:C:H2'   | 85:28:4390:A:C8    | 2.54                     | 0.43              |
| 85:28:4486:C:H2'   | 85:28:4487:A:O4'   | 2.19                     | 0.43              |
| 1:BB:38:ILE:HD11   | 1:BB:150:THR:HG22  | 1.99                     | 0.43              |
| 5:58:148:A:H2'     | 5:58:149:G:H8      | 1.83                     | 0.43              |
| 5:58:155:C:H2'     | 5:58:156:U:C6      | 2.54                     | 0.43              |
| 8:L3:89:ILE:HG21   | 8:L3:197:ALA:HB1   | 2.01                     | 0.43              |
| 9:L4:205:ARG:HG3   | 85:28:2297:G:H5'   | 2.00                     | 0.43              |
| 10:L5:41:LYS:HB2   | 22:21:68:THR:O     | 2.19                     | 0.43              |
| 19:17:48:LEU:O     | 19:17:52:THR:HG23  | 2.19                     | 0.43              |
| 20:19:37:SER:O     | 20:19:41:ILE:HG12  | 2.19                     | 0.43              |
| 43:gg:113:ARG:O    | 43:gg:117:ILE:HG13 | 2.18                     | 0.43              |
| 44:AS:181:LEU:O    | 44:AS:185:VAL:HG23 | 2.19                     | 0.43              |
| 49:F:247:TYR:HB3   | 49:F:302:LEU:HB3   | 2.00                     | 0.43              |
| 58:AA:257:LYS:HD2  | 58:AA:259:TRP:CZ2  | 2.54                     | 0.43              |
| 61:LL:142:ARG:HE   | 61:LL:142:ARG:HB2  | 1.63                     | 0.43              |
| 70:S3:170:THR:HB   | 70:S3:187:LYS:HG2  | 2.01                     | 0.43              |
| 75:GG:38:ASN:C     | 75:GG:69:SER:HB2   | 2.43                     | 0.43              |
| 78:L9:106:GLN:HB2  | 78:L9:111:LEU:HB3  | 2.00                     | 0.43              |
| 79:18:71:G:C8      | 79:18:79:A:C6      | 3.07                     | 0.43              |
| 79:18:678:U:C2     | 79:18:679:A:C8     | 3.07                     | 0.43              |
| 80:v:155:LEU:O     | 80:v:212:VAL:HA    | 2.19                     | 0.43              |
| 85:28:434:A:H2'    | 85:28:435:A:O4'    | 2.18                     | 0.43              |
| 85:28:1370:G:H4'   | 85:28:1371:A:O5'   | 2.19                     | 0.43              |
| 85:28:2730:U:H2'   | 85:28:2731:C:C6    | 2.54                     | 0.43              |
| 85:28:2894:A:H2'   | 85:28:2895:A:H8    | 1.83                     | 0.43              |
| 8:L3:252:ALA:HB3   | 85:28:4457:U:H1'   | 2.01                     | 0.42              |
| 16:14:11:ARG:NH2   | 16:14:61:ILE:HD11  | 2.34                     | 0.42              |
| 16:14:62:LEU:HD13  | 16:14:64:PHE:HE2   | 1.84                     | 0.42              |
| 38:39:44:TRP:CH2   | 38:39:45:ARG:HD3   | 2.54                     | 0.42              |
| 49:F:202:ILE:HB    | 49:F:213:HIS:CD2   | 2.53                     | 0.42              |
| 59:OO:34:LYS:HD3   | 59:OO:107:GLU:HG3  | 2.00                     | 0.42              |
| 65:S6:157:VAL:HG22 | 79:18:75:G:H22     | 1.84                     | 0.42              |
| 75:GG:55:ARG:HH12  | 79:18:954:U:H1'    | 1.83                     | 0.42              |
| 79:18:220:U:C2     | 79:18:221:A:C8     | 3.06                     | 0.42              |
| 79:18:430:C:H2'    | 79:18:431:G:H8     | 1.83                     | 0.42              |
| 79:18:935:G:H2'    | 79:18:936:G:C8     | 2.53                     | 0.42              |
| 79:18:1387:G:C2    | 79:18:1388:A:H1'   | 2.54                     | 0.42              |
| 79:18:1590:C:H3'   | 79:18:1591:C:C6    | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:1787:G:H2'   | 79:18:1788:A:C8    | 2.54                     | 0.42              |
| 85:28:134:G:OP1    | 85:28:134:G:H2'    | 2.19                     | 0.42              |
| 85:28:254:G:H2'    | 85:28:255:C:C6     | 2.54                     | 0.42              |
| 85:28:678:C:H2'    | 85:28:679:C:H6     | 1.83                     | 0.42              |
| 85:28:962:C:H2'    | 85:28:963:G:C8     | 2.53                     | 0.42              |
| 85:28:1617:G:H1'   | 85:28:2513:A:H61   | 1.84                     | 0.42              |
| 85:28:1920:C:H3'   | 85:28:1921:C:H5''  | 2.00                     | 0.42              |
| 85:28:2538:U:H2'   | 85:28:2539:C:H6    | 1.83                     | 0.42              |
| 85:28:2640:G:N3    | 85:28:2641:A:C8    | 2.86                     | 0.42              |
| 2:S2:209:VAL:HG21  | 2:S2:233:LEU:HD11  | 2.01                     | 0.42              |
| 9:L4:66:SER:HA     | 9:L4:77:PRO:HA     | 2.01                     | 0.42              |
| 11:L6:156:LEU:HD13 | 32:ee:105:LEU:HD13 | 2.00                     | 0.42              |
| 14:10:180:GLU:O    | 14:10:184:MET:HG3  | 2.19                     | 0.42              |
| 22:21:80:VAL:O     | 22:21:83:LYS:HG2   | 2.19                     | 0.42              |
| 25:26:59:ARG:HB2   | 25:26:103:LYS:HB3  | 2.02                     | 0.42              |
| 26:27:98:LYS:HE2   | 26:27:98:LYS:HB3   | 1.77                     | 0.42              |
| 27:dd:82:VAL:HB    | 27:dd:86:THR:HG21  | 2.01                     | 0.42              |
| 70:S3:99:ILE:HG12  | 70:S3:100:ALA:N    | 2.34                     | 0.42              |
| 72:WX:20:ARG:HG2   | 72:WX:22:LYS:HE2   | 2.01                     | 0.42              |
| 78:L9:92:MET:HE2   | 78:L9:179:ILE:HG22 | 2.01                     | 0.42              |
| 79:18:191:A:N3     | 79:18:191:A:H2'    | 2.33                     | 0.42              |
| 79:18:1011:A:H2'   | 79:18:1012:A:C8    | 2.53                     | 0.42              |
| 79:18:1856:C:H2'   | 79:18:1857:G:H8    | 1.84                     | 0.42              |
| 80:v:149:GLU:HA    | 80:v:371:LEU:HD13  | 2.01                     | 0.42              |
| 83:A:108:LYS:HD3   | 83:A:108:LYS:HA    | 1.86                     | 0.42              |
| 85:28:228:C:H2'    | 85:28:229:G:H8     | 1.84                     | 0.42              |
| 85:28:262:G:N3     | 85:28:263:G:C8     | 2.87                     | 0.42              |
| 85:28:691:C:H2'    | 85:28:692:A:C8     | 2.54                     | 0.42              |
| 85:28:2060:G:H2'   | 85:28:2061:U:C6    | 2.54                     | 0.42              |
| 85:28:3803:A:C2    | 85:28:3804:G:C8    | 3.06                     | 0.42              |
| 85:28:4356:G:N3    | 85:28:4357:G:C8    | 2.87                     | 0.42              |
| 5:58:71:A:H2'      | 25:26:50:ARG:NH1   | 2.34                     | 0.42              |
| 5:58:108:A:H2'     | 5:58:109:C:O4'     | 2.19                     | 0.42              |
| 15:13:184:MET:HG2  | 85:28:1482:G:H1    | 1.84                     | 0.42              |
| 21:20:30:MET:HE3   | 21:20:32:ILE:HD11  | 2.01                     | 0.42              |
| 42:ff:16:THR:HG22  | 85:28:2876:G:N7    | 2.34                     | 0.42              |
| 45:FF:117:LEU:O    | 45:FF:121:ARG:HG3  | 2.18                     | 0.42              |
| 47:s:192:VAL:HB    | 47:s:199:TYR:HB3   | 2.01                     | 0.42              |
| 48:t:35:LEU:HD11   | 48:t:37:LEU:HB2    | 2.02                     | 0.42              |
| 77:11:95:ARG:HB2   | 77:11:98:ASN:OD1   | 2.20                     | 0.42              |
| 79:18:34:U:H5'     | 79:18:564:A:H4'    | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:18:86:C:H1'     | 79:18:170:A:N1    | 2.34                     | 0.42              |
| 79:18:111:A:H2'    | 79:18:112:U:C6    | 2.54                     | 0.42              |
| 79:18:652:U:H2'    | 79:18:653:A:C8    | 2.54                     | 0.42              |
| 79:18:1083:A:H4'   | 79:18:1085:C:C5   | 2.54                     | 0.42              |
| 79:18:1406:G:H2'   | 79:18:1407:U:H6   | 1.84                     | 0.42              |
| 85:28:648:G:H2'    | 85:28:649:A:C8    | 2.55                     | 0.42              |
| 85:28:930:G:H2'    | 85:28:931:C:O4'   | 2.18                     | 0.42              |
| 85:28:1191:C:H2'   | 85:28:1192:C:C6   | 2.54                     | 0.42              |
| 85:28:1633:G:H5'   | 85:28:1634:A:OP1  | 2.19                     | 0.42              |
| 85:28:1673:U:H2'   | 85:28:1674:C:H6   | 1.85                     | 0.42              |
| 85:28:2611:A:O5'   | 85:28:2688:G:H4'  | 2.20                     | 0.42              |
| 85:28:2678:A:H2'   | 85:28:2679:G:H8   | 1.84                     | 0.42              |
| 85:28:3907:G:H2'   | 85:28:4447:C:O2'  | 2.19                     | 0.42              |
| 85:28:4088:C:H2'   | 85:28:4089:G:H8   | 1.84                     | 0.42              |
| 85:28:4122:G:C6    | 85:28:4123:C:C4   | 3.07                     | 0.42              |
| 2:S2:77:SER:O      | 2:S2:80:GLU:HG2   | 2.19                     | 0.42              |
| 2:S2:256:TRP:CD2   | 72:WX:68:ARG:HD3  | 2.54                     | 0.42              |
| 7:L8:9:ARG:HD2     | 85:28:1628:C:OP2  | 2.20                     | 0.42              |
| 8:L3:293:ILE:HA    | 8:L3:298:LEU:HA   | 2.02                     | 0.42              |
| 9:L4:70:GLY:HA2    | 85:28:3905:A:O3'  | 2.18                     | 0.42              |
| 10:L5:146:LEU:CD1  | 10:L5:163:LEU:HB2 | 2.49                     | 0.42              |
| 10:L5:264:LYS:HE3  | 10:L5:264:LYS:HB2 | 1.90                     | 0.42              |
| 15:13:103:ARG:HH22 | 85:28:73:A:N6     | 2.18                     | 0.42              |
| 16:14:97:ALA:HB2   | 18:bb:203:VAL:HB  | 2.01                     | 0.42              |
| 20:19:59:SER:HA    | 85:28:2634:C:H5'  | 2.00                     | 0.42              |
| 26:27:11:VAL:CG1   | 26:27:80:LEU:HB3  | 2.48                     | 0.42              |
| 32:ee:33:VAL:HG23  | 32:ee:38:GLU:HB2  | 2.01                     | 0.42              |
| 47:s:120:GLU:HG3   | 47:s:159:GLN:HE22 | 1.83                     | 0.42              |
| 48:t:32:ILE:HG22   | 48:t:37:LEU:HB3   | 2.01                     | 0.42              |
| 49:F:22:LYS:HE2    | 49:F:22:LYS:HB3   | 1.93                     | 0.42              |
| 49:F:67:GLU:O      | 49:F:70:MET:HG2   | 2.20                     | 0.42              |
| 54:S5:74:ASN:HD21  | 54:S5:86:LYS:HE3  | 1.84                     | 0.42              |
| 57:CC:3:MET:HE3    | 57:CC:44:HIS:HB3  | 2.01                     | 0.42              |
| 71:RS:105:MET:HE2  | 71:RS:105:MET:HB2 | 1.95                     | 0.42              |
| 78:L9:40:HIS:ND1   | 78:L9:41:ILE:HG13 | 2.34                     | 0.42              |
| 79:18:94:G:C4      | 79:18:95:G:C8     | 3.07                     | 0.42              |
| 79:18:887:U:H2'    | 79:18:888:U:H5''  | 2.01                     | 0.42              |
| 79:18:1369:A:OP1   | 79:18:1369:A:C8   | 2.72                     | 0.42              |
| 79:18:1389:C:H2'   | 79:18:1390:U:C6   | 2.54                     | 0.42              |
| 79:18:1536:G:C2    | 79:18:1537:A:C5   | 3.08                     | 0.42              |
| 80:v:372:LEU:HD22  | 80:v:417:PHE:CZ   | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:324:A:H2'    | 85:28:325:U:C6     | 2.54                     | 0.42              |
| 85:28:489:C:H2'    | 85:28:490:C:H6     | 1.84                     | 0.42              |
| 85:28:2266:C:H4'   | 85:28:2267:U:O5'   | 2.19                     | 0.42              |
| 85:28:4293:U:N3    | 85:28:4294:C:C5    | 2.87                     | 0.42              |
| 85:28:4565:C:H2'   | 85:28:4566:U:C6    | 2.55                     | 0.42              |
| 1:BB:32:PHE:CG     | 79:18:1097:G:H4'   | 2.55                     | 0.42              |
| 5:58:45:C:C2       | 5:58:46:G:C8       | 3.07                     | 0.42              |
| 5:58:126:C:HO2'    | 5:58:127:U:H5      | 1.67                     | 0.42              |
| 13:aa:223:LEU:HA   | 13:aa:223:LEU:HD23 | 1.71                     | 0.42              |
| 17:15:94:PHE:CE2   | 17:15:96:ARG:HB2   | 2.55                     | 0.42              |
| 20:19:155:LEU:HD13 | 20:19:155:LEU:HA   | 1.88                     | 0.42              |
| 21:20:164:LYS:HE2  | 21:20:164:LYS:HB2  | 1.90                     | 0.42              |
| 29:30:77:ASN:OD1   | 29:30:80:GLU:HG2   | 2.20                     | 0.42              |
| 45:FF:113:PHE:O    | 45:FF:117:LEU:HG   | 2.20                     | 0.42              |
| 58:AA:139:LYS:HG3  | 58:AA:140:TYR:CD2  | 2.54                     | 0.42              |
| 64:SS:10:ARG:HB3   | 64:SS:24:VAL:HB    | 2.01                     | 0.42              |
| 64:SS:18:LEU:HD13  | 66:S4:64:ILE:HD11  | 2.01                     | 0.42              |
| 64:SS:111:LYS:HD2  | 79:18:56:G:H5'     | 2.01                     | 0.42              |
| 79:18:351:G:C2     | 79:18:352:U:C6     | 3.07                     | 0.42              |
| 85:28:152:U:C2     | 85:28:153:G:C8     | 3.08                     | 0.42              |
| 85:28:1341:U:C2    | 85:28:1342:A:C8    | 3.08                     | 0.42              |
| 85:28:1586:G:C2    | 85:28:1608:G:C5    | 3.08                     | 0.42              |
| 85:28:2647:A:H62   | 85:28:2686:G:H8    | 1.67                     | 0.42              |
| 85:28:4400:G:C4    | 85:28:4401:G:C8    | 3.07                     | 0.42              |
| 42:ff:50:ARG:HB3   | 42:ff:54:ILE:HD13  | 2.02                     | 0.42              |
| 48:t:142:ASN:HB2   | 48:t:145:GLY:C     | 2.43                     | 0.42              |
| 49:F:81:SER:HB2    | 49:F:107:LYS:HE2   | 2.02                     | 0.42              |
| 70:S3:46:THR:HB    | 70:S3:84:VAL:HA    | 2.01                     | 0.42              |
| 73:S8:143:LYS:HA   | 73:S8:146:GLN:HB3  | 2.02                     | 0.42              |
| 77:11:161:GLU:HA   | 77:11:164:ARG:HG2  | 2.01                     | 0.42              |
| 79:18:298:G:C2     | 79:18:299:A:C8     | 3.07                     | 0.42              |
| 79:18:382:C:C2     | 79:18:383:G:N7     | 2.87                     | 0.42              |
| 79:18:433:A:H2'    | 79:18:434:G:C8     | 2.54                     | 0.42              |
| 79:18:616:A:C2     | 79:18:632:C:H1'    | 2.54                     | 0.42              |
| 79:18:997:A:H2'    | 79:18:998:A:C8     | 2.54                     | 0.42              |
| 79:18:1140:G:H2'   | 79:18:1141:G:C8    | 2.52                     | 0.42              |
| 80:v:396:MET:HB3   | 80:v:485:ILE:HB    | 2.01                     | 0.42              |
| 85:28:959:G:H4'    | 85:28:960:A:O5'    | 2.18                     | 0.42              |
| 85:28:1078:A:H2'   | 85:28:1078:A:N3    | 2.34                     | 0.42              |
| 85:28:1239:C:H4'   | 85:28:1244:G:P     | 2.59                     | 0.42              |
| 85:28:1392:A:H2'   | 85:28:1393:G:C8    | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:2385:U:H2'   | 85:28:2386:U:C6    | 2.55                     | 0.42              |
| 85:28:2454:U:C2    | 85:28:2455:G:C8    | 3.07                     | 0.42              |
| 85:28:2627:C:H41   | 85:28:4649:G:H1    | 1.68                     | 0.42              |
| 85:28:2697:A:C2    | 85:28:2698:G:C8    | 3.08                     | 0.42              |
| 85:28:4068:U:H2'   | 85:28:4069:U:C6    | 2.54                     | 0.42              |
| 85:28:4273:A:H62   | 85:28:4335:C:N4    | 2.16                     | 0.42              |
| 86:23:39:ILE:HG12  | 86:23:61:VAL:HG11  | 2.02                     | 0.42              |
| 1:BB:53:ARG:O      | 1:BB:57:LYS:HG2    | 2.20                     | 0.42              |
| 1:BB:77:ILE:HG12   | 1:BB:99:ILE:HB     | 2.02                     | 0.42              |
| 6:6:59:G:H2'       | 6:6:60:G:H8        | 1.85                     | 0.42              |
| 9:L4:285:LEU:HD22  | 9:L4:285:LEU:HA    | 1.92                     | 0.42              |
| 12:L7:98:ASN:OD1   | 85:28:1897:A:H5''  | 2.19                     | 0.42              |
| 12:L7:219:MET:HB3  | 12:L7:231:ASP:OD2  | 2.20                     | 0.42              |
| 37:38:32:VAL:HG11  | 37:38:53:ALA:HB1   | 2.01                     | 0.42              |
| 58:AA:20:GLN:HG2   | 58:AA:69:VAL:H     | 1.84                     | 0.42              |
| 75:GG:121:ARG:HD2  | 75:GG:121:ARG:HA   | 1.83                     | 0.42              |
| 79:18:27:A:H2'     | 79:18:28:U:C6      | 2.55                     | 0.42              |
| 79:18:193:C:H2'    | 79:18:194:C:H6     | 1.85                     | 0.42              |
| 79:18:1385:G:C4    | 79:18:1386:A:C8    | 3.08                     | 0.42              |
| 79:18:1391:C:H2'   | 79:18:1392:U:C6    | 2.55                     | 0.42              |
| 80:v:207:PRO:HG2   | 80:v:261:TRP:CE2   | 2.54                     | 0.42              |
| 85:28:123:C:H2'    | 85:28:124:C:H6     | 1.85                     | 0.42              |
| 85:28:1170:G:H2'   | 85:28:1171:G:C8    | 2.55                     | 0.42              |
| 85:28:1528:U:H2'   | 85:28:1529:G:H8    | 1.84                     | 0.42              |
| 85:28:1588:U:H2'   | 85:28:1589:C:C6    | 2.55                     | 0.42              |
| 85:28:1933:G:H8    | 85:28:1933:G:O5'   | 2.03                     | 0.42              |
| 85:28:2374:A:H2'   | 85:28:2375:A:H8    | 1.84                     | 0.42              |
| 85:28:4343:U:H2'   | 85:28:4344:U:H6    | 1.83                     | 0.42              |
| 85:28:4595:G:H2'   | 85:28:4596:C:H6    | 1.85                     | 0.42              |
| 85:28:4648:A:C4    | 85:28:4649:G:C8    | 3.08                     | 0.42              |
| 86:23:36:ASN:HD22  | 86:23:36:ASN:HA    | 1.70                     | 0.42              |
| 18:bb:47:PHE:HA    | 18:bb:136:ALA:HB2  | 2.02                     | 0.42              |
| 19:17:27:LYS:O     | 19:17:31:GLU:HG2   | 2.19                     | 0.42              |
| 31:32:89:LEU:HD13  | 31:32:118:LEU:HD22 | 2.02                     | 0.42              |
| 43:gg:93:ILE:HD11  | 43:gg:111:ILE:HA   | 2.01                     | 0.42              |
| 48:t:108:GLU:HA    | 48:t:111:ASN:HD21  | 1.85                     | 0.42              |
| 65:S6:212:LEU:HD12 | 65:S6:215:LYS:HD3  | 2.01                     | 0.42              |
| 68:S7:43:LEU:HD23  | 68:S7:72:PHE:CE1   | 2.55                     | 0.42              |
| 73:S8:129:LEU:HD22 | 73:S8:134:GLU:HB2  | 2.02                     | 0.42              |
| 79:18:92:A:H5'     | 79:18:93:U:C5      | 2.55                     | 0.42              |
| 79:18:639:C:C2     | 79:18:640:A:N7     | 2.88                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 84:ES:2942:C:C2'  | 84:ES:2943:C:H5'   | 2.50                     | 0.42              |
| 85:28:233:U:H6    | 85:28:2304:U:C4    | 2.37                     | 0.42              |
| 85:28:262:G:C2    | 85:28:263:G:C8     | 3.08                     | 0.42              |
| 85:28:294:G:O6    | 85:28:315:G:H1'    | 2.19                     | 0.42              |
| 85:28:385:A:N3    | 85:28:387:G:H5''   | 2.34                     | 0.42              |
| 85:28:949:G:H2'   | 85:28:950:G:H8     | 1.83                     | 0.42              |
| 85:28:1673:U:H2'  | 85:28:1674:C:C6    | 2.54                     | 0.42              |
| 85:28:1958:A:H5'' | 85:28:1962:A:O2'   | 2.19                     | 0.42              |
| 85:28:4674:C:H2'  | 85:28:4675:U:C6    | 2.54                     | 0.42              |
| 85:28:5036:C:H2'  | 85:28:5037:U:C6    | 2.54                     | 0.42              |
| 1:BB:34:MET:HE2   | 1:BB:34:MET:HA     | 2.01                     | 0.42              |
| 5:58:114:G:C4     | 5:58:115:G:C8      | 3.08                     | 0.42              |
| 6:6:60:G:N3       | 6:6:61:G:C8        | 2.87                     | 0.42              |
| 11:L6:179:THR:OG1 | 11:L6:189:LEU:HD23 | 2.19                     | 0.42              |
| 25:26:47:MET:HE1  | 25:26:118:ILE:HB   | 2.02                     | 0.42              |
| 42:ff:52:VAL:HG21 | 85:28:2739:C:H4'   | 2.02                     | 0.42              |
| 44:AS:136:ARG:NH1 | 79:18:941:C:H5''   | 2.35                     | 0.42              |
| 45:FF:49:GLN:O    | 45:FF:53:ILE:HG12  | 2.20                     | 0.42              |
| 54:S5:147:VAL:O   | 54:S5:151:ILE:HG13 | 2.20                     | 0.42              |
| 72:WX:10:ALA:O    | 72:WX:14:ILE:HG13  | 2.20                     | 0.42              |
| 79:18:341:C:H2'   | 79:18:342:C:C6     | 2.55                     | 0.42              |
| 79:18:578:C:C2    | 79:18:579:C:C6     | 3.07                     | 0.42              |
| 79:18:1284:A:OP1  | 79:18:1286:G:H5'   | 2.20                     | 0.42              |
| 80:v:324:ASP:HB3  | 80:v:342:ARG:HH12  | 1.84                     | 0.42              |
| 85:28:758:G:H2'   | 85:28:759:G:O4'    | 2.20                     | 0.42              |
| 85:28:1445:U:H2'  | 85:28:1446:C:C6    | 2.55                     | 0.42              |
| 85:28:1737:A:C4   | 85:28:1738:A:C8    | 3.08                     | 0.42              |
| 85:28:1874:A:H2'  | 85:28:1875:C:C6    | 2.54                     | 0.42              |
| 85:28:2479:G:C2   | 85:28:2480:G:C8    | 3.08                     | 0.42              |
| 85:28:2602:G:O4'  | 85:28:2742:G:H2'   | 2.20                     | 0.42              |
| 85:28:2837:U:N3   | 85:28:2838:G:C8    | 2.88                     | 0.42              |
| 85:28:3734:U:H2'  | 85:28:3735:G:O4'   | 2.20                     | 0.42              |
| 85:28:3760:A:H1'  | 85:28:3761:C:OP1   | 2.20                     | 0.42              |
| 85:28:4562:C:H2'  | 85:28:4563:U:H6    | 1.84                     | 0.42              |
| 85:28:4610:A:C4   | 85:28:4611:A:C8    | 3.08                     | 0.42              |
| 40:41:2:ARG:HD3   | 40:41:5:TRP:NE1    | 2.35                     | 0.42              |
| 47:s:192:VAL:O    | 47:s:198:ILE:HA    | 2.19                     | 0.42              |
| 75:GG:32:HIS:CD2  | 79:18:975:G:H4'    | 2.55                     | 0.42              |
| 75:GG:66:ARG:HB3  | 79:18:962:A:H5''   | 2.01                     | 0.42              |
| 78:L9:12:ILE:HG12 | 78:L9:54:ARG:HA    | 2.02                     | 0.42              |
| 79:18:92:A:H5'    | 79:18:93:U:H5      | 1.85                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:18:1018:U:H2'  | 79:18:1019:C:C6    | 2.55                     | 0.42              |
| 79:18:1675:A:H2'  | 79:18:1676:U:H6    | 1.84                     | 0.42              |
| 79:18:1738:C:H2'  | 79:18:1739:C:C6    | 2.55                     | 0.42              |
| 80:v:200:MET:HE2  | 80:v:200:MET:HB2   | 1.99                     | 0.42              |
| 84:ES:2955:A:H2   | 84:ES:3239:G:H1    | 1.65                     | 0.42              |
| 85:28:318:A:H2'   | 85:28:319:A:C8     | 2.55                     | 0.42              |
| 85:28:1216:C:C4   | 85:28:1217:G:N7    | 2.88                     | 0.42              |
| 85:28:1511:U:H2'  | 85:28:1512:G:H8    | 1.84                     | 0.42              |
| 85:28:1527:A:H2'  | 85:28:1528:U:H6    | 1.83                     | 0.42              |
| 85:28:2556:G:C2   | 85:28:2557:G:C5    | 3.07                     | 0.42              |
| 85:28:2724:G:H5'' | 85:28:2725:A:OP2   | 2.20                     | 0.42              |
| 85:28:3696:C:H2'  | 85:28:3697:U:O4'   | 2.20                     | 0.42              |
| 85:28:3737:A:C4   | 85:28:3738:G:C8    | 3.08                     | 0.42              |
| 85:28:4068:U:H2'  | 85:28:4069:U:H6    | 1.85                     | 0.42              |
| 85:28:4300:U:H2'  | 85:28:4301:U:C6    | 2.55                     | 0.42              |
| 85:28:4642:U:H2'  | 85:28:4643:G:C8    | 2.51                     | 0.42              |
| 85:28:4750:G:H2'  | 85:28:4751:G:C8    | 2.55                     | 0.42              |
| 85:28:4941:G:O2'  | 85:28:4942:C:H5'   | 2.20                     | 0.42              |
| 85:28:5056:A:H2'  | 85:28:5057:C:C6    | 2.55                     | 0.42              |
| 86:23:26:ILE:HG12 | 86:23:37:LEU:HB3   | 2.02                     | 0.42              |
| 2:S2:94:ILE:HD12  | 2:S2:162:ILE:HD11  | 2.02                     | 0.41              |
| 2:S2:253:PRO:HA   | 2:S2:256:TRP:CD1   | 2.56                     | 0.41              |
| 6:6:67:C:OP1      | 10:L5:14:LYS:HG2   | 2.19                     | 0.41              |
| 12:L7:69:ARG:O    | 12:L7:73:MET:HG3   | 2.20                     | 0.41              |
| 13:aa:190:ARG:O   | 13:aa:255:VAL:HA   | 2.20                     | 0.41              |
| 18:bb:81:TRP:HB2  | 18:bb:104:VAL:HG21 | 2.02                     | 0.41              |
| 32:ee:28:LEU:HG   | 32:ee:101:ILE:HD11 | 2.01                     | 0.41              |
| 35:36:34:THR:HB   | 35:36:37:THR:HG23  | 2.02                     | 0.41              |
| 38:39:48:LYS:HD2  | 38:39:48:LYS:HA    | 1.72                     | 0.41              |
| 46:VV:82:LYS:HE2  | 46:VV:82:LYS:HB3   | 1.83                     | 0.41              |
| 50:Q:12:LYS:HG2   | 85:28:2082:G:H5''  | 2.01                     | 0.41              |
| 67:S9:15:THR:HG22 | 67:S9:44:TRP:CZ3   | 2.55                     | 0.41              |
| 72:WX:93:LEU:HB3  | 72:WX:102:ILE:HD11 | 2.02                     | 0.41              |
| 79:18:4:C:H2'     | 79:18:5:U:C6       | 2.54                     | 0.41              |
| 79:18:23:G:C5     | 79:18:24:C:C5      | 3.08                     | 0.41              |
| 79:18:695:C:H2'   | 79:18:696:G:C8     | 2.55                     | 0.41              |
| 79:18:1804:U:H2'  | 79:18:1805:G:O4'   | 2.19                     | 0.41              |
| 79:18:1810:U:H2'  | 79:18:1811:C:C6    | 2.55                     | 0.41              |
| 80:v:176:GLN:O    | 80:v:180:ARG:HG2   | 2.20                     | 0.41              |
| 85:28:48:G:H4'    | 85:28:49:U:O5'     | 2.20                     | 0.41              |
| 85:28:963:G:C2    | 85:28:964:A:C8     | 3.08                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:963:G:O2'    | 85:28:964:A:H8     | 1.99                     | 0.41              |
| 85:28:1205:G:H2'   | 85:28:1206:C:H6    | 1.85                     | 0.41              |
| 85:28:1604:G:H2'   | 85:28:1605:G:C8    | 2.55                     | 0.41              |
| 85:28:4081:G:H2'   | 85:28:4082:G:H8    | 1.84                     | 0.41              |
| 85:28:4419:U:N3    | 85:28:4420:U:C6    | 2.88                     | 0.41              |
| 85:28:4419:U:O2    | 85:28:4419:U:H2'   | 2.19                     | 0.41              |
| 85:28:4958:C:H2'   | 85:28:4959:U:C6    | 2.55                     | 0.41              |
| 5:58:56:G:H2'      | 5:58:57:C:O4'      | 2.20                     | 0.41              |
| 5:58:153:C:H5'     | 13:aa:238:LYS:HE2  | 2.00                     | 0.41              |
| 17:15:68:ARG:HG2   | 17:15:128:LYS:HG3  | 2.01                     | 0.41              |
| 23:22:19:LEU:HD12  | 23:22:77:PRO:HA    | 2.00                     | 0.41              |
| 50:Q:158:THR:HG22  | 50:Q:161:SER:HB3   | 2.01                     | 0.41              |
| 52:EE:58:GLU:HB3   | 52:EE:61:TYR:HB3   | 2.02                     | 0.41              |
| 70:S3:172:VAL:HG13 | 70:S3:185:LYS:HG2  | 2.02                     | 0.41              |
| 73:S8:10:LYS:HB2   | 73:S8:10:LYS:HE3   | 1.81                     | 0.41              |
| 79:18:360:A:C2     | 79:18:362:C:H2'    | 2.55                     | 0.41              |
| 79:18:896:U:H2'    | 79:18:897:U:N1     | 2.36                     | 0.41              |
| 79:18:1043:G:H2'   | 79:18:1044:G:O4'   | 2.20                     | 0.41              |
| 79:18:1265:A:H5''  | 79:18:1266:C:OP2   | 2.20                     | 0.41              |
| 79:18:1724:A:H2'   | 79:18:1725:U:C6    | 2.55                     | 0.41              |
| 79:18:1856:C:H2'   | 79:18:1857:G:C8    | 2.55                     | 0.41              |
| 85:28:424:U:C2     | 85:28:425:U:C5     | 3.08                     | 0.41              |
| 85:28:1200:G:C5    | 85:28:1201:U:C5    | 3.08                     | 0.41              |
| 85:28:1460:C:H2'   | 85:28:1461:C:C6    | 2.54                     | 0.41              |
| 85:28:1468:C:H2'   | 85:28:1469:C:C6    | 2.54                     | 0.41              |
| 85:28:1948:G:H2'   | 85:28:1949:U:C6    | 2.55                     | 0.41              |
| 85:28:1991:A:OP1   | 85:28:1991:A:H4'   | 2.21                     | 0.41              |
| 85:28:2436:U:C2    | 85:28:2783:A:C8    | 3.07                     | 0.41              |
| 85:28:2735:G:N3    | 85:28:2736:G:C8    | 2.88                     | 0.41              |
| 85:28:3720:G:C2    | 85:28:3721:U:C6    | 3.08                     | 0.41              |
| 85:28:3911:C:C2    | 85:28:3912:U:C5    | 3.08                     | 0.41              |
| 85:28:4200:G:C4    | 85:28:4201:G:C8    | 3.07                     | 0.41              |
| 1:BB:3:GLY:HA2     | 3:PP:80:SER:OG     | 2.20                     | 0.41              |
| 7:L8:80:GLU:HG3    | 42:ff:66:GLY:HA2   | 2.02                     | 0.41              |
| 7:L8:132:ASN:OD1   | 85:28:3682:A:H5''  | 2.21                     | 0.41              |
| 11:L6:206:ILE:O    | 11:L6:209:VAL:HG12 | 2.19                     | 0.41              |
| 21:20:34:ALA:HB1   | 21:20:39:VAL:CG2   | 2.50                     | 0.41              |
| 27:dd:40:HIS:HA    | 85:28:1675:C:H1'   | 2.02                     | 0.41              |
| 33:34:56:VAL:HG13  | 33:34:72:LYS:HA    | 2.01                     | 0.41              |
| 35:36:70:LEU:HD22  | 35:36:87:ARG:NH1   | 2.35                     | 0.41              |
| 35:36:90:LEU:O     | 35:36:93:VAL:HG22  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:gg:33:LYS:HD2  | 43:gg:40:TYR:CE1   | 2.55                     | 0.41              |
| 56:II:81:ILE:O    | 56:II:84:ILE:HG12  | 2.20                     | 0.41              |
| 59:OO:67:LYS:HG2  | 62:XX:44:ARG:HH12  | 1.85                     | 0.41              |
| 74:W:107:GLN:O    | 74:W:110:ARG:HG3   | 2.20                     | 0.41              |
| 79:18:75:G:N2     | 79:18:77:A:H5''    | 2.29                     | 0.41              |
| 79:18:475:C:H1'   | 79:18:507:G:O2'    | 2.20                     | 0.41              |
| 80:v:464:VAL:HG21 | 80:v:470:VAL:HB    | 2.02                     | 0.41              |
| 85:28:919:C:H2'   | 85:28:920:C:H6     | 1.85                     | 0.41              |
| 85:28:1537:A:H2'  | 85:28:1538:U:C6    | 2.55                     | 0.41              |
| 85:28:2518:G:H1'  | 85:28:2539:C:H1'   | 2.02                     | 0.41              |
| 85:28:2724:G:H4'  | 85:28:2725:A:OP1   | 2.20                     | 0.41              |
| 85:28:3834:C:H2'  | 85:28:3835:C:C6    | 2.55                     | 0.41              |
| 85:28:3857:G:H2'  | 85:28:3858:C:C6    | 2.56                     | 0.41              |
| 85:28:4175:G:H2'  | 85:28:4176:C:H6    | 1.85                     | 0.41              |
| 85:28:4576:U:H2'  | 85:28:4577:U:C6    | 2.55                     | 0.41              |
| 85:28:4997:G:H2'  | 85:28:4998:G:H8    | 1.85                     | 0.41              |
| 85:28:5055:G:H2'  | 85:28:5056:A:C8    | 2.55                     | 0.41              |
| 6:6:113:G:H2'     | 6:6:114:U:H6       | 1.85                     | 0.41              |
| 10:L5:81:HIS:O    | 10:L5:84:PRO:HD2   | 2.21                     | 0.41              |
| 10:L5:195:HIS:CE1 | 10:L5:199:ILE:HD11 | 2.55                     | 0.41              |
| 57:CC:86:PRO:HA   | 57:CC:87:PRO:HD3   | 1.91                     | 0.41              |
| 64:SS:29:HIS:HE1  | 64:SS:69:THR:HG23  | 1.86                     | 0.41              |
| 66:S4:68:ARG:HG2  | 66:S4:76:VAL:HG11  | 2.02                     | 0.41              |
| 71:RS:11:LYS:HB3  | 71:RS:11:LYS:HE2   | 1.86                     | 0.41              |
| 72:WX:6:VAL:CG1   | 72:WX:29:PRO:HB2   | 2.50                     | 0.41              |
| 79:18:405:G:H2'   | 79:18:406:U:O4'    | 2.20                     | 0.41              |
| 79:18:1820:G:H2'  | 79:18:1821:U:C6    | 2.55                     | 0.41              |
| 80:v:666:THR:HB   | 80:v:669:VAL:HB    | 2.02                     | 0.41              |
| 83:A:102:PHE:CD1  | 83:A:102:PHE:N     | 2.89                     | 0.41              |
| 85:28:284:G:H2'   | 85:28:285:G:H8     | 1.85                     | 0.41              |
| 85:28:1461:C:C2   | 85:28:1462:A:N7    | 2.89                     | 0.41              |
| 85:28:4628:U:C2   | 85:28:4629:U:C5    | 3.09                     | 0.41              |
| 1:BB:74:VAL:HG13  | 1:BB:121:LEU:HB3   | 2.02                     | 0.41              |
| 7:L8:15:VAL:HG21  | 85:28:1628:C:H5''  | 2.01                     | 0.41              |
| 7:L8:225:ILE:HD11 | 7:L8:233:ARG:HG3   | 2.02                     | 0.41              |
| 8:L3:206:PRO:HD2  | 8:L3:209:GLN:HG3   | 2.02                     | 0.41              |
| 8:L3:240:LEU:HB2  | 8:L3:248:LEU:HA    | 2.03                     | 0.41              |
| 31:32:33:ARG:H    | 31:32:33:ARG:HD2   | 1.85                     | 0.41              |
| 45:FF:40:LEU:HD13 | 45:FF:53:ILE:HD11  | 2.02                     | 0.41              |
| 58:AA:17:TRP:O    | 58:AA:36:ARG:HG2   | 2.21                     | 0.41              |
| 60:MM:115:LYS:HA  | 60:MM:121:ARG:HG2  | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:18:34:U:H2'     | 79:18:35:C:C6      | 2.56                     | 0.41              |
| 79:18:118:C:H1'    | 79:18:445:A:C5     | 2.56                     | 0.41              |
| 79:18:399:C:H5     | 79:18:680:G:H5''   | 1.85                     | 0.41              |
| 79:18:640:A:C2     | 79:18:641:A:C5     | 3.08                     | 0.41              |
| 79:18:950:C:H2'    | 79:18:951:C:C6     | 2.56                     | 0.41              |
| 79:18:1367:U:H2'   | 79:18:1368:U:H6    | 1.85                     | 0.41              |
| 79:18:1396:A:N7    | 79:18:1450:G:N2    | 2.68                     | 0.41              |
| 85:28:86:U:H2'     | 85:28:87:A:C8      | 2.55                     | 0.41              |
| 85:28:121:A:H5'    | 85:28:122:U:OP2    | 2.20                     | 0.41              |
| 85:28:268:G:H2'    | 85:28:269:G:C8     | 2.54                     | 0.41              |
| 85:28:1201:U:H2'   | 85:28:1202:C:H6    | 1.85                     | 0.41              |
| 85:28:1693:U:H2'   | 85:28:1694:C:O4'   | 2.19                     | 0.41              |
| 85:28:1884:C:H4'   | 85:28:2070:U:C4    | 2.55                     | 0.41              |
| 85:28:2359:U:H5''  | 85:28:2360:A:OP2   | 2.20                     | 0.41              |
| 85:28:4235:G:C6    | 85:28:4236:G:N7    | 2.88                     | 0.41              |
| 85:28:4564:A:H2'   | 85:28:4565:C:C6    | 2.55                     | 0.41              |
| 85:28:4759:C:H2'   | 85:28:4760:G:O4'   | 2.20                     | 0.41              |
| 85:28:4995:U:H2'   | 85:28:4996:C:H6    | 1.85                     | 0.41              |
| 6:6:58:A:H2'       | 6:6:59:G:C8        | 2.56                     | 0.41              |
| 12:L7:113:LEU:HD21 | 12:L7:120:THR:HG22 | 2.03                     | 0.41              |
| 15:13:105:LYS:HE2  | 15:13:105:LYS:HB3  | 1.86                     | 0.41              |
| 18:bb:126:VAL:HG13 | 18:bb:127:VAL:HG23 | 2.02                     | 0.41              |
| 22:21:96:ILE:HD13  | 22:21:96:ILE:HA    | 1.81                     | 0.41              |
| 23:22:23:LEU:HB3   | 23:22:110:TYR:HB2  | 2.03                     | 0.41              |
| 28:29:28:ARG:HB3   | 85:28:1805:A:C4    | 2.55                     | 0.41              |
| 30:31:23:ARG:HD3   | 30:31:25:TYR:OH    | 2.21                     | 0.41              |
| 49:F:325:LEU:HD13  | 49:F:330:PRO:HB3   | 2.03                     | 0.41              |
| 57:CC:64:TRP:CD1   | 62:XX:23:VAL:HG13  | 2.55                     | 0.41              |
| 65:S6:7:PHE:CD2    | 65:S6:125:THR:HG22 | 2.56                     | 0.41              |
| 75:GG:138:ASP:OD2  | 79:18:985:G:H1'    | 2.21                     | 0.41              |
| 76:UU:12:LYS:HE3   | 76:UU:12:LYS:HB3   | 1.90                     | 0.41              |
| 77:11:35:ARG:O     | 77:11:39:VAL:HG23  | 2.21                     | 0.41              |
| 79:18:155:G:N3     | 79:18:156:G:C8     | 2.89                     | 0.41              |
| 79:18:577:U:H2'    | 79:18:578:C:C6     | 2.55                     | 0.41              |
| 79:18:1192:U:H2'   | 79:18:1193:U:C6    | 2.56                     | 0.41              |
| 79:18:1218:C:H2'   | 79:18:1219:C:C6    | 2.56                     | 0.41              |
| 79:18:1503:C:H2'   | 79:18:1504:U:C6    | 2.56                     | 0.41              |
| 79:18:1639:G:H2'   | 79:18:1640:A:C8    | 2.56                     | 0.41              |
| 80:v:753:GLU:HA    | 80:v:756:VAL:HG23  | 2.02                     | 0.41              |
| 85:28:1373:A:C2    | 85:28:1374:G:C8    | 3.09                     | 0.41              |
| 85:28:2611:A:H2'   | 85:28:2612:G:C8    | 2.56                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:28:2815:A:H2'  | 85:28:2816:G:C8    | 2.55                     | 0.41              |
| 85:28:4474:A:H2'  | 85:28:4476:C:O5'   | 2.21                     | 0.41              |
| 85:28:4519:C:OP1  | 85:28:4520:G:H5''  | 2.21                     | 0.41              |
| 85:28:5000:G:C2   | 85:28:5051:C:C2    | 3.08                     | 0.41              |
| 5:58:62:A:H4'     | 5:58:63:U:O5'      | 2.21                     | 0.41              |
| 6:6:60:G:H2'      | 6:6:61:G:H8        | 1.85                     | 0.41              |
| 9:L4:266:THR:HG22 | 9:L4:269:LYS:HB3   | 2.02                     | 0.41              |
| 14:10:59:GLN:HA   | 14:10:128:ARG:HA   | 2.02                     | 0.41              |
| 16:14:11:ARG:NH1  | 16:14:59:ASP:HA    | 2.35                     | 0.41              |
| 38:39:45:ARG:HA   | 38:39:45:ARG:HD2   | 1.67                     | 0.41              |
| 44:AS:116:LYS:HG2 | 44:AS:117:TRP:CD2  | 2.55                     | 0.41              |
| 47:s:61:MET:O     | 47:s:65:ILE:HG12   | 2.20                     | 0.41              |
| 49:F:86:VAL:HB    | 49:F:308:LEU:HB2   | 2.02                     | 0.41              |
| 54:S5:45:TYR:CE1  | 54:S5:65:GLN:HB2   | 2.56                     | 0.41              |
| 58:AA:291:TRP:CE2 | 58:AA:298:LEU:HD13 | 2.55                     | 0.41              |
| 61:LL:102:GLY:O   | 61:LL:106:LYS:HG2  | 2.21                     | 0.41              |
| 64:SS:13:MET:HB2  | 64:SS:13:MET:HE2   | 1.88                     | 0.41              |
| 70:S3:161:GLY:HA3 | 79:18:1388:A:H61   | 1.84                     | 0.41              |
| 72:WX:4:MET:SD    | 79:18:1159:G:H1'   | 2.60                     | 0.41              |
| 73:S8:176:ALA:HB3 | 79:18:220:U:H4'    | 2.02                     | 0.41              |
| 75:GG:99:ALA:H    | 75:GG:133:THR:HG22 | 1.85                     | 0.41              |
| 79:18:812:A:C4    | 79:18:813:A:C8     | 3.08                     | 0.41              |
| 79:18:955:A:C2    | 79:18:972:A:C6     | 3.09                     | 0.41              |
| 80:v:25:ILE:O     | 80:v:127:VAL:HA    | 2.20                     | 0.41              |
| 80:v:650:TRP:HZ2  | 80:v:672:LEU:HD21  | 1.86                     | 0.41              |
| 85:28:99:A:H2'    | 85:28:100:C:O2     | 2.21                     | 0.41              |
| 85:28:456:C:H2'   | 85:28:457:G:C8     | 2.55                     | 0.41              |
| 85:28:705:G:H2'   | 85:28:706:C:C6     | 2.55                     | 0.41              |
| 85:28:750:U:C2    | 85:28:751:G:C8     | 3.09                     | 0.41              |
| 85:28:1423:U:H2'  | 85:28:1424:G:H8    | 1.85                     | 0.41              |
| 85:28:1469:C:C2   | 85:28:1470:G:C8    | 3.09                     | 0.41              |
| 85:28:1552:G:H1'  | 85:28:1575:A:N6    | 2.36                     | 0.41              |
| 85:28:2529:A:O2'  | 85:28:2530:U:H5''  | 2.21                     | 0.41              |
| 85:28:2587:A:H5'' | 85:28:2588:C:C4    | 2.56                     | 0.41              |
| 85:28:3785:A:C6   | 85:28:4536:C:H1'   | 2.54                     | 0.41              |
| 85:28:3786:U:O2   | 85:28:3814:U:H4'   | 2.20                     | 0.41              |
| 85:28:3923:A:H2'  | 85:28:3924:C:C6    | 2.55                     | 0.41              |
| 85:28:4918:C:H2'  | 85:28:4919:G:C8    | 2.55                     | 0.41              |
| 9:L4:46:LYS:HA    | 9:L4:49:ARG:HD3    | 2.02                     | 0.41              |
| 27:dd:85:GLN:NE2  | 85:28:508:G:H21    | 2.19                     | 0.41              |
| 43:gg:103:HIS:CD2 | 43:gg:106:LEU:HD22 | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:EE:129:LYS:HE3  | 52:EE:129:LYS:HB3  | 1.89                     | 0.41              |
| 59:OO:61:LEU:HD23  | 62:XX:34:TYR:CD2   | 2.55                     | 0.41              |
| 61:LL:61:GLU:O     | 61:LL:64:VAL:HG22  | 2.21                     | 0.41              |
| 67:S9:124:HIS:O    | 67:S9:128:VAL:HG23 | 2.21                     | 0.41              |
| 70:S3:25:LEU:HG    | 70:S3:29:LEU:HD12  | 2.03                     | 0.41              |
| 78:L9:23:ARG:HH22  | 85:28:4763:U:H5''  | 1.85                     | 0.41              |
| 79:18:430:C:H2'    | 79:18:431:G:C8     | 2.56                     | 0.41              |
| 79:18:587:A:H5'    | 79:18:592:C:H41    | 1.86                     | 0.41              |
| 79:18:695:C:H2'    | 79:18:696:G:H8     | 1.85                     | 0.41              |
| 79:18:827:A:C6     | 79:18:828:G:C5     | 3.08                     | 0.41              |
| 85:28:161:G:H2'    | 85:28:162:A:C8     | 2.55                     | 0.41              |
| 85:28:325:U:H2'    | 85:28:326:C:H6     | 1.86                     | 0.41              |
| 85:28:1304:C:H2'   | 85:28:1305:C:C6    | 2.56                     | 0.41              |
| 85:28:1620:U:H2'   | 85:28:1621:A:C8    | 2.56                     | 0.41              |
| 85:28:1672:U:H2'   | 85:28:1673:U:C6    | 2.56                     | 0.41              |
| 85:28:2488:C:H3'   | 85:28:2490:U:O4    | 2.21                     | 0.41              |
| 85:28:2559:G:H2'   | 85:28:2560:C:H6    | 1.84                     | 0.41              |
| 85:28:2750:G:H2'   | 85:28:2751:G:O4'   | 2.20                     | 0.41              |
| 85:28:2757:A:O2'   | 85:28:2758:G:H5'   | 2.21                     | 0.41              |
| 85:28:3633:C:H2'   | 85:28:3634:G:H8    | 1.86                     | 0.41              |
| 85:28:4081:G:H2'   | 85:28:4082:G:C8    | 2.55                     | 0.41              |
| 85:28:4174:U:C2    | 85:28:4175:G:C8    | 3.08                     | 0.41              |
| 85:28:4459:U:H2'   | 85:28:4460:U:H6    | 1.86                     | 0.41              |
| 86:23:106:VAL:HG12 | 86:23:112:MET:HA   | 2.03                     | 0.41              |
| 1:BB:115:ALA:O     | 1:BB:117:ARG:HG2   | 2.21                     | 0.41              |
| 5:58:68:G:C5       | 5:58:69:U:C5       | 3.09                     | 0.41              |
| 6:6:94:C:H2'       | 6:6:95:C:H6        | 1.86                     | 0.41              |
| 8:L3:252:ALA:HB1   | 85:28:4524:G:C2    | 2.56                     | 0.41              |
| 10:L5:180:PHE:HB3  | 10:L5:195:HIS:CD2  | 2.56                     | 0.41              |
| 12:L7:135:VAL:O    | 12:L7:139:ILE:HG12 | 2.20                     | 0.41              |
| 13:aa:217:ILE:O    | 13:aa:221:VAL:HG13 | 2.21                     | 0.41              |
| 18:bb:149:TYR:OH   | 85:28:4583:C:H5''  | 2.21                     | 0.41              |
| 21:20:115:ALA:HB2  | 85:28:2060:G:N2    | 2.36                     | 0.41              |
| 24:cc:148:ASP:O    | 24:cc:152:LYS:HD3  | 2.21                     | 0.41              |
| 28:29:102:PRO:HA   | 28:29:109:ARG:HH22 | 1.86                     | 0.41              |
| 31:32:35:TRP:CH2   | 31:32:55:MET:HG2   | 2.56                     | 0.41              |
| 44:AS:62:LEU:HD23  | 44:AS:91:VAL:HG21  | 2.02                     | 0.41              |
| 44:AS:137:LEU:HG   | 44:AS:215:VAL:HG22 | 2.03                     | 0.41              |
| 44:AS:181:LEU:HA   | 44:AS:184:VAL:HG22 | 2.01                     | 0.41              |
| 49:F:172:LYS:HB3   | 49:F:354:LEU:HD22  | 2.03                     | 0.41              |
| 54:S5:42:LYS:HG2   | 54:S5:43:GLU:HB3   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:S5:166:ILE:HG13 | 79:18:1599:U:N3    | 2.36                     | 0.41              |
| 56:II:19:ALA:HB2   | 56:II:75:GLY:HA3   | 2.03                     | 0.41              |
| 66:S4:100:ARG:HB2  | 66:S4:114:ILE:HD13 | 2.03                     | 0.41              |
| 67:S9:37:LEU:HD23  | 67:S9:42:GLU:HG3   | 2.03                     | 0.41              |
| 68:S7:130:LEU:HB2  | 68:S7:177:TYR:CE1  | 2.56                     | 0.41              |
| 79:18:436:G:H5''   | 79:18:473:A:H62    | 1.85                     | 0.41              |
| 79:18:457:C:C2     | 79:18:458:A:C8     | 3.08                     | 0.41              |
| 79:18:598:G:H2'    | 79:18:599:A:H8     | 1.86                     | 0.41              |
| 79:18:854:A:N3     | 79:18:855:G:C8     | 2.89                     | 0.41              |
| 79:18:934:G:N3     | 79:18:935:G:C8     | 2.89                     | 0.41              |
| 79:18:1050:A:H62   | 79:18:1068:G:H21   | 1.69                     | 0.41              |
| 79:18:1070:A:H2'   | 79:18:1071:G:O4'   | 2.20                     | 0.41              |
| 79:18:1351:G:C2    | 79:18:1352:G:N7    | 2.89                     | 0.41              |
| 79:18:1413:G:C4    | 79:18:1414:A:C8    | 3.09                     | 0.41              |
| 79:18:1678:A:H2'   | 79:18:1679:A:H5'   | 2.03                     | 0.41              |
| 79:18:1687:C:C2    | 79:18:1688:C:C5    | 3.09                     | 0.41              |
| 79:18:1706:G:H2'   | 79:18:1707:U:C6    | 2.54                     | 0.41              |
| 79:18:1723:G:H2'   | 79:18:1724:A:C8    | 2.56                     | 0.41              |
| 80:v:423:THR:HG23  | 80:v:448:GLN:O     | 2.21                     | 0.41              |
| 85:28:223:G:H4'    | 85:28:225:G:C8     | 2.56                     | 0.41              |
| 85:28:247:G:H2'    | 85:28:248:C:C6     | 2.54                     | 0.41              |
| 85:28:1359:G:H3'   | 85:28:1360:G:H8    | 1.84                     | 0.41              |
| 85:28:1494:U:H2'   | 85:28:1495:G:C8    | 2.54                     | 0.41              |
| 85:28:1549:G:C2    | 85:28:1550:G:C8    | 3.09                     | 0.41              |
| 85:28:1589:C:H2'   | 85:28:1590:C:C6    | 2.55                     | 0.41              |
| 85:28:1744:U:H2'   | 85:28:1745:G:H8    | 1.86                     | 0.41              |
| 85:28:2732:G:H2'   | 85:28:2733:C:H6    | 1.86                     | 0.41              |
| 85:28:4233:A:C4    | 85:28:4235:G:N7    | 2.88                     | 0.41              |
| 85:28:4723:A:H2'   | 85:28:4724:A:C8    | 2.55                     | 0.41              |
| 85:28:4728:U:H4'   | 85:28:4966:A:H1'   | 2.01                     | 0.41              |
| 13:aa:210:ILE:HG23 | 13:aa:220:VAL:HG11 | 2.03                     | 0.41              |
| 23:22:24:ASP:HB3   | 23:22:69:LYS:HG3   | 2.03                     | 0.41              |
| 39:40:69:ILE:HD12  | 85:28:4473:A:H5''  | 2.03                     | 0.41              |
| 40:41:3:ALA:HB3    | 79:18:1842:C:OP1   | 2.21                     | 0.41              |
| 48:t:15:LEU:HD11   | 48:t:31:LYS:HE3    | 2.03                     | 0.41              |
| 48:t:64:ILE:HA     | 48:t:69:ALA:HA     | 2.03                     | 0.41              |
| 55:WW:17:VAL:HG23  | 55:WW:30:VAL:HG22  | 2.03                     | 0.41              |
| 60:MM:80:GLY:HA3   | 60:MM:92:PHE:HE1   | 1.85                     | 0.41              |
| 62:XX:16:GLN:CD    | 62:XX:16:GLN:H     | 2.29                     | 0.41              |
| 68:S7:6:ALA:HA     | 68:S7:28:LEU:HD11  | 2.03                     | 0.41              |
| 70:S3:55:THR:O     | 70:S3:58:VAL:HG22  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:18:653:A:H2'   | 79:18:654:A:O4'    | 2.20                     | 0.41              |
| 79:18:1053:C:H2'  | 79:18:1054:G:H8    | 1.86                     | 0.41              |
| 79:18:1506:A:H4'  | 79:18:1507:G:H3'   | 2.03                     | 0.41              |
| 85:28:22:G:H2'    | 85:28:23:C:C6      | 2.56                     | 0.41              |
| 85:28:272:U:H2'   | 85:28:273:U:H6     | 1.86                     | 0.41              |
| 85:28:2273:G:H2'  | 85:28:2274:C:H6    | 1.86                     | 0.41              |
| 85:28:2503:G:H2'  | 85:28:2504:C:C1'   | 2.51                     | 0.41              |
| 85:28:3860:A:H61  | 85:28:4560:C:H5    | 1.67                     | 0.41              |
| 85:28:3927:U:H2'  | 85:28:3928:A:C8    | 2.55                     | 0.41              |
| 85:28:4215:C:C2   | 85:28:4216:G:C8    | 3.09                     | 0.41              |
| 85:28:4433:G:H2'  | 85:28:4434:C:C6    | 2.56                     | 0.41              |
| 85:28:5043:A:C4   | 85:28:5044:A:C8    | 3.09                     | 0.41              |
| 6:6:27:G:N2       | 6:6:54:A:N6        | 2.70                     | 0.40              |
| 13:aa:169:ALA:O   | 13:aa:172:GLU:HG3  | 2.21                     | 0.40              |
| 24:cc:146:ALA:HA  | 24:cc:149:VAL:HG22 | 2.01                     | 0.40              |
| 44:AS:163:GLN:O   | 44:AS:166:LYS:HG2  | 2.21                     | 0.40              |
| 52:EE:92:CYS:HB3  | 52:EE:102:LYS:HB3  | 2.03                     | 0.40              |
| 54:S5:77:MET:HB3  | 54:S5:89:THR:HG21  | 2.03                     | 0.40              |
| 58:AA:36:ARG:O    | 58:AA:65:PHE:HA    | 2.22                     | 0.40              |
| 61:LL:10:GLN:H    | 61:LL:10:GLN:HG2   | 1.76                     | 0.40              |
| 64:SS:76:TYR:CE2  | 64:SS:82:ALA:HA    | 2.56                     | 0.40              |
| 67:S9:78:LEU:HB3  | 67:S9:92:MET:CG    | 2.51                     | 0.40              |
| 71:RS:69:ILE:HG23 | 71:RS:71:ILE:HG23  | 2.03                     | 0.40              |
| 76:UU:10:ARG:HB2  | 76:UU:33:ASP:OD2   | 2.21                     | 0.40              |
| 79:18:196:C:H2'   | 79:18:197:U:C6     | 2.56                     | 0.40              |
| 79:18:220:U:H2'   | 79:18:221:A:C8     | 2.55                     | 0.40              |
| 79:18:1228:A:C2   | 79:18:1229:G:C5    | 3.09                     | 0.40              |
| 79:18:1230:C:H2'  | 79:18:1231:C:H6    | 1.85                     | 0.40              |
| 79:18:1379:A:H2'  | 79:18:1380:C:C6    | 2.56                     | 0.40              |
| 79:18:1390:U:C2   | 79:18:1391:C:C6    | 3.08                     | 0.40              |
| 85:28:263:G:C6    | 85:28:264:C:N4     | 2.89                     | 0.40              |
| 85:28:275:C:H4'   | 85:28:276:C:OP1    | 2.21                     | 0.40              |
| 85:28:441:G:H2'   | 85:28:442:G:C8     | 2.56                     | 0.40              |
| 85:28:726:G:H2'   | 85:28:727:C:H6     | 1.86                     | 0.40              |
| 85:28:956:A:N6    | 85:28:1283:G:H1'   | 2.36                     | 0.40              |
| 85:28:1468:C:C2   | 85:28:1469:C:C5    | 3.09                     | 0.40              |
| 85:28:1735:U:C2   | 85:28:1736:A:C8    | 3.09                     | 0.40              |
| 85:28:1779:U:H2'  | 85:28:1780:A:H8    | 1.86                     | 0.40              |
| 85:28:2102:G:O2'  | 85:28:2103:A:H5'   | 2.22                     | 0.40              |
| 85:28:3698:G:O6   | 85:28:3816:A:H5''  | 2.21                     | 0.40              |
| 85:28:4562:C:H2'  | 85:28:4563:U:C6    | 2.55                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:5000:G:H2'   | 85:28:5001:U:O4'   | 2.21                     | 0.40              |
| 1:BB:89:LYS:HD3    | 1:BB:201:LEU:HG    | 2.03                     | 0.40              |
| 6:6:92:C:H2'       | 6:6:93:G:H8        | 1.86                     | 0.40              |
| 8:L3:252:ALA:HB1   | 85:28:4524:G:N3    | 2.36                     | 0.40              |
| 15:13:48:PRO:HG3   | 34:35:118:LYS:HE3  | 2.03                     | 0.40              |
| 29:30:91:VAL:HG12  | 85:28:2673:G:O2'   | 2.21                     | 0.40              |
| 34:35:96:ASN:N     | 34:35:96:ASN:ND2   | 2.68                     | 0.40              |
| 57:CC:65:ARG:HA    | 57:CC:65:ARG:HD2   | 1.84                     | 0.40              |
| 68:S7:63:PHE:HA    | 68:S7:95:ILE:O     | 2.21                     | 0.40              |
| 71:RS:19:LYS:HD3   | 71:RS:19:LYS:HA    | 1.96                     | 0.40              |
| 79:18:407:G:H2'    | 79:18:407:G:N3     | 2.36                     | 0.40              |
| 79:18:431:G:H2'    | 79:18:432:G:H8     | 1.87                     | 0.40              |
| 79:18:562:U:H3     | 79:18:587:A:H62    | 1.68                     | 0.40              |
| 79:18:1235:G:H5'   | 79:18:1247:C:H42   | 1.86                     | 0.40              |
| 79:18:1522:A:H5'   | 79:18:1523:C:OP2   | 2.21                     | 0.40              |
| 79:18:1611:G:H2'   | 79:18:1612:G:H8    | 1.86                     | 0.40              |
| 79:18:1620:A:OP1   | 83:A:44:ARG:HD3    | 2.21                     | 0.40              |
| 79:18:1708:C:C2    | 79:18:1709:G:C8    | 3.09                     | 0.40              |
| 79:18:1739:C:C2    | 79:18:1740:C:C5    | 3.09                     | 0.40              |
| 85:28:153:G:N3     | 85:28:154:G:C8     | 2.89                     | 0.40              |
| 85:28:516:C:H2'    | 85:28:517:C:C6     | 2.55                     | 0.40              |
| 85:28:909:G:C2     | 85:28:910:G:C8     | 3.09                     | 0.40              |
| 85:28:922(B):C:H3' | 85:28:923:C:H5''   | 2.04                     | 0.40              |
| 85:28:952:G:H2'    | 85:28:953:C:C6     | 2.56                     | 0.40              |
| 85:28:2089:G:H1'   | 85:28:2090:U:OP2   | 2.21                     | 0.40              |
| 85:28:2519:U:H1'   | 85:28:2520:C:C6    | 2.56                     | 0.40              |
| 85:28:3718:A:H2'   | 85:28:3719:A:H8    | 1.87                     | 0.40              |
| 85:28:4291:G:C8    | 85:28:4328:G:C4    | 3.09                     | 0.40              |
| 85:28:4410:G:C2    | 85:28:4411:G:C8    | 3.10                     | 0.40              |
| 85:28:4632:U:H2'   | 85:28:4633:G:O4'   | 2.20                     | 0.40              |
| 85:28:4684:A:H2'   | 85:28:4685:U:O4'   | 2.21                     | 0.40              |
| 5:58:132:G:H2'     | 5:58:133:G:C8      | 2.56                     | 0.40              |
| 5:58:141:C:H5'     | 17:15:113:LEU:HD11 | 2.02                     | 0.40              |
| 10:L5:36:LEU:HD23  | 10:L5:36:LEU:HA    | 1.95                     | 0.40              |
| 17:15:184:ILE:HD12 | 85:28:99:A:H5''    | 2.03                     | 0.40              |
| 22:21:14:MET:HE1   | 22:21:55:LYS:HB2   | 2.03                     | 0.40              |
| 31:32:44:ARG:H     | 31:32:44:ARG:HG3   | 1.57                     | 0.40              |
| 58:AA:150:TRP:HB2  | 58:AA:170:TRP:HB2  | 2.04                     | 0.40              |
| 63:RR:104:GLY:O    | 79:18:648:A:H4'    | 2.20                     | 0.40              |
| 67:S9:171:GLY:O    | 67:S9:175:ARG:HG3  | 2.22                     | 0.40              |
| 68:S7:135:PHE:CG   | 68:S7:136:PRO:HD3  | 2.57                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 68:S7:158:LEU:O    | 68:S7:190:PRO:HD2 | 2.21                     | 0.40              |
| 70:S3:100:ALA:O    | 70:S3:103:GLU:HG3 | 2.21                     | 0.40              |
| 71:RS:7:LYS:O      | 71:RS:11:LYS:HG2  | 2.21                     | 0.40              |
| 76:UU:88:SER:O     | 76:UU:92:ARG:HG3  | 2.21                     | 0.40              |
| 79:18:597:G:H2'    | 79:18:598:G:O4'   | 2.22                     | 0.40              |
| 79:18:623:G:C2     | 79:18:624:C:C6    | 3.10                     | 0.40              |
| 79:18:1716:C:H2'   | 79:18:1717:C:C6   | 2.57                     | 0.40              |
| 85:28:318:A:H2'    | 85:28:319:A:H8    | 1.86                     | 0.40              |
| 85:28:656:C:H2'    | 85:28:657:C:C6    | 2.57                     | 0.40              |
| 85:28:920:C:H2'    | 85:28:921:C:H6    | 1.86                     | 0.40              |
| 85:28:1206:C:H2'   | 85:28:1207:C:C6   | 2.57                     | 0.40              |
| 85:28:1912:G:C6    | 85:28:2057:A:C2   | 3.09                     | 0.40              |
| 85:28:2299:G:C2    | 85:28:2336:G:C5   | 3.09                     | 0.40              |
| 85:28:2654:C:H2'   | 85:28:2655:C:H6   | 1.86                     | 0.40              |
| 85:28:4092:G:C4    | 85:28:4093:G:C8   | 3.10                     | 0.40              |
| 85:28:4483:C:C2    | 85:28:4484:A:C8   | 3.09                     | 0.40              |
| 2:S2:194:ARG:O     | 2:S2:224:THR:HA   | 2.21                     | 0.40              |
| 4:DD:126:VAL:HG13  | 4:DD:142:VAL:HG13 | 2.03                     | 0.40              |
| 8:L3:288:GLY:HA3   | 8:L3:330:PHE:CE1  | 2.56                     | 0.40              |
| 10:L5:53:VAL:HG11  | 10:L5:159:VAL:HA  | 2.02                     | 0.40              |
| 13:aa:314:LEU:O    | 13:aa:318:LEU:HB2 | 2.21                     | 0.40              |
| 25:26:119:LEU:HD13 | 25:26:119:LEU:HA  | 1.95                     | 0.40              |
| 27:dd:57:GLY:HA3   | 50:Q:172:ARG:HD2  | 2.03                     | 0.40              |
| 49:F:57:MET:HE2    | 49:F:57:MET:HA    | 2.02                     | 0.40              |
| 63:RR:29:LYS:HE3   | 63:RR:29:LYS:HB3  | 1.88                     | 0.40              |
| 64:SS:25:ILE:HG13  | 64:SS:57:VAL:HG13 | 2.04                     | 0.40              |
| 65:S6:31:ARG:HG2   | 65:S6:100:CYS:SG  | 2.61                     | 0.40              |
| 79:18:24:C:C2      | 79:18:25:A:N7     | 2.89                     | 0.40              |
| 79:18:24:C:H4'     | 79:18:415:A:H4'   | 2.04                     | 0.40              |
| 79:18:1137:U:H4'   | 79:18:1138:C:OP1  | 2.22                     | 0.40              |
| 79:18:1164:G:O2'   | 79:18:1165:G:H5'  | 2.21                     | 0.40              |
| 79:18:1365:G:C2    | 79:18:1366:G:C5   | 3.09                     | 0.40              |
| 79:18:1545:A:C2    | 79:18:1671:G:H1'  | 2.57                     | 0.40              |
| 79:18:1685:U:C4    | 79:18:1686:G:N7   | 2.89                     | 0.40              |
| 79:18:1836:G:OP1   | 79:18:1839:U:H4'  | 2.21                     | 0.40              |
| 85:28:2:G:H2'      | 85:28:3:C:C6      | 2.57                     | 0.40              |
| 85:28:228:C:H2'    | 85:28:229:G:C8    | 2.56                     | 0.40              |
| 85:28:229:G:H2'    | 85:28:230:G:C8    | 2.56                     | 0.40              |
| 85:28:2292:C:C2    | 85:28:2293:U:C5   | 3.09                     | 0.40              |
| 85:28:2556:G:C2    | 85:28:2557:G:C8   | 3.10                     | 0.40              |
| 85:28:2817:C:H2'   | 85:28:2818:C:C6   | 2.57                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:28:4089:G:H2'   | 85:28:4090:G:C8    | 2.56                     | 0.40              |
| 85:28:4158:C:H2'   | 85:28:4159:C:C6    | 2.56                     | 0.40              |
| 85:28:4177:C:C2    | 85:28:4178:A:C8    | 3.10                     | 0.40              |
| 85:28:4401:G:H2'   | 85:28:4402:C:H6    | 1.86                     | 0.40              |
| 85:28:4511:A:H2'   | 85:28:4512:U:O4'   | 2.21                     | 0.40              |
| 85:28:4749:C:H2'   | 85:28:4750:G:O4'   | 2.21                     | 0.40              |
| 8:L3:77:THR:HG21   | 8:L3:337:VAL:HG22  | 2.04                     | 0.40              |
| 15:13:92:ARG:CZ    | 85:28:109:G:H5'    | 2.51                     | 0.40              |
| 17:15:44:ARG:HH12  | 85:28:280:G:P      | 2.45                     | 0.40              |
| 20:19:106:LEU:HD13 | 20:19:138:LEU:HD21 | 2.03                     | 0.40              |
| 28:29:31:SER:HA    | 85:28:1463:C:H5''  | 2.03                     | 0.40              |
| 44:AS:143:THR:HB   | 44:AS:205:TYR:CE1  | 2.56                     | 0.40              |
| 45:FF:45:LEU:HD12  | 45:FF:45:LEU:HA    | 1.74                     | 0.40              |
| 54:S5:49:LEU:HG    | 56:II:49:TYR:HB2   | 2.04                     | 0.40              |
| 54:S5:119:SER:OG   | 54:S5:189:ALA:HB1  | 2.22                     | 0.40              |
| 61:LL:82:TRP:CD1   | 79:18:1567:G:C6    | 3.10                     | 0.40              |
| 79:18:52:G:H2'     | 79:18:53:C:C6      | 2.57                     | 0.40              |
| 79:18:1512:C:H2'   | 79:18:1513:C:C6    | 2.57                     | 0.40              |
| 85:28:981:U:H2'    | 85:28:982:C:C6     | 2.56                     | 0.40              |
| 85:28:1216:C:C2    | 85:28:1217:G:C8    | 3.09                     | 0.40              |
| 85:28:1311:G:H2'   | 85:28:1312:A:O4'   | 2.22                     | 0.40              |
| 85:28:1384:C:C2    | 85:28:1385:G:C8    | 3.09                     | 0.40              |
| 85:28:1745:G:C2    | 85:28:1746:A:C8    | 3.10                     | 0.40              |
| 85:28:2007:G:H21   | 85:28:2012:A:H62   | 1.69                     | 0.40              |
| 85:28:2294:G:H2'   | 85:28:2295:C:C6    | 2.56                     | 0.40              |
| 85:28:2503:G:N2    | 85:28:4084:G:C8    | 2.89                     | 0.40              |
| 85:28:2728:U:H2'   | 85:28:2729:C:C6    | 2.57                     | 0.40              |
| 85:28:4340:U:C4    | 85:28:4341:C:C5    | 3.10                     | 0.40              |
| 85:28:4530:U:H2'   | 85:28:4531:U:H2'   | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|------------|---------|----------|-------------|-----|
| 1   | BB    | 215/217 (99%)  | 208 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 2   | S2    | 219/221 (99%)  | 217 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 3   | PP    | 81/83 (98%)    | 80 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 4   | DD    | 139/151 (92%)  | 132 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 7   | L8    | 246/248 (99%)  | 239 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 8   | L3    | 392/394 (100%) | 379 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 9   | L4    | 360/362 (99%)  | 354 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 10  | L5    | 291/293 (99%)  | 285 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 11  | L6    | 208/251 (83%)  | 199 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 12  | L7    | 223/225 (99%)  | 214 (96%)  | 8 (4%)  | 1 (0%)   | 30          | 59  |
| 13  | aa    | 229/240 (95%)  | 224 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 14  | 10    | 201/213 (94%)  | 200 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 15  | 13    | 208/211 (99%)  | 202 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 16  | 14    | 136/138 (99%)  | 134 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 17  | 15    | 201/203 (99%)  | 193 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 18  | bb    | 197/199 (99%)  | 196 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 19  | 17    | 151/153 (99%)  | 151 (100%) | 0       | 0        | 100         | 100 |
| 20  | 19    | 178/180 (99%)  | 175 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 21  | 20    | 174/176 (99%)  | 172 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 22  | 21    | 157/159 (99%)  | 156 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 23  | 22    | 97/99 (98%)    | 94 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 24  | cc    | 116/118 (98%)  | 115 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 25  | 26    | 132/134 (98%)  | 132 (100%) | 0       | 0        | 100         | 100 |
| 26  | 27    | 133/135 (98%)  | 129 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 27  | dd    | 145/147 (99%)  | 138 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 28  | 29    | 100/245 (41%)  | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 29  | 30    | 96/98 (98%)    | 95 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 30  | 31    | 105/107 (98%)  | 103 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 31  | 32    | 126/128 (98%)  | 124 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 32  | ee    | 107/109 (98%)  | 103 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 33  | 34    | 112/114 (98%)  | 112 (100%) | 0       | 0        | 100         | 100 |
| 34  | 35    | 120/122 (98%)  | 118 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 35  | 36    | 100/102 (98%) | 99 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 36  | 37    | 84/86 (98%)   | 84 (100%)  | 0       | 0        | 100         | 100 |
| 37  | 38    | 67/69 (97%)   | 66 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 38  | 39    | 48/50 (96%)   | 47 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 39  | 40    | 50/52 (96%)   | 50 (100%)  | 0       | 0        | 100         | 100 |
| 40  | 41    | 23/25 (92%)   | 23 (100%)  | 0       | 0        | 100         | 100 |
| 41  | 42    | 102/104 (98%) | 101 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 42  | ff    | 89/91 (98%)   | 86 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 43  | gg    | 122/124 (98%) | 119 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 44  | AS    | 211/213 (99%) | 207 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 45  | FF    | 147/149 (99%) | 145 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 46  | VV    | 81/83 (98%)   | 79 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 47  | s     | 194/196 (99%) | 188 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 48  | t     | 151/153 (99%) | 143 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 49  | F     | 356/358 (99%) | 349 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 50  | Q     | 185/188 (98%) | 181 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 51  | ZZ    | 66/68 (97%)   | 65 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 52  | EE    | 115/117 (98%) | 109 (95%)  | 6 (5%)  | 0        | 100         | 100 |
| 53  | TT    | 73/75 (97%)   | 69 (94%)   | 4 (6%)  | 0        | 100         | 100 |
| 54  | S5    | 181/191 (95%) | 168 (93%)  | 13 (7%) | 0        | 100         | 100 |
| 55  | WW    | 60/62 (97%)   | 60 (100%)  | 0       | 0        | 100         | 100 |
| 56  | II    | 140/142 (99%) | 137 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 57  | CC    | 94/96 (98%)   | 86 (92%)   | 7 (7%)  | 1 (1%)   | 11          | 36  |
| 58  | AA    | 311/313 (99%) | 297 (96%)  | 14 (4%) | 0        | 100         | 100 |
| 59  | OO    | 98/100 (98%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 60  | MM    | 139/141 (99%) | 135 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 61  | LL    | 142/144 (99%) | 136 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 62  | XX    | 53/55 (96%)   | 52 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 63  | RR    | 139/143 (97%) | 135 (97%)  | 3 (2%)  | 1 (1%)   | 18          | 48  |
| 64  | SS    | 122/124 (98%) | 121 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 65  | S6    | 235/237 (99%) | 234 (100%) | 1 (0%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 66  | S4    | 260/262 (99%)     | 257 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 67  | S9    | 183/185 (99%)     | 179 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 68  | S7    | 181/189 (96%)     | 178 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 69  | YY    | 53/55 (96%)       | 53 (100%)   | 0        | 0        | 100         | 100 |
| 70  | S3    | 212/214 (99%)     | 209 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 71  | RS    | 130/132 (98%)     | 126 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 72  | WX    | 127/129 (98%)     | 123 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 73  | S8    | 204/206 (99%)     | 199 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 74  | W     | 102/121 (84%)     | 101 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 75  | GG    | 133/136 (98%)     | 131 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 76  | UU    | 99/101 (98%)      | 98 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 77  | 11    | 168/170 (99%)     | 166 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 78  | L9    | 188/190 (99%)     | 181 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 80  | v     | 824/857 (96%)     | 809 (98%)   | 15 (2%)  | 0        | 100         | 100 |
| 81  | LA    | 45/1096 (4%)      | 45 (100%)   | 0        | 0        | 100         | 100 |
| 82  | CE    | 71/223 (32%)      | 71 (100%)   | 0        | 0        | 100         | 100 |
| 83  | A     | 119/121 (98%)     | 116 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 86  | 23    | 137/140 (98%)     | 137 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 12809/14451 (89%) | 12518 (98%) | 288 (2%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | RR    | 62  | PRO  |
| 57  | CC    | 65  | ARG  |
| 12  | L7    | 196 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | BB    | 180/181 (99%)  | 167 (93%) | 13 (7%)  | 13          | 39 |
| 2   | S2    | 187/187 (100%) | 180 (96%) | 7 (4%)   | 30          | 64 |
| 3   | PP    | 67/67 (100%)   | 63 (94%)  | 4 (6%)   | 17          | 47 |
| 4   | DD    | 130/136 (96%)  | 124 (95%) | 6 (5%)   | 24          | 57 |
| 7   | L8    | 190/190 (100%) | 182 (96%) | 8 (4%)   | 26          | 60 |
| 8   | L3    | 342/342 (100%) | 327 (96%) | 15 (4%)  | 25          | 59 |
| 9   | L4    | 302/302 (100%) | 293 (97%) | 9 (3%)   | 36          | 70 |
| 10  | L5    | 247/247 (100%) | 240 (97%) | 7 (3%)   | 38          | 72 |
| 11  | L6    | 190/223 (85%)  | 183 (96%) | 7 (4%)   | 30          | 64 |
| 12  | L7    | 196/196 (100%) | 189 (96%) | 7 (4%)   | 31          | 65 |
| 13  | aa    | 200/205 (98%)  | 191 (96%) | 9 (4%)   | 24          | 58 |
| 14  | 10    | 175/180 (97%)  | 171 (98%) | 4 (2%)   | 44          | 76 |
| 15  | 13    | 175/176 (99%)  | 166 (95%) | 9 (5%)   | 21          | 53 |
| 16  | 14    | 117/117 (100%) | 111 (95%) | 6 (5%)   | 21          | 53 |
| 17  | 15    | 171/171 (100%) | 164 (96%) | 7 (4%)   | 27          | 61 |
| 18  | bb    | 171/171 (100%) | 163 (95%) | 8 (5%)   | 23          | 56 |
| 19  | 17    | 134/134 (100%) | 133 (99%) | 1 (1%)   | 76          | 92 |
| 20  | 19    | 159/159 (100%) | 151 (95%) | 8 (5%)   | 22          | 53 |
| 21  | 20    | 157/157 (100%) | 150 (96%) | 7 (4%)   | 24          | 58 |
| 22  | 21    | 139/139 (100%) | 136 (98%) | 3 (2%)   | 45          | 77 |
| 23  | 22    | 89/89 (100%)   | 86 (97%)  | 3 (3%)   | 32          | 66 |
| 24  | cc    | 106/106 (100%) | 105 (99%) | 1 (1%)   | 70          | 90 |
| 25  | 26    | 124/124 (100%) | 117 (94%) | 7 (6%)   | 19          | 50 |
| 26  | 27    | 117/117 (100%) | 114 (97%) | 3 (3%)   | 40          | 73 |
| 27  | dd    | 119/119 (100%) | 117 (98%) | 2 (2%)   | 53          | 82 |
| 28  | 29    | 84/184 (46%)   | 82 (98%)  | 2 (2%)   | 43          | 75 |
| 29  | 30    | 84/84 (100%)   | 82 (98%)  | 2 (2%)   | 43          | 75 |
| 30  | 31    | 98/98 (100%)   | 92 (94%)  | 6 (6%)   | 17          | 46 |
| 31  | 32    | 114/114 (100%) | 108 (95%) | 6 (5%)   | 20          | 52 |
| 32  | ee    | 88/88 (100%)   | 83 (94%)  | 5 (6%)   | 18          | 49 |
| 33  | 34    | 98/98 (100%)   | 97 (99%)  | 1 (1%)   | 68          | 89 |
| 34  | 35    | 109/109 (100%) | 106 (97%) | 3 (3%)   | 38          | 72 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 35  | 36    | 86/86 (100%)   | 82 (95%)  | 4 (5%)   | 23          | 56  |
| 36  | 37    | 73/73 (100%)   | 71 (97%)  | 2 (3%)   | 39          | 73  |
| 37  | 38    | 64/64 (100%)   | 62 (97%)  | 2 (3%)   | 35          | 69  |
| 38  | 39    | 47/47 (100%)   | 47 (100%) | 0        | 100         | 100 |
| 39  | 40    | 48/48 (100%)   | 48 (100%) | 0        | 100         | 100 |
| 40  | 41    | 24/24 (100%)   | 24 (100%) | 0        | 100         | 100 |
| 41  | 42    | 92/92 (100%)   | 90 (98%)  | 2 (2%)   | 45          | 77  |
| 42  | ff    | 74/74 (100%)   | 70 (95%)  | 4 (5%)   | 20          | 51  |
| 43  | gg    | 107/108 (99%)  | 104 (97%) | 3 (3%)   | 38          | 72  |
| 44  | AS    | 194/194 (100%) | 188 (97%) | 6 (3%)   | 35          | 69  |
| 45  | FF    | 130/130 (100%) | 123 (95%) | 7 (5%)   | 20          | 51  |
| 46  | VV    | 75/75 (100%)   | 69 (92%)  | 6 (8%)   | 11          | 34  |
| 47  | s     | 164/164 (100%) | 151 (92%) | 13 (8%)  | 11          | 34  |
| 48  | t     | 126/126 (100%) | 115 (91%) | 11 (9%)  | 9           | 30  |
| 49  | F     | 307/307 (100%) | 295 (96%) | 12 (4%)  | 28          | 63  |
| 50  | Q     | 164/165 (99%)  | 162 (99%) | 2 (1%)   | 63          | 86  |
| 51  | ZZ    | 61/61 (100%)   | 58 (95%)  | 3 (5%)   | 22          | 54  |
| 52  | EE    | 99/99 (100%)   | 96 (97%)  | 3 (3%)   | 36          | 70  |
| 53  | TT    | 66/66 (100%)   | 63 (96%)  | 3 (4%)   | 24          | 58  |
| 54  | S5    | 158/161 (98%)  | 150 (95%) | 8 (5%)   | 21          | 53  |
| 55  | WW    | 55/55 (100%)   | 52 (94%)  | 3 (6%)   | 19          | 50  |
| 56  | II    | 117/117 (100%) | 112 (96%) | 5 (4%)   | 26          | 60  |
| 57  | CC    | 87/87 (100%)   | 84 (97%)  | 3 (3%)   | 32          | 66  |
| 58  | AA    | 272/272 (100%) | 263 (97%) | 9 (3%)   | 33          | 67  |
| 59  | OO    | 92/92 (100%)   | 86 (94%)  | 6 (6%)   | 15          | 44  |
| 60  | MM    | 111/111 (100%) | 108 (97%) | 3 (3%)   | 39          | 73  |
| 61  | LL    | 125/125 (100%) | 117 (94%) | 8 (6%)   | 16          | 44  |
| 62  | XX    | 48/48 (100%)   | 47 (98%)  | 1 (2%)   | 47          | 77  |
| 63  | RR    | 113/115 (98%)  | 108 (96%) | 5 (4%)   | 25          | 59  |
| 64  | SS    | 107/107 (100%) | 100 (94%) | 7 (6%)   | 15          | 44  |
| 65  | S6    | 207/207 (100%) | 201 (97%) | 6 (3%)   | 37          | 71  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 66  | S4    | 224/224 (100%)    | 220 (98%)   | 4 (2%)   | 51          | 80 |
| 67  | S9    | 161/161 (100%)    | 153 (95%)   | 8 (5%)   | 22          | 53 |
| 68  | S7    | 165/169 (98%)     | 159 (96%)   | 6 (4%)   | 31          | 65 |
| 69  | YY    | 46/46 (100%)      | 44 (96%)    | 2 (4%)   | 26          | 60 |
| 70  | S3    | 177/177 (100%)    | 162 (92%)   | 15 (8%)  | 10          | 31 |
| 71  | RS    | 119/119 (100%)    | 110 (92%)   | 9 (8%)   | 12          | 36 |
| 72  | WX    | 112/112 (100%)    | 108 (96%)   | 4 (4%)   | 31          | 65 |
| 73  | S8    | 178/178 (100%)    | 172 (97%)   | 6 (3%)   | 32          | 66 |
| 74  | W     | 86/100 (86%)      | 82 (95%)    | 4 (5%)   | 23          | 56 |
| 75  | GG    | 105/106 (99%)     | 101 (96%)   | 4 (4%)   | 29          | 64 |
| 76  | UU    | 88/88 (100%)      | 86 (98%)    | 2 (2%)   | 44          | 76 |
| 77  | 11    | 143/143 (100%)    | 139 (97%)   | 4 (3%)   | 38          | 72 |
| 78  | L9    | 169/169 (100%)    | 160 (95%)   | 9 (5%)   | 20          | 52 |
| 80  | v     | 705/728 (97%)     | 664 (94%)   | 41 (6%)  | 18          | 49 |
| 81  | LA    | 45/948 (5%)       | 41 (91%)    | 4 (9%)   | 9           | 28 |
| 82  | CE    | 62/190 (33%)      | 59 (95%)    | 3 (5%)   | 23          | 55 |
| 83  | A     | 107/107 (100%)    | 96 (90%)    | 11 (10%) | 7           | 23 |
| 86  | 23    | 106/107 (99%)     | 103 (97%)   | 3 (3%)   | 38          | 72 |
| All | All   | 11150/12382 (90%) | 10678 (96%) | 472 (4%) | 28          | 60 |

All (472) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BB    | 5   | LEU  |
| 1   | BB    | 44  | ASP  |
| 1   | BB    | 51  | LEU  |
| 1   | BB    | 84  | GLN  |
| 1   | BB    | 88  | LEU  |
| 1   | BB    | 136 | GLU  |
| 1   | BB    | 140 | VAL  |
| 1   | BB    | 145 | ILE  |
| 1   | BB    | 157 | VAL  |
| 1   | BB    | 159 | ILE  |
| 1   | BB    | 177 | MET  |
| 1   | BB    | 178 | LEU  |
| 1   | BB    | 208 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 86  | LEU  |
| 2   | S2    | 146 | GLU  |
| 2   | S2    | 165 | VAL  |
| 2   | S2    | 212 | LYS  |
| 2   | S2    | 215 | MET  |
| 2   | S2    | 227 | ARG  |
| 2   | S2    | 252 | THR  |
| 3   | PP    | 32  | ILE  |
| 3   | PP    | 51  | LYS  |
| 3   | PP    | 70  | LEU  |
| 3   | PP    | 72  | LEU  |
| 4   | DD    | 7   | GLU  |
| 4   | DD    | 12  | LYS  |
| 4   | DD    | 16  | ILE  |
| 4   | DD    | 42  | LEU  |
| 4   | DD    | 46  | THR  |
| 4   | DD    | 56  | ILE  |
| 7   | L8    | 42  | LYS  |
| 7   | L8    | 75  | LEU  |
| 7   | L8    | 101 | VAL  |
| 7   | L8    | 158 | ILE  |
| 7   | L8    | 162 | ASN  |
| 7   | L8    | 163 | ARG  |
| 7   | L8    | 165 | VAL  |
| 7   | L8    | 208 | GLU  |
| 8   | L3    | 47  | LEU  |
| 8   | L3    | 56  | ILE  |
| 8   | L3    | 89  | ILE  |
| 8   | L3    | 94  | GLU  |
| 8   | L3    | 95  | THR  |
| 8   | L3    | 158 | GLN  |
| 8   | L3    | 173 | LEU  |
| 8   | L3    | 240 | LEU  |
| 8   | L3    | 246 | ARG  |
| 8   | L3    | 248 | LEU  |
| 8   | L3    | 258 | HIS  |
| 8   | L3    | 262 | VAL  |
| 8   | L3    | 314 | ILE  |
| 8   | L3    | 351 | LEU  |
| 8   | L3    | 362 | LYS  |
| 9   | L4    | 3   | CYS  |
| 9   | L4    | 49  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | L4    | 62  | THR  |
| 9   | L4    | 205 | ARG  |
| 9   | L4    | 227 | ILE  |
| 9   | L4    | 232 | VAL  |
| 9   | L4    | 285 | LEU  |
| 9   | L4    | 294 | LYS  |
| 9   | L4    | 313 | VAL  |
| 10  | L5    | 25  | GLU  |
| 10  | L5    | 35  | ARG  |
| 10  | L5    | 56  | THR  |
| 10  | L5    | 69  | ILE  |
| 10  | L5    | 225 | GLN  |
| 10  | L5    | 249 | GLU  |
| 10  | L5    | 261 | VAL  |
| 11  | L6    | 51  | VAL  |
| 11  | L6    | 112 | LEU  |
| 11  | L6    | 166 | VAL  |
| 11  | L6    | 178 | VAL  |
| 11  | L6    | 197 | VAL  |
| 11  | L6    | 215 | LEU  |
| 11  | L6    | 217 | ASP  |
| 12  | L7    | 34  | LYS  |
| 12  | L7    | 41  | LEU  |
| 12  | L7    | 54  | LYS  |
| 12  | L7    | 97  | ILE  |
| 12  | L7    | 124 | LEU  |
| 12  | L7    | 151 | GLU  |
| 12  | L7    | 189 | LEU  |
| 13  | aa    | 139 | VAL  |
| 13  | aa    | 159 | THR  |
| 13  | aa    | 166 | ARG  |
| 13  | aa    | 193 | VAL  |
| 13  | aa    | 199 | LEU  |
| 13  | aa    | 220 | VAL  |
| 13  | aa    | 226 | LEU  |
| 13  | aa    | 237 | LEU  |
| 13  | aa    | 295 | LEU  |
| 14  | 10    | 44  | ASP  |
| 14  | 10    | 63  | GLU  |
| 14  | 10    | 146 | GLU  |
| 14  | 10    | 163 | GLN  |
| 15  | 13    | 59  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 13    | 63  | THR  |
| 15  | 13    | 67  | HIS  |
| 15  | 13    | 103 | ARG  |
| 15  | 13    | 124 | LEU  |
| 15  | 13    | 144 | LEU  |
| 15  | 13    | 154 | VAL  |
| 15  | 13    | 164 | GLU  |
| 15  | 13    | 205 | GLN  |
| 16  | 14    | 34  | ASN  |
| 16  | 14    | 38  | VAL  |
| 16  | 14    | 59  | ASP  |
| 16  | 14    | 62  | LEU  |
| 16  | 14    | 103 | LYS  |
| 16  | 14    | 137 | LYS  |
| 17  | 15    | 61  | ILE  |
| 17  | 15    | 64  | ILE  |
| 17  | 15    | 66  | VAL  |
| 17  | 15    | 75  | VAL  |
| 17  | 15    | 80  | THR  |
| 17  | 15    | 151 | ILE  |
| 17  | 15    | 198 | LEU  |
| 18  | bb    | 5   | GLN  |
| 18  | bb    | 7   | LEU  |
| 18  | bb    | 12  | ARG  |
| 18  | bb    | 27  | VAL  |
| 18  | bb    | 72  | HIS  |
| 18  | bb    | 113 | ASP  |
| 18  | bb    | 124 | LEU  |
| 18  | bb    | 144 | GLU  |
| 19  | 17    | 103 | GLU  |
| 20  | 19    | 15  | LEU  |
| 20  | 19    | 46  | LYS  |
| 20  | 19    | 50  | ILE  |
| 20  | 19    | 74  | ARG  |
| 20  | 19    | 106 | LEU  |
| 20  | 19    | 145 | LEU  |
| 20  | 19    | 149 | LYS  |
| 20  | 19    | 155 | LEU  |
| 21  | 20    | 1   | MET  |
| 21  | 20    | 7   | LEU  |
| 21  | 20    | 17  | LEU  |
| 21  | 20    | 39  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 20    | 90  | THR  |
| 21  | 20    | 111 | ARG  |
| 21  | 20    | 159 | LEU  |
| 22  | 21    | 69  | GLN  |
| 22  | 21    | 106 | LEU  |
| 22  | 21    | 121 | GLU  |
| 23  | 22    | 23  | LEU  |
| 23  | 22    | 30  | GLU  |
| 23  | 22    | 50  | ASN  |
| 24  | cc    | 147 | LEU  |
| 25  | 26    | 8   | THR  |
| 25  | 26    | 40  | GLN  |
| 25  | 26    | 55  | VAL  |
| 25  | 26    | 79  | VAL  |
| 25  | 26    | 104 | VAL  |
| 25  | 26    | 119 | LEU  |
| 25  | 26    | 120 | GLU  |
| 26  | 27    | 54  | THR  |
| 26  | 27    | 77  | TYR  |
| 26  | 27    | 120 | GLU  |
| 27  | dd    | 86  | THR  |
| 27  | dd    | 103 | VAL  |
| 28  | 29    | 9   | THR  |
| 28  | 29    | 104 | LEU  |
| 29  | 30    | 101 | ASP  |
| 29  | 30    | 105 | ILE  |
| 30  | 31    | 23  | ARG  |
| 30  | 31    | 26  | THR  |
| 30  | 31    | 46  | LEU  |
| 30  | 31    | 96  | GLU  |
| 30  | 31    | 111 | VAL  |
| 30  | 31    | 121 | ASN  |
| 31  | 32    | 4   | LEU  |
| 31  | 32    | 33  | ARG  |
| 31  | 32    | 44  | ARG  |
| 31  | 32    | 48  | ARG  |
| 31  | 32    | 85  | LEU  |
| 31  | 32    | 91  | CYS  |
| 32  | ee    | 18  | LEU  |
| 32  | ee    | 23  | GLU  |
| 32  | ee    | 33  | VAL  |
| 32  | ee    | 103 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | ee    | 105 | LEU  |
| 33  | 34    | 60  | ARG  |
| 34  | 35    | 47  | ILE  |
| 34  | 35    | 96  | ASN  |
| 34  | 35    | 111 | GLU  |
| 35  | 36    | 29  | ARG  |
| 35  | 36    | 42  | ASP  |
| 35  | 36    | 66  | ASP  |
| 35  | 36    | 94  | LEU  |
| 36  | 37    | 58  | THR  |
| 36  | 37    | 83  | THR  |
| 37  | 38    | 12  | LEU  |
| 37  | 38    | 57  | LYS  |
| 41  | 42    | 82  | MET  |
| 41  | 42    | 85  | ILE  |
| 42  | ff    | 52  | VAL  |
| 42  | ff    | 54  | ILE  |
| 42  | ff    | 74  | THR  |
| 42  | ff    | 89  | LEU  |
| 43  | gg    | 90  | LEU  |
| 43  | gg    | 103 | HIS  |
| 43  | gg    | 119 | ARG  |
| 44  | AS    | 60  | ASP  |
| 44  | AS    | 78  | GLU  |
| 44  | AS    | 122 | GLU  |
| 44  | AS    | 134 | LEU  |
| 44  | AS    | 183 | GLU  |
| 44  | AS    | 212 | VAL  |
| 45  | FF    | 22  | VAL  |
| 45  | FF    | 45  | LEU  |
| 45  | FF    | 75  | LEU  |
| 45  | FF    | 102 | LEU  |
| 45  | FF    | 118 | ILE  |
| 45  | FF    | 119 | GLU  |
| 45  | FF    | 142 | GLU  |
| 46  | VV    | 7   | LEU  |
| 46  | VV    | 14  | GLU  |
| 46  | VV    | 29  | ASN  |
| 46  | VV    | 53  | VAL  |
| 46  | VV    | 63  | LEU  |
| 46  | VV    | 73  | LEU  |
| 47  | s     | 29  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | s     | 30  | VAL  |
| 47  | s     | 68  | HIS  |
| 47  | s     | 94  | ASP  |
| 47  | s     | 95  | LEU  |
| 47  | s     | 126 | GLN  |
| 47  | s     | 144 | THR  |
| 47  | s     | 147 | ILE  |
| 47  | s     | 153 | GLU  |
| 47  | s     | 158 | VAL  |
| 47  | s     | 174 | LEU  |
| 47  | s     | 180 | ILE  |
| 47  | s     | 189 | ILE  |
| 48  | t     | 32  | ILE  |
| 48  | t     | 54  | LYS  |
| 48  | t     | 58  | ILE  |
| 48  | t     | 81  | ILE  |
| 48  | t     | 83  | LYS  |
| 48  | t     | 96  | LYS  |
| 48  | t     | 123 | ARG  |
| 48  | t     | 124 | GLU  |
| 48  | t     | 125 | LEU  |
| 48  | t     | 128 | THR  |
| 48  | t     | 146 | ARG  |
| 49  | F     | 21  | TYR  |
| 49  | F     | 51  | LYS  |
| 49  | F     | 82  | VAL  |
| 49  | F     | 131 | GLN  |
| 49  | F     | 177 | PHE  |
| 49  | F     | 209 | GLN  |
| 49  | F     | 226 | VAL  |
| 49  | F     | 287 | LYS  |
| 49  | F     | 319 | PHE  |
| 49  | F     | 350 | GLN  |
| 49  | F     | 353 | GLU  |
| 49  | F     | 354 | LEU  |
| 50  | Q     | 63  | LEU  |
| 50  | Q     | 158 | THR  |
| 51  | ZZ    | 107 | LYS  |
| 51  | ZZ    | 114 | ILE  |
| 51  | ZZ    | 132 | MET  |
| 52  | EE    | 26  | LEU  |
| 52  | EE    | 65  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | EE    | 122 | ASP  |
| 53  | TT    | 58  | LEU  |
| 53  | TT    | 69  | THR  |
| 53  | TT    | 75  | GLU  |
| 54  | S5    | 25  | THR  |
| 54  | S5    | 59  | LYS  |
| 54  | S5    | 81  | ARG  |
| 54  | S5    | 98  | GLU  |
| 54  | S5    | 142 | SER  |
| 54  | S5    | 152 | TRP  |
| 54  | S5    | 154 | LEU  |
| 54  | S5    | 155 | CYS  |
| 55  | WW    | 24  | GLN  |
| 55  | WW    | 28  | THR  |
| 55  | WW    | 57  | THR  |
| 56  | II    | 47  | LEU  |
| 56  | II    | 68  | ILE  |
| 56  | II    | 81  | ILE  |
| 56  | II    | 86  | GLN  |
| 56  | II    | 126 | ARG  |
| 57  | CC    | 11  | ILE  |
| 57  | CC    | 32  | HIS  |
| 57  | CC    | 39  | ASN  |
| 58  | AA    | 17  | TRP  |
| 58  | AA    | 98  | THR  |
| 58  | AA    | 149 | GLU  |
| 58  | AA    | 198 | VAL  |
| 58  | AA    | 206 | LEU  |
| 58  | AA    | 246 | TYR  |
| 58  | AA    | 256 | ILE  |
| 58  | AA    | 257 | LYS  |
| 58  | AA    | 280 | LYS  |
| 59  | OO    | 39  | LEU  |
| 59  | OO    | 44  | LYS  |
| 59  | OO    | 46  | LYS  |
| 59  | OO    | 60  | THR  |
| 59  | OO    | 68  | THR  |
| 59  | OO    | 84  | ILE  |
| 60  | MM    | 43  | LYS  |
| 60  | MM    | 90  | SER  |
| 60  | MM    | 110 | LEU  |
| 61  | LL    | 36  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | LL    | 54  | LYS  |
| 61  | LL    | 75  | ARG  |
| 61  | LL    | 77  | TYR  |
| 61  | LL    | 83  | PHE  |
| 61  | LL    | 98  | VAL  |
| 61  | LL    | 108 | ARG  |
| 61  | LL    | 141 | ARG  |
| 62  | XX    | 50  | ILE  |
| 63  | RR    | 17  | ARG  |
| 63  | RR    | 52  | LEU  |
| 63  | RR    | 81  | ILE  |
| 63  | RR    | 99  | GLU  |
| 63  | RR    | 107 | ARG  |
| 64  | SS    | 4   | THR  |
| 64  | SS    | 29  | HIS  |
| 64  | SS    | 44  | LEU  |
| 64  | SS    | 51  | THR  |
| 64  | SS    | 61  | ARG  |
| 64  | SS    | 110 | ARG  |
| 64  | SS    | 112 | ASN  |
| 65  | S6    | 21  | GLU  |
| 65  | S6    | 24  | LEU  |
| 65  | S6    | 25  | ARG  |
| 65  | S6    | 76  | LEU  |
| 65  | S6    | 146 | ASN  |
| 65  | S6    | 160 | LYS  |
| 66  | S4    | 3   | ARG  |
| 66  | S4    | 42  | LEU  |
| 66  | S4    | 156 | VAL  |
| 66  | S4    | 245 | ARG  |
| 67  | S9    | 3   | VAL  |
| 67  | S9    | 14  | VAL  |
| 67  | S9    | 27  | GLN  |
| 67  | S9    | 59  | GLU  |
| 67  | S9    | 61  | LEU  |
| 67  | S9    | 101 | LYS  |
| 67  | S9    | 106 | LEU  |
| 67  | S9    | 131 | ARG  |
| 68  | S7    | 9   | VAL  |
| 68  | S7    | 18  | GLU  |
| 68  | S7    | 29  | GLU  |
| 68  | S7    | 31  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | S7    | 60  | ILE  |
| 68  | S7    | 121 | THR  |
| 69  | YY    | 107 | ARG  |
| 69  | YY    | 122 | PHE  |
| 70  | S3    | 1   | MET  |
| 70  | S3    | 4   | GLN  |
| 70  | S3    | 44  | THR  |
| 70  | S3    | 45  | ARG  |
| 70  | S3    | 59  | LEU  |
| 70  | S3    | 97  | CYS  |
| 70  | S3    | 99  | ILE  |
| 70  | S3    | 109 | LEU  |
| 70  | S3    | 123 | LEU  |
| 70  | S3    | 124 | ARG  |
| 70  | S3    | 126 | ILE  |
| 70  | S3    | 142 | LEU  |
| 70  | S3    | 157 | MET  |
| 70  | S3    | 167 | TYR  |
| 70  | S3    | 175 | VAL  |
| 71  | RS    | 16  | ILE  |
| 71  | RS    | 18  | GLU  |
| 71  | RS    | 24  | LEU  |
| 71  | RS    | 31  | ASN  |
| 71  | RS    | 69  | ILE  |
| 71  | RS    | 81  | ARG  |
| 71  | RS    | 88  | VAL  |
| 71  | RS    | 107 | LYS  |
| 71  | RS    | 123 | THR  |
| 72  | WX    | 57  | ARG  |
| 72  | WX    | 87  | GLU  |
| 72  | WX    | 103 | VAL  |
| 72  | WX    | 104 | LEU  |
| 73  | S8    | 3   | ILE  |
| 73  | S8    | 6   | ASP  |
| 73  | S8    | 73  | THR  |
| 73  | S8    | 140 | LYS  |
| 73  | S8    | 144 | LYS  |
| 73  | S8    | 178 | ARG  |
| 74  | W     | 30  | GLN  |
| 74  | W     | 82  | ILE  |
| 74  | W     | 94  | ARG  |
| 74  | W     | 97  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | GG    | 52  | THR  |
| 75  | GG    | 76  | LEU  |
| 75  | GG    | 86  | LYS  |
| 75  | GG    | 147 | ARG  |
| 76  | UU    | 43  | ASN  |
| 76  | UU    | 46  | GLU  |
| 77  | 11    | 33  | LEU  |
| 77  | 11    | 46  | GLN  |
| 77  | 11    | 67  | LYS  |
| 77  | 11    | 148 | THR  |
| 78  | L9    | 12  | ILE  |
| 78  | L9    | 20  | LEU  |
| 78  | L9    | 42  | ASN  |
| 78  | L9    | 57  | VAL  |
| 78  | L9    | 74  | CYS  |
| 78  | L9    | 103 | VAL  |
| 78  | L9    | 107 | GLU  |
| 78  | L9    | 141 | LYS  |
| 78  | L9    | 162 | GLN  |
| 80  | v     | 3   | ASN  |
| 80  | v     | 4   | PHE  |
| 80  | v     | 15  | LYS  |
| 80  | v     | 16  | LYS  |
| 80  | v     | 20  | ARG  |
| 80  | v     | 34  | THR  |
| 80  | v     | 75  | ILE  |
| 80  | v     | 77  | LEU  |
| 80  | v     | 99  | LEU  |
| 80  | v     | 140 | GLU  |
| 80  | v     | 164 | LEU  |
| 80  | v     | 211 | THR  |
| 80  | v     | 212 | VAL  |
| 80  | v     | 249 | ARG  |
| 80  | v     | 294 | LEU  |
| 80  | v     | 321 | ILE  |
| 80  | v     | 323 | LEU  |
| 80  | v     | 350 | LEU  |
| 80  | v     | 385 | ILE  |
| 80  | v     | 386 | LYS  |
| 80  | v     | 400 | LYS  |
| 80  | v     | 416 | VAL  |
| 80  | v     | 421 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 80  | v     | 425 | LEU  |
| 80  | v     | 439 | LYS  |
| 80  | v     | 442 | LEU  |
| 80  | v     | 461 | ILE  |
| 80  | v     | 464 | VAL  |
| 80  | v     | 480 | VAL  |
| 80  | v     | 505 | VAL  |
| 80  | v     | 554 | LEU  |
| 80  | v     | 568 | ILE  |
| 80  | v     | 577 | VAL  |
| 80  | v     | 675 | ILE  |
| 80  | v     | 729 | LEU  |
| 80  | v     | 746 | LEU  |
| 80  | v     | 773 | GLU  |
| 80  | v     | 775 | GLN  |
| 80  | v     | 776 | VAL  |
| 80  | v     | 783 | VAL  |
| 80  | v     | 800 | LEU  |
| 81  | LA    | 665 | HIS  |
| 81  | LA    | 683 | LEU  |
| 81  | LA    | 688 | GLN  |
| 81  | LA    | 690 | LEU  |
| 82  | CE    | 33  | GLU  |
| 82  | CE    | 49  | LYS  |
| 82  | CE    | 77  | GLU  |
| 83  | A     | 24  | GLN  |
| 83  | A     | 25  | LEU  |
| 83  | A     | 37  | TYR  |
| 83  | A     | 54  | HIS  |
| 83  | A     | 60  | LEU  |
| 83  | A     | 76  | VAL  |
| 83  | A     | 85  | ILE  |
| 83  | A     | 86  | LEU  |
| 83  | A     | 96  | VAL  |
| 83  | A     | 102 | PHE  |
| 83  | A     | 126 | VAL  |
| 86  | 23    | 16  | ILE  |
| 86  | 23    | 18  | LEU  |
| 86  | 23    | 35  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BB    | 9   | GLN  |
| 1   | BB    | 84  | GLN  |
| 1   | BB    | 111 | GLN  |
| 1   | BB    | 141 | ASN  |
| 2   | S2    | 113 | GLN  |
| 2   | S2    | 136 | HIS  |
| 4   | DD    | 11  | GLN  |
| 4   | DD    | 112 | HIS  |
| 7   | L8    | 22  | HIS  |
| 7   | L8    | 83  | HIS  |
| 7   | L8    | 216 | HIS  |
| 8   | L3    | 109 | HIS  |
| 8   | L3    | 123 | HIS  |
| 8   | L3    | 158 | GLN  |
| 8   | L3    | 175 | GLN  |
| 8   | L3    | 184 | GLN  |
| 8   | L3    | 204 | GLN  |
| 8   | L3    | 258 | HIS  |
| 9   | L4    | 50  | GLN  |
| 9   | L4    | 60  | HIS  |
| 9   | L4    | 178 | ASN  |
| 9   | L4    | 317 | ASN  |
| 9   | L4    | 338 | ASN  |
| 9   | L4    | 346 | ASN  |
| 10  | L5    | 195 | HIS  |
| 10  | L5    | 198 | HIS  |
| 14  | 10    | 95  | HIS  |
| 15  | 13    | 149 | GLN  |
| 16  | 14    | 20  | HIS  |
| 17  | 15    | 109 | HIS  |
| 18  | bb    | 26  | GLN  |
| 18  | bb    | 143 | HIS  |
| 18  | bb    | 150 | GLN  |
| 18  | bb    | 167 | HIS  |
| 18  | bb    | 184 | ASN  |
| 19  | 17    | 21  | ASN  |
| 19  | 17    | 25  | HIS  |
| 19  | 17    | 28  | ASN  |
| 19  | 17    | 56  | GLN  |
| 19  | 17    | 75  | GLN  |
| 19  | 17    | 116 | HIS  |
| 19  | 17    | 118 | GLN  |
| 19  | 17    | 120 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | 17    | 137 | ASN  |
| 20  | 19    | 66  | ASN  |
| 20  | 19    | 143 | HIS  |
| 21  | 20    | 66  | GLN  |
| 21  | 20    | 156 | HIS  |
| 22  | 21    | 98  | HIS  |
| 22  | 21    | 131 | GLN  |
| 23  | 22    | 17  | GLN  |
| 23  | 22    | 38  | ASN  |
| 24  | cc    | 93  | ASN  |
| 25  | 26    | 20  | ASN  |
| 25  | 26    | 61  | HIS  |
| 27  | dd    | 66  | ASN  |
| 27  | dd    | 85  | GLN  |
| 27  | dd    | 120 | GLN  |
| 28  | 29    | 6   | ASN  |
| 28  | 29    | 27  | GLN  |
| 28  | 29    | 61  | ASN  |
| 30  | 31    | 116 | ASN  |
| 33  | 34    | 28  | ASN  |
| 33  | 34    | 112 | GLN  |
| 34  | 35    | 68  | ASN  |
| 34  | 35    | 96  | ASN  |
| 36  | 37    | 13  | ASN  |
| 36  | 37    | 66  | HIS  |
| 37  | 38    | 31  | ASN  |
| 39  | 40    | 64  | ASN  |
| 42  | ff    | 92  | GLN  |
| 43  | gg    | 103 | HIS  |
| 45  | FF    | 69  | ASN  |
| 45  | FF    | 101 | HIS  |
| 46  | VV    | 9   | HIS  |
| 46  | VV    | 29  | ASN  |
| 47  | s     | 68  | HIS  |
| 47  | s     | 71  | ASN  |
| 47  | s     | 72  | ASN  |
| 48  | t     | 97  | ASN  |
| 48  | t     | 137 | GLN  |
| 48  | t     | 142 | ASN  |
| 48  | t     | 147 | HIS  |
| 49  | F     | 29  | ASN  |
| 49  | F     | 113 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | F     | 147 | HIS  |
| 49  | F     | 213 | HIS  |
| 49  | F     | 303 | GLN  |
| 49  | F     | 350 | GLN  |
| 50  | Q     | 57  | ASN  |
| 51  | ZZ    | 139 | HIS  |
| 53  | TT    | 64  | ASN  |
| 54  | S5    | 51  | HIS  |
| 54  | S5    | 74  | ASN  |
| 54  | S5    | 118 | ASN  |
| 54  | S5    | 148 | ASN  |
| 54  | S5    | 203 | ASN  |
| 55  | WW    | 29  | GLN  |
| 57  | CC    | 28  | HIS  |
| 57  | CC    | 32  | HIS  |
| 58  | AA    | 26  | GLN  |
| 60  | MM    | 42  | HIS  |
| 60  | MM    | 126 | GLN  |
| 61  | LL    | 105 | ASN  |
| 63  | RR    | 73  | GLN  |
| 64  | SS    | 19  | GLN  |
| 64  | SS    | 22  | GLN  |
| 64  | SS    | 29  | HIS  |
| 64  | SS    | 112 | ASN  |
| 65  | S6    | 4   | ASN  |
| 65  | S6    | 13  | GLN  |
| 65  | S6    | 59  | GLN  |
| 65  | S6    | 110 | ASN  |
| 66  | S4    | 112 | HIS  |
| 67  | S9    | 75  | ASN  |
| 67  | S9    | 113 | GLN  |
| 67  | S9    | 154 | GLN  |
| 67  | S9    | 177 | ASN  |
| 68  | S7    | 33  | ASN  |
| 68  | S7    | 193 | GLN  |
| 71  | RS    | 56  | HIS  |
| 72  | WX    | 64  | ASN  |
| 72  | WX    | 70  | ASN  |
| 73  | S8    | 7   | ASN  |
| 73  | S8    | 167 | GLN  |
| 74  | W     | 48  | GLN  |
| 75  | GG    | 94  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 77  | 11    | 23  | ASN  |
| 77  | 11    | 71  | HIS  |
| 78  | L9    | 79  | ASN  |
| 78  | L9    | 140 | GLN  |
| 80  | v     | 27  | HIS  |
| 80  | v     | 30  | HIS  |
| 80  | v     | 108 | HIS  |
| 80  | v     | 357 | HIS  |
| 80  | v     | 535 | GLN  |
| 80  | v     | 803 | ASN  |
| 80  | v     | 807 | GLN  |
| 80  | v     | 853 | ASN  |
| 81  | LA    | 680 | ASN  |
| 86  | 23    | 36  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed         | Backbone Outliers | Pucker Outliers |
|-----|-------|------------------|-------------------|-----------------|
| 5   | 58    | 149/156 (95%)    | 20 (13%)          | 1 (0%)          |
| 6   | 6     | 119/120 (99%)    | 9 (7%)            | 0               |
| 79  | 18    | 1675/1688 (99%)  | 300 (17%)         | 14 (0%)         |
| 84  | ES    | 34/5070 (0%)     | 7 (20%)           | 1 (2%)          |
| 85  | 28    | 3479/4808 (72%)  | 581 (16%)         | 48 (1%)         |
| All | All   | 5456/11842 (46%) | 917 (16%)         | 64 (1%)         |

All (917) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 58    | 2   | G    |
| 5   | 58    | 34  | U    |
| 5   | 58    | 35  | C    |
| 5   | 58    | 59  | A    |
| 5   | 58    | 62  | A    |
| 5   | 58    | 63  | U    |
| 5   | 58    | 86  | U    |
| 5   | 58    | 103 | A    |
| 5   | 58    | 105 | C    |
| 5   | 58    | 110 | U    |
| 5   | 58    | 111 | U    |
| 5   | 58    | 112 | G    |
| 5   | 58    | 114 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 58    | 122 | G    |
| 5   | 58    | 123 | U    |
| 5   | 58    | 124 | U    |
| 5   | 58    | 125 | C    |
| 5   | 58    | 126 | C    |
| 5   | 58    | 127 | U    |
| 5   | 58    | 151 | G    |
| 6   | 6     | 7   | G    |
| 6   | 6     | 25  | G    |
| 6   | 6     | 33  | U    |
| 6   | 6     | 53  | U    |
| 6   | 6     | 54  | A    |
| 6   | 6     | 64  | G    |
| 6   | 6     | 100 | A    |
| 6   | 6     | 110 | G    |
| 6   | 6     | 120 | U    |
| 79  | 18    | 2   | A    |
| 79  | 18    | 3   | C    |
| 79  | 18    | 4   | C    |
| 79  | 18    | 25  | A    |
| 79  | 18    | 26  | U    |
| 79  | 18    | 33  | G    |
| 79  | 18    | 36  | U    |
| 79  | 18    | 41  | G    |
| 79  | 18    | 44  | U    |
| 79  | 18    | 45  | A    |
| 79  | 18    | 46  | A    |
| 79  | 18    | 50  | A    |
| 79  | 18    | 51  | U    |
| 79  | 18    | 56  | G    |
| 79  | 18    | 67  | C    |
| 79  | 18    | 74  | G    |
| 79  | 18    | 77  | A    |
| 79  | 18    | 79  | A    |
| 79  | 18    | 93  | U    |
| 79  | 18    | 99  | A    |
| 79  | 18    | 103 | A    |
| 79  | 18    | 111 | A    |
| 79  | 18    | 113 | G    |
| 79  | 18    | 115 | U    |
| 79  | 18    | 116 | U    |
| 79  | 18    | 124 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | 18    | 126 | G    |
| 79  | 18    | 127 | C    |
| 79  | 18    | 142 | C    |
| 79  | 18    | 143 | U    |
| 79  | 18    | 147 | A    |
| 79  | 18    | 155 | G    |
| 79  | 18    | 160 | U    |
| 79  | 18    | 162 | C    |
| 79  | 18    | 163 | U    |
| 79  | 18    | 168 | C    |
| 79  | 18    | 169 | U    |
| 79  | 18    | 182 | C    |
| 79  | 18    | 183 | G    |
| 79  | 18    | 184 | G    |
| 79  | 18    | 191 | A    |
| 79  | 18    | 192 | C    |
| 79  | 18    | 206 | G    |
| 79  | 18    | 292 | A    |
| 79  | 18    | 294 | U    |
| 79  | 18    | 307 | G    |
| 79  | 18    | 308 | G    |
| 79  | 18    | 309 | G    |
| 79  | 18    | 312 | G    |
| 79  | 18    | 319 | C    |
| 79  | 18    | 330 | G    |
| 79  | 18    | 339 | A    |
| 79  | 18    | 340 | C    |
| 79  | 18    | 350 | C    |
| 79  | 18    | 351 | G    |
| 79  | 18    | 360 | A    |
| 79  | 18    | 362 | C    |
| 79  | 18    | 364 | A    |
| 79  | 18    | 368 | U    |
| 79  | 18    | 369 | C    |
| 79  | 18    | 377 | G    |
| 79  | 18    | 385 | G    |
| 79  | 18    | 386 | C    |
| 79  | 18    | 399 | C    |
| 79  | 18    | 400 | C    |
| 79  | 18    | 408 | A    |
| 79  | 18    | 409 | C    |
| 79  | 18    | 418 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | 18    | 435 | A    |
| 79  | 18    | 438 | G    |
| 79  | 18    | 448 | A    |
| 79  | 18    | 450 | C    |
| 79  | 18    | 451 | G    |
| 79  | 18    | 452 | G    |
| 79  | 18    | 465 | A    |
| 79  | 18    | 466 | G    |
| 79  | 18    | 467 | G    |
| 79  | 18    | 472 | C    |
| 79  | 18    | 473 | A    |
| 79  | 18    | 474 | G    |
| 79  | 18    | 487 | U    |
| 79  | 18    | 492 | C    |
| 79  | 18    | 496 | C    |
| 79  | 18    | 500 | A    |
| 79  | 18    | 517 | C    |
| 79  | 18    | 525 | A    |
| 79  | 18    | 532 | C    |
| 79  | 18    | 533 | A    |
| 79  | 18    | 536 | A    |
| 79  | 18    | 537 | C    |
| 79  | 18    | 542 | U    |
| 79  | 18    | 547 | G    |
| 79  | 18    | 554 | A    |
| 79  | 18    | 555 | A    |
| 79  | 18    | 556 | U    |
| 79  | 18    | 559 | G    |
| 79  | 18    | 560 | A    |
| 79  | 18    | 562 | U    |
| 79  | 18    | 564 | A    |
| 79  | 18    | 568 | C    |
| 79  | 18    | 574 | A    |
| 79  | 18    | 576 | A    |
| 79  | 18    | 587 | A    |
| 79  | 18    | 588 | G    |
| 79  | 18    | 590 | A    |
| 79  | 18    | 591 | U    |
| 79  | 18    | 605 | A    |
| 79  | 18    | 606 | G    |
| 79  | 18    | 607 | U    |
| 79  | 18    | 608 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | 18    | 614 | C    |
| 79  | 18    | 629 | A    |
| 79  | 18    | 631 | U    |
| 79  | 18    | 643 | A    |
| 79  | 18    | 644 | G    |
| 79  | 18    | 657 | U    |
| 79  | 18    | 660 | C    |
| 79  | 18    | 668 | A    |
| 79  | 18    | 669 | A    |
| 79  | 18    | 671 | A    |
| 79  | 18    | 672 | A    |
| 79  | 18    | 673 | G    |
| 79  | 18    | 683 | G    |
| 79  | 18    | 688 | U    |
| 79  | 18    | 752 | G    |
| 79  | 18    | 753 | C    |
| 79  | 18    | 754 | G    |
| 79  | 18    | 799 | U    |
| 79  | 18    | 811 | A    |
| 79  | 18    | 821 | G    |
| 79  | 18    | 822 | U    |
| 79  | 18    | 830 | A    |
| 79  | 18    | 847 | A    |
| 79  | 18    | 848 | U    |
| 79  | 18    | 852 | G    |
| 79  | 18    | 853 | C    |
| 79  | 18    | 870 | A    |
| 79  | 18    | 871 | U    |
| 79  | 18    | 872 | A    |
| 79  | 18    | 873 | G    |
| 79  | 18    | 878 | G    |
| 79  | 18    | 879 | C    |
| 79  | 18    | 887 | U    |
| 79  | 18    | 890 | U    |
| 79  | 18    | 893 | U    |
| 79  | 18    | 894 | G    |
| 79  | 18    | 898 | U    |
| 79  | 18    | 901 | G    |
| 79  | 18    | 913 | A    |
| 79  | 18    | 914 | U    |
| 79  | 18    | 920 | A    |
| 79  | 18    | 922 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | 18    | 933  | G    |
| 79  | 18    | 943  | U    |
| 79  | 18    | 955  | A    |
| 79  | 18    | 956  | G    |
| 79  | 18    | 971  | G    |
| 79  | 18    | 978  | G    |
| 79  | 18    | 990  | A    |
| 79  | 18    | 992  | A    |
| 79  | 18    | 999  | G    |
| 79  | 18    | 1002 | U    |
| 79  | 18    | 1023 | A    |
| 79  | 18    | 1045 | U    |
| 79  | 18    | 1060 | A    |
| 79  | 18    | 1062 | A    |
| 79  | 18    | 1083 | A    |
| 79  | 18    | 1085 | C    |
| 79  | 18    | 1100 | A    |
| 79  | 18    | 1113 | A    |
| 79  | 18    | 1115 | U    |
| 79  | 18    | 1116 | C    |
| 79  | 18    | 1117 | C    |
| 79  | 18    | 1118 | C    |
| 79  | 18    | 1120 | U    |
| 79  | 18    | 1131 | G    |
| 79  | 18    | 1133 | A    |
| 79  | 18    | 1138 | C    |
| 79  | 18    | 1139 | C    |
| 79  | 18    | 1150 | A    |
| 79  | 18    | 1153 | C    |
| 79  | 18    | 1154 | U    |
| 79  | 18    | 1155 | U    |
| 79  | 18    | 1157 | G    |
| 79  | 18    | 1158 | G    |
| 79  | 18    | 1195 | A    |
| 79  | 18    | 1207 | G    |
| 79  | 18    | 1212 | G    |
| 79  | 18    | 1215 | C    |
| 79  | 18    | 1216 | C    |
| 79  | 18    | 1224 | G    |
| 79  | 18    | 1242 | U    |
| 79  | 18    | 1251 | A    |
| 79  | 18    | 1253 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | 18    | 1256 | G    |
| 79  | 18    | 1257 | G    |
| 79  | 18    | 1259 | A    |
| 79  | 18    | 1265 | A    |
| 79  | 18    | 1269 | G    |
| 79  | 18    | 1273 | C    |
| 79  | 18    | 1274 | G    |
| 79  | 18    | 1275 | G    |
| 79  | 18    | 1281 | G    |
| 79  | 18    | 1285 | G    |
| 79  | 18    | 1286 | G    |
| 79  | 18    | 1293 | A    |
| 79  | 18    | 1298 | G    |
| 79  | 18    | 1299 | A    |
| 79  | 18    | 1300 | U    |
| 79  | 18    | 1301 | A    |
| 79  | 18    | 1302 | G    |
| 79  | 18    | 1308 | U    |
| 79  | 18    | 1315 | U    |
| 79  | 18    | 1316 | C    |
| 79  | 18    | 1317 | C    |
| 79  | 18    | 1341 | C    |
| 79  | 18    | 1342 | U    |
| 79  | 18    | 1343 | U    |
| 79  | 18    | 1369 | A    |
| 79  | 18    | 1371 | U    |
| 79  | 18    | 1372 | U    |
| 79  | 18    | 1374 | C    |
| 79  | 18    | 1378 | A    |
| 79  | 18    | 1395 | C    |
| 79  | 18    | 1396 | A    |
| 79  | 18    | 1397 | U    |
| 79  | 18    | 1402 | A    |
| 79  | 18    | 1412 | C    |
| 79  | 18    | 1428 | G    |
| 79  | 18    | 1429 | G    |
| 79  | 18    | 1442 | U    |
| 79  | 18    | 1443 | C    |
| 79  | 18    | 1454 | A    |
| 79  | 18    | 1462 | U    |
| 79  | 18    | 1463 | U    |
| 79  | 18    | 1476 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | 18    | 1477 | U    |
| 79  | 18    | 1489 | A    |
| 79  | 18    | 1490 | G    |
| 79  | 18    | 1495 | G    |
| 79  | 18    | 1497 | G    |
| 79  | 18    | 1498 | A    |
| 79  | 18    | 1521 | C    |
| 79  | 18    | 1522 | A    |
| 79  | 18    | 1533 | A    |
| 79  | 18    | 1536 | G    |
| 79  | 18    | 1548 | G    |
| 79  | 18    | 1552 | G    |
| 79  | 18    | 1553 | C    |
| 79  | 18    | 1556 | A    |
| 79  | 18    | 1557 | C    |
| 79  | 18    | 1570 | G    |
| 79  | 18    | 1575 | G    |
| 79  | 18    | 1578 | U    |
| 79  | 18    | 1579 | A    |
| 79  | 18    | 1580 | A    |
| 79  | 18    | 1585 | U    |
| 79  | 18    | 1587 | G    |
| 79  | 18    | 1588 | A    |
| 79  | 18    | 1600 | G    |
| 79  | 18    | 1601 | A    |
| 79  | 18    | 1603 | G    |
| 79  | 18    | 1606 | G    |
| 79  | 18    | 1621 | U    |
| 79  | 18    | 1623 | A    |
| 79  | 18    | 1637 | A    |
| 79  | 18    | 1638 | G    |
| 79  | 18    | 1648 | G    |
| 79  | 18    | 1665 | G    |
| 79  | 18    | 1679 | A    |
| 79  | 18    | 1680 | G    |
| 79  | 18    | 1683 | C    |
| 79  | 18    | 1695 | A    |
| 79  | 18    | 1698 | C    |
| 79  | 18    | 1721 | U    |
| 79  | 18    | 1722 | G    |
| 79  | 18    | 1729 | U    |
| 79  | 18    | 1753 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | 18    | 1756 | C    |
| 79  | 18    | 1757 | G    |
| 79  | 18    | 1774 | C    |
| 79  | 18    | 1779 | G    |
| 79  | 18    | 1783 | C    |
| 79  | 18    | 1784 | G    |
| 79  | 18    | 1785 | C    |
| 79  | 18    | 1793 | A    |
| 79  | 18    | 1805 | G    |
| 79  | 18    | 1823 | A    |
| 79  | 18    | 1824 | A    |
| 79  | 18    | 1825 | A    |
| 79  | 18    | 1836 | G    |
| 79  | 18    | 1838 | U    |
| 79  | 18    | 1849 | G    |
| 79  | 18    | 1851 | A    |
| 79  | 18    | 1861 | G    |
| 79  | 18    | 1862 | G    |
| 79  | 18    | 1863 | A    |
| 79  | 18    | 1865 | C    |
| 79  | 18    | 1867 | U    |
| 79  | 18    | 1869 | A    |
| 84  | ES    | 2941 | G    |
| 84  | ES    | 2942 | C    |
| 84  | ES    | 2943 | C    |
| 84  | ES    | 2958 | C    |
| 84  | ES    | 3237 | G    |
| 84  | ES    | 3238 | C    |
| 84  | ES    | 3247 | A    |
| 85  | 28    | 8    | U    |
| 85  | 28    | 11   | G    |
| 85  | 28    | 13   | U    |
| 85  | 28    | 17   | A    |
| 85  | 28    | 25   | A    |
| 85  | 28    | 39   | A    |
| 85  | 28    | 42   | A    |
| 85  | 28    | 48   | G    |
| 85  | 28    | 49   | U    |
| 85  | 28    | 56   | A    |
| 85  | 28    | 58   | G    |
| 85  | 28    | 59   | A    |
| 85  | 28    | 64   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | 28    | 65  | A    |
| 85  | 28    | 71  | C    |
| 85  | 28    | 73  | A    |
| 85  | 28    | 76  | A    |
| 85  | 28    | 84  | A    |
| 85  | 28    | 91  | G    |
| 85  | 28    | 104 | G    |
| 85  | 28    | 108 | A    |
| 85  | 28    | 109 | G    |
| 85  | 28    | 110 | C    |
| 85  | 28    | 119 | G    |
| 85  | 28    | 120 | A    |
| 85  | 28    | 126 | C    |
| 85  | 28    | 134 | G    |
| 85  | 28    | 135 | G    |
| 85  | 28    | 136 | C    |
| 85  | 28    | 151 | G    |
| 85  | 28    | 157 | U    |
| 85  | 28    | 159 | C    |
| 85  | 28    | 171 | U    |
| 85  | 28    | 172 | C    |
| 85  | 28    | 173 | C    |
| 85  | 28    | 200 | U    |
| 85  | 28    | 201 | C    |
| 85  | 28    | 202 | C    |
| 85  | 28    | 203 | U    |
| 85  | 28    | 209 | U    |
| 85  | 28    | 216 | C    |
| 85  | 28    | 218 | A    |
| 85  | 28    | 220 | C    |
| 85  | 28    | 224 | U    |
| 85  | 28    | 233 | U    |
| 85  | 28    | 234 | G    |
| 85  | 28    | 237 | G    |
| 85  | 28    | 245 | C    |
| 85  | 28    | 246 | G    |
| 85  | 28    | 265 | C    |
| 85  | 28    | 266 | C    |
| 85  | 28    | 276 | C    |
| 85  | 28    | 280 | G    |
| 85  | 28    | 297 | U    |
| 85  | 28    | 306 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 85  | 28    | 309    | C    |
| 85  | 28    | 310    | G    |
| 85  | 28    | 315    | G    |
| 85  | 28    | 316    | U    |
| 85  | 28    | 334    | A    |
| 85  | 28    | 340    | C    |
| 85  | 28    | 350    | C    |
| 85  | 28    | 362    | A    |
| 85  | 28    | 363    | A    |
| 85  | 28    | 386    | A    |
| 85  | 28    | 387    | G    |
| 85  | 28    | 406    | C    |
| 85  | 28    | 407    | A    |
| 85  | 28    | 410    | A    |
| 85  | 28    | 412    | G    |
| 85  | 28    | 413    | G    |
| 85  | 28    | 414    | C    |
| 85  | 28    | 440    | U    |
| 85  | 28    | 449    | C    |
| 85  | 28    | 450    | G    |
| 85  | 28    | 452    | A    |
| 85  | 28    | 453    | G    |
| 85  | 28    | 454    | U    |
| 85  | 28    | 463    | A    |
| 85  | 28    | 467    | U    |
| 85  | 28    | 468    | U    |
| 85  | 28    | 481    | G    |
| 85  | 28    | 481(A) | C    |
| 85  | 28    | 482    | G    |
| 85  | 28    | 483    | G    |
| 85  | 28    | 485    | C    |
| 85  | 28    | 486    | C    |
| 85  | 28    | 492    | U    |
| 85  | 28    | 493    | G    |
| 85  | 28    | 496    | G    |
| 85  | 28    | 497    | G    |
| 85  | 28    | 498    | C    |
| 85  | 28    | 499    | G    |
| 85  | 28    | 505    | G    |
| 85  | 28    | 506    | C    |
| 85  | 28    | 510    | U    |
| 85  | 28    | 666    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 85  | 28    | 667    | A    |
| 85  | 28    | 669    | C    |
| 85  | 28    | 685    | C    |
| 85  | 28    | 686    | A    |
| 85  | 28    | 687    | U    |
| 85  | 28    | 688    | U    |
| 85  | 28    | 691    | C    |
| 85  | 28    | 696    | C    |
| 85  | 28    | 697    | G    |
| 85  | 28    | 704    | C    |
| 85  | 28    | 705    | G    |
| 85  | 28    | 708    | G    |
| 85  | 28    | 719    | C    |
| 85  | 28    | 730    | G    |
| 85  | 28    | 731    | G    |
| 85  | 28    | 738    | C    |
| 85  | 28    | 738(A) | C    |
| 85  | 28    | 739    | G    |
| 85  | 28    | 747    | A    |
| 85  | 28    | 749    | G    |
| 85  | 28    | 758    | G    |
| 85  | 28    | 914    | U    |
| 85  | 28    | 915    | A    |
| 85  | 28    | 916    | C    |
| 85  | 28    | 917    | A    |
| 85  | 28    | 918    | G    |
| 85  | 28    | 923    | C    |
| 85  | 28    | 925    | C    |
| 85  | 28    | 926    | G    |
| 85  | 28    | 929    | A    |
| 85  | 28    | 931    | C    |
| 85  | 28    | 932    | A    |
| 85  | 28    | 933    | G    |
| 85  | 28    | 934    | C    |
| 85  | 28    | 935    | A    |
| 85  | 28    | 935(A) | G    |
| 85  | 28    | 936    | C    |
| 85  | 28    | 938    | C    |
| 85  | 28    | 939    | G    |
| 85  | 28    | 941    | C    |
| 85  | 28    | 943    | A    |
| 85  | 28    | 944    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 945  | U    |
| 85  | 28    | 946  | C    |
| 85  | 28    | 956  | A    |
| 85  | 28    | 959  | G    |
| 85  | 28    | 960  | A    |
| 85  | 28    | 961  | G    |
| 85  | 28    | 964  | A    |
| 85  | 28    | 965  | G    |
| 85  | 28    | 966  | A    |
| 85  | 28    | 967  | C    |
| 85  | 28    | 968  | C    |
| 85  | 28    | 969  | C    |
| 85  | 28    | 970  | G    |
| 85  | 28    | 978  | C    |
| 85  | 28    | 980  | C    |
| 85  | 28    | 983  | U    |
| 85  | 28    | 1070 | G    |
| 85  | 28    | 1072 | C    |
| 85  | 28    | 1073 | G    |
| 85  | 28    | 1079 | C    |
| 85  | 28    | 1081 | C    |
| 85  | 28    | 1083 | U    |
| 85  | 28    | 1179 | U    |
| 85  | 28    | 1195 | G    |
| 85  | 28    | 1211 | G    |
| 85  | 28    | 1212 | G    |
| 85  | 28    | 1214 | C    |
| 85  | 28    | 1215 | C    |
| 85  | 28    | 1234 | G    |
| 85  | 28    | 1235 | G    |
| 85  | 28    | 1236 | C    |
| 85  | 28    | 1237 | C    |
| 85  | 28    | 1238 | A    |
| 85  | 28    | 1239 | C    |
| 85  | 28    | 1277 | G    |
| 85  | 28    | 1280 | C    |
| 85  | 28    | 1283 | G    |
| 85  | 28    | 1284 | G    |
| 85  | 28    | 1285 | U    |
| 85  | 28    | 1287 | G    |
| 85  | 28    | 1292 | C    |
| 85  | 28    | 1293 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 1296 | G    |
| 85  | 28    | 1301 | C    |
| 85  | 28    | 1303 | A    |
| 85  | 28    | 1304 | C    |
| 85  | 28    | 1326 | A    |
| 85  | 28    | 1330 | A    |
| 85  | 28    | 1354 | A    |
| 85  | 28    | 1358 | G    |
| 85  | 28    | 1359 | G    |
| 85  | 28    | 1371 | A    |
| 85  | 28    | 1377 | G    |
| 85  | 28    | 1379 | C    |
| 85  | 28    | 1387 | A    |
| 85  | 28    | 1394 | G    |
| 85  | 28    | 1397 | A    |
| 85  | 28    | 1398 | A    |
| 85  | 28    | 1414 | C    |
| 85  | 28    | 1419 | G    |
| 85  | 28    | 1420 | A    |
| 85  | 28    | 1433 | A    |
| 85  | 28    | 1435 | G    |
| 85  | 28    | 1445 | U    |
| 85  | 28    | 1446 | C    |
| 85  | 28    | 1456 | C    |
| 85  | 28    | 1457 | G    |
| 85  | 28    | 1482 | G    |
| 85  | 28    | 1483 | C    |
| 85  | 28    | 1484 | G    |
| 85  | 28    | 1497 | A    |
| 85  | 28    | 1498 | G    |
| 85  | 28    | 1502 | G    |
| 85  | 28    | 1504 | G    |
| 85  | 28    | 1516 | G    |
| 85  | 28    | 1523 | A    |
| 85  | 28    | 1534 | A    |
| 85  | 28    | 1547 | A    |
| 85  | 28    | 1566 | C    |
| 85  | 28    | 1574 | G    |
| 85  | 28    | 1578 | U    |
| 85  | 28    | 1591 | U    |
| 85  | 28    | 1596 | U    |
| 85  | 28    | 1612 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 1613 | A    |
| 85  | 28    | 1624 | G    |
| 85  | 28    | 1625 | G    |
| 85  | 28    | 1631 | A    |
| 85  | 28    | 1633 | G    |
| 85  | 28    | 1634 | A    |
| 85  | 28    | 1638 | A    |
| 85  | 28    | 1641 | G    |
| 85  | 28    | 1654 | G    |
| 85  | 28    | 1661 | C    |
| 85  | 28    | 1676 | C    |
| 85  | 28    | 1677 | U    |
| 85  | 28    | 1726 | U    |
| 85  | 28    | 1731 | C    |
| 85  | 28    | 1742 | A    |
| 85  | 28    | 1752 | G    |
| 85  | 28    | 1755 | C    |
| 85  | 28    | 1756 | U    |
| 85  | 28    | 1757 | U    |
| 85  | 28    | 1760 | G    |
| 85  | 28    | 1761 | G    |
| 85  | 28    | 1764 | G    |
| 85  | 28    | 1765 | A    |
| 85  | 28    | 1769 | G    |
| 85  | 28    | 1772 | C    |
| 85  | 28    | 1773 | U    |
| 85  | 28    | 1776 | A    |
| 85  | 28    | 1781 | U    |
| 85  | 28    | 1787 | A    |
| 85  | 28    | 1804 | A    |
| 85  | 28    | 1805 | A    |
| 85  | 28    | 1807 | C    |
| 85  | 28    | 1821 | G    |
| 85  | 28    | 1822 | U    |
| 85  | 28    | 1828 | C    |
| 85  | 28    | 1832 | C    |
| 85  | 28    | 1836 | G    |
| 85  | 28    | 1837 | A    |
| 85  | 28    | 1842 | G    |
| 85  | 28    | 1855 | G    |
| 85  | 28    | 1869 | G    |
| 85  | 28    | 1883 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 1897 | A    |
| 85  | 28    | 1918 | U    |
| 85  | 28    | 1920 | C    |
| 85  | 28    | 1921 | C    |
| 85  | 28    | 1922 | G    |
| 85  | 28    | 1931 | C    |
| 85  | 28    | 1940 | G    |
| 85  | 28    | 1948 | G    |
| 85  | 28    | 1951 | G    |
| 85  | 28    | 1955 | G    |
| 85  | 28    | 1957 | U    |
| 85  | 28    | 1958 | A    |
| 85  | 28    | 1960 | A    |
| 85  | 28    | 1961 | G    |
| 85  | 28    | 1962 | A    |
| 85  | 28    | 1976 | G    |
| 85  | 28    | 1979 | A    |
| 85  | 28    | 1980 | U    |
| 85  | 28    | 1984 | A    |
| 85  | 28    | 1985 | G    |
| 85  | 28    | 1987 | C    |
| 85  | 28    | 1988 | G    |
| 85  | 28    | 1991 | A    |
| 85  | 28    | 1992 | U    |
| 85  | 28    | 1993 | C    |
| 85  | 28    | 1997 | U    |
| 85  | 28    | 2001 | G    |
| 85  | 28    | 2002 | A    |
| 85  | 28    | 2003 | G    |
| 85  | 28    | 2004 | U    |
| 85  | 28    | 2010 | A    |
| 85  | 28    | 2011 | C    |
| 85  | 28    | 2025 | A    |
| 85  | 28    | 2026 | A    |
| 85  | 28    | 2046 | G    |
| 85  | 28    | 2047 | A    |
| 85  | 28    | 2048 | U    |
| 85  | 28    | 2055 | G    |
| 85  | 28    | 2056 | G    |
| 85  | 28    | 2069 | A    |
| 85  | 28    | 2084 | U    |
| 85  | 28    | 2090 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 2092 | G    |
| 85  | 28    | 2093 | G    |
| 85  | 28    | 2094 | C    |
| 85  | 28    | 2097 | A    |
| 85  | 28    | 2098 | G    |
| 85  | 28    | 2100 | G    |
| 85  | 28    | 2102 | G    |
| 85  | 28    | 2104 | A    |
| 85  | 28    | 2107 | A    |
| 85  | 28    | 2108 | G    |
| 85  | 28    | 2109 | A    |
| 85  | 28    | 2267 | U    |
| 85  | 28    | 2268 | A    |
| 85  | 28    | 2275 | G    |
| 85  | 28    | 2279 | A    |
| 85  | 28    | 2289 | C    |
| 85  | 28    | 2300 | A    |
| 85  | 28    | 2301 | G    |
| 85  | 28    | 2306 | G    |
| 85  | 28    | 2313 | A    |
| 85  | 28    | 2314 | G    |
| 85  | 28    | 2333 | G    |
| 85  | 28    | 2348 | G    |
| 85  | 28    | 2351 | C    |
| 85  | 28    | 2360 | A    |
| 85  | 28    | 2395 | A    |
| 85  | 28    | 2422 | C    |
| 85  | 28    | 2425 | U    |
| 85  | 28    | 2433 | G    |
| 85  | 28    | 2441 | C    |
| 85  | 28    | 2470 | C    |
| 85  | 28    | 2471 | G    |
| 85  | 28    | 2475 | G    |
| 85  | 28    | 2488 | C    |
| 85  | 28    | 2489 | C    |
| 85  | 28    | 2490 | U    |
| 85  | 28    | 2491 | C    |
| 85  | 28    | 2503 | G    |
| 85  | 28    | 2504 | C    |
| 85  | 28    | 2505 | C    |
| 85  | 28    | 2506 | G    |
| 85  | 28    | 2507 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 2513 | A    |
| 85  | 28    | 2529 | A    |
| 85  | 28    | 2537 | A    |
| 85  | 28    | 2544 | G    |
| 85  | 28    | 2545 | U    |
| 85  | 28    | 2546 | G    |
| 85  | 28    | 2547 | G    |
| 85  | 28    | 2553 | A    |
| 85  | 28    | 2554 | U    |
| 85  | 28    | 2566 | G    |
| 85  | 28    | 2575 | U    |
| 85  | 28    | 2583 | C    |
| 85  | 28    | 2587 | A    |
| 85  | 28    | 2627 | C    |
| 85  | 28    | 2638 | G    |
| 85  | 28    | 2653 | C    |
| 85  | 28    | 2669 | C    |
| 85  | 28    | 2686 | G    |
| 85  | 28    | 2687 | U    |
| 85  | 28    | 2694 | G    |
| 85  | 28    | 2695 | A    |
| 85  | 28    | 2696 | A    |
| 85  | 28    | 2703 | G    |
| 85  | 28    | 2707 | U    |
| 85  | 28    | 2708 | U    |
| 85  | 28    | 2709 | C    |
| 85  | 28    | 2711 | G    |
| 85  | 28    | 2712 | G    |
| 85  | 28    | 2714 | G    |
| 85  | 28    | 2716 | C    |
| 85  | 28    | 2725 | A    |
| 85  | 28    | 2726 | G    |
| 85  | 28    | 2735 | G    |
| 85  | 28    | 2740 | U    |
| 85  | 28    | 2743 | A    |
| 85  | 28    | 2760 | G    |
| 85  | 28    | 2763 | U    |
| 85  | 28    | 2764 | A    |
| 85  | 28    | 2769 | U    |
| 85  | 28    | 2787 | A    |
| 85  | 28    | 2788 | U    |
| 85  | 28    | 2790 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 2826 | U    |
| 85  | 28    | 2842 | G    |
| 85  | 28    | 2855 | G    |
| 85  | 28    | 2869 | U    |
| 85  | 28    | 3625 | G    |
| 85  | 28    | 3626 | G    |
| 85  | 28    | 3635 | A    |
| 85  | 28    | 3644 | U    |
| 85  | 28    | 3646 | A    |
| 85  | 28    | 3662 | A    |
| 85  | 28    | 3664 | G    |
| 85  | 28    | 3711 | A    |
| 85  | 28    | 3712 | A    |
| 85  | 28    | 3713 | U    |
| 85  | 28    | 3714 | G    |
| 85  | 28    | 3729 | U    |
| 85  | 28    | 3748 | A    |
| 85  | 28    | 3753 | G    |
| 85  | 28    | 3760 | A    |
| 85  | 28    | 3761 | C    |
| 85  | 28    | 3773 | U    |
| 85  | 28    | 3776 | G    |
| 85  | 28    | 3777 | G    |
| 85  | 28    | 3784 | A    |
| 85  | 28    | 3786 | U    |
| 85  | 28    | 3810 | C    |
| 85  | 28    | 3811 | G    |
| 85  | 28    | 3814 | U    |
| 85  | 28    | 3817 | A    |
| 85  | 28    | 3819 | G    |
| 85  | 28    | 3839 | G    |
| 85  | 28    | 3840 | U    |
| 85  | 28    | 3860 | A    |
| 85  | 28    | 3877 | A    |
| 85  | 28    | 3878 | C    |
| 85  | 28    | 3879 | G    |
| 85  | 28    | 3897 | G    |
| 85  | 28    | 3901 | A    |
| 85  | 28    | 3905 | A    |
| 85  | 28    | 3906 | A    |
| 85  | 28    | 3907 | G    |
| 85  | 28    | 3908 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 3915 | U    |
| 85  | 28    | 3923 | A    |
| 85  | 28    | 3938 | G    |
| 85  | 28    | 4073 | A    |
| 85  | 28    | 4076 | G    |
| 85  | 28    | 4086 | G    |
| 85  | 28    | 4094 | G    |
| 85  | 28    | 4116 | C    |
| 85  | 28    | 4119 | C    |
| 85  | 28    | 4120 | U    |
| 85  | 28    | 4121 | G    |
| 85  | 28    | 4122 | G    |
| 85  | 28    | 4127 | A    |
| 85  | 28    | 4158 | C    |
| 85  | 28    | 4162 | C    |
| 85  | 28    | 4163 | U    |
| 85  | 28    | 4170 | A    |
| 85  | 28    | 4183 | G    |
| 85  | 28    | 4184 | G    |
| 85  | 28    | 4191 | G    |
| 85  | 28    | 4203 | A    |
| 85  | 28    | 4229 | U    |
| 85  | 28    | 4233 | A    |
| 85  | 28    | 4251 | A    |
| 85  | 28    | 4253 | A    |
| 85  | 28    | 4254 | G    |
| 85  | 28    | 4266 | G    |
| 85  | 28    | 4268 | A    |
| 85  | 28    | 4273 | A    |
| 85  | 28    | 4281 | A    |
| 85  | 28    | 4291 | G    |
| 85  | 28    | 4297 | G    |
| 85  | 28    | 4305 | G    |
| 85  | 28    | 4306 | U    |
| 85  | 28    | 4314 | C    |
| 85  | 28    | 4317 | A    |
| 85  | 28    | 4330 | G    |
| 85  | 28    | 4332 | C    |
| 85  | 28    | 4348 | A    |
| 85  | 28    | 4349 | C    |
| 85  | 28    | 4354 | U    |
| 85  | 28    | 4377 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 4378 | A    |
| 85  | 28    | 4380 | A    |
| 85  | 28    | 4387 | C    |
| 85  | 28    | 4394 | A    |
| 85  | 28    | 4395 | U    |
| 85  | 28    | 4419 | U    |
| 85  | 28    | 4422 | A    |
| 85  | 28    | 4426 | C    |
| 85  | 28    | 4444 | C    |
| 85  | 28    | 4448 | G    |
| 85  | 28    | 4449 | A    |
| 85  | 28    | 4453 | C    |
| 85  | 28    | 4464 | A    |
| 85  | 28    | 4466 | C    |
| 85  | 28    | 4475 | G    |
| 85  | 28    | 4476 | C    |
| 85  | 28    | 4500 | U    |
| 85  | 28    | 4512 | U    |
| 85  | 28    | 4513 | A    |
| 85  | 28    | 4519 | C    |
| 85  | 28    | 4524 | G    |
| 85  | 28    | 4548 | A    |
| 85  | 28    | 4549 | G    |
| 85  | 28    | 4554 | G    |
| 85  | 28    | 4560 | C    |
| 85  | 28    | 4567 | G    |
| 85  | 28    | 4570 | G    |
| 85  | 28    | 4573 | G    |
| 85  | 28    | 4574 | U    |
| 85  | 28    | 4575 | G    |
| 85  | 28    | 4586 | G    |
| 85  | 28    | 4590 | A    |
| 85  | 28    | 4627 | U    |
| 85  | 28    | 4636 | U    |
| 85  | 28    | 4656 | A    |
| 85  | 28    | 4670 | C    |
| 85  | 28    | 4671 | C    |
| 85  | 28    | 4672 | A    |
| 85  | 28    | 4677 | U    |
| 85  | 28    | 4700 | A    |
| 85  | 28    | 4709 | U    |
| 85  | 28    | 4719 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 4720 | C    |
| 85  | 28    | 4729 | A    |
| 85  | 28    | 4730 | C    |
| 85  | 28    | 4731 | G    |
| 85  | 28    | 4732 | G    |
| 85  | 28    | 4733 | C    |
| 85  | 28    | 4734 | A    |
| 85  | 28    | 4751 | G    |
| 85  | 28    | 4754 | G    |
| 85  | 28    | 4757 | C    |
| 85  | 28    | 4759 | C    |
| 85  | 28    | 4761 | G    |
| 85  | 28    | 4765 | G    |
| 85  | 28    | 4771 | C    |
| 85  | 28    | 4870 | G    |
| 85  | 28    | 4872 | G    |
| 85  | 28    | 4875 | G    |
| 85  | 28    | 4877 | G    |
| 85  | 28    | 4882 | U    |
| 85  | 28    | 4883 | C    |
| 85  | 28    | 4885 | U    |
| 85  | 28    | 4895 | C    |
| 85  | 28    | 4902 | C    |
| 85  | 28    | 4906 | C    |
| 85  | 28    | 4910 | A    |
| 85  | 28    | 4912 | G    |
| 85  | 28    | 4914 | G    |
| 85  | 28    | 4915 | G    |
| 85  | 28    | 4918 | C    |
| 85  | 28    | 4919 | G    |
| 85  | 28    | 4921 | C    |
| 85  | 28    | 4922 | C    |
| 85  | 28    | 4923 | U    |
| 85  | 28    | 4925 | U    |
| 85  | 28    | 4926 | C    |
| 85  | 28    | 4927 | G    |
| 85  | 28    | 4928 | C    |
| 85  | 28    | 4929 | C    |
| 85  | 28    | 4931 | G    |
| 85  | 28    | 4935 | C    |
| 85  | 28    | 4937 | C    |
| 85  | 28    | 4943 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 4944 | C    |
| 85  | 28    | 4948 | C    |
| 85  | 28    | 4949 | G    |
| 85  | 28    | 4950 | U    |
| 85  | 28    | 4951 | G    |
| 85  | 28    | 4960 | G    |
| 85  | 28    | 4965 | U    |
| 85  | 28    | 4966 | A    |
| 85  | 28    | 4976 | U    |
| 85  | 28    | 4979 | A    |
| 85  | 28    | 4988 | U    |
| 85  | 28    | 4990 | C    |
| 85  | 28    | 5006 | U    |
| 85  | 28    | 5007 | A    |
| 85  | 28    | 5017 | G    |
| 85  | 28    | 5029 | C    |
| 85  | 28    | 5041 | G    |
| 85  | 28    | 5050 | C    |
| 85  | 28    | 5053 | U    |
| 85  | 28    | 5054 | C    |
| 85  | 28    | 5061 | A    |
| 85  | 28    | 5062 | G    |

All (64) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | 58    | 124  | U    |
| 79  | 18    | 110  | U    |
| 79  | 18    | 291  | G    |
| 79  | 18    | 434  | G    |
| 79  | 18    | 465  | A    |
| 79  | 18    | 642  | U    |
| 79  | 18    | 752  | G    |
| 79  | 18    | 870  | A    |
| 79  | 18    | 1137 | U    |
| 79  | 18    | 1394 | G    |
| 79  | 18    | 1395 | C    |
| 79  | 18    | 1520 | G    |
| 79  | 18    | 1637 | A    |
| 79  | 18    | 1664 | A    |
| 79  | 18    | 1862 | G    |
| 84  | ES    | 3236 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 12   | A    |
| 85  | 28    | 47   | A    |
| 85  | 28    | 48   | G    |
| 85  | 28    | 125  | C    |
| 85  | 28    | 134  | G    |
| 85  | 28    | 217  | C    |
| 85  | 28    | 245  | C    |
| 85  | 28    | 265  | C    |
| 85  | 28    | 275  | C    |
| 85  | 28    | 385  | A    |
| 85  | 28    | 406  | C    |
| 85  | 28    | 449  | C    |
| 85  | 28    | 480  | C    |
| 85  | 28    | 485  | C    |
| 85  | 28    | 492  | U    |
| 85  | 28    | 504  | G    |
| 85  | 28    | 684  | G    |
| 85  | 28    | 930  | G    |
| 85  | 28    | 959  | G    |
| 85  | 28    | 1072 | C    |
| 85  | 28    | 1211 | G    |
| 85  | 28    | 1238 | A    |
| 85  | 28    | 1291 | G    |
| 85  | 28    | 1329 | G    |
| 85  | 28    | 1370 | G    |
| 85  | 28    | 1445 | U    |
| 85  | 28    | 1455 | G    |
| 85  | 28    | 1633 | G    |
| 85  | 28    | 1804 | A    |
| 85  | 28    | 1979 | A    |
| 85  | 28    | 2046 | G    |
| 85  | 28    | 2089 | G    |
| 85  | 28    | 2266 | C    |
| 85  | 28    | 2502 | A    |
| 85  | 28    | 2546 | G    |
| 85  | 28    | 2695 | A    |
| 85  | 28    | 2724 | G    |
| 85  | 28    | 3760 | A    |
| 85  | 28    | 3876 | A    |
| 85  | 28    | 3904 | G    |
| 85  | 28    | 4119 | C    |
| 85  | 28    | 4232 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 28    | 4448 | G    |
| 85  | 28    | 4699 | U    |
| 85  | 28    | 4884 | G    |
| 85  | 28    | 4925 | U    |
| 85  | 28    | 4936 | G    |
| 85  | 28    | 4947 | U    |

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

1 non-standard protein/DNA/RNA residue is 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 | $\# Z  > 2$ |
| 80  | DDE  | v     | 715 | 80   | 18,20,21     | 1.03 | 1 (5%)      | 17,28,30    | 0.85 | 1 (5%)      |

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  | DDE  | v     | 715 | 80   | -       | 9/20/21/23 | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 80  | v     | 715 | DDE  | CD2-CG | 2.57 | 1.41        | 1.36     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 80  | v     | 715 | DDE  | CAU-CBW-CBI | -2.29 | 106.75      | 111.22   |

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 80  | v     | 715 | DDE  | C-CA-CB-CG      |
| 80  | v     | 715 | DDE  | NAD-CBI-CBW-CAU |
| 80  | v     | 715 | DDE  | CAT-CAU-CBW-CBI |
| 80  | v     | 715 | DDE  | CAT-CAU-CBW-NCB |
| 80  | v     | 715 | DDE  | OAG-CBI-CBW-CAU |
| 80  | v     | 715 | DDE  | CA-CB-CG-ND1    |
| 80  | v     | 715 | DDE  | CA-CB-CG-CD2    |
| 80  | v     | 715 | DDE  | N-CA-CB-CG      |
| 80  | v     | 715 | DDE  | CE1-CAT-CAU-CBW |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 88  | GDP  | v     | 900 | -    | 29,30,30     | 3.49 | 12 (41%)    | 45,47,47    | 1.89 | 12 (26%)    |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 88  | GDP  | v     | 900 | -    | -       | 0/16/32/32 | 0/3/3/3 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 88  | v     | 900 | GDP  | O6-C6   | 9.57  | 1.41        | 1.23     |
| 88  | v     | 900 | GDP  | C2'-C3' | -8.18 | 1.31        | 1.53     |
| 88  | v     | 900 | GDP  | O4'-C4' | -6.89 | 1.29        | 1.45     |
| 88  | v     | 900 | GDP  | O4'-C1' | 5.72  | 1.55        | 1.42     |
| 88  | v     | 900 | GDP  | C2-N2   | 4.69  | 1.45        | 1.34     |
| 88  | v     | 900 | GDP  | C1'-N9  | -4.29 | 1.35        | 1.47     |
| 88  | v     | 900 | GDP  | PA-O3A  | 4.22  | 1.64        | 1.59     |
| 88  | v     | 900 | GDP  | C3'-C4' | 3.55  | 1.62        | 1.53     |
| 88  | v     | 900 | GDP  | C6-N1   | -3.33 | 1.32        | 1.38     |
| 88  | v     | 900 | GDP  | O2'-C2' | 3.02  | 1.50        | 1.43     |
| 88  | v     | 900 | GDP  | C8-N9   | -2.18 | 1.32        | 1.37     |
| 88  | v     | 900 | GDP  | C2-N1   | -2.07 | 1.32        | 1.37     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 88  | v     | 900 | GDP  | C5-C4-N3    | -6.03 | 118.79      | 128.39   |
| 88  | v     | 900 | GDP  | C2-N3-C4    | 5.04  | 120.98      | 112.30   |
| 88  | v     | 900 | GDP  | N9-C4-N3    | 4.17  | 134.29      | 125.95   |
| 88  | v     | 900 | GDP  | C8-N7-C5    | 2.92  | 109.46      | 104.26   |
| 88  | v     | 900 | GDP  | C4-C5-N7    | -2.91 | 106.06      | 110.67   |
| 88  | v     | 900 | GDP  | C6-C5-N7    | 2.83  | 135.44      | 130.29   |
| 88  | v     | 900 | GDP  | N9-C8-N7    | -2.61 | 108.55      | 113.40   |
| 88  | v     | 900 | GDP  | C3'-C2'-C1' | 2.45  | 106.09      | 101.46   |
| 88  | v     | 900 | GDP  | O6-C6-C5    | -2.42 | 120.14      | 126.53   |
| 88  | v     | 900 | GDP  | C2-N1-C6    | -2.31 | 120.92      | 125.11   |
| 88  | v     | 900 | GDP  | C4'-O4'-C1' | -2.31 | 104.37      | 109.47   |
| 88  | v     | 900 | GDP  | C5-C6-N1    | 2.28  | 119.07      | 113.25   |

There are no chirality outliers.

There are no torsion outliers.

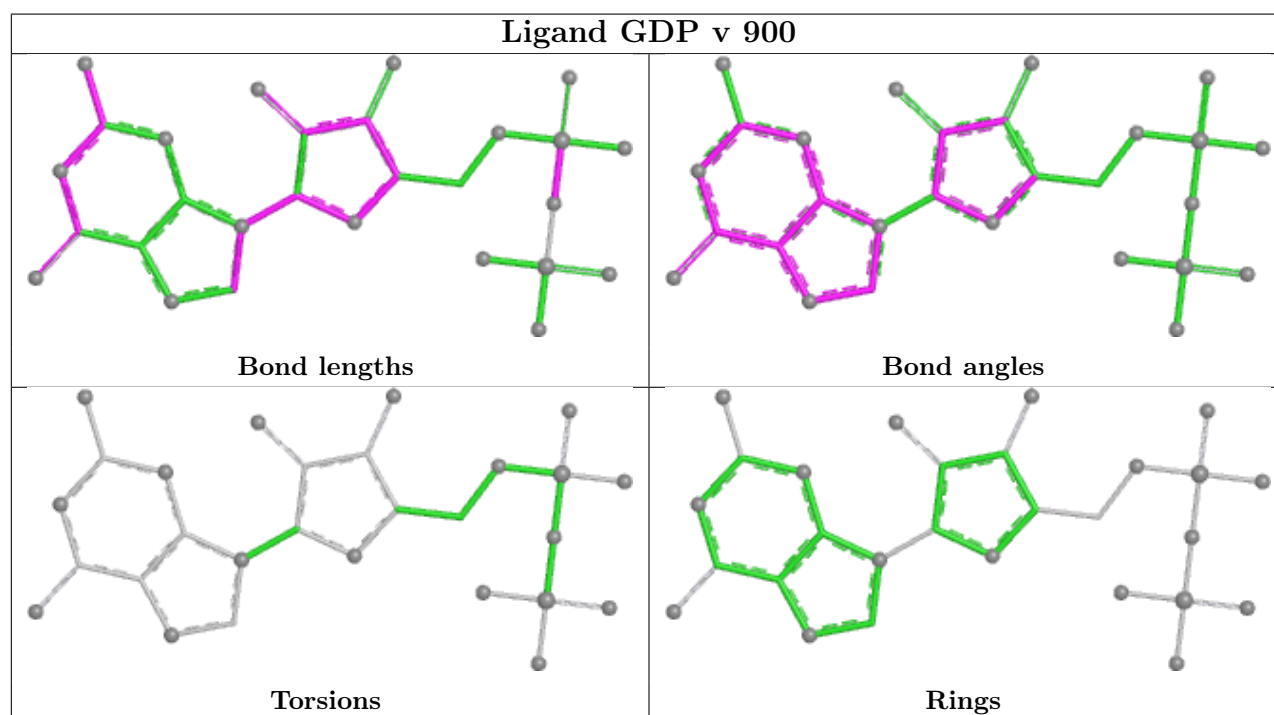
There are no ring outliers.

1 monomer is involved in 1 short contact:

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



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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 79  | 18    | 12               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 18    | 756:C     | O3'    | 788:G     | P      | 20.22        |
| 1     | 18    | 697:G     | O3'    | 729:C     | P      | 19.25        |
| 1     | 18    | 1417:C    | O3'    | 1423:C    | P      | 17.97        |
| 1     | 18    | 321:C     | O3'    | 329:G     | P      | 16.66        |
| 1     | 18    | 1759:G    | O3'    | 1773:C    | P      | 16.39        |
| 1     | 18    | 834:C     | O3'    | 841:G     | P      | 16.28        |
| 1     | 18    | 130:G     | O3'    | 141:A     | P      | 15.80        |
| 1     | 18    | 547:G     | O3'    | 551:U     | P      | 13.14        |
| 1     | 18    | 745:C     | O3'    | 749:U     | P      | 8.25         |
| 1     | 18    | 736:C     | O3'    | 743:U     | P      | 7.88         |
| 1     | 18    | 225:G     | O3'    | 287:U     | P      | 4.28         |
| 1     | 18    | 1432:U    | O3'    | 1438:A    | P      | 3.64         |

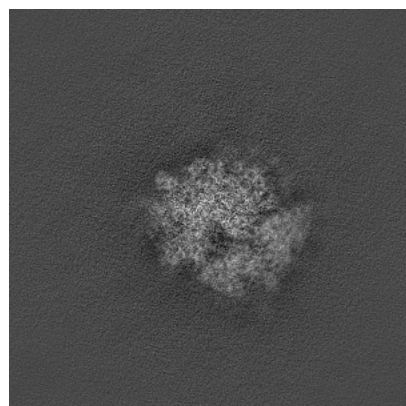
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75689. These allow visual inspection of the internal detail of the map and identification of artifacts.

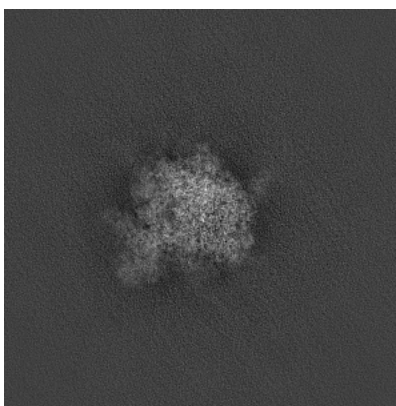
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

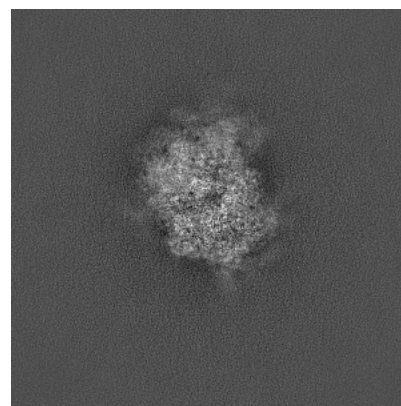
#### 6.1.1 Primary map



X

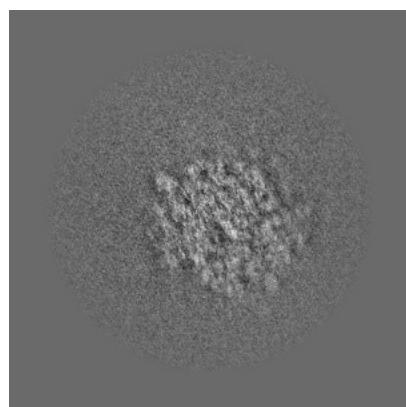


Y

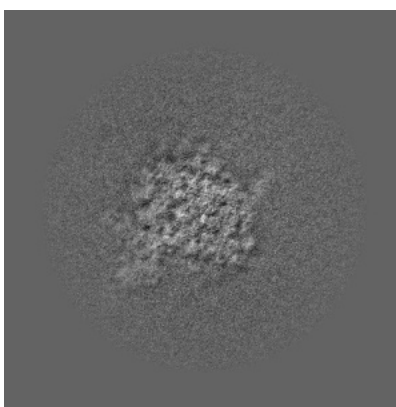


Z

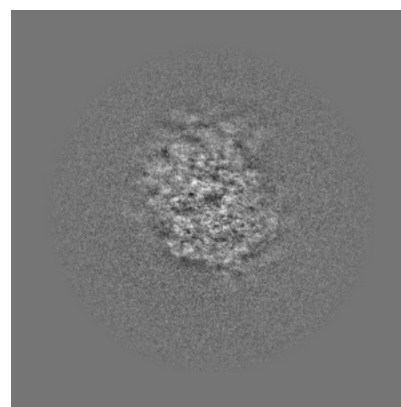
#### 6.1.2 Raw map



X



Y

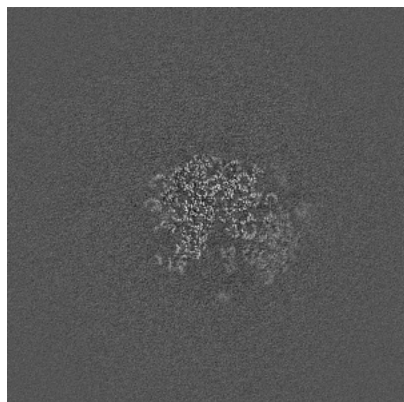


Z

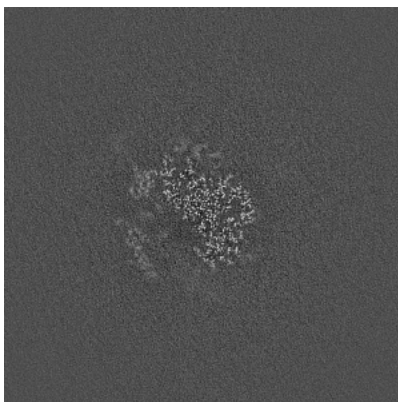
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

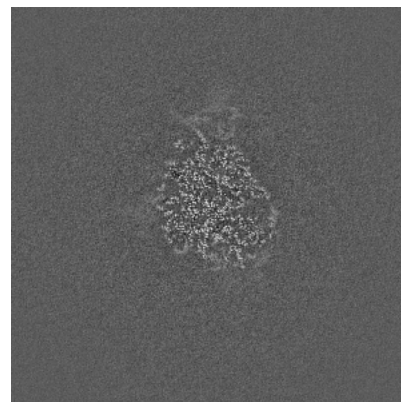
### 6.2.1 Primary map



X Index: 400

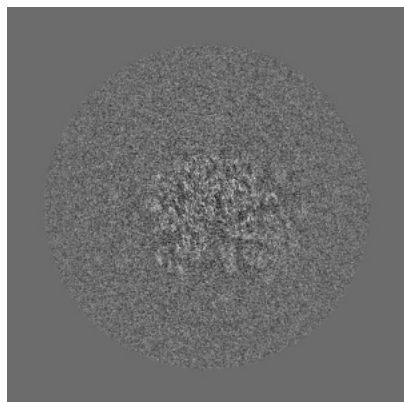


Y Index: 400

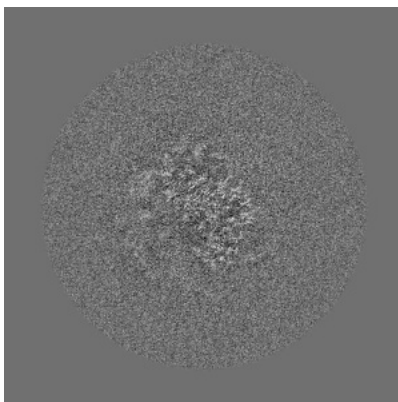


Z Index: 400

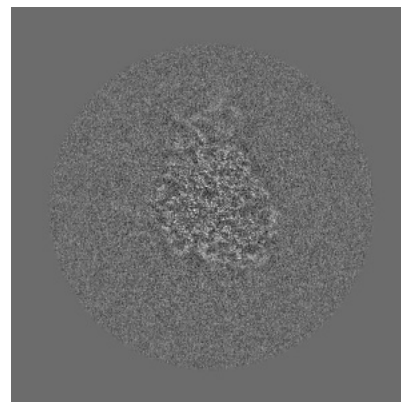
### 6.2.2 Raw map



X Index: 400



Y Index: 400

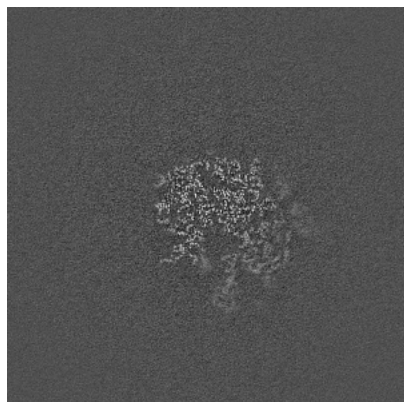


Z Index: 400

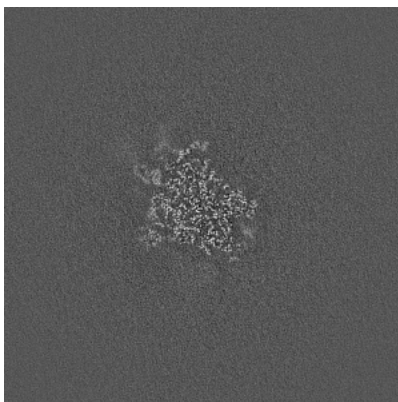
The images above show central slices of the map in three orthogonal directions.

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

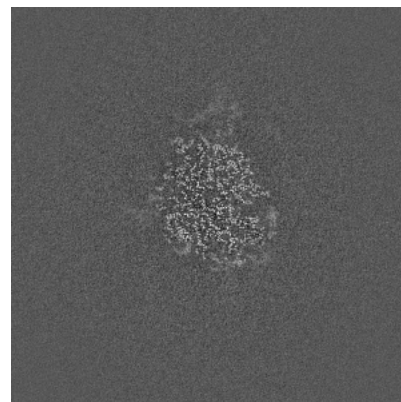
### 6.3.1 Primary map



X Index: 385

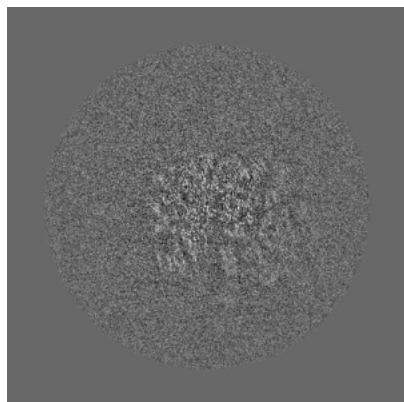


Y Index: 376

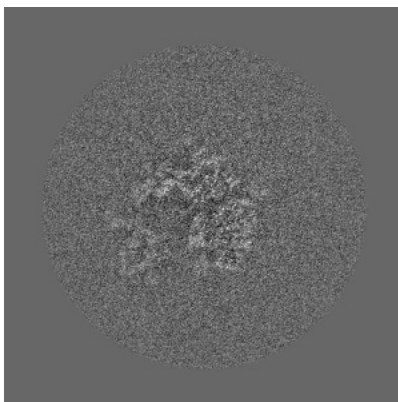


Z Index: 403

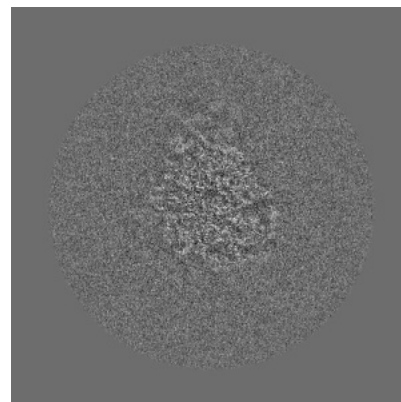
### 6.3.2 Raw map



X Index: 396



Y Index: 420



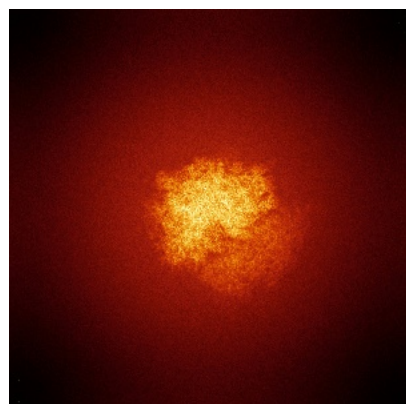
Z Index: 402

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

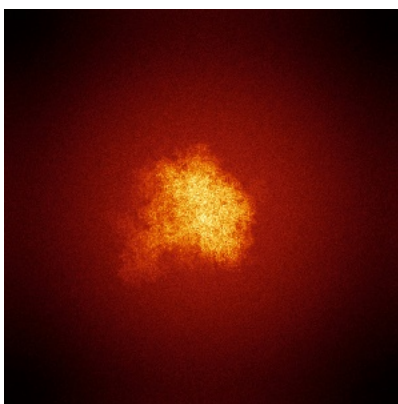


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

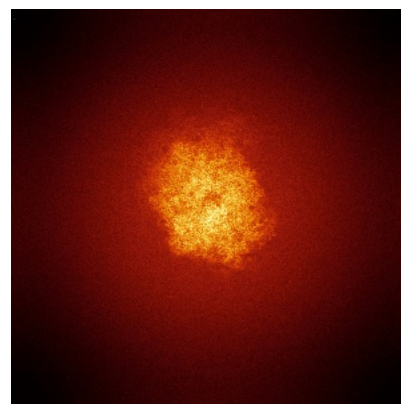
### 6.4.1 Primary map



X

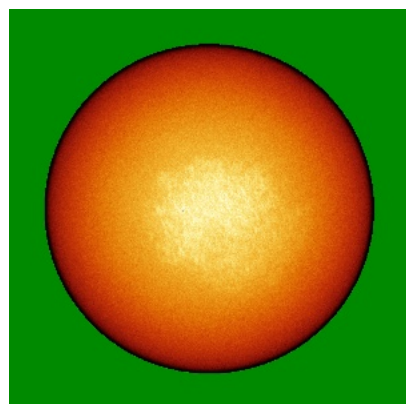


Y

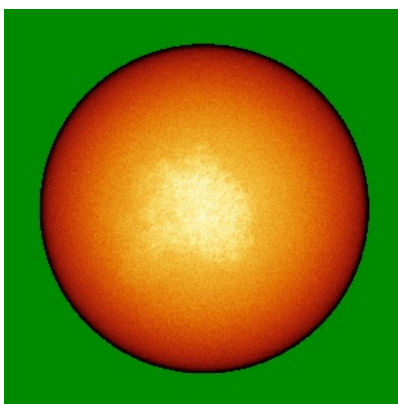


Z

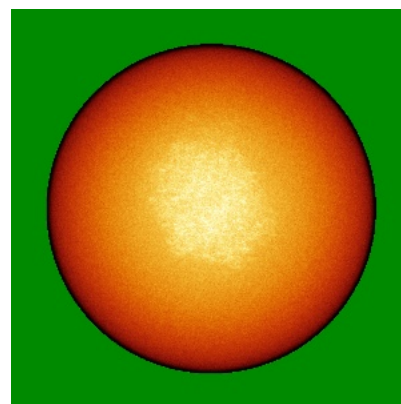
### 6.4.2 Raw map



X



Y

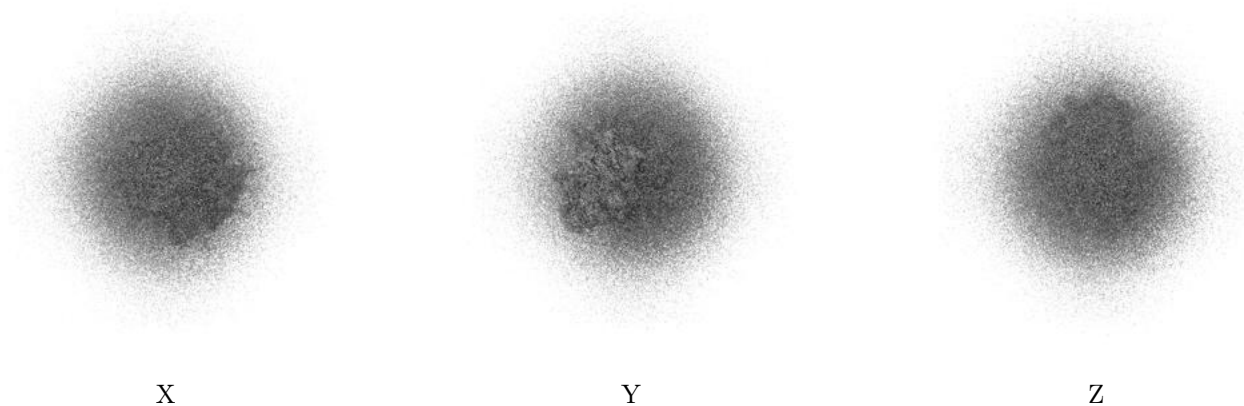


Z

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

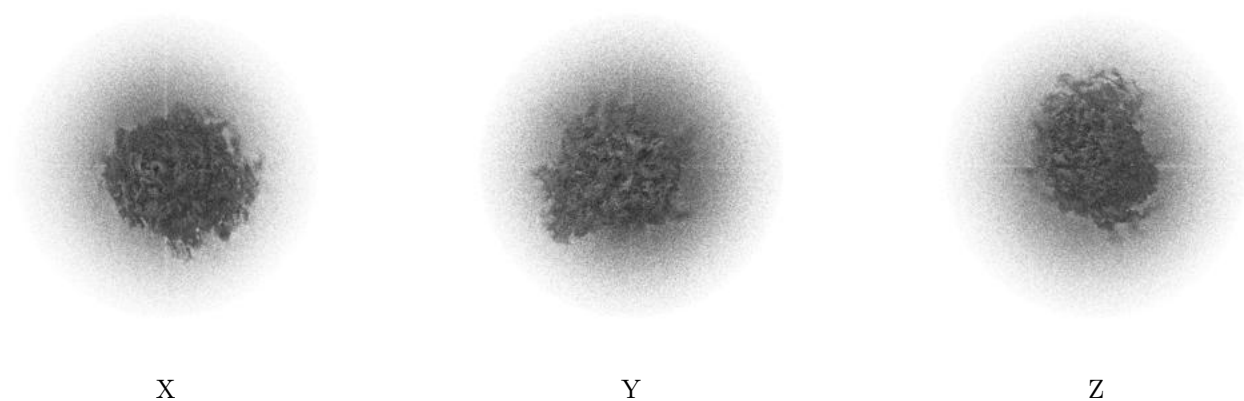
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

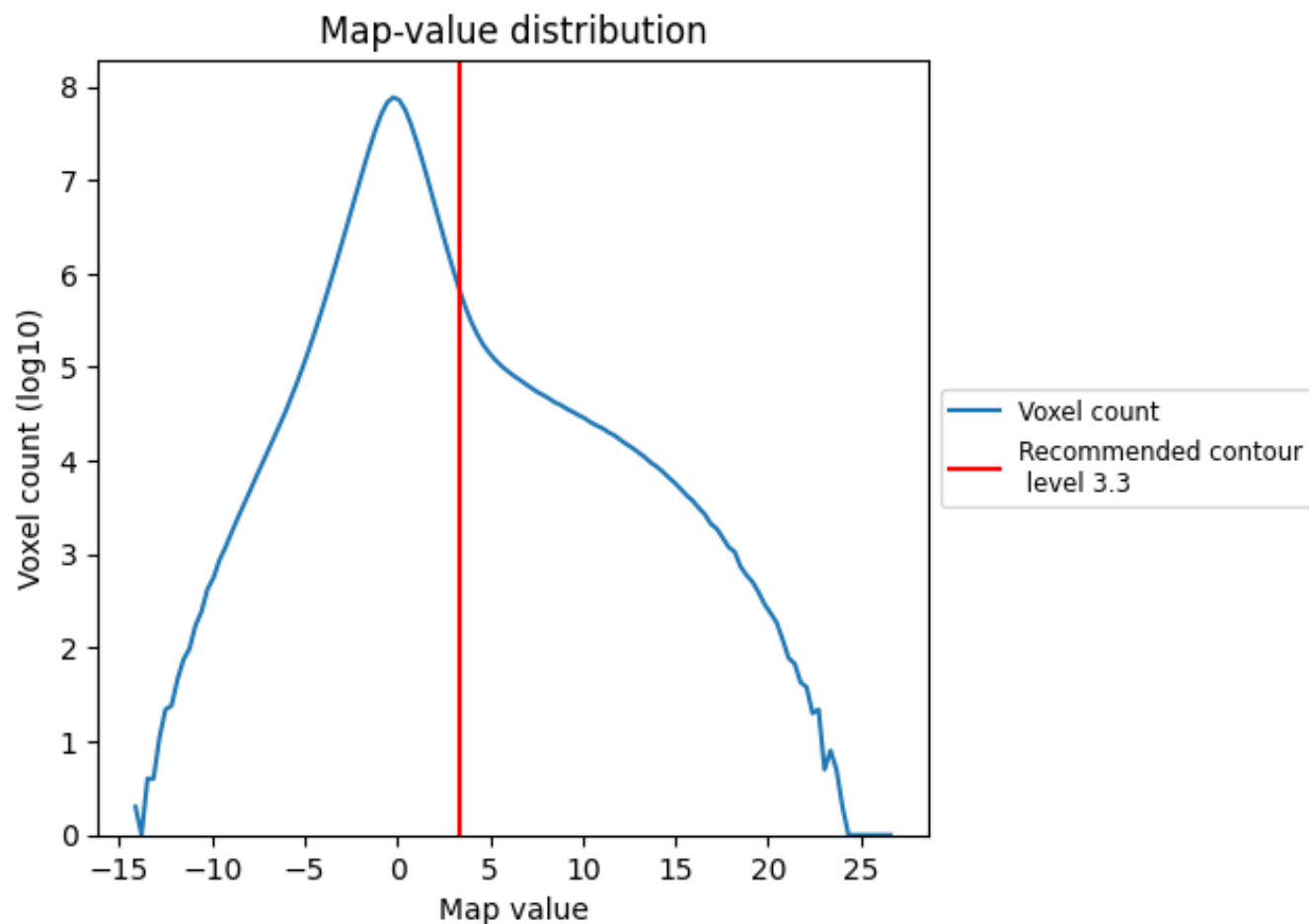
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

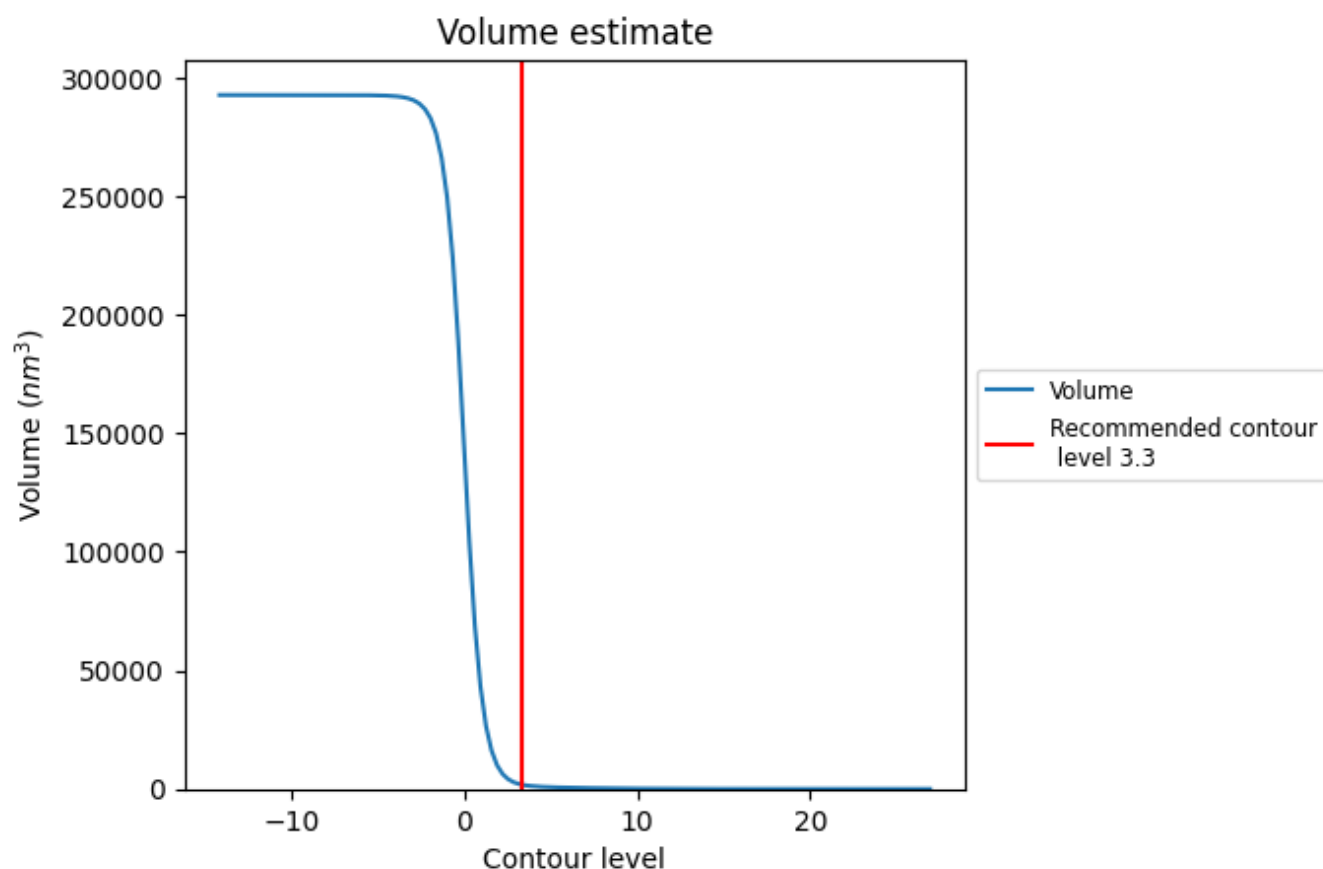
### 7.1 Map-value distribution [i](#)



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.



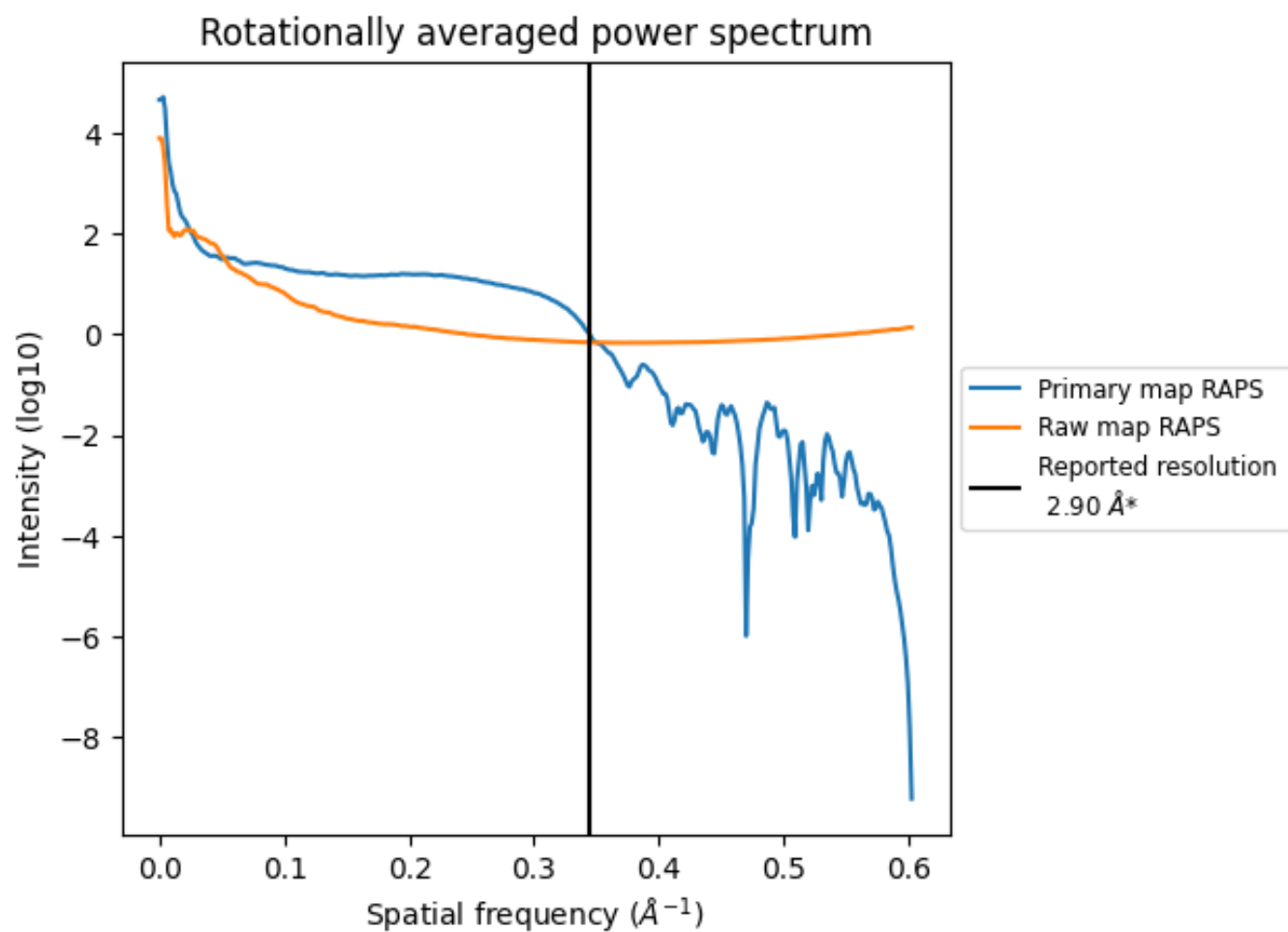
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1898  $\text{nm}^3$ ; this corresponds to an approximate mass of 1715 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

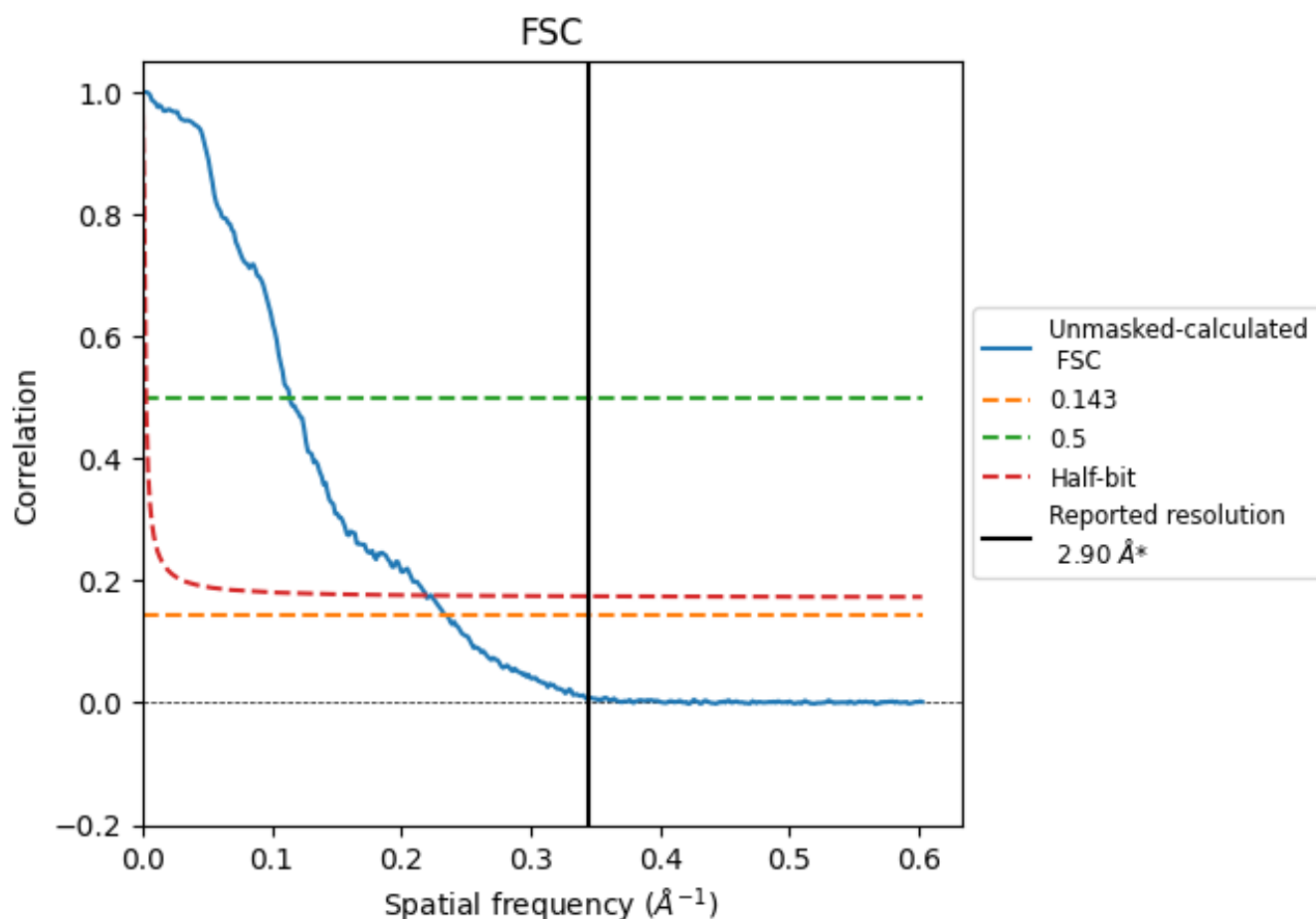


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

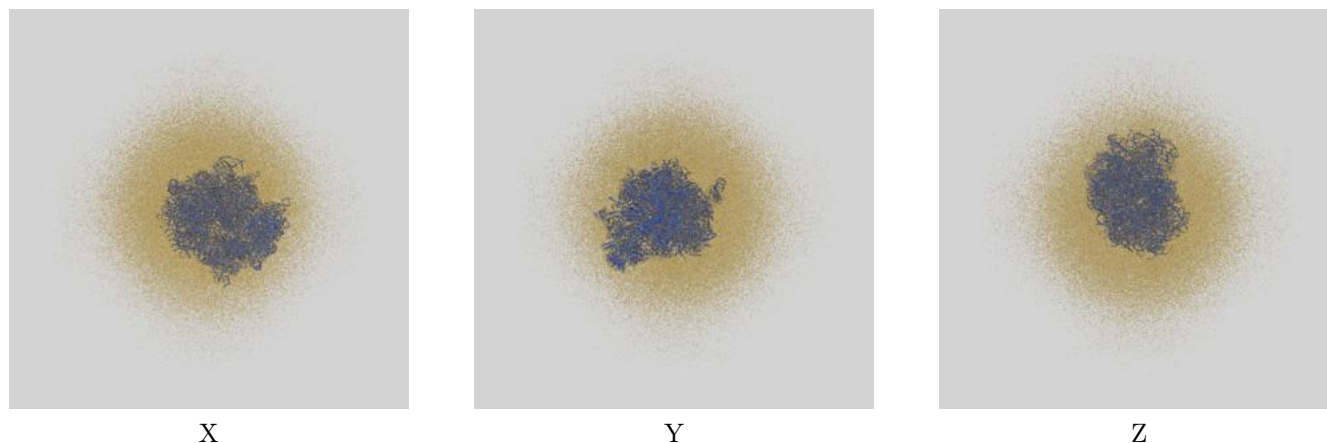
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.25                               | 8.78 | 4.56     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 2.9 by more than 10 %

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

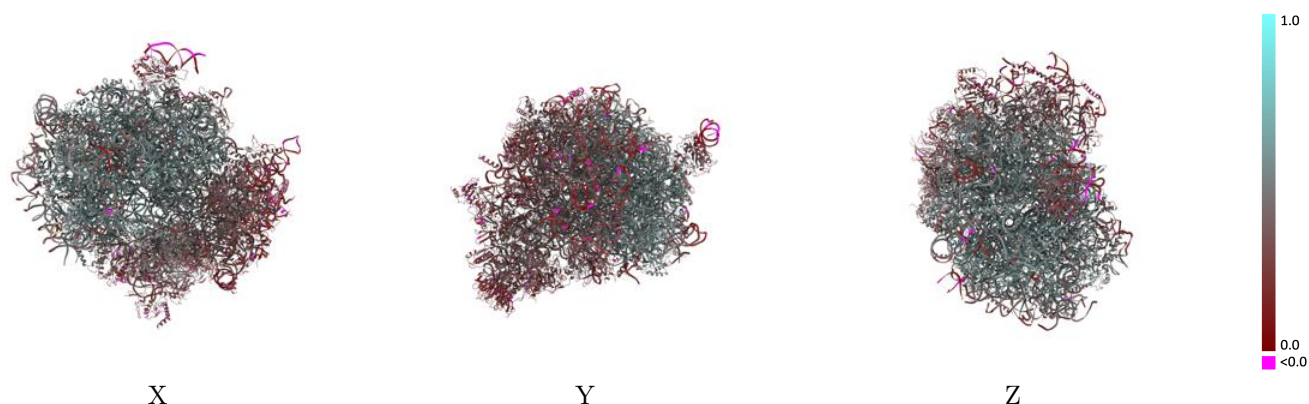
This section contains information regarding the fit between EMDB map EMD-75689 and PDB model 11HG. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



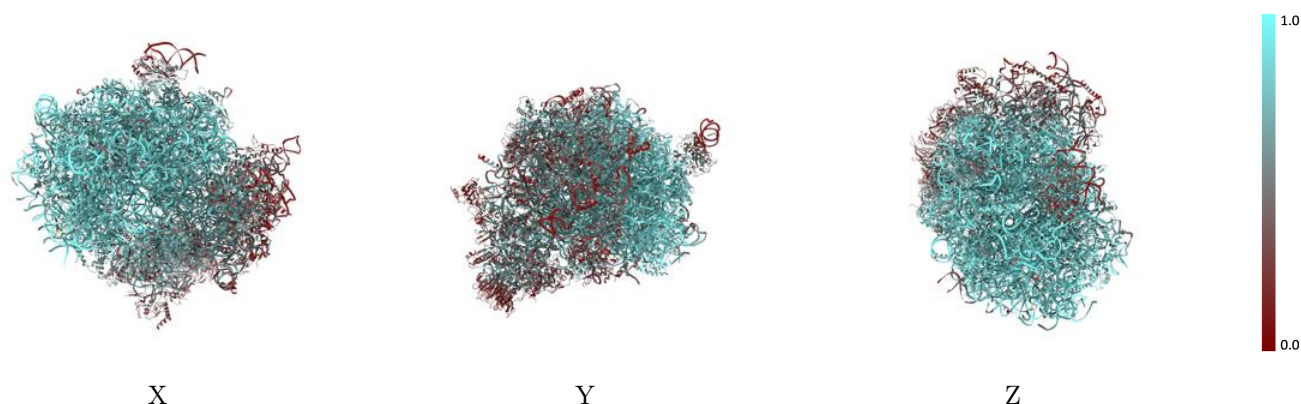
The images above show the 3D surface view of the map at the recommended contour level 3.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



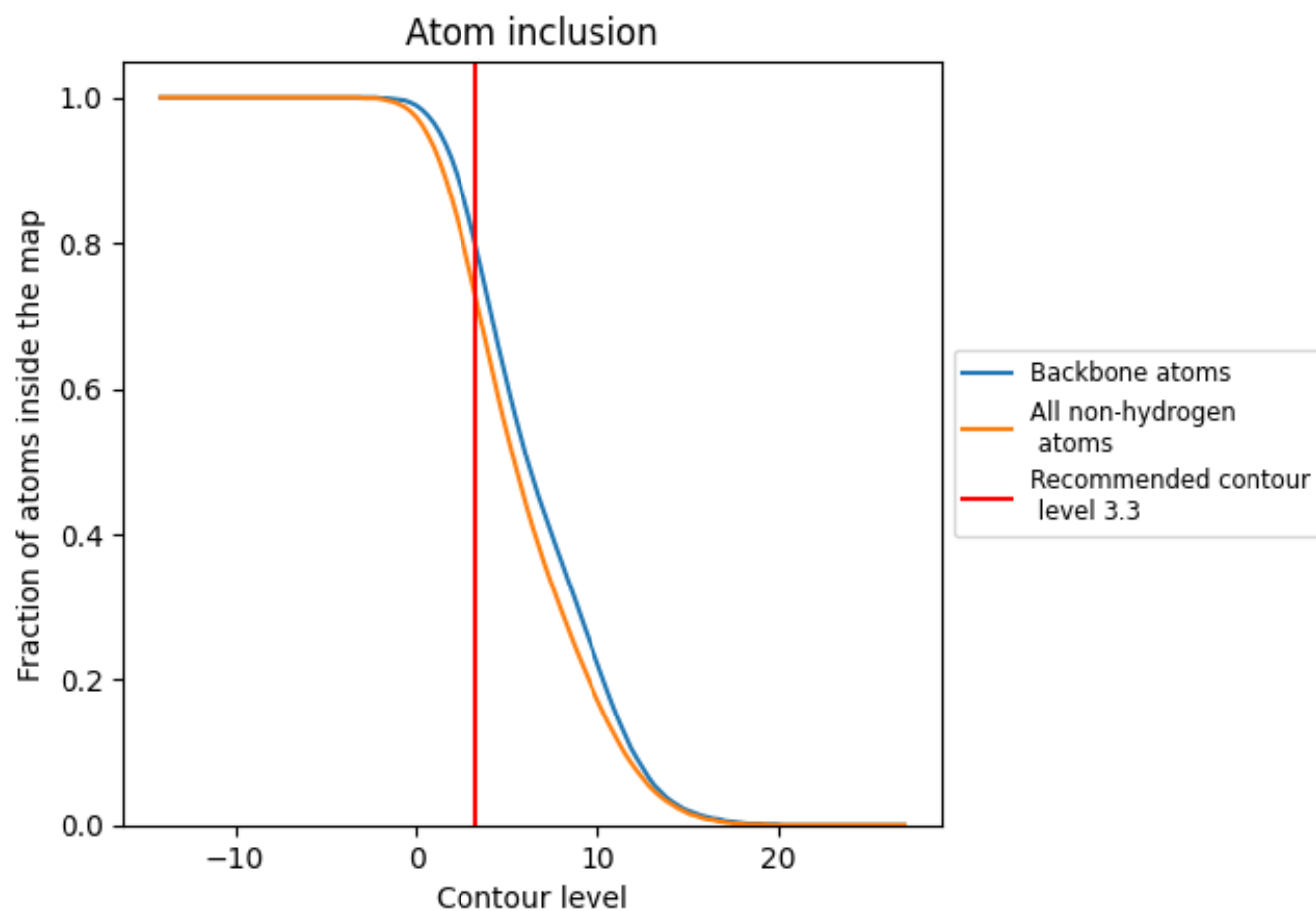
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 72% 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 (3.3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7230   |  0.4420   |
| 10    |  0.8140   |  0.5240   |
| 11    |  0.7250   |  0.4540   |
| 13    |  0.8000   |  0.5120   |
| 14    |  0.8250   |  0.5140   |
| 15    |  0.8640   |  0.5650   |
| 17    |  0.8380   |  0.5420   |
| 18    |  0.6610   |  0.3730   |
| 19    |  0.7440   |  0.4780   |
| 20    |  0.8520   |  0.5420   |
| 21    |  0.8160   |  0.5180   |
| 22    |  0.6880   |  0.4230   |
| 23    |  0.7780   |  0.5200   |
| 26    |  0.8120   |  0.5180   |
| 27    |  0.8040  |  0.5130  |
| 28    |  0.8810 |  0.5040 |
| 29    |  0.7470 |  0.4800 |
| 30    |  0.7750 |  0.5000 |
| 31    |  0.7880 |  0.4920 |
| 32    |  0.8610 |  0.5550 |
| 34    |  0.7950 |  0.5160 |
| 35    |  0.7850 |  0.5110 |
| 36    |  0.8140 |  0.5100 |
| 37    |  0.8650 |  0.5570 |
| 38    |  0.7200 |  0.4570 |
| 39    |  0.8240 |  0.5260 |
| 40    |  0.7850 |  0.5060 |
| 41    |  0.7250 |  0.4510 |
| 42    |  0.7880 |  0.5150 |
| 58    |  0.8940 |  0.5170 |
| 6     |  0.9330 |  0.5430 |
| A     |  0.5330 |  0.3280 |
| AA    |  0.2430 |  0.2290 |
| AS    |  0.4930 |  0.3670 |
| BB    |  0.4030 |  0.3340 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| CC    |  0.4730   |  0.3120   |
| CE    |  0.3390   |  0.2980   |
| DD    |  0.4610   |  0.3730   |
| EE    |  0.2460   |  0.2150   |
| ES    |  0.1350   |  0.0620   |
| F     |  0.4420   |  0.3130   |
| FF    |  0.4890   |  0.3710   |
| GG    |  0.5780   |  0.3760   |
| II    |  0.4330   |  0.3240   |
| L3    |  0.8210   |  0.5340   |
| L4    |  0.8560   |  0.5420   |
| L5    |  0.8010   |  0.4940   |
| L6    |  0.8140   |  0.5000   |
| L7    |  0.8310   |  0.5440   |
| L8    |  0.8390   |  0.5540   |
| L9    |  0.7890   |  0.5050   |
| LA    |  0.3300   |  0.2710   |
| LL    |  0.4910  |  0.3030  |
| MM    |  0.4490 |  0.3120 |
| OO    |  0.4160 |  0.3240 |
| PP    |  0.3760 |  0.2930 |
| Q     |  0.8580 |  0.5540 |
| RR    |  0.5270 |  0.3710 |
| RS    |  0.3830 |  0.3070 |
| S2    |  0.4600 |  0.3460 |
| S3    |  0.4530 |  0.3200 |
| S4    |  0.3340 |  0.2970 |
| S5    |  0.4600 |  0.3230 |
| S6    |  0.3410 |  0.2710 |
| S7    |  0.3210 |  0.2960 |
| S8    |  0.4190 |  0.3440 |
| S9    |  0.3690 |  0.3000 |
| SS    |  0.3050 |  0.2670 |
| TT    |  0.3840 |  0.2960 |
| UU    |  0.5430 |  0.3760 |
| VV    |  0.3870 |  0.3380 |
| W     |  0.5580 |  0.3860 |
| WW    |  0.4210 |  0.3170 |
| WX    |  0.4450 |  0.3590 |
| XX    |  0.5740 |  0.3960 |
| YY    |  0.3500 |  0.2870 |
| ZZ    |  0.2830 |  0.2210 |

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*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| aa    |  0.7630 |  0.4810 |
| bb    |  0.8520 |  0.5370 |
| cc    |  0.7960 |  0.5150 |
| dd    |  0.8530 |  0.5580 |
| ee    |  0.8400 |  0.5460 |
| ff    |  0.7950 |  0.5120 |
| gg    |  0.8340 |  0.5330 |
| s     |  0.5250 |  0.3450 |
| t     |  0.3210 |  0.2140 |
| v     |  0.5600 |  0.3700 |