



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:43 PM UTC

PDB ID : 7NRC / pdb\_00007nrc  
EMDB ID : EMD-12534  
Title : Structure of the yeast Gcn1 bound to a leading stalled 80S ribosome with Rbg2, Gir2, A- and P-tRNA and eIF5A  
Authors : Pochopien, A.A.; Beckert, B.; Wilson, D.N.  
Deposited on : 2021-03-03  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

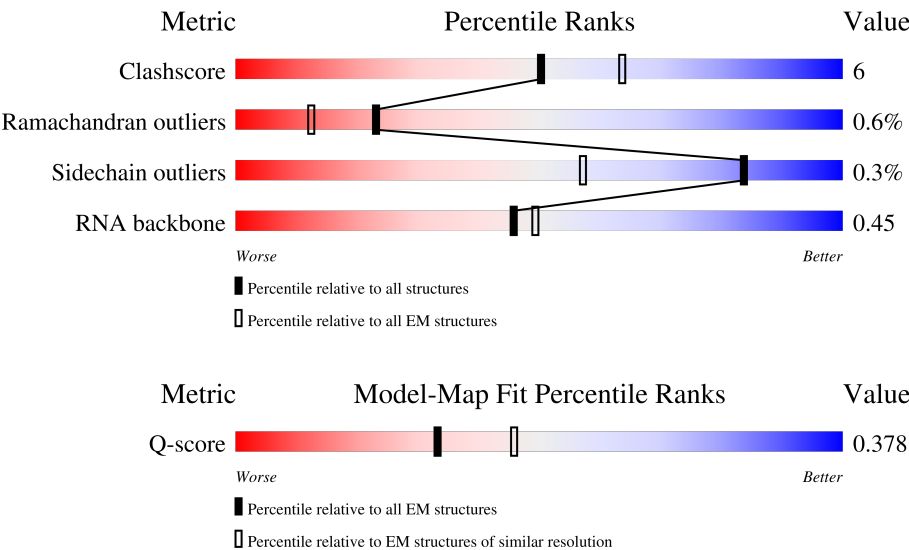
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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                       | 8855 ( 3.40 - 4.40 )                                     |

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   | S2    | 1800   |                  |
| 2   | Sl    | 6      |                  |
| 3   | SP    | 206    |                  |

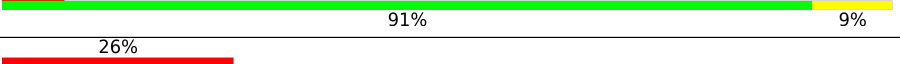
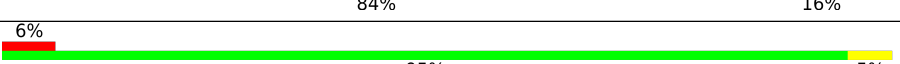
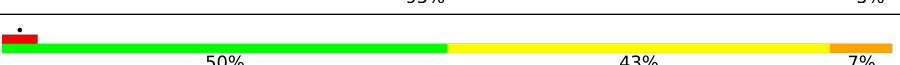
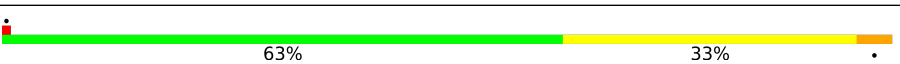
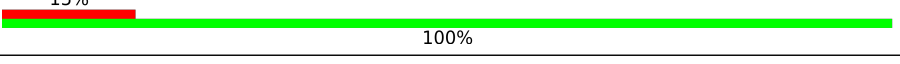
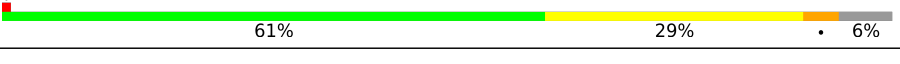
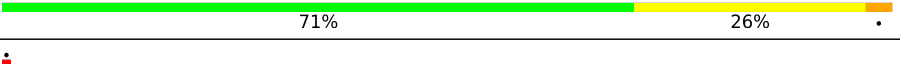
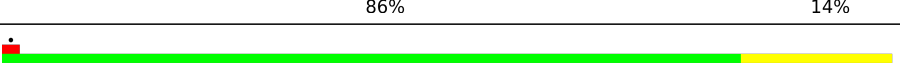
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | SQ    | 232    |                  |
| 5   | SE    | 117    |                  |
| 6   | SR    | 216    |                  |
| 7   | SA    | 222    |                  |
| 8   | SS    | 258    |                  |
| 9   | SB    | 206    |                  |
| 10  | ST    | 228    |                  |
| 11  | SU    | 184    |                  |
| 12  | SV    | 198    |                  |
| 13  | SW    | 184    |                  |
| 14  | SC    | 92     |                  |
| 15  | SX    | 142    |                  |
| 16  | SD    | 121    |                  |
| 17  | SY    | 150    |                  |
| 18  | SZ    | 127    |                  |
| 19  | SF    | 141    |                  |
| 20  | SG    | 125    |                  |
| 21  | SH    | 145    |                  |
| 22  | SI    | 143    |                  |
| 23  | SJ    | 100    |                  |
| 24  | Sa    | 87     |                  |
| 25  | Sb    | 129    |                  |
| 26  | Sc    | 144    |                  |
| 27  | Sd    | 134    |                  |
| 28  | SK    | 82     |                  |

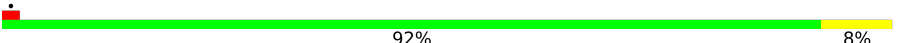
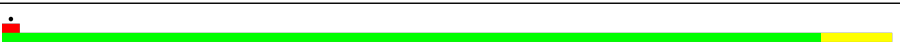
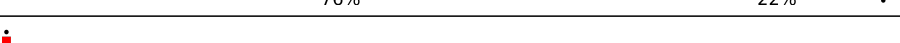
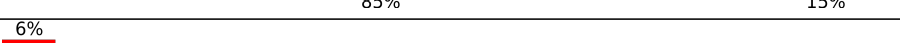
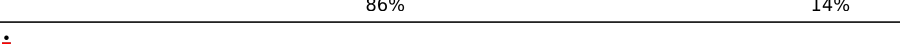
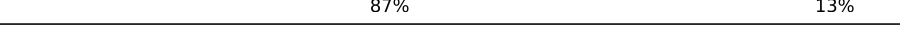
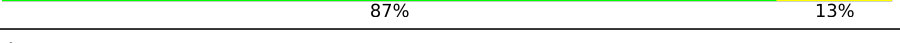
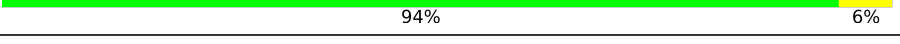
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | Se    | 97     |    |
| 30  | Sf    | 81     |    |
| 31  | SM    | 53     |    |
| 32  | Sg    | 57     |    |
| 33  | SN    | 73     |    |
| 34  | SO    | 312    |    |
| 35  | SL    | 63     |    |
| 36  | Sm    | 76     |    |
| 37  | Sn    | 75     |    |
| 38  | So    | 366    |    |
| 39  | Sp    | 48     |   |
| 40  | LA    | 3394   |  |
| 41  | LB    | 121    |  |
| 42  | LC    | 158    |  |
| 43  | LD    | 251    |  |
| 44  | LE    | 386    |  |
| 45  | LF    | 361    |  |
| 46  | LG    | 294    |  |
| 47  | LH    | 175    |  |
| 48  | LI    | 222    |  |
| 49  | LJ    | 233    |  |
| 50  | LK    | 191    |  |
| 51  | LL    | 218    |  |
| 52  | LM    | 169    |  |
| 53  | LN    | 193    |  |

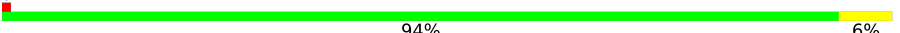
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | LO    | 136    |    |
| 55  | LP    | 203    |    |
| 56  | LQ    | 197    |    |
| 57  | LR    | 183    |    |
| 58  | LS    | 185    |    |
| 59  | LT    | 188    |    |
| 60  | LU    | 171    |    |
| 61  | LV    | 159    |    |
| 62  | LW    | 100    |    |
| 63  | LX    | 136    |    |
| 64  | LY    | 65     |    |
| 65  | LZ    | 121    |    |
| 66  | La    | 125    |  |
| 67  | Lb    | 135    |  |
| 68  | Lc    | 148    |  |
| 69  | Ld    | 58     |  |
| 70  | Le    | 96     |  |
| 71  | Lf    | 109    |  |
| 72  | Lg    | 127    |  |
| 73  | Lh    | 106    |  |
| 74  | Li    | 112    |  |
| 75  | Lj    | 119    |  |
| 76  | Lk    | 99     |  |
| 77  | Ll    | 81     |  |
| 78  | Lm    | 77     |  |

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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 79  | Ln    | 50     |  68% 32%         |
| 80  | Lo    | 52     |  83% 17%         |
| 81  | Lp    | 25     |  92% 8%          |
| 82  | Lq    | 103    |  94% 6%          |
| 83  | Lr    | 91     |  79% 20% .       |
| 84  | Ls    | 154    |  13% 65% 32% .   |
| 85  | Lt    | 210    |  7% 98% .        |
| 86  | A     | 1209   |  71% 75% 21% . . |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 84  | 5CT  | Ls    | 51  | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 213576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA (1771-MER).

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | S2    | 1771     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 37739 | 16872 | 6683 | 12413 | 1771 |         |       |

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*UP\*GP\*AP\*AP\*A)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 2   | Sl    | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 131   | 59 | 27 | 39 | 6 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | SP    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1603  | 1030 | 284 | 287 | 2 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | SQ    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1798  | 1139 | 330 | 325 | 4 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | SE    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 583 | 171 | 155 | 7 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | SR    | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1626  | 1042 | 287 | 295 | 2 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | SA    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1729  | 1098 | 312 | 313 | 6 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | SS    | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2056  | 1308 | 387 | 358 | 3 |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | SB    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1605  | 1005 | 299 | 298 | 3 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | ST    | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1815  | 1138 | 351 | 323 | 3 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 11  | SU    | 184      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1473  | 946 | 263 | 264 |  |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | SV    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1476  | 916 | 295 | 263 | 2 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | SW    | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1479  | 935 | 285 | 258 | 1 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | SC    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 752   | 487 | 122 | 141 | 2 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | SX    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1142  | 733 | 217 | 189 | 3 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | SD    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 551 | 153 | 169 | 2 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | SY    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | SZ    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 923   | 568 | 185 | 167 | 3 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 19  | SF    | 141      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1105  | 708 | 203 | 194 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | SG    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 948   | 596 | 179 | 171 | 2 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | SH    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1188  | 741 | 237 | 208 | 2 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | SI    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | SJ    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 797   | 506 | 144 | 146 | 1 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Sa    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 673   | 415 | 125 | 131 | 2 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Sb    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Sc    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 27  | Sd    | 134      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1032  | 651 | 195 | 186 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28  | SK    | 82       | Total | C   | N   | O   |         |       |
|     |       |          | 651   | 416 | 123 | 112 | 0       | 0     |

- Molecule 29 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | Se    | 97       | Total | C   | N   | O   | S |         |       |
|     |       |          | 765   | 473 | 160 | 127 | 5 | 0       | 0     |

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Sf    | 81       | Total | C   | N   | O   | S |         |       |
|     |       |          | 610   | 382 | 110 | 113 | 5 | 0       | 0     |

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | SM    | 53       | Total | C   | N  | O  | S |         |       |
|     |       |          | 442   | 274 | 92 | 72 | 4 | 0       | 0     |

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | Sg    | 57       | Total | C   | N  | O  | S |         |       |
|     |       |          | 451   | 284 | 93 | 73 | 1 | 0       | 0     |

- Molecule 33 is a protein called 40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33  | SN    | 73       | Total | C   | N   | O  | S |         |       |
|     |       |          | 556   | 352 | 105 | 95 | 4 | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| SN    | 97      | ALA      | LYS    | variant | UNP P05759 |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | SO    | 312      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2383  | 1514 | 409 | 452 | 8 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | SL    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 491   | 303 | 96 | 91 | 1 |         |       |

- Molecule 36 is a RNA chain called tRNA (76-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 36  | Sm    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1611  | 721 | 281 | 534 | 75 |         |       |

- Molecule 37 is a RNA chain called tRNA (75-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 37  | Sn    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1606  | 716 | 297 | 518 | 75 |         |       |

- Molecule 38 is a protein called Ribosome-interacting GTPase 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 38  | So    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2729  | 1723 | 478 | 518 | 10 |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| So    | 62      | ALA      | LYS    | variant | UNP P53295 |
| So    | 92      | ALA      | ILE    | variant | UNP P53295 |
| So    | 94      | GLU      | HIS    | variant | UNP P53295 |
| So    | 96      | GLU      | ALA    | variant | UNP P53295 |
| So    | 134     | LYS      | ARG    | variant | UNP P53295 |
| So    | 271     | ALA      | THR    | variant | UNP P53295 |
| So    | 299     | ALA      | TYR    | variant | UNP P53295 |
| So    | 303     | ALA      | ARG    | variant | UNP P53295 |
| So    | 318     | ASP      | ASN    | variant | UNP P53295 |
| So    | 361     | GLU      | ASP    | variant | UNP P53295 |

- Molecule 39 is a protein called GIR2.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 39  | Sp    | 48       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 240   | 144 | 48 | 48 |         |       |

- Molecule 40 is a RNA chain called 25S rRNA (3184-MER).

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 40  | LA    | 3184     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 68091 | 30415 | 12259 | 22233 | 3184 |         |       |

- Molecule 41 is a RNA chain called 5S rRNA (121-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 41  | LB    | 121      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |       |

- Molecule 42 is a RNA chain called 5.8S rRNA (158-MER).

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 42  | LC    | 158      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43  | LD    | 251      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1899  | 1182 | 385 | 331 | 1 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44  | LE    | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45  | LF    | 361      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | LG    | 294      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2351  | 1484 | 410 | 455 | 2 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L6-B.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 47  | LH    | 167      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1307  | 843 | 234 | 230 |  |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| LH    | 120     | LYS      | ASN    | variant | UNP P05739 |

- Molecule 48 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | LI    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | LJ    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | LK    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 957 | 274 | 273 | 4 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | LL    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1117 | 334 | 306 | 7 |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | LM    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 843 | 252 | 247 | 4 |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | LN    | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |   |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | LO    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | LP    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | LQ    | 197      | Total | C    | N   | O   | S | 197     | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | LR    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1416  | 879 | 284 | 253 |   |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | LS    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 59  | LT    | 188      | Total | C   | N   | O   |         |       |
|     |       |          | 1515  | 932 | 323 | 260 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | LU    | 171      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1437  | 925 | 266 | 243 | 3 | 0       | 0     |

- Molecule 61 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | LV    | 159      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1272  | 802 | 245 | 221 | 4 | 0       | 0     |

- Molecule 62 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 62  | LW    | 100      | Total | C   | N   | O   |         |       |
|     |       |          | 796   | 516 | 131 | 149 | 0       | 0     |

- Molecule 63 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | LX    | 136      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1003  | 628 | 189 | 179 | 7 | 0       | 0     |

- Molecule 64 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 64  | LY    | 65       | Total | C   | N   | O  | S |         |       |
|     |       |          | 528   | 339 | 104 | 84 | 1 | 0       | 0     |

- Molecule 65 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | LZ    | 121      | Total | C   | N   | O   | S |         |       |
|     |       |          | 964   | 620 | 169 | 173 | 2 | 0       | 0     |

- Molecule 66 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 66  | La    | 125      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 984   | 620 | 191 | 173 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 67  | Lb    | 135      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1080  | 701 | 199 | 180 |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | Lc    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1169  | 747 | 231 | 188 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 69  | Ld    | 58       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | Le    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 476 | 123 | 137 | 1 |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 556 | 167 | 152 | 1 |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | Lg    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1017  | 644 | 205 | 167 | 1 |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | Lh    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Li    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | Lj    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | Lk    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 766   | 478 | 154 | 132 | 2 |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Ll    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 645   | 393 | 141 | 106 | 5 |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 78  | Lm    | 77       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |         |       |

- Molecule 79 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 79  | Ln    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | Lo    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 410   | 254 | 86 | 65 | 5 |         |       |

- Molecule 81 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 81  | Lp    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 229   | 139 | 62 | 27 | 1 |         |       |

- Molecule 82 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | Lq    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 824   | 517 | 167 | 135 | 5 |         |       |

- Molecule 83 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | Lr    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |       |

- Molecule 84 is a protein called eiF5A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | Ls    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 709 | 195 | 230 | 9 |         |       |

- Molecule 85 is a protein called L1 60S ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 85  | Lt    | 210      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1050  | 630 | 210 | 210 |         |       |

- Molecule 86 is a protein called GCN1.

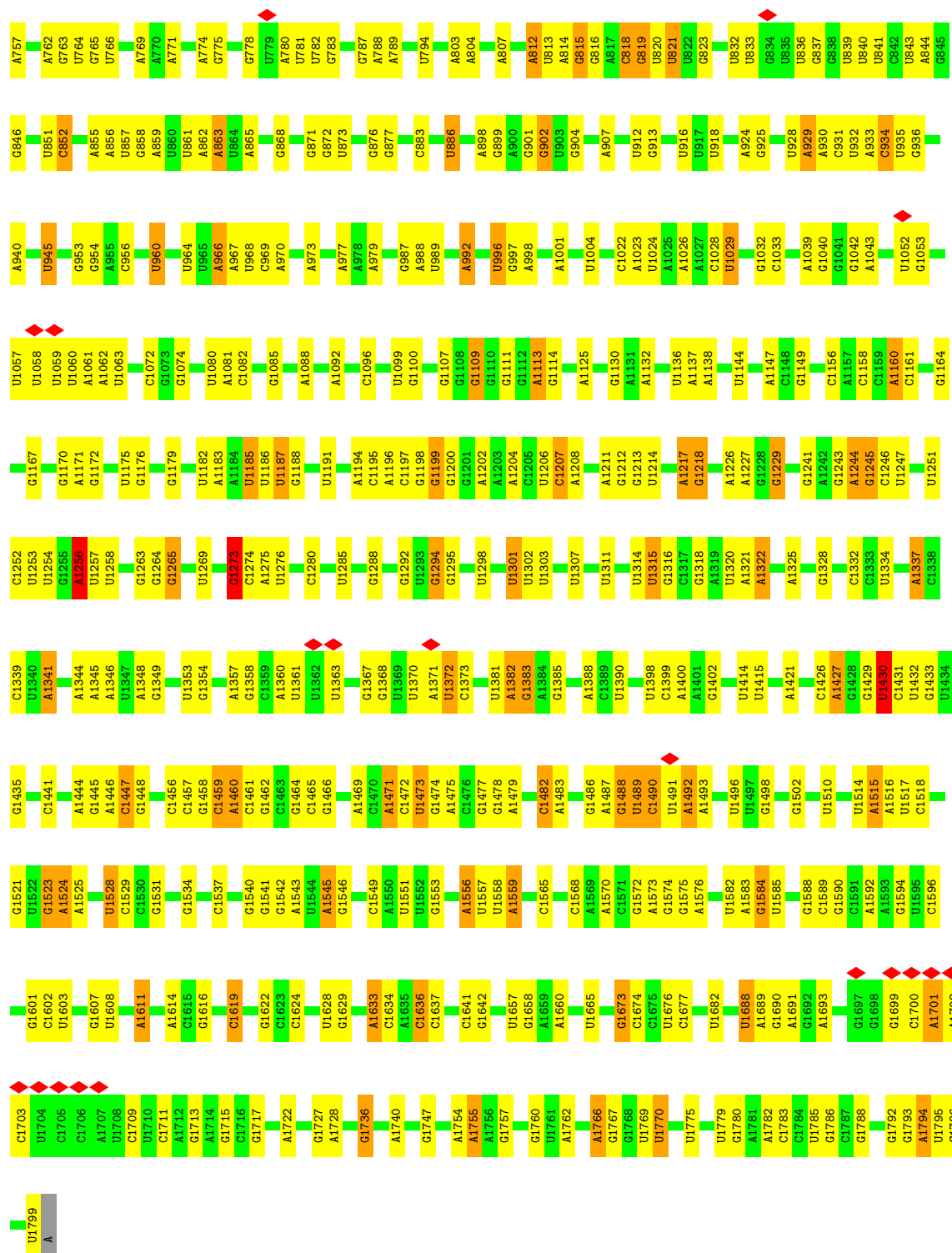
| Mol | Chain | Residues | Atoms |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 86  | A     | 1209     | Total | C    | N    | O    | 1       | 0     |
|     |       |          | 6029  | 3609 | 1210 | 1210 |         |       |

### 3 Residue-property plots

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

#### • Molecule 1: 18S rRNA (1771-MER)





• Molecule 2: RNA (5'-R(P\*AP\*UP\*GP\*AP\*AP\*A)-3')

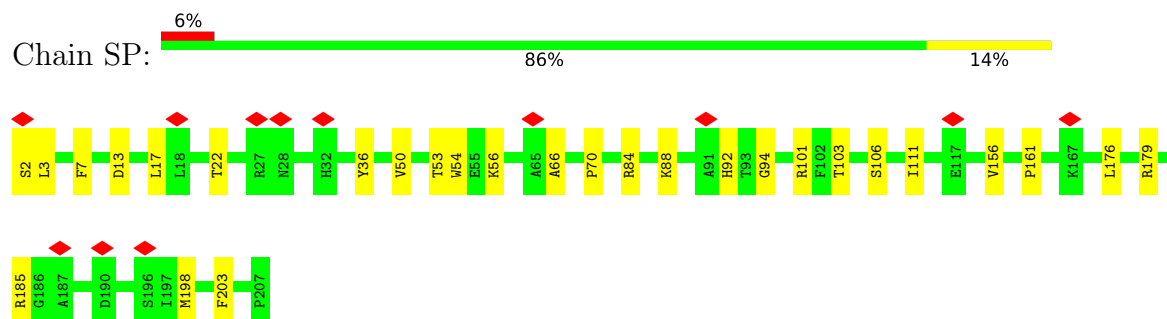
Chain S1:

83%

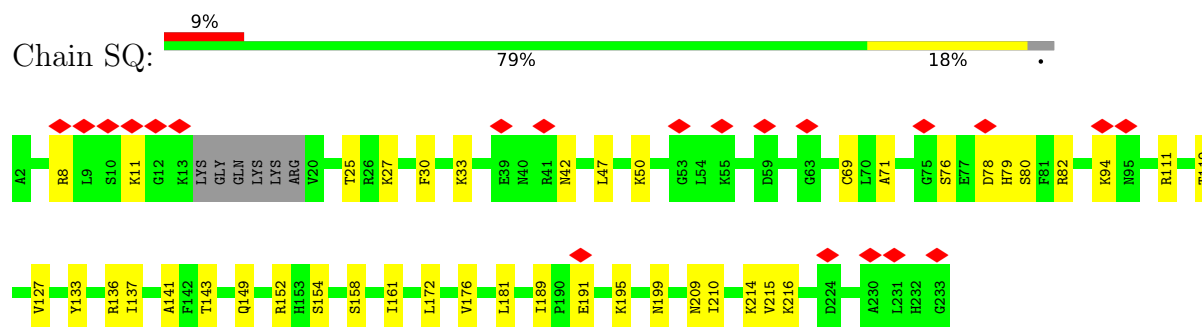
17%



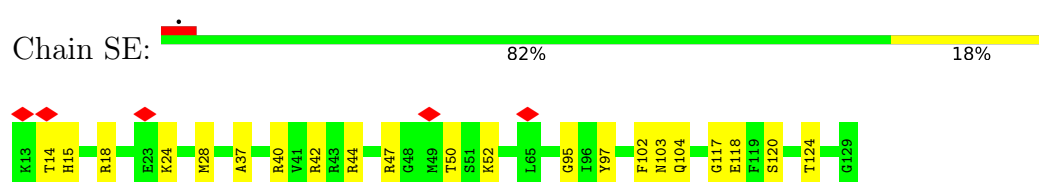
- Molecule 3: 40S ribosomal protein S0-A



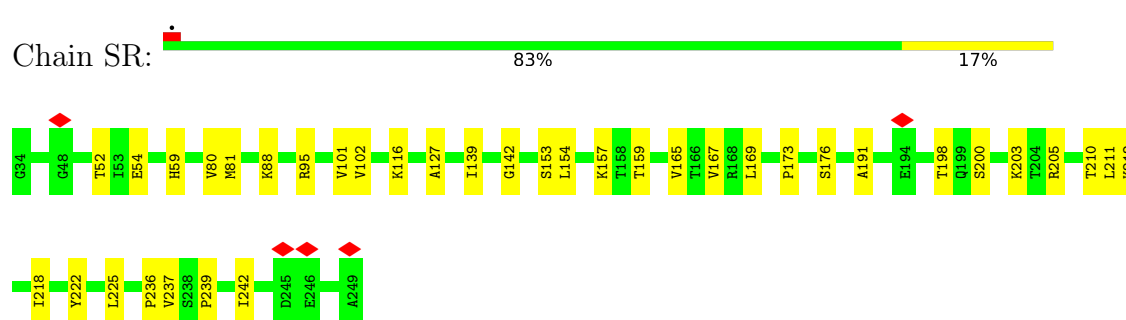
- Molecule 4: 40S ribosomal protein S1-A



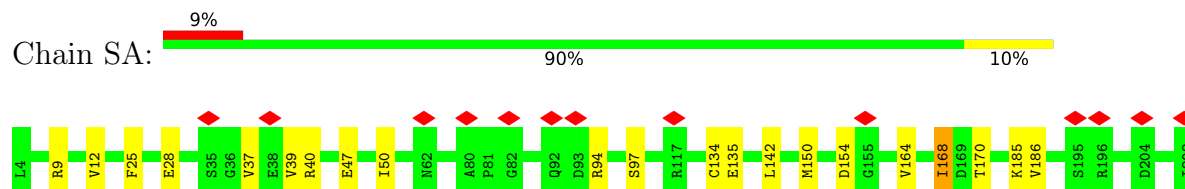
- Molecule 5: 40S ribosomal protein S15

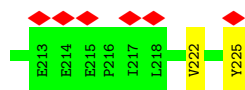


- Molecule 6: 40S ribosomal protein S2



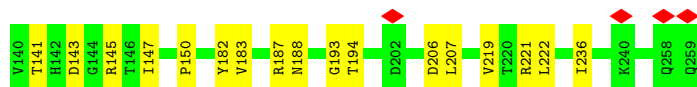
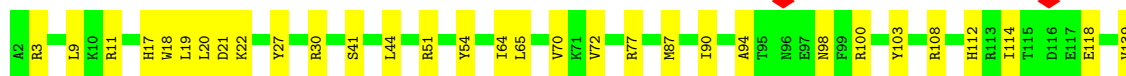
- Molecule 7: 40S ribosomal protein S3





- Molecule 8: 40S ribosomal protein S4-A

Chain SS: 81% 19%



- Molecule 9: 40S ribosomal protein S5

Chain SB: 9% 84% 16%



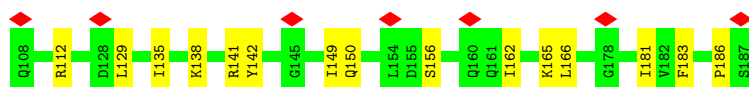
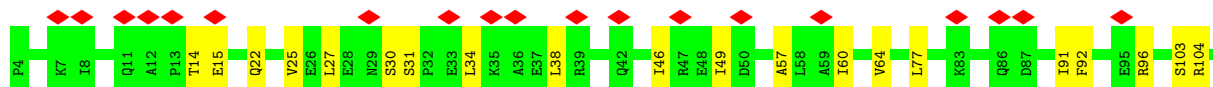
- Molecule 10: 40S ribosomal protein S6-A

Chain ST: 86% 14%



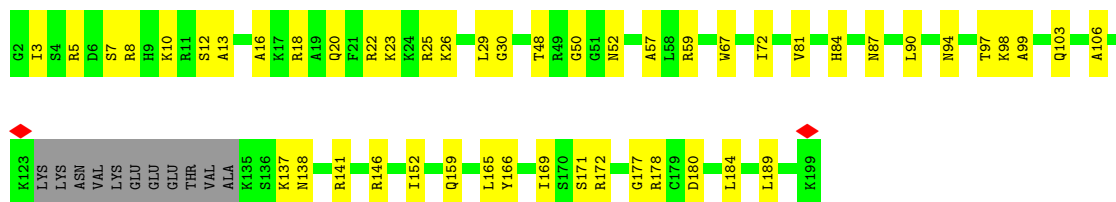
- Molecule 11: 40S ribosomal protein S7-A

Chain SU: 14% 81% 19%



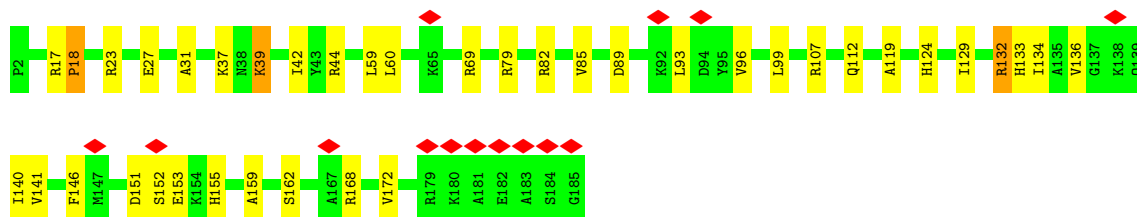
- Molecule 12: 40S ribosomal protein S8-A

Chain SV:  70% 25% 6%



- Molecule 13: 40S ribosomal protein S9-A

Chain SW:  8% 79% 20%



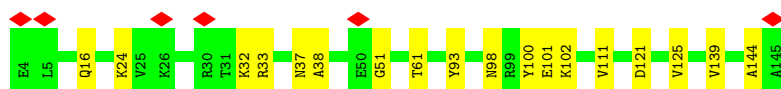
- Molecule 14: 40S ribosomal protein S10-A

Chain SC:  10% 85% 14%



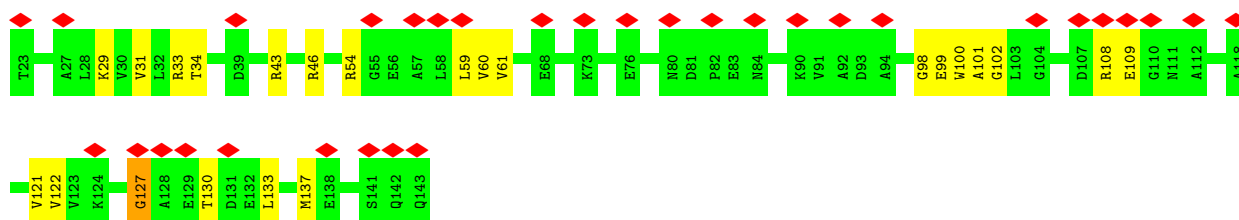
- Molecule 15: 40S ribosomal protein S11-A

Chain SX:  87% 13%



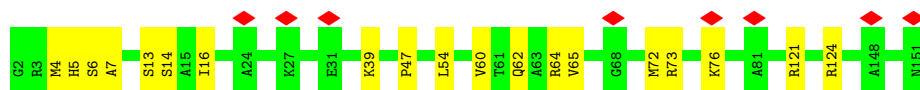
- Molecule 16: 40S ribosomal protein S12

Chain SD:  26% 81% 18%

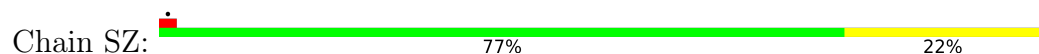


- Molecule 17: 40S ribosomal protein S13

Chain SY:  5% 87% 13%



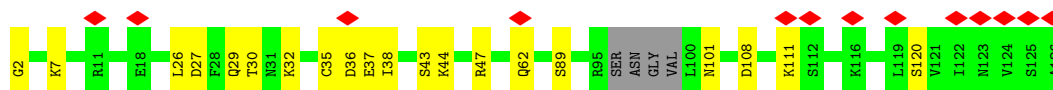
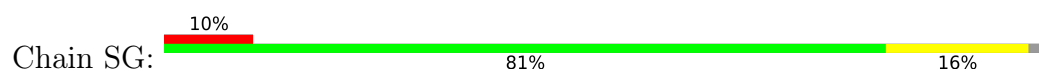
- Molecule 18: 40S ribosomal protein S14-B



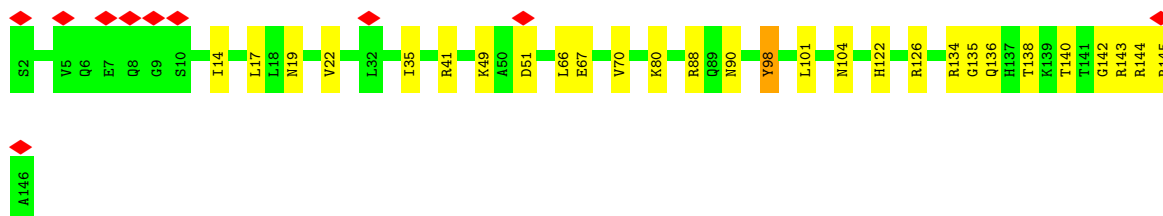
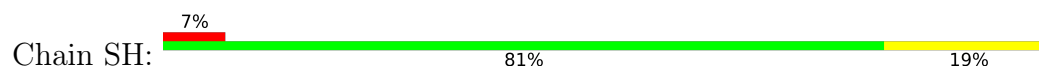
- Molecule 19: 40S ribosomal protein S16-A



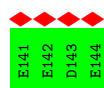
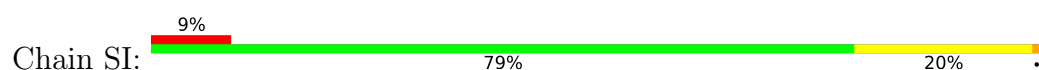
- Molecule 20: 40S ribosomal protein S17-B



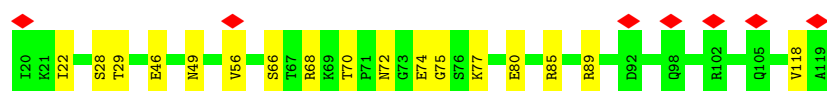
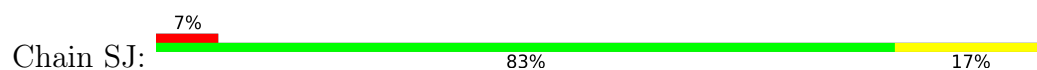
- Molecule 21: 40S ribosomal protein S18-A



- Molecule 22: 40S ribosomal protein S19-A



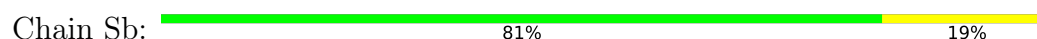
- Molecule 23: 40S ribosomal protein S20



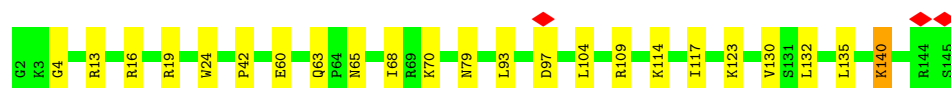
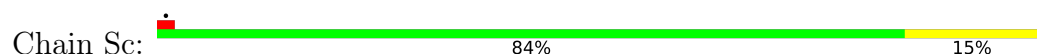
- Molecule 24: 40S ribosomal protein S21-A



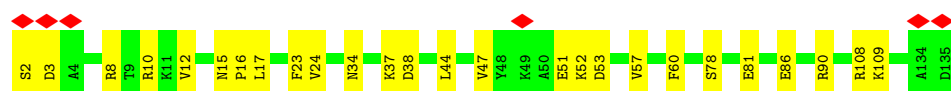
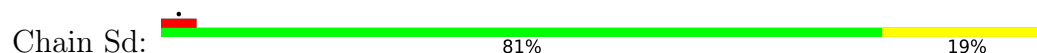
- Molecule 25: 40S ribosomal protein S22-A



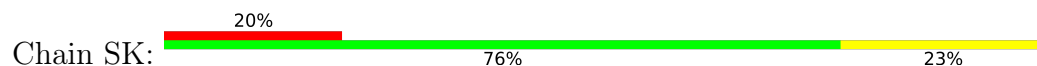
- Molecule 26: 40S ribosomal protein S23-A



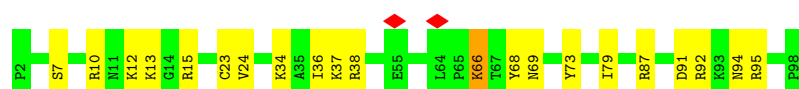
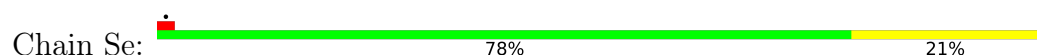
- Molecule 27: 40S ribosomal protein S24-A



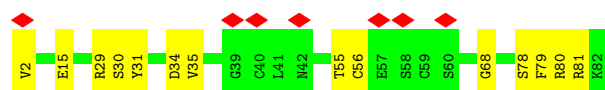
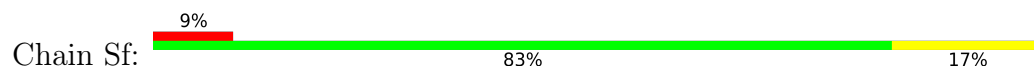
- Molecule 28: 40S ribosomal protein S25-A



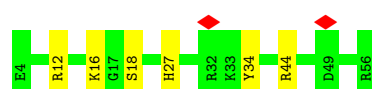
- Molecule 29: 40S ribosomal protein S26-B



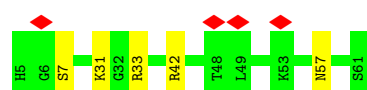
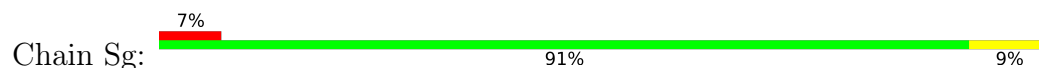
- Molecule 30: 40S ribosomal protein S27-A



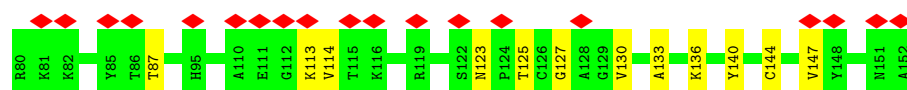
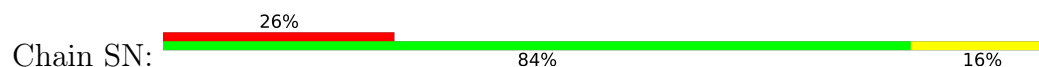
- Molecule 31: 40S ribosomal protein S29-A



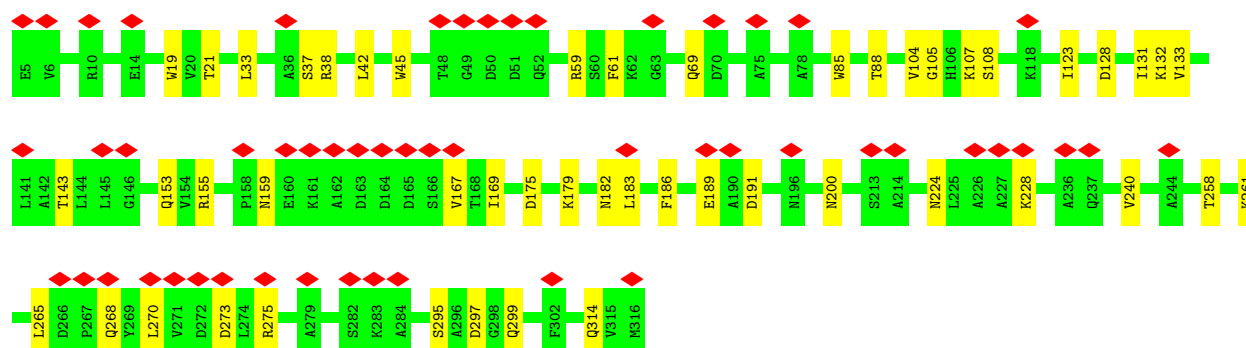
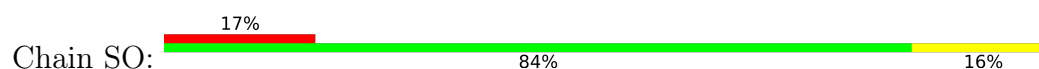
- Molecule 32: 40S ribosomal protein S30-A



- Molecule 33: 40S ribosomal protein S31



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



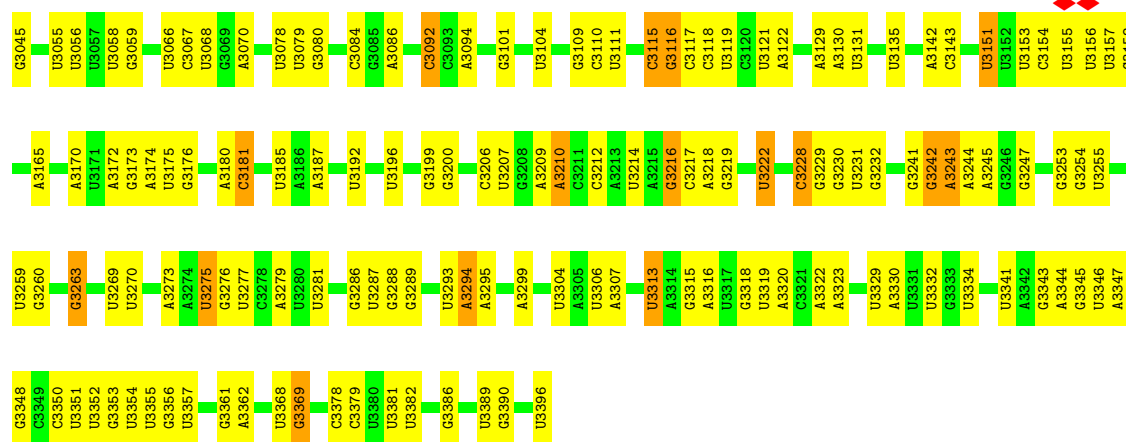
- Molecule 35: 40S ribosomal protein S28-A







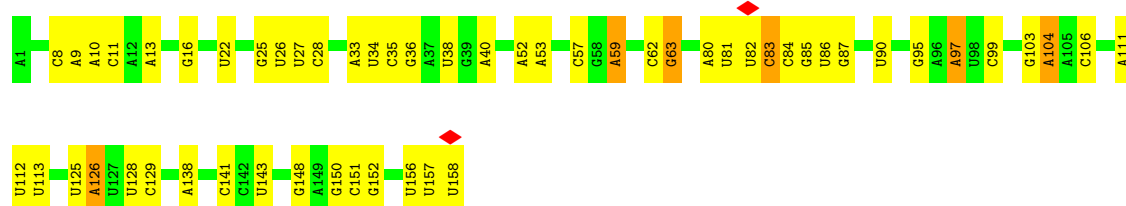




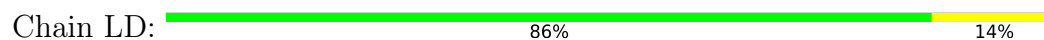
• Molecule 41: 5S rRNA (121-MER)



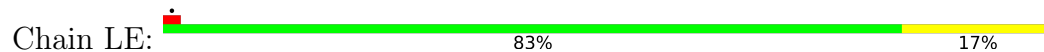
• Molecule 42: 5.8S rRNA (158-MER)

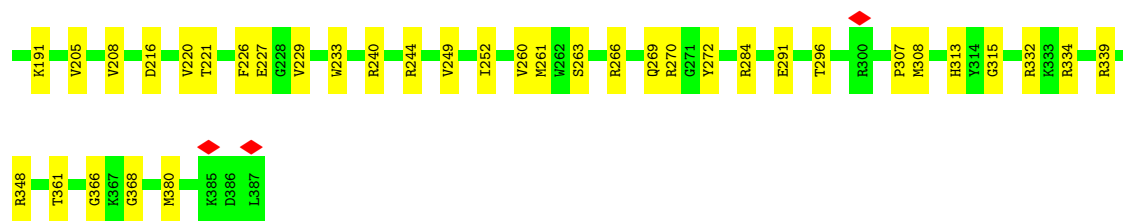


• Molecule 43: 60S ribosomal protein L2-A



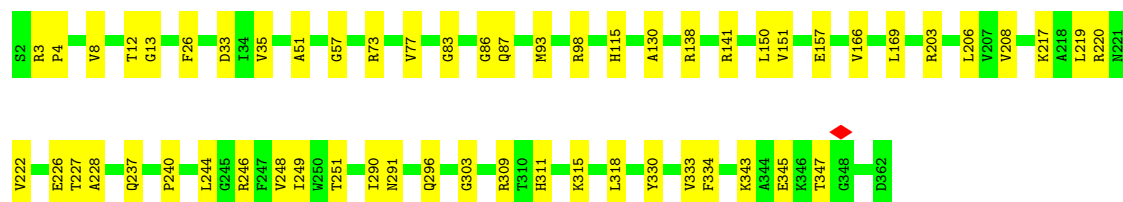
• Molecule 44: 60S ribosomal protein L3





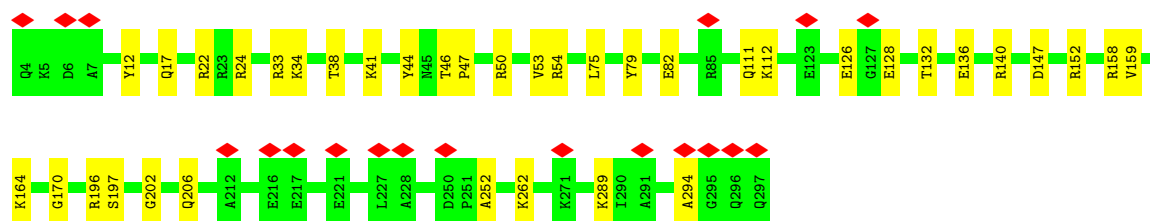
- Molecule 45: 60S ribosomal protein L4-A

Chain LF: 84% 16%



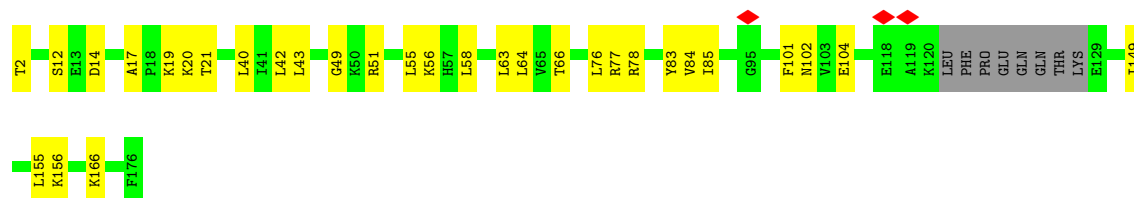
- Molecule 46: 60S ribosomal protein L5

Chain LG: 6% 87% 13%



- Molecule 47: 60S ribosomal protein L6-B

Chain LH: 78% 18% 5%



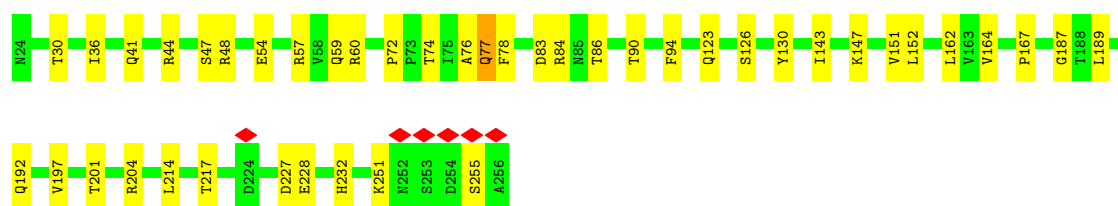
- Molecule 48: 60S ribosomal protein L7-A

Chain LI: 89% 11%

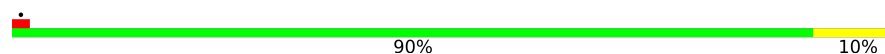


- Molecule 49: 60S ribosomal protein L8-A

Chain LJ:  82% 18%



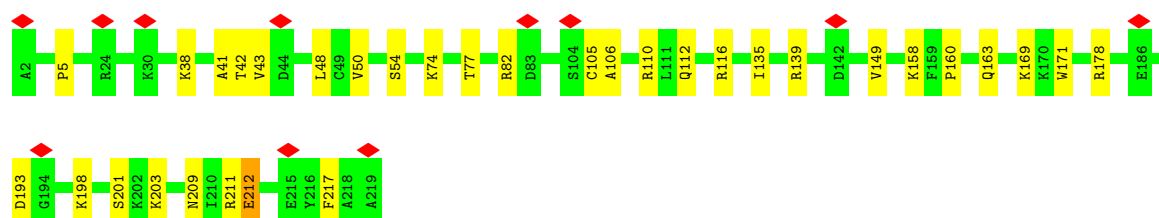
- Molecule 50: 60S ribosomal protein L9-A

Chain LK:  90% 10%



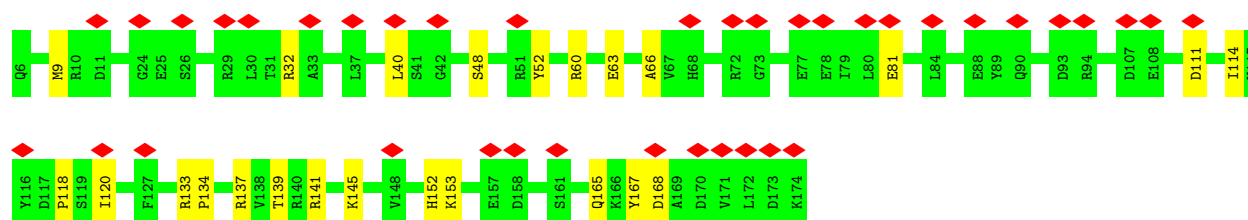
- Molecule 51: 60S ribosomal protein L10

Chain LL:  5% 85% 15%



- Molecule 52: 60S ribosomal protein L11-B

Chain LM:  22% 86% 14%



- Molecule 53: 60S ribosomal protein L13-A

Chain LN:  87% 13%

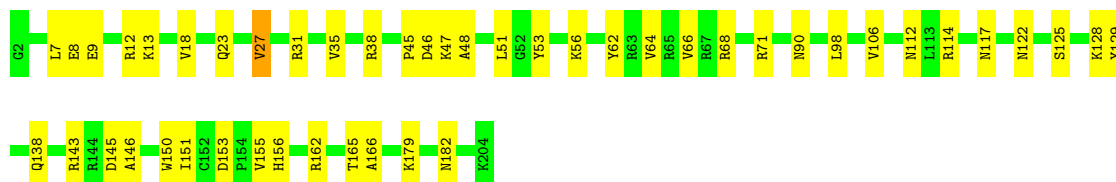
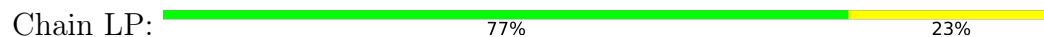


- Molecule 54: 60S ribosomal protein L14-A

Chain LO:  86% 14%



- Molecule 55: 60S ribosomal protein L15-A



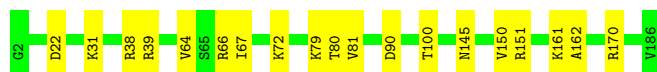
- Molecule 56: 60S ribosomal protein L16-A



- Molecule 57: 60S ribosomal protein L17-A



- Molecule 58: 60S ribosomal protein L18-A



- Molecule 59: 60S ribosomal protein L19-A

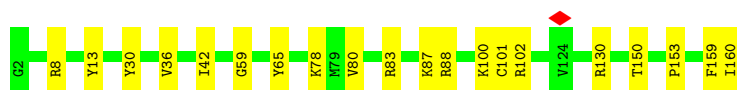


- Molecule 60: 60S ribosomal protein L20-A



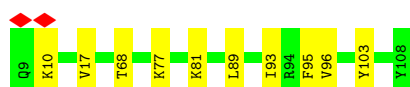
- Molecule 61: 60S ribosomal protein L21-A

Chain LV:  87% 13%



- Molecule 62: 60S ribosomal protein L22-A

Chain LW:  90% 10%



- Molecule 63: 60S ribosomal protein L23-A

Chain LX:  82% 18%



- Molecule 64: 60S ribosomal protein L24-A

Chain LY:  83% 17%



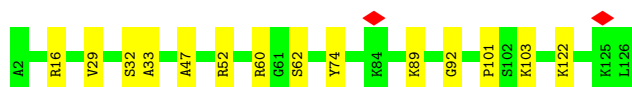
- Molecule 65: 60S ribosomal protein L25

Chain LZ:  92% 8%



- Molecule 66: 60S ribosomal protein L26-A

Chain La:  89% 11%

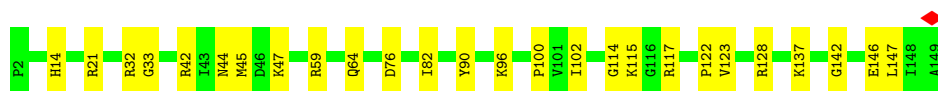
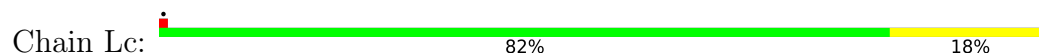


- Molecule 67: 60S ribosomal protein L27-A

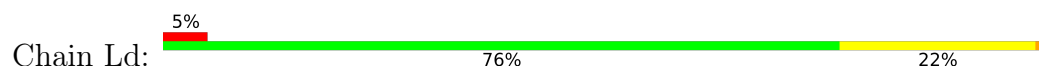
Chain Lb:  86% 14%



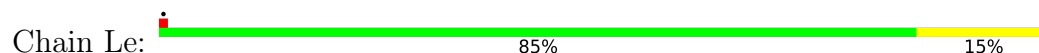
- Molecule 68: 60S ribosomal protein L28



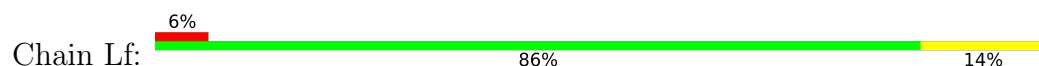
- Molecule 69: 60S ribosomal protein L29



- Molecule 70: 60S ribosomal protein L30



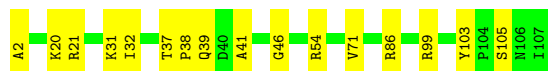
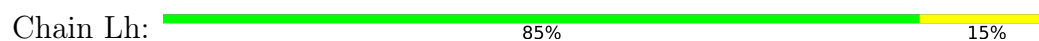
- Molecule 71: 60S ribosomal protein L31-A



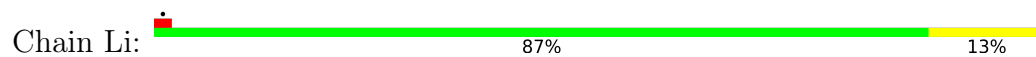
- Molecule 72: 60S ribosomal protein L32



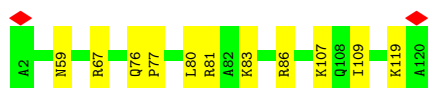
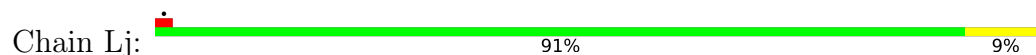
- Molecule 73: 60S ribosomal protein L33-A



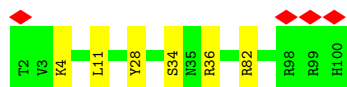
- Molecule 74: 60S ribosomal protein L34-A



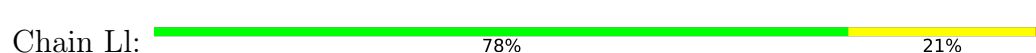
- Molecule 75: 60S ribosomal protein L35-A



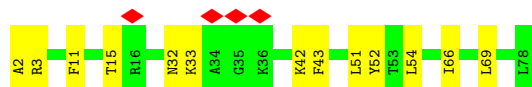
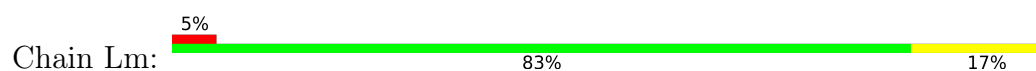
- Molecule 76: 60S ribosomal protein L36-A



- Molecule 77: 60S ribosomal protein L37-A



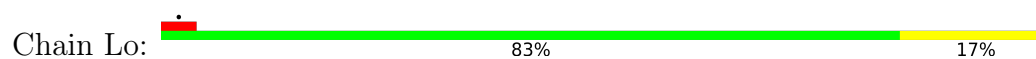
- Molecule 78: 60S ribosomal protein L38



- Molecule 79: 60S ribosomal protein L39



- Molecule 80: 60S ribosomal protein L40-A



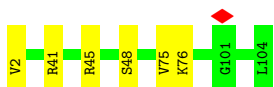
- Molecule 81: 60S ribosomal protein L41-A

Chain Lp:  92% 8%



- Molecule 82: 60S ribosomal protein L42-A

Chain Lq:  94% 6%



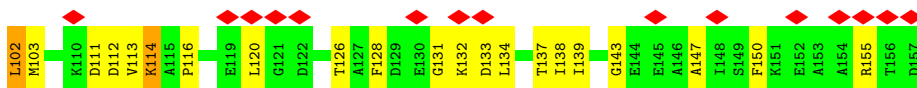
- Molecule 83: 60S ribosomal protein L43-A

Chain Lr:  79% 20%



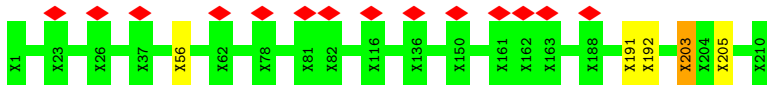
- Molecule 84: eiF5A

Chain Ls:  13% 65% 32%



- Molecule 85: L1 60S ribosomal protein

Chain Lt:  7% 98%



- Molecule 86: GCN1

Chain A:  71% 75% 21%





|       |       |       |       |
|-------|-------|-------|-------|
| A2409 | A2349 | A2287 | A2227 |
| A2410 | A2350 | A2288 | A2228 |
| A2411 | A2351 | A2289 | A2229 |
| A2412 | A2352 | A2290 | A2230 |
| A2413 | A2353 | A2291 | A2231 |
| A2414 | A2354 | A2292 | A2232 |
| A2415 | A2355 | A2293 | A2233 |
| A2416 | A2356 | A2294 | A2234 |
| A2417 | A2357 | A2295 | A2235 |
| A2418 | A2358 | A2296 | A2236 |
| A2419 | A2359 | A2297 | A2237 |
| A2420 | A2360 | A2298 | A2238 |
| A2421 | A2361 | A2299 | A2239 |
| A2422 | A2362 | A2300 | A2240 |
| A2423 | A2363 | A2301 | A2241 |
| A2424 | A2364 | A2302 | A2242 |
| A2425 | A2365 | A2303 | A2243 |
| A2426 | A2366 | A2304 | A2244 |
| A2427 | A2367 | A2305 | A2245 |
| A2428 | A2368 | A2306 | A2246 |
|       | A2369 | A2307 | A2247 |
|       | A2370 | A2308 | A2248 |
|       | A2371 | A2309 | A2249 |
|       | A2372 | A2310 | A2250 |
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|       | A2374 | A2312 | A2252 |
|       | A2375 | A2313 | A2253 |
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|       | A2378 | A2316 | A2256 |
|       | A2379 | A2317 | A2257 |
|       | A2380 | A2320 | A2258 |
|       | A2381 | A2321 | A2259 |
|       | A2382 | A2322 | A2260 |
|       | A2383 | A2323 | A2261 |
|       | A2384 | A2324 | A2262 |
|       | A2385 | A2325 | A2263 |
|       | A2386 | A2326 | A2264 |
|       | A2387 | A2327 | A2265 |
|       | A2388 | A2328 | A2266 |
|       | A2389 | A2329 | A2267 |
|       | A2390 | A2330 | A2268 |
|       | A2391 | A2331 | A2269 |
|       | A2392 | A2332 | A2270 |
|       | A2393 | A2333 | A2271 |
|       | A2394 | A2334 | A2272 |
|       | A2395 | A2335 | A2273 |
|       | A2396 | A2336 | A2274 |
|       | A2397 | A2337 | A2275 |
|       | A2398 | A2338 | A2276 |
|       | A2399 | A2339 | A2277 |
|       | A2400 | A2340 | A2278 |
|       | A2401 | A2341 | A2279 |
|       | A2402 | A2342 | A2280 |
|       | A2403 | A2343 | A2281 |
|       | A2404 | A2344 | A2282 |
|       | A2405 | A2345 | A2283 |
|       | A2406 | A2346 | A2284 |
|       | A2407 | A2347 | A2285 |
|       | A2408 | A2348 | A2286 |

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 30016                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 2.5                                     | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.512                                   | Depositor |
| Minimum map value                    | -0.389                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.008                                   | Depositor |
| Recommended contour level            | 0.03                                    | Depositor |
| Map size (Å)                         | 758.8, 758.8, 758.8                     | wwPDB     |
| Map dimensions                       | 700, 700, 700                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.084, 1.084, 1.084                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5CT

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   | S2    | 0.28         | 0/42211     | 0.59        | 14/65773 (0.0%) |
| 2   | SI    | 0.26         | 0/147       | 0.46        | 0/227           |
| 3   | SP    | 0.34         | 0/1644      | 0.79        | 0/2249          |
| 4   | SQ    | 0.37         | 0/1823      | 0.90        | 3/2447 (0.1%)   |
| 5   | SE    | 0.37         | 0/936       | 0.87        | 0/1259          |
| 6   | SR    | 0.38         | 0/1656      | 0.85        | 0/2251          |
| 7   | SA    | 0.33         | 0/1754      | 0.78        | 0/2361          |
| 8   | SS    | 0.38         | 0/2097      | 0.87        | 0/2823          |
| 9   | SB    | 0.36         | 0/1625      | 0.83        | 2/2197 (0.1%)   |
| 10  | ST    | 0.35         | 0/1839      | 0.85        | 0/2460          |
| 11  | SU    | 0.39         | 0/1498      | 0.88        | 0/2019          |
| 12  | SV    | 0.31         | 0/1501      | 0.78        | 0/2006          |
| 13  | SW    | 0.33         | 0/1504      | 0.83        | 1/2016 (0.0%)   |
| 14  | SC    | 0.37         | 0/769       | 0.85        | 0/1039          |
| 15  | SX    | 0.30         | 0/1168      | 0.75        | 0/1575          |
| 16  | SD    | 0.40         | 0/883       | 0.95        | 0/1199          |
| 17  | SY    | 0.35         | 0/1215      | 0.83        | 0/1638          |
| 18  | SZ    | 0.36         | 0/934       | 0.86        | 2/1257 (0.2%)   |
| 19  | SF    | 0.33         | 0/1125      | 0.84        | 0/1510          |
| 20  | SG    | 0.33         | 0/957       | 0.75        | 0/1283          |
| 21  | SH    | 0.34         | 0/1207      | 0.86        | 0/1623          |
| 22  | SI    | 0.36         | 0/1130      | 0.83        | 2/1517 (0.1%)   |
| 23  | SJ    | 0.34         | 0/807       | 0.78        | 0/1091          |
| 24  | Sa    | 0.29         | 0/682       | 0.78        | 1/921 (0.1%)    |
| 25  | Sb    | 0.38         | 0/1038      | 0.87        | 0/1395          |
| 26  | Sc    | 0.36         | 0/1139      | 0.86        | 2/1518 (0.1%)   |
| 27  | Sd    | 0.34         | 0/1046      | 0.80        | 0/1401          |
| 28  | SK    | 0.38         | 0/661       | 0.92        | 1/888 (0.1%)    |
| 29  | Se    | 0.32         | 0/778       | 0.81        | 0/1042          |
| 30  | Sf    | 0.29         | 0/620       | 0.82        | 0/838           |
| 31  | SM    | 0.32         | 0/452       | 0.83        | 0/600           |
| 32  | Sg    | 0.32         | 0/459       | 0.89        | 0/611           |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 33  | SN    | 0.33         | 0/567   | 0.89        | 1/764 (0.1%)     |
| 34  | SO    | 0.32         | 0/2436  | 0.84        | 0/3318           |
| 35  | SL    | 0.36         | 0/493   | 0.96        | 0/663            |
| 36  | Sm    | 0.32         | 0/1799  | 0.69        | 0/2801           |
| 37  | Sn    | 0.31         | 0/1796  | 0.62        | 0/2799           |
| 38  | So    | 0.25         | 0/2769  | 0.67        | 0/3736           |
| 40  | LA    | 0.28         | 0/76214 | 0.55        | 10/118821 (0.0%) |
| 41  | LB    | 0.25         | 0/2883  | 0.51        | 1/4491 (0.0%)    |
| 42  | LC    | 0.28         | 0/3746  | 0.55        | 0/5832           |
| 43  | LD    | 0.33         | 0/1933  | 0.79        | 0/2598           |
| 44  | LE    | 0.33         | 0/3146  | 0.78        | 1/4228 (0.0%)    |
| 45  | LF    | 0.34         | 0/2800  | 0.80        | 0/3790           |
| 46  | LG    | 0.33         | 0/2400  | 0.77        | 2/3239 (0.1%)    |
| 47  | LH    | 0.35         | 0/1329  | 0.81        | 1/1794 (0.1%)    |
| 48  | LI    | 0.35         | 0/1821  | 0.78        | 0/2451           |
| 49  | LJ    | 0.35         | 0/1836  | 0.79        | 0/2481           |
| 50  | LK    | 0.32         | 0/1529  | 0.77        | 0/2060           |
| 51  | LL    | 0.32         | 0/1801  | 0.80        | 5/2416 (0.2%)    |
| 52  | LM    | 0.35         | 0/1367  | 0.85        | 0/1834           |
| 53  | LN    | 0.32         | 0/1568  | 0.78        | 1/2106 (0.0%)    |
| 54  | LO    | 0.32         | 0/1068  | 0.77        | 0/1438           |
| 55  | LP    | 0.38         | 0/1757  | 0.80        | 0/2354           |
| 56  | LQ    | 0.37         | 0/1585  | 0.75        | 0/2128           |
| 57  | LR    | 0.32         | 0/1439  | 0.72        | 0/1938           |
| 58  | LS    | 0.32         | 0/1465  | 0.79        | 0/1965           |
| 59  | LT    | 0.30         | 0/1532  | 0.72        | 0/2043           |
| 60  | LU    | 0.32         | 0/1473  | 0.75        | 0/1980           |
| 61  | LV    | 0.32         | 0/1296  | 0.76        | 0/1739           |
| 62  | LW    | 0.34         | 0/812   | 0.77        | 0/1099           |
| 63  | LX    | 0.30         | 0/1018  | 0.71        | 0/1369           |
| 64  | LY    | 0.23         | 0/540   | 0.66        | 0/717            |
| 65  | LZ    | 0.31         | 0/979   | 0.79        | 0/1321           |
| 66  | La    | 0.28         | 0/995   | 0.73        | 0/1329           |
| 67  | Lb    | 0.29         | 0/1106  | 0.78        | 0/1485           |
| 68  | Lc    | 0.33         | 0/1200  | 0.78        | 0/1607           |
| 69  | Ld    | 0.31         | 0/473   | 0.79        | 0/629            |
| 70  | Le    | 0.30         | 0/745   | 0.76        | 0/1001           |
| 71  | Lf    | 0.34         | 0/890   | 0.81        | 0/1196           |
| 72  | Lg    | 0.30         | 0/1038  | 0.71        | 0/1390           |
| 73  | Lh    | 0.32         | 0/868   | 0.79        | 1/1168 (0.1%)    |
| 74  | Li    | 0.38         | 0/890   | 0.82        | 0/1189           |
| 75  | Lj    | 0.31         | 0/978   | 0.74        | 0/1301           |
| 76  | Lk    | 0.31         | 0/772   | 0.77        | 0/1026           |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 77  | Ll    | 0.43         | 0/660            | 0.94        | 0/875             |
| 78  | Lm    | 0.34         | 0/618            | 0.74        | 0/826             |
| 79  | Ln    | 0.32         | 0/443            | 0.81        | 0/588             |
| 80  | Lo    | 0.30         | 0/416            | 0.84        | 0/553             |
| 81  | Lp    | 0.37         | 0/230            | 0.87        | 0/296             |
| 82  | Lq    | 0.33         | 0/836            | 0.80        | 0/1104            |
| 83  | Lr    | 0.33         | 0/701            | 0.80        | 1/934 (0.1%)      |
| 84  | Ls    | 0.43         | 0/1142           | 1.26        | 18/1537 (1.2%)    |
| 86  | A     | 1.43         | 24/6015 (0.4%)   | 1.76        | 69/8386 (0.8%)    |
| All | All   | 0.38         | 24/227518 (0.0%) | 0.72        | 139/333767 (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 |
|-----|-------|---------------------|---------------------|
| 8   | SS    | 0                   | 1                   |
| 9   | SB    | 0                   | 2                   |
| 11  | SU    | 0                   | 1                   |
| 16  | SD    | 0                   | 1                   |
| 18  | SZ    | 0                   | 1                   |
| 19  | SF    | 0                   | 1                   |
| 22  | SI    | 0                   | 1                   |
| 25  | Sb    | 0                   | 1                   |
| 33  | SN    | 0                   | 1                   |
| 45  | LF    | 0                   | 3                   |
| 48  | LI    | 0                   | 1                   |
| 49  | LJ    | 0                   | 3                   |
| 58  | LS    | 0                   | 1                   |
| 68  | Lc    | 0                   | 2                   |
| 69  | Ld    | 0                   | 2                   |
| 70  | Le    | 0                   | 1                   |
| 71  | Lf    | 0                   | 1                   |
| 75  | Lj    | 0                   | 1                   |
| 84  | Ls    | 1                   | 2                   |
| 85  | Lt    | 0                   | 4                   |
| 86  | A     | 0                   | 12                  |
| All | All   | 1                   | 43                  |

All (24) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 86  | A     | 2351 | ALA  | N-CA  | 20.84 | 1.70        | 1.46     |
| 86  | A     | 1840 | ALA  | N-CA  | 20.80 | 1.70        | 1.46     |
| 86  | A     | 2040 | ALA  | N-CA  | 20.79 | 1.70        | 1.46     |
| 86  | A     | 2240 | ALA  | N-CA  | 20.75 | 1.70        | 1.46     |
| 86  | A     | 2300 | ALA  | N-CA  | 18.20 | 1.69        | 1.46     |
| 86  | A     | 2411 | ALA  | N-CA  | 18.19 | 1.69        | 1.46     |
| 86  | A     | 1900 | ALA  | N-CA  | 18.13 | 1.69        | 1.46     |
| 86  | A     | 1361 | PRO  | N-CA  | 18.05 | 1.70        | 1.47     |
| 86  | A     | 1421 | PRO  | N-CA  | 17.36 | 1.69        | 1.47     |
| 86  | A     | 1223 | PRO  | N-CA  | 17.22 | 1.69        | 1.47     |
| 86  | A     | 2239 | ALA  | C-N   | 10.06 | 1.46        | 1.33     |
| 86  | A     | 2350 | ALA  | C-N   | 10.03 | 1.45        | 1.33     |
| 86  | A     | 2039 | ALA  | C-N   | 10.02 | 1.45        | 1.33     |
| 86  | A     | 1839 | ALA  | C-N   | 9.99  | 1.45        | 1.33     |
| 86  | A     | 2410 | ALA  | C-N   | 8.55  | 1.45        | 1.33     |
| 86  | A     | 2299 | ALA  | C-N   | 8.54  | 1.45        | 1.33     |
| 86  | A     | 1899 | ALA  | C-N   | 8.52  | 1.45        | 1.33     |
| 86  | A     | 1616 | ALA  | C-O   | 8.42  | 1.34        | 1.24     |
| 86  | A     | 1163 | LEU  | C-O   | -6.70 | 1.15        | 1.24     |
| 86  | A     | 1181 | GLU  | C-N   | 6.65  | 1.49        | 1.33     |
| 86  | A     | 1162 | ALA  | C-O   | 6.22  | 1.31        | 1.24     |
| 86  | A     | 1256 | LEU  | C-N   | 5.59  | 1.41        | 1.33     |
| 86  | A     | 1360 | GLY  | C-N   | 5.11  | 1.45        | 1.33     |
| 86  | A     | 1420 | VAL  | C-N   | 5.06  | 1.45        | 1.33     |

All (139) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 86  | A     | 1181 | GLU  | CA-C-N | 20.41  | 145.35      | 119.84   |
| 86  | A     | 1181 | GLU  | C-N-CA | 20.41  | 145.35      | 119.84   |
| 86  | A     | 1420 | VAL  | CA-C-N | 17.02  | 141.12      | 119.84   |
| 86  | A     | 1420 | VAL  | C-N-CA | 17.02  | 141.12      | 119.84   |
| 86  | A     | 1360 | GLY  | CA-C-N | 15.08  | 138.70      | 119.84   |
| 86  | A     | 1360 | GLY  | C-N-CA | 15.08  | 138.70      | 119.84   |
| 86  | A     | 1340 | LYS  | O-C-N  | -14.67 | 103.08      | 122.59   |
| 86  | A     | 2019 | ALA  | O-C-N  | -14.62 | 103.15      | 122.59   |
| 86  | A     | 1819 | ALA  | O-C-N  | -14.59 | 103.18      | 122.59   |
| 86  | A     | 2330 | ALA  | O-C-N  | -14.57 | 103.21      | 122.59   |
| 86  | A     | 2039 | ALA  | CA-C-N | 12.86  | 138.67      | 120.79   |
| 86  | A     | 2039 | ALA  | C-N-CA | 12.86  | 138.67      | 120.79   |
| 86  | A     | 2350 | ALA  | CA-C-N | 12.84  | 138.64      | 120.79   |
| 86  | A     | 2350 | ALA  | C-N-CA | 12.84  | 138.64      | 120.79   |
| 86  | A     | 1839 | ALA  | CA-C-N | 12.84  | 138.64      | 120.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 86  | A     | 1839 | ALA  | C-N-CA      | 12.84 | 138.64      | 120.79   |
| 86  | A     | 2239 | ALA  | CA-C-N      | 12.84 | 138.64      | 120.79   |
| 86  | A     | 2239 | ALA  | C-N-CA      | 12.84 | 138.64      | 120.79   |
| 86  | A     | 2232 | ALA  | CA-C-N      | 11.15 | 139.26      | 122.65   |
| 86  | A     | 2232 | ALA  | C-N-CA      | 11.15 | 139.26      | 122.65   |
| 86  | A     | 2343 | ALA  | CA-C-N      | 11.14 | 139.25      | 122.65   |
| 86  | A     | 2343 | ALA  | C-N-CA      | 11.14 | 139.25      | 122.65   |
| 86  | A     | 1353 | GLN  | CA-C-N      | 11.14 | 139.25      | 122.65   |
| 86  | A     | 1353 | GLN  | C-N-CA      | 11.14 | 139.25      | 122.65   |
| 86  | A     | 2032 | ALA  | CA-C-N      | 11.14 | 139.24      | 122.65   |
| 86  | A     | 2032 | ALA  | C-N-CA      | 11.14 | 139.24      | 122.65   |
| 86  | A     | 1832 | ALA  | CA-C-N      | 11.12 | 139.22      | 122.65   |
| 86  | A     | 1832 | ALA  | C-N-CA      | 11.12 | 139.22      | 122.65   |
| 86  | A     | 1899 | ALA  | CA-C-N      | 10.25 | 141.11      | 121.54   |
| 86  | A     | 1899 | ALA  | C-N-CA      | 10.25 | 141.11      | 121.54   |
| 86  | A     | 2410 | ALA  | CA-C-N      | 10.22 | 141.06      | 121.54   |
| 86  | A     | 2410 | ALA  | C-N-CA      | 10.22 | 141.06      | 121.54   |
| 86  | A     | 2299 | ALA  | CA-C-N      | 10.20 | 141.03      | 121.54   |
| 86  | A     | 2299 | ALA  | C-N-CA      | 10.20 | 141.03      | 121.54   |
| 86  | A     | 2015 | ALA  | CA-C-N      | -9.00 | 109.50      | 122.19   |
| 86  | A     | 2015 | ALA  | C-N-CA      | -9.00 | 109.50      | 122.19   |
| 86  | A     | 1815 | ALA  | CA-C-N      | -8.98 | 109.52      | 122.19   |
| 86  | A     | 1815 | ALA  | C-N-CA      | -8.98 | 109.52      | 122.19   |
| 86  | A     | 2326 | ALA  | CA-C-N      | -8.97 | 109.53      | 122.19   |
| 86  | A     | 2326 | ALA  | C-N-CA      | -8.97 | 109.53      | 122.19   |
| 84  | Ls    | 132  | LYS  | N-CA-C      | 7.96  | 120.97      | 111.02   |
| 84  | Ls    | 111  | ASP  | CA-C-N      | 7.63  | 136.12      | 121.54   |
| 84  | Ls    | 111  | ASP  | C-N-CA      | 7.63  | 136.12      | 121.54   |
| 86  | A     | 1615 | ALA  | O-C-N       | -7.54 | 113.01      | 123.11   |
| 86  | A     | 1162 | ALA  | CA-C-N      | 7.33  | 135.53      | 121.54   |
| 86  | A     | 1162 | ALA  | C-N-CA      | 7.33  | 135.53      | 121.54   |
| 1   | S2    | 400  | A    | C2'-C3'-O3' | 6.79  | 119.69      | 109.50   |
| 86  | A     | 1690 | ALA  | CA-C-N      | 6.62  | 134.17      | 121.54   |
| 86  | A     | 1690 | ALA  | C-N-CA      | 6.62  | 134.17      | 121.54   |
| 86  | A     | 1319 | ILE  | CA-C-O      | -6.60 | 116.89      | 122.63   |
| 40  | LA    | 2541 | U    | P-O3'-C3'   | 6.57  | 130.06      | 120.20   |
| 86  | A     | 1629 | ALA  | N-CA-C      | -6.49 | 104.29      | 111.36   |
| 86  | A     | 1235 | ALA  | O-C-N       | 6.39  | 129.93      | 122.20   |
| 1   | S2    | 400  | A    | P-O3'-C3'   | 6.30  | 129.65      | 120.20   |
| 13  | SW    | 132  | ARG  | CA-CB-CG    | 6.26  | 126.63      | 114.10   |
| 86  | A     | 1805 | ALA  | N-CA-C      | -6.20 | 106.94      | 114.75   |
| 86  | A     | 1326 | LYS  | N-CA-C      | -6.18 | 106.96      | 114.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 86  | A     | 2205 | ALA  | N-CA-C      | -6.17 | 106.98      | 114.75   |
| 86  | A     | 2005 | ALA  | N-CA-C      | -6.16 | 106.99      | 114.75   |
| 40  | LA    | 1582 | C    | P-O3'-C3'   | 6.12  | 129.38      | 120.20   |
| 1   | S2    | 322  | G    | C2'-C3'-O3' | 6.07  | 118.61      | 109.50   |
| 86  | A     | 1704 | ALA  | CA-C-N      | -6.06 | 112.62      | 122.26   |
| 86  | A     | 1704 | ALA  | C-N-CA      | -6.06 | 112.62      | 122.26   |
| 44  | LE    | 291  | GLU  | CA-CB-CG    | 6.05  | 126.19      | 114.10   |
| 86  | A     | 1519 | ALA  | N-CA-C      | -5.99 | 105.83      | 113.02   |
| 86  | A     | 2219 | ALA  | N-CA-C      | 5.99  | 117.81      | 111.28   |
| 73  | Lh    | 86   | ARG  | CA-CB-CG    | 5.88  | 125.87      | 114.10   |
| 40  | LA    | 1716 | U    | P-O3'-C3'   | 5.86  | 128.99      | 120.20   |
| 86  | A     | 1239 | HIS  | CA-C-N      | -5.83 | 111.33      | 122.53   |
| 86  | A     | 1239 | HIS  | C-N-CA      | -5.83 | 111.33      | 122.53   |
| 1   | S2    | 1633 | A    | P-O3'-C3'   | 5.82  | 128.94      | 120.20   |
| 1   | S2    | 1256 | A    | P-O3'-C3'   | 5.82  | 128.92      | 120.20   |
| 4   | SQ    | 214  | LYS  | N-CA-C      | 5.73  | 117.94      | 110.43   |
| 40  | LA    | 2537 | U    | P-O3'-C3'   | 5.67  | 128.70      | 120.20   |
| 86  | A     | 1137 | PRO  | N-CA-C      | 5.67  | 124.15      | 112.47   |
| 24  | Sa    | 10   | GLU  | CA-CB-CG    | 5.65  | 125.41      | 114.10   |
| 33  | SN    | 136  | LYS  | CA-CB-CG    | 5.62  | 125.33      | 114.10   |
| 84  | Ls    | 143  | GLY  | N-CA-C      | 5.58  | 122.52      | 114.10   |
| 47  | LH    | 77   | ARG  | N-CA-CB     | 5.57  | 120.93      | 111.57   |
| 83  | Lr    | 85   | ARG  | CA-CB-CG    | 5.56  | 125.22      | 114.10   |
| 1   | S2    | 224  | C    | P-O3'-C3'   | 5.56  | 128.53      | 120.20   |
| 1   | S2    | 215  | A    | P-O3'-C3'   | 5.54  | 128.52      | 120.20   |
| 86  | A     | 1256 | LEU  | CA-C-N      | -5.51 | 111.02      | 121.54   |
| 86  | A     | 1256 | LEU  | C-N-CA      | -5.51 | 111.02      | 121.54   |
| 51  | LL    | 112  | GLN  | CA-C-N      | 5.50  | 132.05      | 121.54   |
| 51  | LL    | 112  | GLN  | C-N-CA      | 5.50  | 132.05      | 121.54   |
| 22  | SI    | 52   | GLY  | CA-C-N      | 5.50  | 132.04      | 121.54   |
| 22  | SI    | 52   | GLY  | C-N-CA      | 5.50  | 132.04      | 121.54   |
| 1   | S2    | 639  | U    | P-O3'-C3'   | 5.46  | 128.38      | 120.20   |
| 84  | Ls    | 103  | MET  | CB-CG-SD    | 5.45  | 129.05      | 112.70   |
| 84  | Ls    | 114  | LYS  | CA-CB-CG    | 5.40  | 124.90      | 114.10   |
| 40  | LA    | 2514 | U    | P-O3'-C3'   | 5.39  | 128.29      | 120.20   |
| 84  | Ls    | 113  | VAL  | N-CA-C      | 5.39  | 120.55      | 109.34   |
| 84  | Ls    | 120  | LEU  | CA-C-N      | 5.39  | 125.96      | 119.98   |
| 84  | Ls    | 120  | LEU  | C-N-CA      | 5.39  | 125.96      | 119.98   |
| 86  | A     | 1223 | PRO  | N-CA-C      | -5.37 | 101.42      | 112.47   |
| 40  | LA    | 1815 | U    | P-O3'-C3'   | 5.36  | 128.25      | 120.20   |
| 86  | A     | 1624 | ALA  | CA-C-N      | 5.35  | 127.45      | 120.28   |
| 86  | A     | 1624 | ALA  | C-N-CA      | 5.35  | 127.45      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 84  | Ls    | 7    | THR  | CA-C-N      | 5.34  | 131.74      | 121.54   |
| 84  | Ls    | 7    | THR  | C-N-CA      | 5.34  | 131.74      | 121.54   |
| 4   | SQ    | 214  | LYS  | CA-C-N      | 5.33  | 131.57      | 121.97   |
| 4   | SQ    | 214  | LYS  | C-N-CA      | 5.33  | 131.57      | 121.97   |
| 9   | SB    | 124  | LEU  | CA-C-N      | 5.33  | 131.72      | 121.54   |
| 9   | SB    | 124  | LEU  | C-N-CA      | 5.33  | 131.72      | 121.54   |
| 26  | Sc    | 4    | GLY  | CA-C-N      | 5.32  | 128.44      | 120.83   |
| 26  | Sc    | 4    | GLY  | C-N-CA      | 5.32  | 128.44      | 120.83   |
| 86  | A     | 1632 | ALA  | N-CA-C      | -5.31 | 105.57      | 111.36   |
| 40  | LA    | 1562 | C    | P-O3'-C3'   | 5.31  | 128.16      | 120.20   |
| 86  | A     | 1489 | ALA  | N-CA-C      | -5.29 | 105.43      | 111.14   |
| 1   | S2    | 77   | U    | P-O3'-C3'   | 5.28  | 128.12      | 120.20   |
| 40  | LA    | 763  | G    | P-O3'-C3'   | 5.25  | 128.07      | 120.20   |
| 18  | SZ    | 17   | ALA  | CA-C-N      | 5.24  | 131.56      | 121.54   |
| 18  | SZ    | 17   | ALA  | C-N-CA      | 5.24  | 131.56      | 121.54   |
| 40  | LA    | 1562 | C    | C4'-C3'-O3' | 5.22  | 117.22      | 109.40   |
| 86  | A     | 1226 | ARG  | N-CA-C      | -5.22 | 105.49      | 111.07   |
| 84  | Ls    | 131  | GLY  | CA-C-N      | 5.15  | 130.61      | 122.78   |
| 84  | Ls    | 131  | GLY  | C-N-CA      | 5.15  | 130.61      | 122.78   |
| 41  | LB    | 52   | G    | P-O3'-C3'   | 5.14  | 127.92      | 120.20   |
| 1   | S2    | 1273 | G    | P-O3'-C3'   | 5.11  | 127.86      | 120.20   |
| 1   | S2    | 322  | G    | P-O3'-C3'   | 5.11  | 127.86      | 120.20   |
| 86  | A     | 1659 | ALA  | N-CA-C      | -5.10 | 106.22      | 112.90   |
| 46  | LG    | 136  | GLU  | CA-C-N      | 5.10  | 131.28      | 121.54   |
| 46  | LG    | 136  | GLU  | C-N-CA      | 5.10  | 131.28      | 121.54   |
| 51  | LL    | 5    | PRO  | N-CA-C      | 5.10  | 119.49      | 111.38   |
| 51  | LL    | 212  | GLU  | CA-C-N      | 5.10  | 134.24      | 121.80   |
| 51  | LL    | 212  | GLU  | C-N-CA      | 5.10  | 134.24      | 121.80   |
| 1   | S2    | 1382 | A    | P-O3'-C3'   | 5.09  | 127.83      | 120.20   |
| 40  | LA    | 2112 | U    | P-O3'-C3'   | 5.08  | 127.82      | 120.20   |
| 84  | Ls    | 155  | ARG  | CA-C-N      | 5.06  | 129.37      | 122.34   |
| 84  | Ls    | 155  | ARG  | C-N-CA      | 5.06  | 129.37      | 122.34   |
| 28  | SK    | 77   | ARG  | NE-CZ-NH2   | 5.03  | 123.72      | 119.20   |
| 86  | A     | 1653 | ALA  | N-CA-C      | -5.02 | 106.32      | 112.90   |
| 1   | S2    | 139  | C    | P-O3'-C3'   | 5.01  | 127.72      | 120.20   |
| 84  | Ls    | 150  | PHE  | N-CA-CB     | -5.01 | 103.79      | 111.56   |
| 84  | Ls    | 126  | THR  | CA-C-N      | 5.01  | 127.49      | 120.28   |
| 84  | Ls    | 126  | THR  | C-N-CA      | 5.01  | 127.49      | 120.28   |
| 53  | LN    | 137  | GLN  | N-CA-C      | 5.00  | 117.36      | 110.35   |
| 1   | S2    | 1430 | U    | C2'-C3'-O3' | 5.00  | 121.20      | 113.70   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 84  | Ls    | 51  | 5CT  | C2   |

All (43) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 86  | A     | 1198 | SER  | Peptide   |
| 86  | A     | 1256 | LEU  | Mainchain |
| 86  | A     | 1340 | LYS  | Mainchain |
| 86  | A     | 1580 | ALA  | Peptide   |
| 86  | A     | 1615 | ALA  | Mainchain |
| 86  | A     | 1639 | ALA  | Peptide   |
| 86  | A     | 1705 | ALA  | Peptide   |
| 86  | A     | 1819 | ALA  | Mainchain |
| 86  | A     | 2019 | ALA  | Mainchain |
| 86  | A     | 2330 | ALA  | Mainchain |
| 86  | A     | 950  | ALA  | Mainchain |
| 86  | A     | 982  | ALA  | Peptide   |
| 45  | LF    | 13   | GLY  | Peptide   |
| 45  | LF    | 3    | ARG  | Peptide   |
| 45  | LF    | 318  | LEU  | Peptide   |
| 48  | LI    | 232  | ARG  | Peptide   |
| 49  | LJ    | 30   | THR  | Peptide   |
| 49  | LJ    | 76   | ALA  | Peptide   |
| 49  | LJ    | 77   | GLN  | Peptide   |
| 58  | LS    | 161  | LYS  | Peptide   |
| 68  | Lc    | 115  | LYS  | Peptide   |
| 68  | Lc    | 14   | HIS  | Peptide   |
| 69  | Ld    | 19   | ASN  | Peptide   |
| 69  | Ld    | 20   | GLY  | Peptide   |
| 70  | Le    | 47   | ASN  | Peptide   |
| 71  | Lf    | 7    | VAL  | Peptide   |
| 75  | Lj    | 83   | LYS  | Peptide   |
| 84  | Ls    | 112  | ASP  | Peptide   |
| 84  | Ls    | 97   | ASP  | Peptide   |
| 85  | Lt    | 191  | UNK  | Peptide   |
| 85  | Lt    | 192  | UNK  | Peptide   |
| 85  | Lt    | 203  | UNK  | Peptide   |
| 85  | Lt    | 56   | UNK  | Peptide   |
| 9   | SB    | 125  | THR  | Peptide   |
| 9   | SB    | 42   | LEU  | Peptide   |
| 16  | SD    | 108  | ARG  | Peptide   |
| 19  | SF    | 40   | GLU  | Peptide   |
| 22  | SI    | 120  | GLY  | Peptide   |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 33  | SN    | 147 | VAL  | Peptide |
| 8   | SS    | 193 | GLY  | Peptide |
| 11  | SU    | 64  | VAL  | Peptide |
| 18  | SZ    | 90  | ARG  | Peptide |
| 25  | Sb    | 54  | ASP  | Peptide |

## 5.2 Too-close contacts [i](#)

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   | S2    | 37739 | 0        | 18988    | 295     | 0            |
| 2   | SI    | 131   | 0        | 66       | 0       | 0            |
| 3   | SP    | 1603  | 0        | 1610     | 19      | 0            |
| 4   | SQ    | 1798  | 0        | 1890     | 26      | 0            |
| 5   | SE    | 916   | 0        | 941      | 17      | 0            |
| 6   | SR    | 1626  | 0        | 1715     | 24      | 0            |
| 7   | SA    | 1729  | 0        | 1812     | 17      | 0            |
| 8   | SS    | 2056  | 0        | 2140     | 33      | 0            |
| 9   | SB    | 1605  | 0        | 1669     | 20      | 0            |
| 10  | ST    | 1815  | 0        | 1894     | 25      | 0            |
| 11  | SU    | 1473  | 0        | 1555     | 20      | 0            |
| 12  | SV    | 1476  | 0        | 1501     | 37      | 0            |
| 13  | SW    | 1479  | 0        | 1556     | 26      | 0            |
| 14  | SC    | 752   | 0        | 719      | 9       | 0            |
| 15  | SX    | 1142  | 0        | 1209     | 13      | 0            |
| 16  | SD    | 875   | 0        | 878      | 12      | 0            |
| 17  | SY    | 1192  | 0        | 1255     | 14      | 0            |
| 18  | SZ    | 923   | 0        | 948      | 20      | 0            |
| 19  | SF    | 1105  | 0        | 1166     | 15      | 0            |
| 20  | SG    | 948   | 0        | 990      | 13      | 0            |
| 21  | SH    | 1188  | 0        | 1218     | 25      | 0            |
| 22  | SI    | 1112  | 0        | 1122     | 67      | 0            |
| 23  | SJ    | 797   | 0        | 863      | 13      | 0            |
| 24  | Sa    | 673   | 0        | 662      | 10      | 0            |
| 25  | Sb    | 1021  | 0        | 1060     | 17      | 0            |
| 26  | Sc    | 1121  | 0        | 1196     | 17      | 0            |
| 27  | Sd    | 1032  | 0        | 1044     | 18      | 0            |
| 28  | SK    | 651   | 0        | 682      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | Se    | 765   | 0        | 814      | 16      | 0            |
| 30  | Sf    | 610   | 0        | 633      | 10      | 0            |
| 31  | SM    | 442   | 0        | 432      | 5       | 0            |
| 32  | Sg    | 451   | 0        | 494      | 6       | 0            |
| 33  | SN    | 556   | 0        | 552      | 7       | 0            |
| 34  | SO    | 2383  | 0        | 2332     | 30      | 0            |
| 35  | SL    | 491   | 0        | 524      | 3       | 0            |
| 36  | Sm    | 1611  | 0        | 817      | 5       | 0            |
| 37  | Sn    | 1606  | 0        | 816      | 8       | 0            |
| 38  | So    | 2729  | 0        | 2780     | 33      | 0            |
| 39  | Sp    | 240   | 0        | 50       | 0       | 0            |
| 40  | LA    | 68091 | 0        | 34217    | 406     | 0            |
| 41  | LB    | 2579  | 0        | 1304     | 19      | 0            |
| 42  | LC    | 3353  | 0        | 1695     | 32      | 0            |
| 43  | LD    | 1899  | 0        | 1957     | 29      | 0            |
| 44  | LE    | 3075  | 0        | 3142     | 48      | 0            |
| 45  | LF    | 2748  | 0        | 2859     | 39      | 0            |
| 46  | LG    | 2351  | 0        | 2294     | 26      | 0            |
| 47  | LH    | 1307  | 0        | 1377     | 22      | 0            |
| 48  | LI    | 1784  | 0        | 1862     | 15      | 0            |
| 49  | LJ    | 1804  | 0        | 1877     | 32      | 0            |
| 50  | LK    | 1508  | 0        | 1572     | 12      | 0            |
| 51  | LL    | 1764  | 0        | 1804     | 22      | 0            |
| 52  | LM    | 1346  | 0        | 1370     | 23      | 0            |
| 53  | LN    | 1543  | 0        | 1608     | 20      | 0            |
| 54  | LO    | 1053  | 0        | 1149     | 14      | 0            |
| 55  | LP    | 1720  | 0        | 1779     | 36      | 0            |
| 56  | LQ    | 1555  | 0        | 1659     | 13      | 0            |
| 57  | LR    | 1416  | 0        | 1433     | 15      | 0            |
| 58  | LS    | 1441  | 0        | 1543     | 17      | 0            |
| 59  | LT    | 1515  | 0        | 1606     | 14      | 0            |
| 60  | LU    | 1437  | 0        | 1475     | 13      | 0            |
| 61  | LV    | 1272  | 0        | 1312     | 17      | 0            |
| 62  | LW    | 796   | 0        | 812      | 6       | 0            |
| 63  | LX    | 1003  | 0        | 1048     | 16      | 0            |
| 64  | LY    | 528   | 0        | 546      | 9       | 0            |
| 65  | LZ    | 964   | 0        | 1025     | 7       | 0            |
| 66  | La    | 984   | 0        | 1075     | 10      | 0            |
| 67  | Lb    | 1080  | 0        | 1122     | 11      | 0            |
| 68  | Lc    | 1169  | 0        | 1211     | 24      | 0            |
| 69  | Ld    | 462   | 0        | 491      | 11      | 0            |
| 70  | Le    | 737   | 0        | 792      | 7       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 71  | Lf    | 876    | 0        | 912      | 7       | 0            |
| 72  | Lg    | 1017   | 0        | 1081     | 12      | 0            |
| 73  | Lh    | 850    | 0        | 880      | 10      | 0            |
| 74  | Li    | 880    | 0        | 945      | 16      | 0            |
| 75  | Lj    | 969    | 0        | 1078     | 7       | 0            |
| 76  | Lk    | 766    | 0        | 844      | 5       | 0            |
| 77  | Ll    | 645    | 0        | 649      | 14      | 0            |
| 78  | Lm    | 612    | 0        | 682      | 8       | 0            |
| 79  | Ln    | 436    | 0        | 475      | 15      | 0            |
| 80  | Lo    | 410    | 0        | 446      | 7       | 0            |
| 81  | Lp    | 229    | 0        | 273      | 2       | 0            |
| 82  | Lq    | 824    | 0        | 892      | 6       | 0            |
| 83  | Lr    | 694    | 0        | 738      | 17      | 0            |
| 84  | Ls    | 1143   | 0        | 1104     | 25      | 0            |
| 85  | Lt    | 1050   | 0        | 230      | 1       | 0            |
| 86  | A     | 6029   | 0        | 5195     | 439     | 0            |
| All | All   | 213576 | 0        | 158033   | 1993    | 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 6.

All (1993) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:SI:138:GLN:HG2  | 86:A:1303:GLU:CA  | 1.24                     | 1.55              |
| 86:A:2240:ALA:N    | 86:A:2240:ALA:CA  | 1.70                     | 1.54              |
| 86:A:2411:ALA:N    | 86:A:2411:ALA:CA  | 1.69                     | 1.54              |
| 86:A:1421:PRO:N    | 86:A:1421:PRO:CA  | 1.69                     | 1.53              |
| 86:A:2040:ALA:N    | 86:A:2040:ALA:CA  | 1.70                     | 1.53              |
| 86:A:2300:ALA:N    | 86:A:2300:ALA:CA  | 1.69                     | 1.53              |
| 86:A:1840:ALA:N    | 86:A:1840:ALA:CA  | 1.70                     | 1.53              |
| 22:SI:138:GLN:HG2  | 86:A:1303:GLU:CB  | 1.09                     | 1.52              |
| 86:A:1223:PRO:N    | 86:A:1223:PRO:CA  | 1.69                     | 1.51              |
| 86:A:1900:ALA:N    | 86:A:1900:ALA:CA  | 1.69                     | 1.51              |
| 86:A:2351:ALA:N    | 86:A:2351:ALA:CA  | 1.70                     | 1.51              |
| 86:A:1361:PRO:N    | 86:A:1361:PRO:CA  | 1.70                     | 1.49              |
| 86:A:987:ALA:HB1   | 86:A:988:ALA:N    | 1.30                     | 1.45              |
| 22:SI:138:GLN:CG   | 86:A:1303:GLU:CB  | 1.93                     | 1.45              |
| 22:SI:138:GLN:HE21 | 86:A:1302:LYS:C   | 1.22                     | 1.43              |
| 22:SI:24:ARG:NE    | 86:A:1338:PRO:CB  | 1.83                     | 1.40              |
| 86:A:2294:ALA:CB   | 86:A:2306:ALA:HB1 | 1.57                     | 1.34              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 86:A:2094:ALA:CB  | 86:A:2106:ALA:HB1 | 1.57                     | 1.34              |
| 86:A:1241:THR:CB  | 86:A:1242:GLY:N   | 1.88                     | 1.34              |
| 86:A:1894:ALA:CB  | 86:A:1906:ALA:HB1 | 1.57                     | 1.33              |
| 86:A:1415:ALA:CB  | 86:A:1427:ALA:HB1 | 1.59                     | 1.32              |
| 22:SI:138:GLN:CG  | 86:A:1303:GLU:CA  | 2.06                     | 1.32              |
| 86:A:2405:ALA:CB  | 86:A:2417:ALA:HB1 | 1.57                     | 1.32              |
| 86:A:1668:ALA:O   | 86:A:1672:ALA:HB2 | 1.14                     | 1.30              |
| 22:SI:24:ARG:CG   | 86:A:1338:PRO:CB  | 2.12                     | 1.27              |
| 22:SI:21:PHE:CZ   | 86:A:1299:ASP:HA  | 1.69                     | 1.27              |
| 22:SI:24:ARG:HG2  | 86:A:1338:PRO:CB  | 1.65                     | 1.25              |
| 86:A:1428:ALA:CB  | 86:A:1461:ALA:HA  | 1.70                     | 1.21              |
| 86:A:1221:ALA:HB1 | 86:A:1222:VAL:N   | 1.58                     | 1.19              |
| 86:A:2104:ALA:CB  | 86:A:2215:ALA:HB2 | 1.72                     | 1.19              |
| 22:SI:138:GLN:CG  | 86:A:1303:GLU:N   | 2.06                     | 1.18              |
| 86:A:2094:ALA:HB1 | 86:A:2106:ALA:HB1 | 1.24                     | 1.17              |
| 86:A:1241:THR:CB  | 86:A:1242:GLY:CA  | 2.22                     | 1.17              |
| 86:A:965:ALA:O    | 86:A:969:ALA:CB   | 1.93                     | 1.16              |
| 83:Lr:53:GLY:HA2  | 83:Lr:66:GLY:O    | 1.43                     | 1.15              |
| 86:A:1894:ALA:HB1 | 86:A:1906:ALA:HB1 | 1.24                     | 1.15              |
| 86:A:1668:ALA:O   | 86:A:1672:ALA:CB  | 1.95                     | 1.15              |
| 83:Lr:53:GLY:CA   | 83:Lr:66:GLY:O    | 1.95                     | 1.14              |
| 86:A:1415:ALA:HB1 | 86:A:1427:ALA:HB1 | 1.24                     | 1.14              |
| 22:SI:138:GLN:NE2 | 86:A:1302:LYS:C   | 2.06                     | 1.13              |
| 86:A:2100:ALA:HA  | 86:A:2216:ALA:N   | 1.26                     | 1.13              |
| 86:A:1482:ALA:HB1 | 86:A:1493:ALA:HB1 | 1.25                     | 1.11              |
| 22:SI:24:ARG:CD   | 86:A:1338:PRO:CB  | 2.26                     | 1.11              |
| 86:A:987:ALA:CB   | 86:A:988:ALA:N    | 2.13                     | 1.11              |
| 86:A:1221:ALA:C   | 86:A:1222:VAL:N   | 2.08                     | 1.11              |
| 86:A:2405:ALA:HB1 | 86:A:2417:ALA:HB1 | 1.24                     | 1.10              |
| 86:A:2294:ALA:HB1 | 86:A:2306:ALA:HB1 | 1.24                     | 1.08              |
| 22:SI:21:PHE:HZ   | 86:A:1299:ASP:HA  | 0.94                     | 1.08              |
| 86:A:1241:THR:CB  | 86:A:1242:GLY:HA2 | 1.82                     | 1.08              |
| 86:A:1705:ALA:HB1 | 86:A:1815:ALA:O   | 1.51                     | 1.08              |
| 86:A:2314:ALA:CB  | 86:A:2321:ALA:HB3 | 1.82                     | 1.08              |
| 86:A:1523:ALA:H   | 86:A:1527:ALA:HB2 | 0.90                     | 1.06              |
| 64:LY:4:GLU:O     | 64:LY:12:LYS:HA   | 1.51                     | 1.06              |
| 86:A:2321:ALA:O   | 86:A:2325:ALA:HB2 | 1.56                     | 1.06              |
| 86:A:2314:ALA:HB1 | 86:A:2321:ALA:HB3 | 1.12                     | 1.05              |
| 86:A:1221:ALA:CB  | 86:A:1222:VAL:N   | 2.18                     | 1.05              |
| 86:A:1487:ALA:O   | 86:A:1491:ALA:N   | 1.88                     | 1.05              |
| 86:A:2010:ALA:O   | 86:A:2014:ALA:HB2 | 1.56                     | 1.05              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 86:A:2104:ALA:HB2  | 86:A:2215:ALA:HB2 | 1.12                     | 1.05              |
| 86:A:2325:ALA:O    | 86:A:2326:ALA:HB2 | 1.55                     | 1.05              |
| 86:A:1810:ALA:O    | 86:A:1814:ALA:HB2 | 1.56                     | 1.05              |
| 86:A:948:ALA:HB3   | 86:A:983:ALA:HB1  | 1.36                     | 1.04              |
| 86:A:2209:ALA:O    | 86:A:2213:ALA:CB  | 2.06                     | 1.03              |
| 86:A:1428:ALA:HB2  | 86:A:1461:ALA:HA  | 1.34                     | 1.02              |
| 86:A:2209:ALA:O    | 86:A:2213:ALA:N   | 1.91                     | 1.02              |
| 86:A:1894:ALA:HB2  | 86:A:1906:ALA:HB1 | 1.40                     | 1.02              |
| 22:SI:138:GLN:HE21 | 86:A:1303:GLU:N   | 1.56                     | 1.01              |
| 86:A:2094:ALA:HB2  | 86:A:2106:ALA:HB1 | 1.40                     | 1.01              |
| 86:A:2100:ALA:CA   | 86:A:2216:ALA:N   | 2.23                     | 1.01              |
| 86:A:2294:ALA:HB2  | 86:A:2306:ALA:HB1 | 1.41                     | 1.01              |
| 86:A:2405:ALA:HB2  | 86:A:2417:ALA:HB1 | 1.40                     | 1.01              |
| 4:SQ:136:ARG:O     | 4:SQ:215:VAL:HA   | 1.61                     | 1.00              |
| 86:A:1523:ALA:N    | 86:A:1527:ALA:HB2 | 1.75                     | 1.00              |
| 86:A:2014:ALA:O    | 86:A:2015:ALA:HB2 | 1.55                     | 1.00              |
| 21:SH:51:ASP:HB3   | 86:A:1378:SER:O   | 1.62                     | 1.00              |
| 86:A:1814:ALA:O    | 86:A:1815:ALA:HB2 | 1.55                     | 0.99              |
| 86:A:1162:ALA:O    | 86:A:1166:PHE:CB  | 2.10                     | 0.99              |
| 86:A:2104:ALA:HB2  | 86:A:2215:ALA:CB  | 1.93                     | 0.99              |
| 40:LA:2844:C:H42   | 40:LA:2898:G:H22  | 1.10                     | 0.99              |
| 86:A:1482:ALA:CB   | 86:A:1493:ALA:HB1 | 1.91                     | 0.99              |
| 86:A:2325:ALA:O    | 86:A:2326:ALA:CB  | 2.12                     | 0.97              |
| 1:S2:395:U:H3      | 1:S2:399:A:H62    | 1.00                     | 0.97              |
| 22:SI:24:ARG:HE    | 86:A:1338:PRO:CB  | 1.64                     | 0.97              |
| 86:A:2014:ALA:O    | 86:A:2015:ALA:CB  | 2.12                     | 0.96              |
| 40:LA:2448:G:H1    | 40:LA:2498:U:H3   | 1.03                     | 0.96              |
| 86:A:1814:ALA:O    | 86:A:1815:ALA:CB  | 2.12                     | 0.96              |
| 86:A:1415:ALA:HB2  | 86:A:1427:ALA:HB1 | 1.43                     | 0.96              |
| 40:LA:3232:G:H1    | 40:LA:3255:U:H3   | 1.05                     | 0.95              |
| 86:A:1485:ALA:O    | 86:A:1490:ALA:HB1 | 1.65                     | 0.95              |
| 22:SI:138:GLN:HG2  | 86:A:1303:GLU:HA  | 1.49                     | 0.95              |
| 86:A:1523:ALA:H    | 86:A:1527:ALA:CB  | 1.80                     | 0.95              |
| 22:SI:138:GLN:HG3  | 86:A:1303:GLU:N   | 1.77                     | 0.95              |
| 86:A:2373:ALA:HB2  | 86:A:2413:ALA:HB1 | 1.49                     | 0.94              |
| 86:A:2062:ALA:HB2  | 86:A:2102:ALA:HB1 | 1.49                     | 0.94              |
| 22:SI:138:GLN:CB   | 86:A:1303:GLU:CB  | 2.46                     | 0.94              |
| 86:A:1458:ALA:HB3  | 86:A:1461:ALA:HB3 | 1.49                     | 0.94              |
| 14:SC:23:ALA:O     | 14:SC:64:TYR:HB2  | 1.67                     | 0.94              |
| 40:LA:2844:C:H42   | 40:LA:2898:G:N2   | 1.65                     | 0.94              |
| 86:A:1675:ALA:HB1  | 86:A:1714:ALA:HB2 | 1.45                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 86:A:1894:ALA:HB1 | 86:A:1906:ALA:CB  | 1.98                     | 0.94              |
| 86:A:2094:ALA:HB1 | 86:A:2106:ALA:CB  | 1.97                     | 0.93              |
| 86:A:2294:ALA:HB1 | 86:A:2306:ALA:CB  | 1.98                     | 0.93              |
| 86:A:2262:ALA:HB2 | 86:A:2302:ALA:HB1 | 1.49                     | 0.93              |
| 22:SI:138:GLN:HG3 | 86:A:1303:GLU:H   | 1.29                     | 0.93              |
| 86:A:2405:ALA:HB1 | 86:A:2417:ALA:CB  | 1.98                     | 0.93              |
| 86:A:1415:ALA:HB1 | 86:A:1427:ALA:CB  | 1.99                     | 0.93              |
| 86:A:2100:ALA:HA  | 86:A:2216:ALA:H   | 1.30                     | 0.93              |
| 22:SI:21:PHE:HZ   | 86:A:1299:ASP:CA  | 1.82                     | 0.92              |
| 86:A:927:ALA:HB3  | 86:A:933:ALA:CB   | 1.99                     | 0.92              |
| 86:A:1636:ALA:CB  | 86:A:1674:ALA:HB1 | 2.00                     | 0.92              |
| 86:A:1463:ALA:HB2 | 86:A:1499:ALA:HB1 | 1.50                     | 0.91              |
| 86:A:1862:ALA:HB2 | 86:A:1902:ALA:HB1 | 1.49                     | 0.91              |
| 22:SI:25:GLN:HG3  | 86:A:1298:ASN:CB  | 2.00                     | 0.91              |
| 86:A:965:ALA:O    | 86:A:969:ALA:N    | 2.03                     | 0.90              |
| 86:A:2314:ALA:HB1 | 86:A:2321:ALA:CB  | 1.98                     | 0.90              |
| 86:A:2100:ALA:H   | 86:A:2216:ALA:HA  | 1.34                     | 0.90              |
| 86:A:965:ALA:O    | 86:A:969:ALA:HB3  | 1.67                     | 0.90              |
| 22:SI:21:PHE:CZ   | 86:A:1299:ASP:CA  | 2.55                     | 0.89              |
| 1:S2:1229:G:H21   | 1:S2:1256:A:H62   | 1.12                     | 0.89              |
| 86:A:1523:ALA:O   | 86:A:1527:ALA:HB3 | 1.71                     | 0.89              |
| 86:A:1458:ALA:HB3 | 86:A:1461:ALA:CB  | 2.02                     | 0.88              |
| 83:Lr:53:GLY:HA3  | 83:Lr:66:GLY:O    | 1.74                     | 0.88              |
| 22:SI:138:GLN:NE2 | 86:A:1303:GLU:N   | 2.21                     | 0.87              |
| 86:A:1428:ALA:HB1 | 86:A:1461:ALA:HA  | 1.54                     | 0.87              |
| 22:SI:138:GLN:HG2 | 86:A:1303:GLU:N   | 1.83                     | 0.86              |
| 86:A:1637:ALA:H   | 86:A:1676:ALA:HB3 | 1.40                     | 0.86              |
| 86:A:2211:ALA:O   | 86:A:2215:ALA:HB2 | 1.74                     | 0.86              |
| 1:S2:1229:G:H21   | 1:S2:1256:A:N6    | 1.71                     | 0.86              |
| 86:A:1523:ALA:HB3 | 86:A:1527:ALA:H   | 1.41                     | 0.85              |
| 22:SI:138:GLN:OE1 | 86:A:1300:SER:CB  | 2.24                     | 0.85              |
| 86:A:965:ALA:O    | 86:A:969:ALA:HB2  | 1.76                     | 0.85              |
| 1:S2:1187:U:H3    | 1:S2:1198:G:H1    | 1.21                     | 0.85              |
| 86:A:1862:ALA:HB2 | 86:A:1902:ALA:CB  | 2.07                     | 0.85              |
| 86:A:1331:LEU:O   | 86:A:1335:ILE:CB  | 2.25                     | 0.84              |
| 86:A:2262:ALA:HB2 | 86:A:2302:ALA:CB  | 2.07                     | 0.84              |
| 86:A:1487:ALA:O   | 86:A:1491:ALA:CB  | 2.25                     | 0.84              |
| 40:LA:2844:C:N4   | 40:LA:2898:G:H22  | 1.73                     | 0.84              |
| 86:A:2062:ALA:HB2 | 86:A:2102:ALA:CB  | 2.07                     | 0.83              |
| 86:A:2373:ALA:HB2 | 86:A:2413:ALA:CB  | 2.07                     | 0.83              |
| 86:A:2209:ALA:O   | 86:A:2213:ALA:HB2 | 1.76                     | 0.83              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:LA:3222:U:H3    | 40:LA:3263:G:H1   | 1.23                     | 0.83              |
| 86:A:927:ALA:HB3   | 86:A:933:ALA:HB3  | 1.61                     | 0.83              |
| 86:A:965:ALA:H     | 86:A:969:ALA:HB2  | 1.41                     | 0.82              |
| 86:A:1482:ALA:HB1  | 86:A:1493:ALA:CB  | 2.08                     | 0.82              |
| 86:A:1637:ALA:H    | 86:A:1676:ALA:CB  | 1.92                     | 0.82              |
| 22:SI:138:GLN:HE22 | 86:A:1300:SER:CB  | 1.93                     | 0.82              |
| 86:A:1432:GLY:CA   | 86:A:1468:ALA:HB2 | 2.09                     | 0.82              |
| 86:A:2097:ALA:HB1  | 86:A:2103:ALA:CB  | 2.10                     | 0.81              |
| 22:SI:138:GLN:HE22 | 86:A:1300:SER:CA  | 1.93                     | 0.81              |
| 86:A:1636:ALA:HB2  | 86:A:1677:ALA:HB2 | 1.60                     | 0.81              |
| 86:A:1482:ALA:CA   | 86:A:1493:ALA:HB1 | 2.10                     | 0.81              |
| 1:S2:1229:G:N2     | 1:S2:1256:A:H62   | 1.78                     | 0.81              |
| 52:LM:165:GLN:HB3  | 86:A:1601:ALA:CB  | 2.11                     | 0.80              |
| 86:A:1221:ALA:CA   | 86:A:1222:VAL:N   | 2.44                     | 0.80              |
| 86:A:1260:ALA:O    | 86:A:1264:LYS:N   | 2.13                     | 0.80              |
| 86:A:927:ALA:HB3   | 86:A:933:ALA:H    | 1.46                     | 0.80              |
| 86:A:2094:ALA:CB   | 86:A:2106:ALA:CB  | 2.52                     | 0.80              |
| 86:A:1293:ILE:CB   | 86:A:1313:LYS:CB  | 2.60                     | 0.79              |
| 86:A:2211:ALA:O    | 86:A:2215:ALA:CB  | 2.30                     | 0.79              |
| 86:A:2349:ALA:O    | 86:A:2350:ALA:CB  | 2.31                     | 0.79              |
| 86:A:1599:ALA:HB2  | 86:A:1604:ALA:HB2 | 1.64                     | 0.79              |
| 86:A:1217:ASN:HA   | 86:A:1230:ALA:HB2 | 1.63                     | 0.79              |
| 86:A:1537:ALA:O    | 86:A:1539:ALA:N   | 2.16                     | 0.79              |
| 86:A:1838:ALA:O    | 86:A:1839:ALA:HB2 | 1.83                     | 0.78              |
| 86:A:1485:ALA:C    | 86:A:1490:ALA:HB1 | 2.08                     | 0.78              |
| 86:A:1216:LYS:O    | 86:A:1230:ALA:N   | 2.15                     | 0.78              |
| 1:S2:415:C:O2      | 1:S2:418:G:N1     | 2.17                     | 0.78              |
| 86:A:1838:ALA:O    | 86:A:1839:ALA:CB  | 2.31                     | 0.78              |
| 86:A:1636:ALA:HB3  | 86:A:1674:ALA:HB1 | 1.65                     | 0.78              |
| 86:A:2038:ALA:O    | 86:A:2039:ALA:HB2 | 1.83                     | 0.78              |
| 86:A:2038:ALA:O    | 86:A:2039:ALA:CB  | 2.31                     | 0.78              |
| 86:A:2238:ALA:O    | 86:A:2239:ALA:CB  | 2.31                     | 0.78              |
| 86:A:2349:ALA:O    | 86:A:2350:ALA:HB2 | 1.83                     | 0.77              |
| 86:A:1428:ALA:HB1  | 86:A:1464:ALA:HB3 | 1.66                     | 0.77              |
| 86:A:1523:ALA:HB3  | 86:A:1527:ALA:N   | 1.99                     | 0.77              |
| 52:LM:168:ASP:OD2  | 86:A:1562:ALA:HA  | 1.84                     | 0.77              |
| 86:A:1810:ALA:O    | 86:A:1814:ALA:CB  | 2.32                     | 0.77              |
| 86:A:2100:ALA:N    | 86:A:2216:ALA:HA  | 1.98                     | 0.77              |
| 1:S2:1502:G:N7     | 22:SI:102:ARG:NH2 | 2.34                     | 0.76              |
| 86:A:2238:ALA:O    | 86:A:2239:ALA:HB2 | 1.83                     | 0.76              |
| 86:A:2321:ALA:O    | 86:A:2325:ALA:CB  | 2.32                     | 0.76              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:LC:63:G:H1     | 42:LC:97:A:H61     | 1.32                     | 0.76              |
| 86:A:2010:ALA:O   | 86:A:2014:ALA:CB   | 2.32                     | 0.76              |
| 86:A:1223:PRO:N   | 86:A:1223:PRO:CB   | 2.49                     | 0.76              |
| 86:A:1487:ALA:O   | 86:A:1491:ALA:HB2  | 1.86                     | 0.75              |
| 52:LM:165:GLN:HB2 | 86:A:1601:ALA:HB3  | 1.67                     | 0.75              |
| 52:LM:165:GLN:CB  | 86:A:1601:ALA:HB3  | 2.17                     | 0.74              |
| 22:SI:138:GLN:CD  | 86:A:1303:GLU:HA   | 2.12                     | 0.74              |
| 86:A:1705:ALA:O   | 86:A:1815:ALA:HB1  | 1.88                     | 0.74              |
| 86:A:2097:ALA:HB1 | 86:A:2103:ALA:HB1  | 1.68                     | 0.74              |
| 86:A:920:ALA:O    | 86:A:924:ALA:HB3   | 1.87                     | 0.74              |
| 86:A:1589:ALA:HB1 | 86:A:1627:ALA:HB2  | 1.69                     | 0.74              |
| 86:A:1675:ALA:HB1 | 86:A:1714:ALA:CB   | 2.17                     | 0.74              |
| 86:A:1894:ALA:CB  | 86:A:1906:ALA:CB   | 2.52                     | 0.74              |
| 86:A:948:ALA:HB3  | 86:A:983:ALA:CB    | 2.15                     | 0.73              |
| 86:A:1421:PRO:N   | 86:A:1421:PRO:CB   | 2.51                     | 0.73              |
| 86:A:1705:ALA:C   | 86:A:1815:ALA:HB1  | 2.13                     | 0.73              |
| 86:A:1488:ALA:HA  | 86:A:1491:ALA:HB3  | 1.71                     | 0.73              |
| 86:A:1537:ALA:C   | 86:A:1539:ALA:H    | 1.97                     | 0.73              |
| 22:SI:138:GLN:CD  | 86:A:1303:GLU:CA   | 2.60                     | 0.73              |
| 86:A:960:ALA:HB2  | 86:A:972:ALA:HB1   | 1.69                     | 0.73              |
| 86:A:1486:ALA:O   | 86:A:1487:ALA:N    | 2.22                     | 0.73              |
| 84:Ls:86:LYS:O    | 84:Ls:139:ILE:HA   | 1.89                     | 0.72              |
| 86:A:1564:ALA:HB1 | 86:A:1598:ALA:HB1  | 1.70                     | 0.72              |
| 21:SH:22:VAL:HG22 | 21:SH:35:ILE:HD11  | 1.71                     | 0.72              |
| 1:S2:1295:G:H1    | 1:S2:1302:U:H3     | 1.38                     | 0.72              |
| 86:A:1668:ALA:O   | 86:A:1672:ALA:CA   | 2.37                     | 0.72              |
| 22:SI:138:GLN:NE2 | 86:A:1300:SER:CB   | 2.53                     | 0.72              |
| 86:A:1520:ALA:O   | 86:A:1521:ALA:HB3  | 1.90                     | 0.71              |
| 40:LA:1580:A:OP2  | 40:LA:2522:G:N2    | 2.22                     | 0.71              |
| 86:A:2405:ALA:CB  | 86:A:2417:ALA:CB   | 2.52                     | 0.71              |
| 44:LE:205:VAL:HA  | 44:LE:208:VAL:HG12 | 1.73                     | 0.71              |
| 51:LL:160:PRO:O   | 51:LL:163:GLN:NE2  | 2.23                     | 0.71              |
| 86:A:2100:ALA:O   | 86:A:2102:ALA:N    | 2.23                     | 0.70              |
| 40:LA:2442:G:H1   | 40:LA:2505:U:H3    | 1.38                     | 0.70              |
| 40:LA:1634:G:N7   | 67:Lb:17:ARG:NH1   | 2.39                     | 0.70              |
| 41:LB:44:C:H4'    | 46:LG:152:ARG:HG3  | 1.74                     | 0.70              |
| 86:A:1463:ALA:CB  | 86:A:1499:ALA:HB1  | 2.21                     | 0.70              |
| 86:A:1218:LEU:CB  | 86:A:1226:ARG:CB   | 2.70                     | 0.69              |
| 86:A:1869:ALA:HB2 | 86:A:1909:ALA:HB1  | 1.74                     | 0.69              |
| 86:A:2103:ALA:HB3 | 86:A:2215:ALA:HA   | 1.73                     | 0.69              |
| 21:SH:101:LEU:H   | 21:SH:104:ASN:HB2  | 1.56                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:A:2100:ALA:N    | 86:A:2216:ALA:CA   | 2.51                     | 0.69              |
| 22:SI:24:ARG:CB    | 86:A:1338:PRO:CB   | 2.71                     | 0.69              |
| 40:LA:1621:A:H62   | 40:LA:1820:U:H3    | 1.40                     | 0.69              |
| 86:A:925:ALA:HB1   | 86:A:968:ALA:HB2   | 1.75                     | 0.69              |
| 86:A:1223:PRO:N    | 86:A:1223:PRO:C    | 2.50                     | 0.69              |
| 86:A:2269:ALA:HB2  | 86:A:2309:ALA:HB1  | 1.74                     | 0.69              |
| 86:A:2209:ALA:O    | 86:A:2213:ALA:CA   | 2.41                     | 0.69              |
| 86:A:1429:ARG:HA   | 86:A:1464:ALA:HB1  | 1.74                     | 0.69              |
| 8:SS:100:ARG:HB3   | 8:SS:112:HIS:HB3   | 1.76                     | 0.68              |
| 86:A:965:ALA:O     | 86:A:969:ALA:CA    | 2.41                     | 0.68              |
| 86:A:1218:LEU:HA   | 86:A:1226:ARG:CB   | 2.23                     | 0.68              |
| 8:SS:94:ALA:HB1    | 27:Sd:16:PRO:HB2   | 1.74                     | 0.68              |
| 86:A:1636:ALA:HA   | 86:A:1676:ALA:HB3  | 1.74                     | 0.68              |
| 86:A:2069:ALA:HB2  | 86:A:2109:ALA:HB1  | 1.74                     | 0.68              |
| 40:LA:1492:G:N7    | 79:Ln:2:ALA:N      | 2.42                     | 0.68              |
| 1:S2:1541:G:H21    | 1:S2:1570:A:H62    | 1.39                     | 0.68              |
| 13:SW:129:ILE:HD13 | 13:SW:134:ILE:HG21 | 1.75                     | 0.68              |
| 1:S2:868:G:OP1     | 17:SY:121:ARG:NH1  | 2.27                     | 0.68              |
| 22:SI:138:GLN:CD   | 86:A:1303:GLU:N    | 2.51                     | 0.68              |
| 40:LA:1656:A:OP2   | 74:Li:37:LYS:NZ    | 2.26                     | 0.68              |
| 49:LJ:54:GLU:HG2   | 49:LJ:57:ARG:HH21  | 1.58                     | 0.68              |
| 9:SB:121:ILE:O     | 9:SB:124:LEU:O     | 2.12                     | 0.68              |
| 86:A:923:ALA:O     | 86:A:926:ALA:N     | 2.27                     | 0.67              |
| 52:LM:165:GLN:CB   | 86:A:1601:ALA:CB   | 2.71                     | 0.67              |
| 22:SI:138:GLN:CG   | 86:A:1303:GLU:HA   | 2.10                     | 0.67              |
| 86:A:1593:ALA:HB2  | 86:A:1627:ALA:HB1  | 1.75                     | 0.67              |
| 86:A:1361:PRO:N    | 86:A:1361:PRO:CB   | 2.56                     | 0.67              |
| 86:A:2380:ALA:HB2  | 86:A:2420:ALA:HB1  | 1.74                     | 0.67              |
| 1:S2:868:G:H1      | 1:S2:960:U:H3      | 1.42                     | 0.66              |
| 1:S2:1489:U:OP2    | 7:SA:9:ARG:NH2     | 2.28                     | 0.66              |
| 40:LA:1169:A:H4'   | 48:LI:219:LYS:HE2  | 1.78                     | 0.66              |
| 86:A:1260:ALA:CB   | 86:A:1264:LYS:CB   | 2.73                     | 0.66              |
| 86:A:1485:ALA:C    | 86:A:1490:ALA:CB   | 2.67                     | 0.66              |
| 15:SX:100:TYR:OH   | 25:Sb:80:ASN:ND2   | 2.29                     | 0.66              |
| 69:Ld:16:ALA:O     | 69:Ld:20:GLY:CA    | 2.44                     | 0.66              |
| 44:LE:10:ARG:NH2   | 44:LE:11:HIS:O     | 2.29                     | 0.66              |
| 86:A:1222:VAL:C    | 86:A:1223:PRO:CA   | 2.63                     | 0.66              |
| 23:SJ:68:ARG:HH12  | 23:SJ:77:LYS:HG3   | 1.61                     | 0.66              |
| 86:A:1222:VAL:O    | 86:A:1226:ARG:CB   | 2.44                     | 0.66              |
| 41:LB:13:A:O2'     | 46:LG:24:ARG:NH1   | 2.29                     | 0.66              |
| 86:A:1485:ALA:O    | 86:A:1490:ALA:CB   | 2.43                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:A:2100:ALA:O    | 86:A:2101:ALA:C    | 2.37                     | 0.66              |
| 22:SI:24:ARG:CZ    | 86:A:1338:PRO:CB   | 2.73                     | 0.65              |
| 43:LD:47:GLN:HE21  | 43:LD:60:LYS:HD2   | 1.60                     | 0.65              |
| 86:A:1428:ALA:C    | 86:A:1464:ALA:CB   | 2.69                     | 0.65              |
| 25:Sb:15:ASN:ND2   | 25:Sb:72:CYS:O     | 2.30                     | 0.65              |
| 1:S2:1429:G:N3     | 23:SJ:72:ASN:ND2   | 2.44                     | 0.65              |
| 86:A:1429:ARG:N    | 86:A:1464:ALA:HB1  | 2.12                     | 0.65              |
| 86:A:1705:ALA:HA   | 86:A:1815:ALA:HB1  | 1.79                     | 0.65              |
| 86:A:2100:ALA:O    | 86:A:2103:ALA:N    | 2.30                     | 0.65              |
| 12:SV:5:ARG:NH1    | 12:SV:29:LEU:O     | 2.30                     | 0.65              |
| 86:A:1260:ALA:HB1  | 86:A:1264:LYS:CB   | 2.26                     | 0.65              |
| 86:A:1705:ALA:O    | 86:A:1815:ALA:O    | 2.14                     | 0.65              |
| 22:SI:138:GLN:NE2  | 86:A:1303:GLU:CA   | 2.60                     | 0.65              |
| 57:LR:107:LEU:HD23 | 57:LR:152:GLU:HG3  | 1.79                     | 0.65              |
| 86:A:924:ALA:HA    | 86:A:933:ALA:C     | 2.21                     | 0.65              |
| 86:A:1428:ALA:C    | 86:A:1464:ALA:HB1  | 2.21                     | 0.65              |
| 86:A:2380:ALA:HB2  | 86:A:2420:ALA:CB   | 2.26                     | 0.65              |
| 22:SI:138:GLN:CD   | 86:A:1300:SER:CB   | 2.70                     | 0.65              |
| 33:SN:123:ASN:ND2  | 33:SN:144:CYS:SG   | 2.71                     | 0.65              |
| 45:LF:330:TYR:O    | 45:LF:334:PHE:HB2  | 1.97                     | 0.65              |
| 86:A:1705:ALA:O    | 86:A:1815:ALA:C    | 2.40                     | 0.65              |
| 86:A:1218:LEU:CA   | 86:A:1226:ARG:CB   | 2.75                     | 0.64              |
| 1:S2:185:U:OP1     | 12:SV:146:ARG:NH2  | 2.30                     | 0.64              |
| 86:A:2104:ALA:HB1  | 86:A:2210:ALA:O    | 1.97                     | 0.64              |
| 86:A:2269:ALA:HB2  | 86:A:2309:ALA:CB   | 2.26                     | 0.64              |
| 86:A:1458:ALA:O    | 86:A:1460:ALA:N    | 2.29                     | 0.64              |
| 86:A:1869:ALA:HB2  | 86:A:1909:ALA:CB   | 2.26                     | 0.64              |
| 1:S2:902:G:N7      | 18:SZ:24:ASN:ND2   | 2.45                     | 0.64              |
| 40:LA:269:G:OP1    | 55:LP:47:LYS:NZ    | 2.30                     | 0.64              |
| 42:LC:53:A:O2'     | 79:Ln:40:LYS:NZ    | 2.30                     | 0.64              |
| 1:S2:265:A:N7      | 10:ST:190:GLN:NE2  | 2.46                     | 0.64              |
| 1:S2:415:C:O2      | 1:S2:418:G:C6      | 2.49                     | 0.64              |
| 40:LA:2294:U:OP2   | 63:LX:71:LYS:NZ    | 2.30                     | 0.64              |
| 34:SO:123:ILE:HG22 | 34:SO:133:VAL:HG12 | 1.79                     | 0.64              |
| 49:LJ:72:PRO:HG3   | 55:LP:18:VAL:HA    | 1.80                     | 0.64              |
| 86:A:1482:ALA:C    | 86:A:1493:ALA:HB1  | 2.22                     | 0.64              |
| 86:A:1599:ALA:HB2  | 86:A:1604:ALA:CB   | 2.28                     | 0.64              |
| 1:S2:1213:G:O2'    | 1:S2:1244:A:N7     | 2.30                     | 0.64              |
| 40:LA:1156:C:OP2   | 48:LI:94:LYS:NZ    | 2.31                     | 0.64              |
| 40:LA:1613:A:OP1   | 78:Lm:2:ALA:N      | 2.31                     | 0.64              |
| 45:LF:150:LEU:HD23 | 45:LF:249:ILE:HG12 | 1.79                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 86:A:1636:ALA:HB1 | 86:A:1674:ALA:HB1  | 1.80                     | 0.64              |
| 86:A:1637:ALA:N   | 86:A:1676:ALA:HB3  | 2.11                     | 0.64              |
| 86:A:2069:ALA:HB2 | 86:A:2109:ALA:CB   | 2.26                     | 0.64              |
| 6:SR:88:LYS:HD2   | 6:SR:95:ARG:HD3    | 1.79                     | 0.64              |
| 86:A:1429:ARG:CA  | 86:A:1464:ALA:HB1  | 2.28                     | 0.63              |
| 40:LA:2617:U:O2'  | 51:LL:116:ARG:NH2  | 2.31                     | 0.63              |
| 60:LU:154:HIS:HA  | 60:LU:170:THR:HB   | 1.80                     | 0.63              |
| 1:S2:780:A:H2     | 27:Sd:10:ARG:HG2   | 1.63                     | 0.63              |
| 22:SI:77:ASN:HB3  | 22:SI:95:ASP:HB3   | 1.81                     | 0.63              |
| 11:SU:27:LEU:O    | 11:SU:30:SER:O     | 2.17                     | 0.63              |
| 86:A:927:ALA:HB3  | 86:A:933:ALA:N     | 2.12                     | 0.63              |
| 22:SI:42:GLY:HA2  | 22:SI:84:LYS:HD3   | 1.81                     | 0.63              |
| 1:S2:629:U:OP2    | 1:S2:969:C:N4      | 2.31                     | 0.63              |
| 22:SI:138:GLN:NE2 | 86:A:1303:GLU:HA   | 2.12                     | 0.63              |
| 43:LD:27:ALA:O    | 43:LD:128:ARG:NH2  | 2.31                     | 0.63              |
| 67:Lb:68:ILE:O    | 67:Lb:115:LYS:NZ   | 2.32                     | 0.63              |
| 1:S2:532:U:O2     | 27:Sd:34:ASN:ND2   | 2.32                     | 0.63              |
| 1:S2:764:U:OP2    | 13:SW:82:ARG:NH1   | 2.31                     | 0.63              |
| 40:LA:2679:A:HO2' | 52:LM:52:TYR:HH    | 1.47                     | 0.63              |
| 42:LC:52:A:OP1    | 79:Ln:21:ARG:NH1   | 2.31                     | 0.63              |
| 42:LC:83:C:H42    | 66:La:52:ARG:HH22  | 1.46                     | 0.63              |
| 42:LC:141:C:O2    | 55:LP:112:ASN:ND2  | 2.31                     | 0.63              |
| 86:A:929:ALA:C    | 86:A:932:ALA:H     | 2.07                     | 0.63              |
| 86:A:1482:ALA:O   | 86:A:1493:ALA:HB3  | 1.98                     | 0.63              |
| 40:LA:640:U:OP1   | 68:Lc:21:ARG:NH2   | 2.29                     | 0.62              |
| 40:LA:2800:G:O6   | 68:Lc:42:ARG:NH2   | 2.32                     | 0.62              |
| 57:LR:56:ARG:NH1  | 57:LR:75:GLU:OE2   | 2.32                     | 0.62              |
| 1:S2:1195:C:OP1   | 23:SJ:77:LYS:NZ    | 2.33                     | 0.62              |
| 10:ST:154:ARG:HG2 | 10:ST:178:LEU:HD11 | 1.80                     | 0.62              |
| 40:LA:283:G:OP1   | 82:Lq:45:ARG:NH1   | 2.31                     | 0.62              |
| 40:LA:901:G:OP1   | 77:Ll:13:ASN:ND2   | 2.32                     | 0.62              |
| 40:LA:1659:U:H3   | 40:LA:1790:G:H1    | 1.47                     | 0.62              |
| 83:Lr:51:ALA:HB3  | 83:Lr:54:ILE:HD12  | 1.81                     | 0.62              |
| 1:S2:1582:U:OP1   | 19:SF:135:ARG:NH1  | 2.31                     | 0.62              |
| 34:SO:42:LEU:HB2  | 34:SO:61:PHE:HB2   | 1.81                     | 0.62              |
| 40:LA:364:G:N7    | 77:Ll:56:ARG:NH2   | 2.48                     | 0.62              |
| 86:A:1429:ARG:N   | 86:A:1464:ALA:CB   | 2.63                     | 0.62              |
| 1:S2:229:U:O4     | 1:S2:237:C:N3      | 2.32                     | 0.62              |
| 45:LF:77:VAL:O    | 45:LF:86:GLY:N     | 2.33                     | 0.62              |
| 1:S2:1542:G:H1    | 1:S2:1568:C:HO2'   | 1.45                     | 0.62              |
| 1:S2:1673:G:O6    | 1:S2:1728:A:N1     | 2.33                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:LA:1579:C:OP1   | 43:LD:68:LYS:NZ   | 2.33                     | 0.62              |
| 67:Lb:90:GLU:HA    | 67:Lb:93:LYS:HE2  | 1.82                     | 0.62              |
| 86:A:1456:ALA:O    | 86:A:1457:ALA:HB3 | 1.98                     | 0.62              |
| 1:S2:1435:G:H8     | 14:SC:62:GLN:HE22 | 1.46                     | 0.62              |
| 40:LA:388:G:H1'    | 57:LR:97:ASN:HD21 | 1.65                     | 0.62              |
| 40:LA:1363:A:OP1   | 48:LI:160:ARG:NH1 | 2.32                     | 0.62              |
| 44:LE:14:LEU:HA    | 44:LE:17:LEU:HD13 | 1.82                     | 0.62              |
| 86:A:1668:ALA:C    | 86:A:1672:ALA:HB2 | 2.17                     | 0.61              |
| 1:S2:395:U:H3      | 1:S2:399:A:N6     | 1.85                     | 0.61              |
| 46:LG:41:LYS:NZ    | 61:LV:30:TYR:O    | 2.33                     | 0.61              |
| 65:LZ:117:ASN:O    | 79:Ln:18:LYS:NZ   | 2.33                     | 0.61              |
| 68:Lc:96:LYS:HG2   | 68:Lc:122:PRO:HG2 | 1.82                     | 0.61              |
| 86:A:1216:LYS:O    | 86:A:1229:THR:CB  | 2.48                     | 0.61              |
| 86:A:1458:ALA:O    | 86:A:1461:ALA:N   | 2.29                     | 0.61              |
| 86:A:2209:ALA:O    | 86:A:2213:ALA:HB3 | 1.97                     | 0.61              |
| 16:SD:43:ARG:NH2   | 16:SD:102:GLY:O   | 2.30                     | 0.61              |
| 22:SI:138:GLN:HA   | 86:A:1303:GLU:CB  | 2.30                     | 0.61              |
| 40:LA:68:C:OP2     | 40:LA:301:G:N2    | 2.34                     | 0.61              |
| 40:LA:509:U:H3     | 40:LA:582:G:H1    | 1.48                     | 0.61              |
| 1:S2:393:C:N4      | 1:S2:401:A:OP2    | 2.33                     | 0.61              |
| 1:S2:1358:G:OP1    | 22:SI:130:ARG:NH1 | 2.34                     | 0.61              |
| 45:LF:237:GLN:O    | 45:LF:246:ARG:NH1 | 2.33                     | 0.61              |
| 86:A:2072:ALA:C    | 86:A:2074:ALA:H   | 2.09                     | 0.61              |
| 3:SP:70:PRO:HG3    | 3:SP:185:ARG:HH12 | 1.65                     | 0.61              |
| 8:SS:19:LEU:HD12   | 8:SS:51:ARG:HH22  | 1.65                     | 0.61              |
| 22:SI:65:ILE:O     | 22:SI:68:ARG:O    | 2.19                     | 0.61              |
| 72:Lg:83:GLU:HA    | 72:Lg:86:THR:HG23 | 1.81                     | 0.61              |
| 86:A:1487:ALA:O    | 86:A:1491:ALA:CA  | 2.48                     | 0.61              |
| 86:A:1640:ALA:C    | 86:A:1642:ALA:H   | 2.07                     | 0.61              |
| 47:LH:63:LEU:O     | 47:LH:78:ARG:HA   | 2.00                     | 0.61              |
| 52:LM:165:GLN:HB3  | 86:A:1601:ALA:HB2 | 1.83                     | 0.61              |
| 40:LA:936:A:OP1    | 68:Lc:32:ARG:NH2  | 2.33                     | 0.61              |
| 40:LA:2756:C:O2    | 61:LV:8:ARG:NH2   | 2.33                     | 0.61              |
| 40:LA:2835:U:OP1   | 80:Lo:98:LYS:NZ   | 2.33                     | 0.61              |
| 40:LA:2838:A:H4'   | 51:LL:74:LYS:HG2  | 1.83                     | 0.61              |
| 42:LC:52:A:H62     | 79:Ln:27:ILE:HD13 | 1.66                     | 0.61              |
| 46:LG:111:GLN:HE22 | 46:LG:252:ALA:HB2 | 1.66                     | 0.61              |
| 55:LP:98:LEU:HD22  | 55:LP:128:LYS:HD2 | 1.83                     | 0.61              |
| 1:S2:1339:C:O2'    | 1:S2:1341:A:N7    | 2.34                     | 0.61              |
| 9:SB:121:ILE:O     | 9:SB:124:LEU:C    | 2.43                     | 0.61              |
| 1:S2:821:U:H3      | 1:S2:852:C:N4     | 1.99                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:2852:C:N3    | 51:LL:158:LYS:NZ   | 2.49                     | 0.61              |
| 41:LB:6:C:OP2      | 46:LG:22:ARG:NH1   | 2.34                     | 0.61              |
| 52:LM:139:THR:O    | 52:LM:145:LYS:NZ   | 2.33                     | 0.61              |
| 55:LP:138:GLN:HA   | 55:LP:143:ARG:HH21 | 1.65                     | 0.61              |
| 86:A:1432:GLY:C    | 86:A:1468:ALA:HB2  | 2.26                     | 0.61              |
| 40:LA:120:G:N2     | 49:LJ:126:SER:O    | 2.33                     | 0.60              |
| 40:LA:2666:C:OP2   | 40:LA:2687:G:N1    | 2.34                     | 0.60              |
| 11:SU:46:ILE:HD13  | 11:SU:60:ILE:HG13  | 1.84                     | 0.60              |
| 86:A:2383:ALA:C    | 86:A:2385:ALA:H    | 2.09                     | 0.60              |
| 15:SX:102:LYS:O    | 26:Sc:13:ARG:NH2   | 2.30                     | 0.60              |
| 40:LA:1915:A:H5''  | 59:LT:84:THR:HG22  | 1.83                     | 0.60              |
| 55:LP:114:ARG:NH1  | 55:LP:151:ILE:O    | 2.32                     | 0.60              |
| 1:S2:329:G:H5''    | 12:SV:98:LYS:HB3   | 1.83                     | 0.60              |
| 20:SG:26:LEU:HD11  | 20:SG:62:GLN:HG3   | 1.83                     | 0.60              |
| 40:LA:2282:U:OP1   | 40:LA:2973:G:O2'   | 2.18                     | 0.60              |
| 86:A:1872:ALA:C    | 86:A:1874:ALA:H    | 2.09                     | 0.60              |
| 86:A:2314:ALA:CB   | 86:A:2321:ALA:CB   | 2.70                     | 0.60              |
| 1:S2:67:A:N6       | 1:S2:83:G:O2'      | 2.35                     | 0.60              |
| 1:S2:554:C:N4      | 1:S2:571:G:O6      | 2.34                     | 0.60              |
| 1:S2:815:G:O2'     | 59:LT:162:ARG:NH2  | 2.34                     | 0.60              |
| 8:SS:100:ARG:NH2   | 8:SS:118:GLU:O     | 2.35                     | 0.60              |
| 42:LC:126:A:O2'    | 42:LC:129:C:N4     | 2.34                     | 0.60              |
| 51:LL:209:ASN:O    | 51:LL:212:GLU:C    | 2.45                     | 0.60              |
| 82:Lq:75:VAL:HG23  | 82:Lq:76:LYS:HD2   | 1.84                     | 0.60              |
| 86:A:927:ALA:CB    | 86:A:933:ALA:HB3   | 2.30                     | 0.60              |
| 86:A:1393:ALA:C    | 86:A:1395:LEU:H    | 2.09                     | 0.60              |
| 40:LA:2185:G:O2'   | 40:LA:2314:U:OP2   | 2.19                     | 0.60              |
| 86:A:987:ALA:CB    | 86:A:988:ALA:CB    | 2.79                     | 0.60              |
| 24:Sa:17:CYS:SG    | 24:Sa:18:SER:N     | 2.75                     | 0.60              |
| 40:LA:1390:A:N6    | 40:LA:1418:A:O2'   | 2.34                     | 0.60              |
| 40:LA:1488:G:H21   | 74:Li:12:PRO:HG3   | 1.65                     | 0.60              |
| 40:LA:3092:C:O2'   | 40:LA:3094:A:OP2   | 2.20                     | 0.60              |
| 36:Sm:37:A:O2'     | 40:LA:2256:A:N1    | 2.35                     | 0.60              |
| 40:LA:744:A:H5'    | 58:LS:66:ARG:HH22  | 1.67                     | 0.60              |
| 86:A:1432:GLY:HA3  | 86:A:1468:ALA:HB2  | 1.82                     | 0.60              |
| 21:SH:19:ASN:ND2   | 52:LM:111:ASP:OD1  | 2.34                     | 0.60              |
| 38:So:342:VAL:HG22 | 38:So:344:GLY:H    | 1.67                     | 0.60              |
| 40:LA:89:A:OP2     | 58:LS:170:ARG:NH2  | 2.35                     | 0.60              |
| 46:LG:75:LEU:O     | 46:LG:112:LYS:NZ   | 2.32                     | 0.60              |
| 86:A:1428:ALA:HB2  | 86:A:1461:ALA:CA   | 2.22                     | 0.60              |
| 14:SC:12:HIS:HA    | 14:SC:15:LEU:HD12  | 1.83                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S2:480:G:H1      | 1:S2:508:U:H3      | 1.48                     | 0.59              |
| 3:SP:36:TYR:OH     | 24:Sa:70:ASN:ND2   | 2.33                     | 0.59              |
| 40:LA:1055:A:N3    | 41:LB:81:U:O2'     | 2.34                     | 0.59              |
| 40:LA:1833:G:O2'   | 79:Ln:3:ALA:O      | 2.21                     | 0.59              |
| 40:LA:2452:G:O6    | 40:LA:2493:U:C4    | 2.55                     | 0.59              |
| 5:SE:18:ARG:NH1    | 21:SH:90:ASN:O     | 2.35                     | 0.59              |
| 8:SS:54:TYR:O      | 27:Sd:15:ASN:ND2   | 2.35                     | 0.59              |
| 86:A:1636:ALA:HB1  | 86:A:1677:ALA:H    | 1.67                     | 0.59              |
| 1:S2:1553:G:N1     | 1:S2:1556:A:OP2    | 2.35                     | 0.59              |
| 55:LP:9:GLU:OE2    | 55:LP:13:LYS:NZ    | 2.35                     | 0.59              |
| 1:S2:638:U:H1'     | 11:SU:112:ARG:HH22 | 1.65                     | 0.59              |
| 33:SN:123:ASN:ND2  | 33:SN:125:THR:OG1  | 2.35                     | 0.59              |
| 40:LA:2588:U:OP1   | 49:LJ:48:ARG:NH2   | 2.35                     | 0.59              |
| 86:A:1520:ALA:O    | 86:A:1521:ALA:CB   | 2.49                     | 0.59              |
| 40:LA:199:A:H5''   | 66:La:60:ARG:HD2   | 1.82                     | 0.59              |
| 49:LJ:90:THR:HG22  | 49:LJ:214:LEU:HD21 | 1.84                     | 0.59              |
| 52:LM:81:GLU:OE1   | 52:LM:167:TYR:OH   | 2.21                     | 0.59              |
| 86:A:925:ALA:CB    | 86:A:968:ALA:HB2   | 2.32                     | 0.59              |
| 3:SP:36:TYR:OH     | 3:SP:56:LYS:NZ     | 2.34                     | 0.59              |
| 26:Sc:42:PRO:O     | 26:Sc:79:ASN:ND2   | 2.35                     | 0.59              |
| 40:LA:1157:G:O2'   | 40:LA:1169:A:N3    | 2.35                     | 0.59              |
| 40:LA:1369:A:OP1   | 68:Lc:21:ARG:NH1   | 2.35                     | 0.59              |
| 41:LB:3:U:O2'      | 41:LB:25:G:N3      | 2.33                     | 0.59              |
| 41:LB:64:A:OP2     | 46:LG:289:LYS:NZ   | 2.36                     | 0.59              |
| 45:LF:291:ASN:HA   | 45:LF:296:GLN:HE21 | 1.68                     | 0.59              |
| 86:A:1639:ALA:HB1  | 86:A:1641:ALA:H    | 1.68                     | 0.59              |
| 71:Lf:13:THR:OG1   | 71:Lf:72:ARG:NH1   | 2.36                     | 0.59              |
| 86:A:1636:ALA:C    | 86:A:1638:ALA:H    | 2.10                     | 0.59              |
| 1:S2:298:C:O2'     | 8:SS:30:ARG:NH1    | 2.35                     | 0.59              |
| 1:S2:1487:A:OP1    | 31:SM:34:TYR:OH    | 2.18                     | 0.59              |
| 29:Se:37:LYS:O     | 29:Se:38:ARG:NH1   | 2.36                     | 0.59              |
| 77:Ll:36:SER:HA    | 77:Ll:45:ARG:HH21  | 1.67                     | 0.59              |
| 86:A:960:ALA:CB    | 86:A:972:ALA:HB1   | 2.32                     | 0.59              |
| 86:A:2272:ALA:C    | 86:A:2274:ALA:H    | 2.09                     | 0.59              |
| 1:S2:567:A:OP1     | 26:Sc:70:LYS:NZ    | 2.35                     | 0.59              |
| 1:S2:1551:U:O4     | 5:SE:40:ARG:NH1    | 2.36                     | 0.59              |
| 40:LA:2196:C:O2'   | 40:LA:2270:A:N3    | 2.31                     | 0.59              |
| 40:LA:3216:G:OP2   | 73:Lh:2:ALA:N      | 2.35                     | 0.59              |
| 49:LJ:162:LEU:HD23 | 55:LP:7:LEU:HD21   | 1.85                     | 0.59              |
| 34:SO:153:GLN:OE1  | 34:SO:155:ARG:NH1  | 2.36                     | 0.58              |
| 3:SP:53:THR:HG22   | 3:SP:161:PRO:HG2   | 1.84                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:So:335:ASP:O    | 63:LX:128:ARG:NH1  | 2.36                     | 0.58              |
| 40:LA:967:A:OP1    | 68:Lc:47:LYS:NZ    | 2.36                     | 0.58              |
| 40:LA:1566:A:N1    | 40:LA:1571:A:N6    | 2.50                     | 0.58              |
| 40:LA:2608:G:OP1   | 43:LD:2:GLY:N      | 2.37                     | 0.58              |
| 51:LL:201:SER:OG   | 51:LL:203:LYS:O    | 2.22                     | 0.58              |
| 86:A:1456:ALA:O    | 86:A:1457:ALA:CB   | 2.51                     | 0.58              |
| 1:S2:694:U:N3      | 11:SU:96:ARG:O     | 2.35                     | 0.58              |
| 1:S2:1594:G:OP2    | 1:S2:1596:C:N4     | 2.36                     | 0.58              |
| 40:LA:1488:G:O2'   | 74:Li:10:ARG:O     | 2.22                     | 0.58              |
| 45:LF:219:LEU:HA   | 45:LF:222:VAL:HG22 | 1.85                     | 0.58              |
| 40:LA:291:C:OP2    | 55:LP:128:LYS:NZ   | 2.37                     | 0.58              |
| 41:LB:13:A:OP2     | 41:LB:67:G:N2      | 2.36                     | 0.58              |
| 54:LO:37:GLU:OE2   | 54:LO:74:ARG:NH2   | 2.36                     | 0.58              |
| 86:A:1705:ALA:CB   | 86:A:1815:ALA:O    | 2.39                     | 0.58              |
| 1:S2:1459:C:OP2    | 21:SH:138:THR:OG1  | 2.21                     | 0.58              |
| 13:SW:27:GLU:HG3   | 13:SW:39:LYS:HE2   | 1.85                     | 0.58              |
| 40:LA:1385:C:OP1   | 45:LF:141:ARG:NH2  | 2.31                     | 0.58              |
| 40:LA:2194:G:OP1   | 43:LD:247:ARG:NH1  | 2.36                     | 0.58              |
| 49:LJ:77:GLN:HE22  | 49:LJ:167:PRO:HG2  | 1.68                     | 0.58              |
| 84:Ls:87:ARG:HA    | 84:Ls:138:ILE:O    | 2.04                     | 0.58              |
| 86:A:1636:ALA:CA   | 86:A:1676:ALA:HB3  | 2.32                     | 0.58              |
| 86:A:2097:ALA:HB1  | 86:A:2103:ALA:HB2  | 1.84                     | 0.58              |
| 1:S2:647:G:H22     | 1:S2:687:G:H1      | 1.52                     | 0.58              |
| 40:LA:508:U:H3     | 40:LA:583:G:H1     | 1.50                     | 0.58              |
| 18:SZ:16:VAL:HG12  | 18:SZ:80:HIS:HB2   | 1.86                     | 0.58              |
| 22:SI:73:VAL:O     | 22:SI:77:ASN:ND2   | 2.36                     | 0.58              |
| 40:LA:524:U:OP1    | 54:LO:77:ARG:NH2   | 2.37                     | 0.58              |
| 40:LA:649:A:OP2    | 40:LA:2868:U:O2'   | 2.22                     | 0.58              |
| 1:S2:330:G:OP2     | 12:SV:172:ARG:NH1  | 2.36                     | 0.58              |
| 9:SB:94:THR:HG22   | 9:SB:114:ILE:HG13  | 1.86                     | 0.58              |
| 18:SZ:82:LYS:NZ    | 18:SZ:116:GLU:OE1  | 2.36                     | 0.58              |
| 40:LA:114:A:N1     | 40:LA:266:A:O2'    | 2.36                     | 0.58              |
| 40:LA:593:C:OP2    | 47:LH:19:LYS:NZ    | 2.36                     | 0.58              |
| 86:A:948:ALA:O     | 86:A:984:ALA:HB3   | 2.04                     | 0.58              |
| 19:SF:89:LEU:HG    | 19:SF:105:LEU:HD21 | 1.86                     | 0.58              |
| 60:LU:124:LEU:HD23 | 61:LV:153:PRO:HB2  | 1.86                     | 0.58              |
| 1:S2:883:C:N3      | 1:S2:945:U:O4      | 2.37                     | 0.58              |
| 1:S2:1175:U:H3     | 1:S2:1464:G:H1     | 1.52                     | 0.58              |
| 13:SW:59:LEU:HD12  | 13:SW:69:ARG:HA    | 1.86                     | 0.57              |
| 24:Sa:87:ARG:HH12  | 30:Sf:2:VAL:HG11   | 1.67                     | 0.57              |
| 27:Sd:44:LEU:HA    | 27:Sd:47:VAL:HG12  | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:1302:A:N7    | 40:LA:2857:C:O2'   | 2.35                     | 0.57              |
| 52:LM:133:ARG:NH1  | 52:LM:153:LYS:O    | 2.37                     | 0.57              |
| 1:S2:1795:U:H5'    | 29:Se:79:ILE:HD11  | 1.85                     | 0.57              |
| 24:Sa:15:ARG:NH1   | 24:Sa:33:GLN:OE1   | 2.37                     | 0.57              |
| 41:LB:6:C:OP1      | 46:LG:54:ARG:NE    | 2.36                     | 0.57              |
| 83:Lr:46:THR:HG1   | 83:Lr:57:CYS:HG    | 1.51                     | 0.57              |
| 40:LA:67:A:N6      | 40:LA:271:C:O2'    | 2.31                     | 0.57              |
| 40:LA:120:G:N2     | 49:LJ:123:GLN:O    | 2.37                     | 0.57              |
| 53:LN:70:ARG:NH1   | 53:LN:71:ALA:O     | 2.37                     | 0.57              |
| 57:LR:119:VAL:HG22 | 57:LR:146:ILE:HG12 | 1.86                     | 0.57              |
| 70:Le:22:LYS:NZ    | 70:Le:94:GLU:OE2   | 2.38                     | 0.57              |
| 86:A:1523:ALA:CB   | 86:A:1526:ALA:HB3  | 2.34                     | 0.57              |
| 22:SI:65:ILE:O     | 22:SI:68:ARG:C     | 2.47                     | 0.57              |
| 40:LA:364:G:OP2    | 77:Ll:52:LYS:NZ    | 2.37                     | 0.57              |
| 51:LL:209:ASN:O    | 51:LL:212:GLU:O    | 2.22                     | 0.57              |
| 7:SA:28:GLU:OE2    | 14:SC:58:GLN:NE2   | 2.34                     | 0.57              |
| 53:LN:4:SER:O      | 68:Lc:44:ASN:ND2   | 2.34                     | 0.57              |
| 1:S2:463:U:O2'     | 1:S2:527:A:N6      | 2.37                     | 0.57              |
| 3:SP:88:LYS:O      | 3:SP:92:HIS:ND1    | 2.37                     | 0.57              |
| 40:LA:1268:G:O2'   | 40:LA:1269:U:O2    | 2.23                     | 0.57              |
| 51:LL:171:TRP:HE3  | 51:LL:178:ARG:HG3  | 1.68                     | 0.57              |
| 86:A:1583:ALA:C    | 86:A:1585:ALA:H    | 2.13                     | 0.57              |
| 1:S2:763:G:OP2     | 13:SW:79:ARG:NH2   | 2.38                     | 0.57              |
| 1:S2:1674:C:OP1    | 10:ST:92:ARG:NH2   | 2.36                     | 0.57              |
| 22:SI:24:ARG:HB3   | 86:A:1338:PRO:CB   | 2.34                     | 0.57              |
| 40:LA:1348:U:OP1   | 58:LS:39:ARG:NH1   | 2.38                     | 0.57              |
| 50:LK:114:VAL:HB   | 50:LK:124:ARG:HB2  | 1.87                     | 0.57              |
| 40:LA:533:A:O2'    | 40:LA:535:G:OP2    | 2.23                     | 0.57              |
| 40:LA:804:C:OP1    | 45:LF:98:ARG:NH1   | 2.37                     | 0.57              |
| 43:LD:95:SER:OG    | 43:LD:97:ASN:ND2   | 2.38                     | 0.57              |
| 51:LL:105:CYS:SG   | 51:LL:106:ALA:N    | 2.77                     | 0.57              |
| 1:S2:151:G:N3      | 10:ST:13:GLN:NE2   | 2.52                     | 0.57              |
| 1:S2:1337:A:OP1    | 19:SF:123:ARG:NH2  | 2.36                     | 0.57              |
| 1:S2:1461:C:OP1    | 21:SH:144:ARG:NH1  | 2.37                     | 0.57              |
| 3:SP:13:ASP:OD1    | 3:SP:179:ARG:NH2   | 2.38                     | 0.57              |
| 7:SA:37:VAL:HG12   | 7:SA:50:ILE:HG12   | 1.85                     | 0.57              |
| 38:So:135:GLN:NE2  | 40:LA:3027:A:N7    | 2.53                     | 0.57              |
| 40:LA:1385:C:O2    | 47:LH:2:THR:N      | 2.37                     | 0.57              |
| 44:LE:252:ILE:HD12 | 44:LE:266:ARG:HH12 | 1.70                     | 0.57              |
| 57:LR:128:ARG:HG3  | 57:LR:136:ILE:HG23 | 1.87                     | 0.57              |
| 77:Ll:19:CYS:SG    | 77:Ll:20:ASN:N     | 2.78                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:SR:52:THR:OG1    | 6:SR:54:GLU:OE1    | 2.22                     | 0.57              |
| 22:SI:138:GLN:HE22 | 86:A:1300:SER:C    | 2.12                     | 0.57              |
| 40:LA:2712:U:HO2'  | 40:LA:2743:A:HO2'  | 1.51                     | 0.57              |
| 40:LA:3212:C:OP2   | 54:LO:124:ARG:NH2  | 2.38                     | 0.57              |
| 50:LK:4:ILE:H      | 60:LU:142:GLN:HE21 | 1.52                     | 0.57              |
| 68:Lc:100:PRO:HG2  | 68:Lc:123:VAL:HG23 | 1.87                     | 0.57              |
| 18:SZ:17:ALA:O     | 18:SZ:29:HIS:O     | 2.23                     | 0.56              |
| 40:LA:1355:A:H2    | 58:LS:38:ARG:HH12  | 1.53                     | 0.56              |
| 11:SU:27:LEU:O     | 11:SU:30:SER:C     | 2.47                     | 0.56              |
| 40:LA:284:A:OP2    | 82:Lq:41:ARG:NH1   | 2.38                     | 0.56              |
| 43:LD:97:ASN:OD1   | 83:Lr:87:ARG:NH1   | 2.38                     | 0.56              |
| 7:SA:134:CYS:SG    | 7:SA:135:GLU:N     | 2.78                     | 0.56              |
| 25:Sb:79:PHE:O     | 25:Sb:124:LYS:HA   | 2.05                     | 0.56              |
| 38:So:341:LEU:HB3  | 38:So:367:SER:HB3  | 1.86                     | 0.56              |
| 40:LA:216:G:OP1    | 66:La:16:ARG:NH1   | 2.37                     | 0.56              |
| 40:LA:271:C:O2     | 76:Lk:82:ARG:NH2   | 2.34                     | 0.56              |
| 40:LA:292:U:OP2    | 55:LP:68:ARG:NH1   | 2.38                     | 0.56              |
| 40:LA:2896:A:O2'   | 80:Lo:122:ARG:NH2  | 2.38                     | 0.56              |
| 40:LA:3070:A:OP1   | 59:LT:62:ARG:NH2   | 2.38                     | 0.56              |
| 86:A:1840:ALA:N    | 86:A:1840:ALA:C    | 2.59                     | 0.56              |
| 86:A:2300:ALA:N    | 86:A:2300:ALA:CB   | 2.62                     | 0.56              |
| 1:S2:247:A:O2'     | 15:SX:37:ASN:O     | 2.24                     | 0.56              |
| 1:S2:1113:A:N6     | 1:S2:1132:A:OP2    | 2.38                     | 0.56              |
| 8:SS:18:TRP:NE1    | 8:SS:41:SER:O      | 2.38                     | 0.56              |
| 15:SX:121:ASP:HA   | 15:SX:144:ALA:HB3  | 1.86                     | 0.56              |
| 24:Sa:1:MET:N      | 24:Sa:10:GLU:OE2   | 2.37                     | 0.56              |
| 40:LA:3228:C:OP1   | 54:LO:137:LYS:NZ   | 2.38                     | 0.56              |
| 86:A:2294:ALA:CB   | 86:A:2306:ALA:CB   | 2.52                     | 0.56              |
| 42:LC:26:U:O2'     | 45:LF:51:ALA:O     | 2.22                     | 0.56              |
| 1:S2:23:G:O2'      | 1:S2:368:U:OP1     | 2.23                     | 0.56              |
| 1:S2:1029:U:OP2    | 29:Se:12:LYS:NZ    | 2.39                     | 0.56              |
| 1:S2:1534:G:OP2    | 28:SK:74:SER:OG    | 2.22                     | 0.56              |
| 1:S2:1368:G:OP1    | 22:SI:69:LYS:NZ    | 2.35                     | 0.56              |
| 18:SZ:26:THR:HG21  | 18:SZ:97:GLY:HA3   | 1.87                     | 0.56              |
| 22:SI:134:ARG:HB3  | 86:A:1300:SER:O    | 2.06                     | 0.56              |
| 26:Sc:70:LYS:HB3   | 26:Sc:93:LEU:HD22  | 1.88                     | 0.56              |
| 78:Lm:2:ALA:N      | 78:Lm:51:LEU:O     | 2.39                     | 0.56              |
| 86:A:2351:ALA:N    | 86:A:2351:ALA:C    | 2.59                     | 0.56              |
| 1:S2:956:C:OP1     | 1:S2:1072:C:O2'    | 2.23                     | 0.56              |
| 1:S2:1254:U:OP2    | 16:SD:46:ARG:NH2   | 2.38                     | 0.56              |
| 1:S2:1334:U:O2'    | 23:SJ:85:ARG:NH2   | 2.37                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:SQ:76:SER:OG     | 4:SQ:78:ASP:OD1    | 2.22                     | 0.56              |
| 19:SF:129:PHE:O    | 19:SF:137:ARG:NH1  | 2.36                     | 0.56              |
| 30:Sf:34:ASP:O     | 30:Sf:79:PHE:HA    | 2.05                     | 0.56              |
| 40:LA:164:A:N1     | 40:LA:258:G:C6     | 2.74                     | 0.56              |
| 40:LA:1592:G:OP1   | 74:Li:58:ARG:NH2   | 2.39                     | 0.56              |
| 40:LA:2424:A:OP1   | 55:LP:90:ASN:ND2   | 2.36                     | 0.56              |
| 86:A:929:ALA:O     | 86:A:931:ALA:N     | 2.39                     | 0.56              |
| 1:S2:334:G:O6      | 12:SV:5:ARG:NH2    | 2.39                     | 0.56              |
| 1:S2:930:A:H1'     | 4:SQ:111:ARG:HH12  | 1.71                     | 0.56              |
| 6:SR:59:HIS:NE2    | 6:SR:237:VAL:O     | 2.39                     | 0.56              |
| 12:SV:99:ALA:N     | 12:SV:169:ILE:O    | 2.39                     | 0.56              |
| 14:SC:70:GLU:HA    | 14:SC:73:VAL:HG12  | 1.86                     | 0.56              |
| 40:LA:1591:G:H5''  | 74:Li:37:LYS:HZ1   | 1.71                     | 0.56              |
| 41:LB:44:C:OP2     | 52:LM:137:ARG:NH2  | 2.38                     | 0.56              |
| 46:LG:294:ALA:HB1  | 51:LL:217:PHE:HB3  | 1.88                     | 0.56              |
| 84:Ls:92:LEU:HB3   | 84:Ls:134:LEU:O    | 2.06                     | 0.56              |
| 1:S2:415:C:O2      | 1:S2:418:G:O6      | 2.24                     | 0.56              |
| 1:S2:444:C:OP2     | 27:Sd:108:ARG:NH2  | 2.38                     | 0.56              |
| 1:S2:907:A:N3      | 1:S2:997:G:O2'     | 2.34                     | 0.56              |
| 38:So:340:ALA:O    | 38:So:354:CYS:HB3  | 2.06                     | 0.56              |
| 43:LD:101:VAL:HG22 | 43:LD:165:VAL:HG22 | 1.87                     | 0.56              |
| 1:S2:1490:C:OP2    | 7:SA:9:ARG:NH1     | 2.39                     | 0.55              |
| 8:SS:87:MET:HE1    | 8:SS:236:ILE:HG21  | 1.88                     | 0.55              |
| 27:Sd:78:SER:OG    | 27:Sd:81:GLU:OE1   | 2.22                     | 0.55              |
| 38:So:103:VAL:HG21 | 38:So:117:VAL:HA   | 1.87                     | 0.55              |
| 40:LA:1448:U:OP1   | 57:LR:82:ARG:NH2   | 2.39                     | 0.55              |
| 40:LA:1805:C:H2'   | 40:LA:1806:A:H8    | 1.71                     | 0.55              |
| 27:Sd:38:ASP:O     | 27:Sd:52:LYS:NZ    | 2.38                     | 0.55              |
| 40:LA:59:G:H2'     | 42:LC:33:A:H2'     | 1.88                     | 0.55              |
| 40:LA:729:C:O2'    | 58:LS:79:LYS:NZ    | 2.37                     | 0.55              |
| 40:LA:3041:U:OP1   | 63:LX:12:ARG:NH1   | 2.38                     | 0.55              |
| 46:LG:53:VAL:HG21  | 46:LG:159:VAL:HG23 | 1.88                     | 0.55              |
| 69:Ld:56:ALA:O     | 69:Ld:59:LYS:NZ    | 2.36                     | 0.55              |
| 86:A:1900:ALA:N    | 86:A:1900:ALA:CB   | 2.62                     | 0.55              |
| 86:A:2040:ALA:N    | 86:A:2040:ALA:C    | 2.59                     | 0.55              |
| 5:SE:102:PHE:O     | 5:SE:104:GLN:NE2   | 2.39                     | 0.55              |
| 9:SB:91:GLU:O      | 9:SB:95:ASN:ND2    | 2.40                     | 0.55              |
| 13:SW:31:ALA:HB2   | 13:SW:42:ILE:HD11  | 1.88                     | 0.55              |
| 40:LA:1141:C:O2'   | 40:LA:1153:A:N3    | 2.39                     | 0.55              |
| 40:LA:3109:G:OP1   | 80:Lo:93:LYS:NZ    | 2.39                     | 0.55              |
| 86:A:948:ALA:O     | 86:A:984:ALA:CB    | 2.54                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:S2:1298:U:O3'    | 6:SR:212:LYS:NZ   | 2.39                     | 0.55              |
| 5:SE:44:ARG:O      | 5:SE:47:ARG:C     | 2.49                     | 0.55              |
| 40:LA:1361:U:O2    | 48:LI:159:GLN:NE2 | 2.38                     | 0.55              |
| 40:LA:2241:U:HO2'  | 43:LD:243:THR:H   | 1.54                     | 0.55              |
| 40:LA:2722:U:OP1   | 69:Ld:33:LYS:NZ   | 2.39                     | 0.55              |
| 1:S2:1273:G:O2'    | 1:S2:1430:U:OP2   | 2.23                     | 0.55              |
| 28:SK:35:ARG:O     | 28:SK:37:GLN:NE2  | 2.39                     | 0.55              |
| 44:LE:137:TYR:O    | 44:LE:139:GLN:NE2 | 2.39                     | 0.55              |
| 60:LU:9:VAL:HG22   | 60:LU:61:ILE:HG13 | 1.87                     | 0.55              |
| 75:Lj:76:GLN:O     | 75:Lj:81:ARG:NH2  | 2.40                     | 0.55              |
| 1:S2:143:G:N7      | 10:ST:177:ARG:NH1 | 2.53                     | 0.55              |
| 40:LA:1940:G:OP1   | 59:LT:80:LYS:NZ   | 2.38                     | 0.55              |
| 40:LA:2688:U:OP1   | 46:LG:12:TYR:OH   | 2.24                     | 0.55              |
| 56:LQ:126[A]:VAL:O | 60:LU:154:HIS:NE2 | 2.31                     | 0.55              |
| 71:Lf:4:LEU:O      | 71:Lf:79:ARG:NH2  | 2.40                     | 0.55              |
| 86:A:1361:PRO:N    | 86:A:1361:PRO:C   | 2.59                     | 0.55              |
| 1:S2:1466:G:O2'    | 1:S2:1602:C:OP1   | 2.25                     | 0.55              |
| 6:SR:81:MET:HB2    | 6:SR:101:VAL:HG13 | 1.87                     | 0.55              |
| 23:SJ:80:GLU:OE1   | 31:SM:44:ARG:NH1  | 2.39                     | 0.55              |
| 34:SO:258:THR:HG22 | 34:SO:275:ARG:HD3 | 1.88                     | 0.55              |
| 34:SO:265:LEU:O    | 34:SO:268:GLN:NE2 | 2.40                     | 0.55              |
| 38:So:107:LEU:HB3  | 38:So:114:ILE:HB  | 1.89                     | 0.55              |
| 40:LA:401:U:O2'    | 79:Ln:36:ARG:NH2  | 2.40                     | 0.55              |
| 55:LP:155:VAL:O    | 55:LP:162:ARG:NH2 | 2.39                     | 0.55              |
| 86:A:927:ALA:HB1   | 86:A:930:ALA:H    | 1.71                     | 0.55              |
| 86:A:1675:ALA:CB   | 86:A:1714:ALA:HB2 | 2.30                     | 0.55              |
| 12:SV:103:GLN:HE21 | 12:SV:166:TYR:HE1 | 1.53                     | 0.55              |
| 31:SM:16:LYS:O     | 31:SM:27:HIS:ND1  | 2.40                     | 0.55              |
| 34:SO:270:LEU:HD21 | 34:SO:273:ASP:HB2 | 1.89                     | 0.55              |
| 1:S2:486:G:N2      | 1:S2:501:U:O2'    | 2.40                     | 0.55              |
| 6:SR:159:THR:HA    | 6:SR:167:VAL:O    | 2.07                     | 0.55              |
| 9:SB:154:ALA:O     | 9:SB:156:ARG:NH1  | 2.40                     | 0.55              |
| 42:LC:156:U:OP2    | 49:LJ:84:ARG:NH2  | 2.39                     | 0.55              |
| 61:LV:80:VAL:O     | 61:LV:83:ARG:NH1  | 2.39                     | 0.55              |
| 1:S2:447:U:O2'     | 8:SS:27:TYR:O     | 2.24                     | 0.55              |
| 1:S2:992:A:O2'     | 1:S2:1785:U:O2    | 2.20                     | 0.55              |
| 1:S2:1549:C:OP1    | 5:SE:42:ARG:NH2   | 2.39                     | 0.55              |
| 21:SH:142:GLY:O    | 21:SH:145:ARG:NH2 | 2.40                     | 0.55              |
| 38:So:152:ALA:HA   | 38:So:155:SER:HB3 | 1.88                     | 0.55              |
| 40:LA:1551:C:HO2'  | 40:LA:2170:U:HO2' | 1.54                     | 0.55              |
| 40:LA:2261:G:O2'   | 40:LA:2263:C:N4   | 2.40                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:LA:2679:A:O2'   | 52:LM:52:TYR:OH   | 2.23                     | 0.55              |
| 47:LH:42:LEU:O     | 47:LH:49:GLY:N    | 2.38                     | 0.55              |
| 63:LX:104:ASN:OD1  | 63:LX:108:GLU:N   | 2.40                     | 0.55              |
| 1:S2:458:G:OP1     | 27:Sd:109:LYS:NZ  | 2.38                     | 0.54              |
| 3:SP:103:THR:O     | 3:SP:106:SER:OG   | 2.25                     | 0.54              |
| 40:LA:689:U:H3     | 45:LF:227:THR:HG1 | 1.55                     | 0.54              |
| 40:LA:2989:U:H1'   | 44:LE:266:ARG:HG2 | 1.88                     | 0.54              |
| 64:LY:4:GLU:O      | 64:LY:12:LYS:CA   | 2.41                     | 0.54              |
| 40:LA:3348:G:H1    | 40:LA:3357:U:H3   | 1.54                     | 0.54              |
| 86:A:1260:ALA:HB3  | 86:A:1264:LYS:CB  | 2.36                     | 0.54              |
| 22:SI:138:GLN:HE21 | 86:A:1303:GLU:CA  | 2.21                     | 0.54              |
| 40:LA:408:A:N3     | 40:LA:655:C:O2'   | 2.36                     | 0.54              |
| 40:LA:1595:U:O2'   | 40:LA:1606:U:O2   | 2.26                     | 0.54              |
| 40:LA:1863:G:H4'   | 59:LT:82:LYS:HD3  | 1.87                     | 0.54              |
| 86:A:1639:ALA:HB1  | 86:A:1641:ALA:HB3 | 1.88                     | 0.54              |
| 45:LF:33:ASP:HB3   | 58:LS:22:ASP:HB2  | 1.90                     | 0.54              |
| 53:LN:180:ARG:HH11 | 76:Lk:11:LEU:HD22 | 1.73                     | 0.54              |
| 1:S2:1462:G:OP2    | 21:SH:143:ARG:NH1 | 2.39                     | 0.54              |
| 8:SS:139:VAL:HG13  | 8:SS:150:PRO:HG3  | 1.89                     | 0.54              |
| 83:Lr:33:GLN:OE1   | 83:Lr:49:ARG:NH1  | 2.40                     | 0.54              |
| 7:SA:164:VAL:HG23  | 7:SA:168:ILE:HD13 | 1.89                     | 0.54              |
| 22:SI:125:SER:OG   | 22:SI:127:ASN:OD1 | 2.20                     | 0.54              |
| 40:LA:592:A:O2'    | 47:LH:20:LYS:NZ   | 2.32                     | 0.54              |
| 40:LA:1178:G:N3    | 40:LA:1328:C:O2'  | 2.39                     | 0.54              |
| 40:LA:1886:A:O2'   | 44:LE:226:PHE:O   | 2.26                     | 0.54              |
| 40:LA:3275:U:O2'   | 73:Lh:99:ARG:NH1  | 2.40                     | 0.54              |
| 1:S2:1211:A:N3     | 5:SE:97:TYR:OH    | 2.39                     | 0.54              |
| 1:S2:1217:A:O3'    | 14:SC:44:LYS:NZ   | 2.39                     | 0.54              |
| 40:LA:20:A:OP2     | 75:Lj:86:ARG:NH2  | 2.40                     | 0.54              |
| 44:LE:227:GLU:HG2  | 44:LE:270:ARG:HE  | 1.73                     | 0.54              |
| 86:A:924:ALA:HA    | 86:A:933:ALA:O    | 2.07                     | 0.54              |
| 1:S2:105:A:O2'     | 12:SV:8:ARG:NH1   | 2.35                     | 0.54              |
| 1:S2:859:A:N1      | 17:SY:76:LYS:NZ   | 2.56                     | 0.54              |
| 40:LA:908:G:N2     | 40:LA:2415:C:OP2  | 2.41                     | 0.54              |
| 40:LA:2522:G:O6    | 43:LD:72:ARG:NH1  | 2.41                     | 0.54              |
| 40:LA:3039:C:O2'   | 63:LX:10:LYS:O    | 2.24                     | 0.54              |
| 47:LH:12:SER:OG    | 47:LH:14:ASP:OD1  | 2.26                     | 0.54              |
| 84:Ls:18:THR:HB    | 84:Ls:83:PRO:HA   | 1.89                     | 0.54              |
| 1:S2:1179:G:H21    | 1:S2:1460:A:H62   | 1.56                     | 0.54              |
| 12:SV:184:LEU:HD23 | 12:SV:189:LEU:HA  | 1.88                     | 0.54              |
| 16:SD:59:LEU:HD21  | 16:SD:137:MET:HE1 | 1.88                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:LI:86:VAL:O    | 48:LI:114:GLY:HA2  | 2.07                     | 0.54              |
| 86:A:1383:ARG:CB  | 86:A:1423:THR:CB   | 2.86                     | 0.54              |
| 1:S2:1546:G:N7    | 21:SH:134:ARG:NH2  | 2.56                     | 0.54              |
| 1:S2:1559:A:H5''  | 21:SH:135:GLY:HA3  | 1.90                     | 0.54              |
| 12:SV:23:LYS:O    | 12:SV:25:ARG:NH1   | 2.41                     | 0.54              |
| 12:SV:84:HIS:NE2  | 12:SV:97:THR:OG1   | 2.38                     | 0.54              |
| 22:SI:138:GLN:CA  | 86:A:1303:GLU:CB   | 2.85                     | 0.54              |
| 37:Sn:15:G:H22    | 37:Sn:48:C:H42     | 1.56                     | 0.54              |
| 41:LB:33:U:H1'    | 46:LG:206:GLN:HE22 | 1.73                     | 0.54              |
| 42:LC:11:C:O3'    | 57:LR:3:ARG:NH1    | 2.41                     | 0.54              |
| 86:A:1523:ALA:O   | 86:A:1527:ALA:CB   | 2.51                     | 0.54              |
| 19:SF:14:LYS:O    | 19:SF:123:ARG:NH1  | 2.41                     | 0.53              |
| 40:LA:2814:G:OP1  | 45:LF:73:ARG:NH1   | 2.35                     | 0.53              |
| 40:LA:3185:U:HO2' | 60:LU:170:THR:HG1  | 1.56                     | 0.53              |
| 43:LD:95:SER:O    | 43:LD:100:ASN:ND2  | 2.38                     | 0.53              |
| 86:A:917:ALA:HA   | 86:A:920:ALA:HB3   | 1.90                     | 0.53              |
| 86:A:1636:ALA:HB3 | 86:A:1674:ALA:CB   | 2.35                     | 0.53              |
| 86:A:1655:ALA:HB3 | 86:A:1658:ALA:HB2  | 1.89                     | 0.53              |
| 86:A:1705:ALA:CA  | 86:A:1815:ALA:HB1  | 2.37                     | 0.53              |
| 37:Sn:16:U:O4'    | 84:Ls:87:ARG:NH1   | 2.40                     | 0.53              |
| 63:LX:4:ASN:HD21  | 63:LX:57:MET:HE1   | 1.72                     | 0.53              |
| 86:A:1705:ALA:O   | 86:A:1815:ALA:CB   | 2.56                     | 0.53              |
| 9:SB:29:ILE:HB    | 9:SB:34:GLN:HE21   | 1.74                     | 0.53              |
| 26:Sc:68:ILE:HD12 | 32:Sg:7:SER:HB2    | 1.90                     | 0.53              |
| 40:LA:2554:A:H5'' | 74:Li:91:ARG:HH22  | 1.73                     | 0.53              |
| 86:A:965:ALA:C    | 86:A:969:ALA:HB2   | 2.33                     | 0.53              |
| 86:A:1482:ALA:O   | 86:A:1493:ALA:CB   | 2.56                     | 0.53              |
| 1:S2:1673:G:H1    | 1:S2:1728:A:H2     | 1.53                     | 0.53              |
| 28:SK:95:HIS:ND1  | 28:SK:96:SER:O     | 2.41                     | 0.53              |
| 33:SN:133:ALA:HB3 | 33:SN:140:TYR:HB3  | 1.90                     | 0.53              |
| 42:LC:150:G:H21   | 49:LJ:59:GLN:HE22  | 1.57                     | 0.53              |
| 6:SR:222:TYR:OH   | 24:Sa:11:LEU:O     | 2.21                     | 0.53              |
| 34:SO:295:SER:OG  | 34:SO:297:ASP:OD1  | 2.27                     | 0.53              |
| 40:LA:1778:G:O2'  | 40:LA:1780:G:OP2   | 2.26                     | 0.53              |
| 84:Ls:46:THR:HG22 | 84:Ls:57:VAL:HG22  | 1.89                     | 0.53              |
| 12:SV:3:ILE:O     | 12:SV:30:GLY:N     | 2.41                     | 0.53              |
| 16:SD:33:ARG:NH2  | 16:SD:99:GLU:O     | 2.42                     | 0.53              |
| 23:SJ:66:SER:HA   | 23:SJ:80:GLU:O     | 2.09                     | 0.53              |
| 73:Lh:46:GLY:N    | 73:Lh:71:VAL:O     | 2.41                     | 0.53              |
| 1:S2:1292:G:H21   | 3:SP:111:ILE:HD11  | 1.73                     | 0.53              |
| 34:SO:105:GLY:O   | 34:SO:107:LYS:NZ   | 2.42                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:LA:1447:G:OP2   | 57:LR:27:LYS:NZ   | 2.41                     | 0.53              |
| 40:LA:3306:U:OP1   | 44:LE:269:GLN:NE2 | 2.39                     | 0.53              |
| 45:LF:83:GLY:O     | 45:LF:87:GLN:NE2  | 2.41                     | 0.53              |
| 1:S2:142:G:H22     | 1:S2:173:A:H2     | 1.54                     | 0.53              |
| 1:S2:1445:G:N2     | 33:SN:87:THR:OG1  | 2.42                     | 0.53              |
| 4:SQ:79:HIS:NE2    | 4:SQ:189:ILE:O    | 2.42                     | 0.53              |
| 13:SW:107:ARG:NH1  | 13:SW:153:GLU:OE2 | 2.41                     | 0.53              |
| 40:LA:3210:A:OP1   | 54:LO:109:ARG:NH1 | 2.40                     | 0.53              |
| 60:LU:26:ARG:NH1   | 61:LV:150:THR:OG1 | 2.42                     | 0.53              |
| 86:A:1392:MET:O    | 86:A:1395:LEU:CB  | 2.57                     | 0.53              |
| 1:S2:7:G:OP2       | 6:SR:205:ARG:NH2  | 2.41                     | 0.53              |
| 19:SF:143:ARG:NH1  | 37:Sn:33:U:OP2    | 2.40                     | 0.53              |
| 26:Sc:130:VAL:HG13 | 26:Sc:140:LYS:HE2 | 1.91                     | 0.53              |
| 40:LA:591:G:O2'    | 47:LH:17:ALA:O    | 2.26                     | 0.53              |
| 40:LA:801:A:H61    | 53:LN:19:GLN:HE22 | 1.55                     | 0.53              |
| 40:LA:2654:C:OP2   | 82:Lq:2:VAL:N     | 2.42                     | 0.53              |
| 42:LC:13:A:O2'     | 57:LR:121:GLN:O   | 2.22                     | 0.53              |
| 50:LK:165:CYS:SG   | 50:LK:179:ILE:N   | 2.79                     | 0.53              |
| 1:S2:1311:U:O3'    | 20:SG:2:GLY:N     | 2.42                     | 0.53              |
| 8:SS:194:THR:OG1   | 8:SS:194:THR:O    | 2.27                     | 0.53              |
| 38:So:298:VAL:HB   | 38:So:363:GLU:HA  | 1.91                     | 0.53              |
| 40:LA:798:G:OP1    | 68:Lc:33:GLY:N    | 2.41                     | 0.53              |
| 40:LA:1468:A:N1    | 40:LA:1880:U:O2'  | 2.40                     | 0.53              |
| 44:LE:216:ASP:OD2  | 44:LE:339:ARG:NH2 | 2.42                     | 0.53              |
| 52:LM:60:ARG:N     | 52:LM:63:GLU:OE1  | 2.42                     | 0.53              |
| 65:LZ:115:ARG:O    | 65:LZ:118:GLY:N   | 2.42                     | 0.53              |
| 69:Ld:16:ALA:O     | 69:Ld:20:GLY:HA3  | 2.09                     | 0.53              |
| 84:Ls:33:VAL:HB    | 84:Ls:81:GLU:HG3  | 1.91                     | 0.53              |
| 86:A:1216:LYS:O    | 86:A:1226:ARG:O   | 2.27                     | 0.53              |
| 86:A:2100:ALA:HB1  | 86:A:2220:ALA:HB2 | 1.91                     | 0.53              |
| 1:S2:967:A:OP2     | 17:SY:124:ARG:NH2 | 2.42                     | 0.52              |
| 1:S2:1175:U:H2'    | 1:S2:1176:G:H8    | 1.75                     | 0.52              |
| 5:SE:50:THR:HG22   | 5:SE:52:LYS:HE3   | 1.91                     | 0.52              |
| 86:A:927:ALA:HB3   | 86:A:933:ALA:HB2  | 1.90                     | 0.52              |
| 1:S2:551:G:H2'     | 1:S2:552:G:H8     | 1.73                     | 0.52              |
| 1:S2:1775:U:OP1    | 81:Lp:11:ARG:NH1  | 2.41                     | 0.52              |
| 52:LM:134:PRO:O    | 52:LM:152:HIS:NE2 | 2.41                     | 0.52              |
| 66:La:33:ALA:HB2   | 66:La:101:PRO:HB2 | 1.91                     | 0.52              |
| 11:SU:22:GLN:HA    | 11:SU:25:VAL:HG22 | 1.92                     | 0.52              |
| 40:LA:3230:G:H4'   | 54:LO:132:LYS:HD3 | 1.91                     | 0.52              |
| 42:LC:27:U:H4'     | 45:LF:51:ALA:HB3  | 1.92                     | 0.52              |

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| Atom-1               | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 46:LG:50:ARG:NH1     | 46:LG:147:ASP:OD2     | 2.43                     | 0.52              |
| 73:Lh:38:PRO:HA      | 73:Lh:41:ALA:HB3      | 1.91                     | 0.52              |
| 1:S2:438:A:O2'       | 1:S2:465:G:N2         | 2.41                     | 0.52              |
| 1:S2:821:U:H3        | 1:S2:852:C:H42        | 1.56                     | 0.52              |
| 42:LC:143:U:OP1      | 55:LP:38:ARG:NH2      | 2.42                     | 0.52              |
| 49:LJ:143:ILE:HD11   | 49:LJ:151:VAL:HG11    | 1.91                     | 0.52              |
| 51:LL:50:VAL:HG11    | 51:LL:149:VAL:HG12    | 1.91                     | 0.52              |
| 51:LL:193:ASP:OD1    | 51:LL:198:LYS:NZ      | 2.42                     | 0.52              |
| 86:A:927:ALA:CB      | 86:A:933:ALA:H        | 2.21                     | 0.52              |
| 1:S2:636:A:H5''      | 25:Sb:31:SER:HB3      | 1.91                     | 0.52              |
| 1:S2:1245:G:O2'      | 1:S2:1247:U:OP2       | 2.22                     | 0.52              |
| 1:S2:1357:A:N3       | 22:SI:129:GLN:NE2     | 2.56                     | 0.52              |
| 40:LA:2564:G:OP2     | 67:Lb:55:LYS:NZ       | 2.41                     | 0.52              |
| 40:LA:3231:U:H2'     | 40:LA:3232:G:H8       | 1.73                     | 0.52              |
| 52:LM:165:GLN:OE1    | 86:A:1603:ALA:HB2     | 2.10                     | 0.52              |
| 86:A:1458:ALA:HB3    | 86:A:1461:ALA:HB2     | 1.86                     | 0.52              |
| 86:A:2240:ALA:N      | 86:A:2240:ALA:C       | 2.59                     | 0.52              |
| 1:S2:217:A:N1        | 1:S2:844:A:O2'        | 2.40                     | 0.52              |
| 1:S2:930:A:N3        | 4:SQ:111:ARG:NH2      | 2.57                     | 0.52              |
| 1:S2:1218:G:O2'      | 1:S2:1265:G:N2        | 2.43                     | 0.52              |
| 1:S2:1465:C:H5'      | 19:SF:139:GLN:HG2     | 1.91                     | 0.52              |
| 1:S2:1722:A:H1'      | 10:ST:67:VAL:HA       | 1.90                     | 0.52              |
| 8:SS:11:ARG:NH2      | 8:SS:21:ASP:O         | 2.43                     | 0.52              |
| 38:So:122:ILE:HG21   | 38:So:169:VAL:HG11    | 1.91                     | 0.52              |
| 40:LA:860:G:OP1      | 83:Lr:17:ARG:NH2      | 2.42                     | 0.52              |
| 40:LA:2722:U:O2'     | 61:LV:88:ARG:O        | 2.25                     | 0.52              |
| 41:LB:2:G:H1         | 41:LB:119:U:H3        | 1.57                     | 0.52              |
| 55:LP:27:VAL:HG13    | 55:LP:31:ARG:HH21     | 1.75                     | 0.52              |
| 56:LQ:125[A]:ARG:HG3 | 56:LQ:129[A]:LEU:HD12 | 1.91                     | 0.52              |
| 1:S2:139:C:O2'       | 1:S2:177:U:O2         | 2.25                     | 0.52              |
| 9:SB:77:TYR:HD1      | 9:SB:83:ARG:HG2       | 1.74                     | 0.52              |
| 9:SB:196:GLU:O       | 9:SB:200:ASN:ND2      | 2.43                     | 0.52              |
| 26:Sc:114:LYS:HB3    | 26:Sc:117:ILE:HD11    | 1.92                     | 0.52              |
| 34:SO:182:ASN:O      | 34:SO:186:PHE:N       | 2.43                     | 0.52              |
| 34:SO:299:GLN:O      | 34:SO:314:GLN:HA      | 2.10                     | 0.52              |
| 36:Sm:27:G:H22       | 36:Sm:43:U:H3         | 1.58                     | 0.52              |
| 40:LA:1604:G:H4'     | 40:LA:1835:A:H4'      | 1.91                     | 0.52              |
| 70:Le:40:LYS:HB3     | 70:Le:101:LEU:HD11    | 1.91                     | 0.52              |
| 78:Lm:66:ILE:HA      | 78:Lm:69:LEU:HD12     | 1.91                     | 0.52              |
| 86:A:1803:ALA:HA     | 86:A:1806:ALA:HB3     | 1.92                     | 0.52              |
| 1:S2:278:U:O2        | 1:S2:279:G:N1         | 2.43                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:S2:1603:U:OP2     | 19:SF:132:LYS:NZ    | 2.36                     | 0.52              |
| 4:SQ:82:ARG:NH1     | 4:SQ:191:GLU:OE2    | 2.42                     | 0.52              |
| 29:Se:87:ARG:NH1    | 29:Se:91:ASP:O      | 2.43                     | 0.52              |
| 40:LA:286:U:O2'     | 55:LP:179:LYS:O     | 2.28                     | 0.52              |
| 86:A:1282:LEU:O     | 86:A:1286:VAL:N     | 2.36                     | 0.52              |
| 1:S2:1204:A:OP1     | 1:S2:1456:C:N4      | 2.43                     | 0.52              |
| 4:SQ:141:ALA:HA     | 4:SQ:209:ASN:O      | 2.10                     | 0.52              |
| 15:SX:125:VAL:HG12  | 15:SX:139:VAL:HG12  | 1.92                     | 0.52              |
| 38:So:354:CYS:SG    | 38:So:355:GLY:N     | 2.83                     | 0.52              |
| 40:LA:874:U:N3      | 40:LA:2978:U:OP1    | 2.34                     | 0.52              |
| 40:LA:2382:G:N7     | 56:LQ:91[A]:LYS:NZ  | 2.58                     | 0.52              |
| 56:LQ:49[A]:ARG:HD2 | 56:LQ:53[A]:LYS:HE3 | 1.91                     | 0.52              |
| 61:LV:78:LYS:HD3    | 61:LV:87:LYS:HZ2    | 1.75                     | 0.52              |
| 63:LX:93:LEU:HA     | 64:LY:20:LEU:O      | 2.10                     | 0.52              |
| 86:A:1535:ALA:O     | 86:A:1539:ALA:HB2   | 2.10                     | 0.52              |
| 1:S2:395:U:O4       | 1:S2:399:A:N7       | 2.43                     | 0.52              |
| 40:LA:938:C:O2      | 40:LA:2813:A:O2'    | 2.27                     | 0.52              |
| 40:LA:1016:C:N4     | 40:LA:2671:A:OP1    | 2.42                     | 0.52              |
| 40:LA:1410:U:H4'    | 72:Lg:75:LEU:HD11   | 1.92                     | 0.52              |
| 40:LA:2144:A:OP1    | 40:LA:2323:G:N2     | 2.42                     | 0.52              |
| 40:LA:2404:A:N7     | 40:LA:2872:A:N6     | 2.58                     | 0.52              |
| 40:LA:3000:A:O2'    | 44:LE:118:PHE:O     | 2.28                     | 0.52              |
| 43:LD:39:GLY:HA3    | 49:LJ:36:ILE:HD13   | 1.92                     | 0.52              |
| 43:LD:150:LEU:O     | 43:LD:153:GLY:N     | 2.43                     | 0.52              |
| 47:LH:149:ILE:HG23  | 47:LH:155:LEU:HD23  | 1.92                     | 0.52              |
| 49:LJ:251:LYS:O     | 49:LJ:255:SER:OG    | 2.24                     | 0.52              |
| 86:A:927:ALA:H      | 86:A:933:ALA:HB3    | 1.75                     | 0.52              |
| 86:A:2203:ALA:HA    | 86:A:2206:ALA:HB3   | 1.92                     | 0.52              |
| 1:S2:343:C:H2'      | 1:S2:344:A:H8       | 1.76                     | 0.51              |
| 1:S2:1473:U:OP2     | 9:SB:189:THR:OG1    | 2.26                     | 0.51              |
| 11:SU:27:LEU:O      | 11:SU:31:SER:OG     | 2.22                     | 0.51              |
| 11:SU:77:LEU:HD22   | 11:SU:92:PHE:HZ     | 1.74                     | 0.51              |
| 28:SK:50:ILE:HG22   | 28:SK:69:LEU:HD13   | 1.92                     | 0.51              |
| 29:Se:7:SER:OG      | 29:Se:10:ARG:O      | 2.27                     | 0.51              |
| 40:LA:280:U:O2'     | 55:LP:182:ASN:ND2   | 2.41                     | 0.51              |
| 84:Ls:72:ASP:OD1    | 84:Ls:72:ASP:N      | 2.42                     | 0.51              |
| 86:A:1428:ALA:CB    | 86:A:1464:ALA:HB3   | 2.38                     | 0.51              |
| 13:SW:136:VAL:HB    | 13:SW:152:SER:HB3   | 1.91                     | 0.51              |
| 40:LA:3153:U:OP2    | 40:LA:3293:U:O2'    | 2.23                     | 0.51              |
| 86:A:2411:ALA:N     | 86:A:2411:ALA:CB    | 2.62                     | 0.51              |
| 1:S2:918:U:O3'      | 18:SZ:18:ARG:NH1    | 2.42                     | 0.51              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:S2:1303:U:O2'   | 1:S2:1322:A:OP2     | 2.28                     | 0.51              |
| 86:A:1163:LEU:O   | 86:A:1165:GLU:N     | 2.44                     | 0.51              |
| 86:A:1538:ALA:HB3 | 86:A:1574:ALA:HB1   | 1.93                     | 0.51              |
| 40:LA:398:A:N7    | 57:LR:3:ARG:NH2     | 2.59                     | 0.51              |
| 40:LA:2183:A:H5'' | 43:LD:7:ASN:HB3     | 1.92                     | 0.51              |
| 40:LA:2768:U:H2'  | 40:LA:2769:A:H8     | 1.75                     | 0.51              |
| 51:LL:38:LYS:HG3  | 51:LL:41:ALA:HB2    | 1.93                     | 0.51              |
| 1:S2:936:G:N7     | 29:Se:15:ARG:NH2    | 2.59                     | 0.51              |
| 1:S2:1471:A:H2    | 1:S2:1474:G:H21     | 1.58                     | 0.51              |
| 4:SQ:78:ASP:OD1   | 4:SQ:79:HIS:ND1     | 2.41                     | 0.51              |
| 4:SQ:195:LYS:O    | 4:SQ:199:ASN:ND2    | 2.43                     | 0.51              |
| 6:SR:225:LEU:HD12 | 24:Sa:23:ILE:HG12   | 1.92                     | 0.51              |
| 37:Sn:15:G:N2     | 37:Sn:48:C:H42      | 2.08                     | 0.51              |
| 40:LA:1348:U:OP2  | 58:LS:38:ARG:NH2    | 2.44                     | 0.51              |
| 40:LA:1928:G:N2   | 40:LA:2320:A:O2'    | 2.41                     | 0.51              |
| 40:LA:2555:G:OP2  | 74:Li:91:ARG:NH2    | 2.43                     | 0.51              |
| 40:LA:3214:U:H6   | 47:LH:166:LYS:HE2   | 1.76                     | 0.51              |
| 45:LF:330:TYR:HA  | 45:LF:333:VAL:HG22  | 1.92                     | 0.51              |
| 48:LI:30:ARG:HA   | 48:LI:33:ARG:HE     | 1.76                     | 0.51              |
| 6:SR:142:GLY:N    | 6:SR:153:SER:O      | 2.41                     | 0.51              |
| 10:ST:79:LYS:HB3  | 10:ST:86:PRO:HG3    | 1.92                     | 0.51              |
| 20:SG:44:LYS:HG3  | 20:SG:47:ARG:HH21   | 1.75                     | 0.51              |
| 34:SO:224:ASN:O   | 34:SO:228:LYS:N     | 2.43                     | 0.51              |
| 40:LA:104:G:O2'   | 40:LA:698:U:O2      | 2.28                     | 0.51              |
| 40:LA:718:G:OP1   | 68:Lc:117:ARG:NH2   | 2.43                     | 0.51              |
| 40:LA:876:A:H5''  | 40:LA:1890:U:H5''   | 1.93                     | 0.51              |
| 40:LA:3008:A:OP2  | 56:LQ:74[A]:ARG:NH1 | 2.44                     | 0.51              |
| 1:S2:588:U:O2     | 32:Sg:57:ASN:ND2    | 2.44                     | 0.51              |
| 1:S2:752:A:O2'    | 8:SS:221:ARG:NE     | 2.44                     | 0.51              |
| 40:LA:1795:U:N3   | 83:Lr:50:GLY:O      | 2.42                     | 0.51              |
| 42:LC:57:C:OP2    | 77:Ll:68:LYS:NZ     | 2.43                     | 0.51              |
| 53:LN:27:ASP:O    | 53:LN:31:LYS:HB2    | 2.11                     | 0.51              |
| 86:A:1221:ALA:C   | 86:A:1222:VAL:CA    | 2.82                     | 0.51              |
| 1:S2:428:A:N3     | 1:S2:440:U:O2'      | 2.39                     | 0.51              |
| 40:LA:2349:U:O2'  | 40:LA:3307:A:N3     | 2.43                     | 0.51              |
| 69:Ld:16:ALA:O    | 69:Ld:20:GLY:HA2    | 2.11                     | 0.51              |
| 86:A:987:ALA:HB2  | 86:A:988:ALA:HB2    | 1.92                     | 0.51              |
| 86:A:2271:ALA:O   | 86:A:2274:ALA:CB    | 2.59                     | 0.51              |
| 1:S2:1795:U:O4    | 29:Se:34:LYS:NZ     | 2.44                     | 0.51              |
| 13:SW:60:LEU:HB2  | 13:SW:93:LEU:HD23   | 1.92                     | 0.51              |
| 38:So:184:LYS:NZ  | 38:So:218:ASN:OD1   | 2.44                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:2745:G:N2    | 40:LA:2748:A:OP2   | 2.38                     | 0.51              |
| 72:Lg:97:ALA:O     | 72:Lg:105:ARG:NH2  | 2.44                     | 0.51              |
| 78:Lm:3:ARG:HD2    | 78:Lm:52:TYR:HE1   | 1.76                     | 0.51              |
| 1:S2:354:C:H5''    | 12:SV:16:ALA:HB2   | 1.93                     | 0.51              |
| 1:S2:1206:U:H3'    | 1:S2:1207:C:H2'    | 1.93                     | 0.51              |
| 22:SI:65:ILE:HD13  | 22:SI:71:VAL:HG22  | 1.93                     | 0.51              |
| 40:LA:169:U:H4'    | 53:LN:128:ARG:HH11 | 1.76                     | 0.51              |
| 40:LA:769:G:O2'    | 53:LN:168:ARG:NH1  | 2.39                     | 0.51              |
| 44:LE:163:HIS:HA   | 44:LE:177:HIS:O    | 2.11                     | 0.51              |
| 44:LE:368:GLY:O    | 64:LY:17:ARG:NH1   | 2.44                     | 0.51              |
| 45:LF:33:ASP:N     | 45:LF:33:ASP:OD1   | 2.41                     | 0.51              |
| 45:LF:203:ARG:NH1  | 45:LF:226:GLU:OE2  | 2.44                     | 0.51              |
| 54:LO:94:TRP:O     | 54:LO:97:SER:OG    | 2.28                     | 0.51              |
| 55:LP:27:VAL:O     | 55:LP:31:ARG:HB2   | 2.11                     | 0.51              |
| 63:LX:10:LYS:NZ    | 63:LX:56:ASP:OD1   | 2.42                     | 0.51              |
| 83:Lr:46:THR:O     | 83:Lr:57:CYS:HA    | 2.10                     | 0.51              |
| 86:A:2003:ALA:HA   | 86:A:2006:ALA:HB3  | 1.92                     | 0.51              |
| 86:A:2104:ALA:CB   | 86:A:2210:ALA:O    | 2.59                     | 0.51              |
| 86:A:2382:ALA:O    | 86:A:2385:ALA:CB   | 2.59                     | 0.51              |
| 1:S2:397:A:H4'     | 12:SV:50:GLY:HA2   | 1.92                     | 0.50              |
| 1:S2:1584:G:N2     | 1:S2:1611:A:OP2    | 2.45                     | 0.50              |
| 40:LA:2854:U:H4'   | 51:LL:160:PRO:HD3  | 1.93                     | 0.50              |
| 44:LE:66:LYS:NZ    | 63:LX:9:THR:OG1    | 2.43                     | 0.50              |
| 47:LH:56:LYS:NZ    | 47:LH:101:PHE:O    | 2.44                     | 0.50              |
| 73:Lh:31:LYS:NZ    | 73:Lh:32:ILE:O     | 2.37                     | 0.50              |
| 86:A:921:ALA:O     | 86:A:925:ALA:CB    | 2.59                     | 0.50              |
| 86:A:1482:ALA:C    | 86:A:1493:ALA:CB   | 2.84                     | 0.50              |
| 1:S2:66:U:H5''     | 10:ST:173:PRO:HA   | 1.92                     | 0.50              |
| 47:LH:102:ASN:ND2  | 47:LH:104:GLU:OE1  | 2.44                     | 0.50              |
| 78:Lm:32:ASN:OD1   | 78:Lm:33:LYS:N     | 2.44                     | 0.50              |
| 4:SQ:69:CYS:SG     | 18:SZ:114:ARG:NH1  | 2.85                     | 0.50              |
| 11:SU:34:LEU:HD22  | 11:SU:38:LEU:HD21  | 1.93                     | 0.50              |
| 49:LJ:162:LEU:HD21 | 55:LP:45:PRO:HG2   | 1.93                     | 0.50              |
| 86:A:927:ALA:CB    | 86:A:933:ALA:CB    | 2.82                     | 0.50              |
| 86:A:2071:ALA:O    | 86:A:2074:ALA:CB   | 2.59                     | 0.50              |
| 86:A:2100:ALA:HA   | 86:A:2215:ALA:C    | 2.21                     | 0.50              |
| 40:LA:3045:G:OP1   | 44:LE:19:ARG:NH2   | 2.41                     | 0.50              |
| 44:LE:17:LEU:HD11  | 44:LE:233:TRP:HH2  | 1.75                     | 0.50              |
| 84:Ls:116:PRO:HG3  | 84:Ls:147:ALA:HB3  | 1.94                     | 0.50              |
| 86:A:1871:ALA:O    | 86:A:1874:ALA:CB   | 2.59                     | 0.50              |
| 7:SA:9:ARG:HA      | 7:SA:12:VAL:HG22   | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:SW:96:VAL:HA    | 13:SW:99:LEU:HG    | 1.93                     | 0.50              |
| 20:SG:27:ASP:HB3   | 20:SG:30:THR:HG22  | 1.94                     | 0.50              |
| 45:LF:345:GLU:OE1  | 45:LF:347:THR:OG1  | 2.29                     | 0.50              |
| 50:LK:173:ARG:NH1  | 80:Lo:125:LYS:O    | 2.45                     | 0.50              |
| 1:S2:127:G:O6      | 10:ST:202:ARG:NH2  | 2.44                     | 0.50              |
| 1:S2:467:G:O2'     | 1:S2:469:C:OP2     | 2.29                     | 0.50              |
| 15:SX:101:GLU:OE1  | 26:Sc:16:ARG:NH1   | 2.45                     | 0.50              |
| 37:Sn:76:A:OP1     | 40:LA:2808:A:N6    | 2.45                     | 0.50              |
| 44:LE:43:LEU:HB2   | 44:LE:208:VAL:HG23 | 1.94                     | 0.50              |
| 44:LE:88:GLY:HA2   | 44:LE:105:VAL:O    | 2.11                     | 0.50              |
| 86:A:1187:SER:CB   | 86:A:1225:VAL:CB   | 2.89                     | 0.50              |
| 21:SH:49:LYS:NZ    | 21:SH:80:LYS:O     | 2.44                     | 0.50              |
| 36:Sm:53:G:N7      | 36:Sm:54:U:N3      | 2.60                     | 0.50              |
| 38:So:342:VAL:HG23 | 38:So:366:VAL:HG22 | 1.94                     | 0.50              |
| 40:LA:1861:G:O2'   | 40:LA:3066:U:OP1   | 2.27                     | 0.50              |
| 40:LA:3241:G:OP2   | 44:LE:153:LYS:NZ   | 2.44                     | 0.50              |
| 42:LC:8:C:H2'      | 42:LC:9:A:H8       | 1.76                     | 0.50              |
| 1:S2:861:U:OP2     | 1:S2:862:A:N6      | 2.44                     | 0.50              |
| 40:LA:1523:U:OP2   | 40:LA:1604:G:O2'   | 2.30                     | 0.50              |
| 40:LA:2808:A:H2'   | 84:Ls:51:5CT:H9    | 1.94                     | 0.50              |
| 40:LA:2901:G:O2'   | 40:LA:3024:A:N1    | 2.43                     | 0.50              |
| 44:LE:26:ARG:HD3   | 44:LE:177:HIS:HD2  | 1.77                     | 0.50              |
| 86:A:1706:ALA:O    | 86:A:1708:ALA:N    | 2.44                     | 0.50              |
| 1:S2:1315:U:OP2    | 1:S2:1328:G:N1     | 2.39                     | 0.50              |
| 5:SE:24:LYS:HB3    | 5:SE:28:MET:HE2    | 1.94                     | 0.50              |
| 13:SW:151:ASP:O    | 13:SW:155:HIS:ND1  | 2.45                     | 0.50              |
| 40:LA:939:U:O2'    | 40:LA:2402:A:N1    | 2.41                     | 0.50              |
| 40:LA:1497:C:O2'   | 40:LA:1602:A:N3    | 2.38                     | 0.50              |
| 48:LI:184:LEU:HD21 | 48:LI:202:LEU:HD21 | 1.94                     | 0.50              |
| 51:LL:211:ARG:NH1  | 51:LL:212:GLU:OE2  | 2.44                     | 0.50              |
| 55:LP:62:TYR:HD2   | 55:LP:106:VAL:HG13 | 1.77                     | 0.50              |
| 72:Lg:59:SER:HB2   | 72:Lg:64:LYS:HG3   | 1.94                     | 0.50              |
| 84:Ls:43:ASP:HB2   | 84:Ls:60:VAL:HB    | 1.94                     | 0.50              |
| 40:LA:351:A:N6     | 79:Ln:37:TYR:O     | 2.30                     | 0.49              |
| 40:LA:646:A:H61    | 40:LA:2371:G:H21   | 1.60                     | 0.49              |
| 40:LA:1899:G:O2'   | 40:LA:2334:U:O4    | 2.25                     | 0.49              |
| 40:LA:1914:G:N2    | 59:LT:81:ARG:O     | 2.41                     | 0.49              |
| 47:LH:2:THR:OG1    | 72:Lg:81:ASP:OD2   | 2.23                     | 0.49              |
| 59:LT:105:LEU:HD23 | 59:LT:138:LEU:HD23 | 1.94                     | 0.49              |
| 86:A:965:ALA:C     | 86:A:969:ALA:CB    | 2.80                     | 0.49              |
| 1:S2:64:U:O2'      | 1:S2:168:A:N3      | 2.40                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:S2:572:C:OP1     | 26:Sc:109:ARG:NH1   | 2.45                     | 0.49              |
| 1:S2:705:U:O2'     | 1:S2:706:A:O5'      | 2.29                     | 0.49              |
| 1:S2:1688:U:H3     | 1:S2:1713:G:H1      | 1.60                     | 0.49              |
| 10:ST:44:GLU:O     | 10:ST:119:GLN:NE2   | 2.44                     | 0.49              |
| 12:SV:138:ASN:OD1  | 12:SV:141:ARG:NH2   | 2.45                     | 0.49              |
| 12:SV:152:ILE:HG23 | 15:SX:24:LYS:HE3    | 1.93                     | 0.49              |
| 17:SY:47:PRO:HG2   | 17:SY:72:MET:HE2    | 1.94                     | 0.49              |
| 40:LA:1268:G:N2    | 40:LA:1269:U:O4     | 2.45                     | 0.49              |
| 44:LE:284:ARG:HH22 | 44:LE:296:THR:HG22  | 1.77                     | 0.49              |
| 49:LJ:162:LEU:HA   | 55:LP:7:LEU:HD11    | 1.94                     | 0.49              |
| 68:Lc:76:ASP:OD1   | 68:Lc:76:ASP:N      | 2.44                     | 0.49              |
| 40:LA:348:A:N3     | 40:LA:352:A:O2'     | 2.46                     | 0.49              |
| 40:LA:2742:C:H2'   | 40:LA:2743:A:H8     | 1.77                     | 0.49              |
| 40:LA:2948:C:OP1   | 44:LE:244:ARG:NH2   | 2.45                     | 0.49              |
| 40:LA:3135:U:OP1   | 56:LQ:148[A]:LYS:NZ | 2.39                     | 0.49              |
| 70:Le:9:SER:OG     | 70:Le:10:ILE:N      | 2.43                     | 0.49              |
| 84:Ls:94:ASP:HA    | 84:Ls:128:PHE:HZ    | 1.76                     | 0.49              |
| 86:A:1637:ALA:H    | 86:A:1676:ALA:HB2   | 1.76                     | 0.49              |
| 40:LA:3009:G:N2    | 44:LE:15:GLY:O      | 2.36                     | 0.49              |
| 68:Lc:96:LYS:NZ    | 68:Lc:142:GLY:O     | 2.45                     | 0.49              |
| 86:A:2212:ALA:HA   | 86:A:2215:ALA:HB3   | 1.94                     | 0.49              |
| 1:S2:1747:G:O2'    | 40:LA:2303:A:O2'    | 2.27                     | 0.49              |
| 14:SC:47:GLN:O     | 14:SC:50:THR:OG1    | 2.29                     | 0.49              |
| 40:LA:86:G:O2'     | 40:LA:98:G:O6       | 2.29                     | 0.49              |
| 40:LA:98:G:N7      | 53:LN:13:HIS:NE2    | 2.60                     | 0.49              |
| 40:LA:3026:G:N2    | 40:LA:3029:A:OP2    | 2.46                     | 0.49              |
| 58:LS:67:ILE:HG23  | 58:LS:81:VAL:HG21   | 1.95                     | 0.49              |
| 74:Li:41:ARG:O     | 74:Li:43:LYS:NZ     | 2.45                     | 0.49              |
| 86:A:2072:ALA:O    | 86:A:2074:ALA:N     | 2.44                     | 0.49              |
| 1:S2:861:U:OP1     | 17:SY:64:ARG:NH2    | 2.46                     | 0.49              |
| 6:SR:81:MET:HG3    | 6:SR:211:LEU:HD11   | 1.94                     | 0.49              |
| 40:LA:2307:G:O2'   | 40:LA:2310:U:OP2    | 2.31                     | 0.49              |
| 40:LA:2452:G:O6    | 40:LA:2493:U:N3     | 2.46                     | 0.49              |
| 40:LA:2848:G:OP1   | 80:Lo:100:TYR:OH    | 2.29                     | 0.49              |
| 48:LI:88:ARG:NH1   | 48:LI:108:LEU:O     | 2.41                     | 0.49              |
| 72:Lg:101:SER:OG   | 72:Lg:104:ASN:OD1   | 2.31                     | 0.49              |
| 86:A:1635:ALA:O    | 86:A:1639:ALA:HB3   | 2.13                     | 0.49              |
| 1:S2:195:G:N7      | 12:SV:137:LYS:NZ    | 2.51                     | 0.49              |
| 1:S2:611:U:OP1     | 26:Sc:19:ARG:NH1    | 2.42                     | 0.49              |
| 25:Sb:90:THR:HA    | 25:Sb:94:LEU:HD23   | 1.93                     | 0.49              |
| 41:LB:72:A:O2'     | 41:LB:74:C:OP1      | 2.29                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 84:Ls:97:ASP:O     | 84:Ls:99:PHE:N     | 2.46                     | 0.49              |
| 86:A:2104:ALA:HB1  | 86:A:2210:ALA:C    | 2.37                     | 0.49              |
| 1:S2:385:A:H5''    | 12:SV:22:ARG:HG2   | 1.93                     | 0.49              |
| 12:SV:152:ILE:HD12 | 15:SX:24:LYS:HE3   | 1.94                     | 0.49              |
| 14:SC:11:ILE:HD11  | 14:SC:42:VAL:HG22  | 1.95                     | 0.49              |
| 25:Sb:3:ARG:NH1    | 25:Sb:9:ASP:OD2    | 2.46                     | 0.49              |
| 40:LA:2785:A:O2'   | 82:Lq:41:ARG:NH2   | 2.45                     | 0.49              |
| 1:S2:258:C:O2      | 12:SV:178:ARG:NH2  | 2.41                     | 0.49              |
| 1:S2:388:G:O3'     | 1:S2:425:A:N6      | 2.45                     | 0.49              |
| 1:S2:929:A:OP1     | 1:S2:931:C:N4      | 2.45                     | 0.49              |
| 4:SQ:25:THR:O      | 4:SQ:50:LYS:NZ     | 2.46                     | 0.49              |
| 40:LA:2101:C:O2'   | 40:LA:2102:U:O5'   | 2.29                     | 0.49              |
| 45:LF:330:TYR:O    | 45:LF:334:PHE:CB   | 2.61                     | 0.49              |
| 71:Lf:20:LEU:HD11  | 71:Lf:32:ALA:HB2   | 1.95                     | 0.49              |
| 84:Ls:89:GLU:HA    | 84:Ls:137:THR:HG22 | 1.95                     | 0.49              |
| 84:Ls:90:TYR:HB3   | 84:Ls:102:LEU:HB3  | 1.94                     | 0.49              |
| 86:A:988:ALA:C     | 86:A:990:ALA:H     | 2.19                     | 0.49              |
| 1:S2:1332:C:OP1    | 20:SG:43:SER:OG    | 2.30                     | 0.49              |
| 8:SS:65:LEU:HD13   | 8:SS:70:VAL:HG11   | 1.95                     | 0.49              |
| 40:LA:90:C:O2'     | 40:LA:282:G:OP1    | 2.30                     | 0.49              |
| 40:LA:542:G:H1     | 40:LA:549:U:H3     | 1.61                     | 0.49              |
| 40:LA:990:U:H1'    | 61:LV:101:CYS:HB3  | 1.95                     | 0.49              |
| 40:LA:1907:C:O2    | 44:LE:240:ARG:NH2  | 2.26                     | 0.49              |
| 40:LA:3111:U:OP1   | 50:LK:184:LYS:NZ   | 2.46                     | 0.49              |
| 40:LA:3243:A:H4'   | 44:LE:95:THR:HG22  | 1.93                     | 0.49              |
| 86:A:2383:ALA:O    | 86:A:2385:ALA:N    | 2.45                     | 0.49              |
| 1:S2:812:A:O4'     | 1:S2:858:G:N2      | 2.45                     | 0.48              |
| 11:SU:135:ILE:HD11 | 11:SU:138:LYS:HD3  | 1.95                     | 0.48              |
| 40:LA:528:U:H2'    | 40:LA:529:A:C8     | 2.48                     | 0.48              |
| 40:LA:839:C:H4'    | 40:LA:1724:U:H2'   | 1.94                     | 0.48              |
| 40:LA:925:A:N6     | 40:LA:2415:C:OP1   | 2.46                     | 0.48              |
| 55:LP:23:GLN:NE2   | 55:LP:122:ASN:OD1  | 2.46                     | 0.48              |
| 1:S2:61:A:O2'      | 1:S2:62:A:O4'      | 2.31                     | 0.48              |
| 12:SV:57:ALA:HB2   | 12:SV:177:GLY:HA2  | 1.95                     | 0.48              |
| 40:LA:38:U:H4'     | 68:Lc:32:ARG:HD2   | 1.93                     | 0.48              |
| 40:LA:838:G:O6     | 83:Lr:4:ARG:NH1    | 2.39                     | 0.48              |
| 42:LC:104:A:OP1    | 77:Ll:21:ARG:NH1   | 2.46                     | 0.48              |
| 68:Lc:82:ILE:HD11  | 68:Lc:102:ILE:HD11 | 1.95                     | 0.48              |
| 86:A:1840:ALA:N    | 86:A:1840:ALA:CB   | 2.67                     | 0.48              |
| 1:S2:788:A:N1      | 8:SS:51:ARG:NH2    | 2.61                     | 0.48              |
| 1:S2:979:A:N3      | 1:S2:1775:U:O2'    | 2.47                     | 0.48              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:S2:1042:G:H2'     | 1:S2:1043:A:H8       | 1.78                     | 0.48              |
| 1:S2:1182:U:H4'     | 5:SE:124:THR:HB      | 1.95                     | 0.48              |
| 1:S2:1528:U:O2'     | 19:SF:42:GLU:OE1     | 2.23                     | 0.48              |
| 7:SA:142:LEU:HD13   | 7:SA:150:MET:HE3     | 1.95                     | 0.48              |
| 8:SS:17:HIS:HB2     | 8:SS:108:ARG:HA      | 1.96                     | 0.48              |
| 17:SY:62:GLN:HG3    | 17:SY:65:VAL:HG22    | 1.96                     | 0.48              |
| 86:A:1457:ALA:O     | 86:A:1461:ALA:HB3    | 2.13                     | 0.48              |
| 86:A:2351:ALA:N     | 86:A:2351:ALA:CB     | 2.67                     | 0.48              |
| 1:S2:498:G:O2'      | 1:S2:499:U:O2        | 2.26                     | 0.48              |
| 15:SX:93:TYR:OH     | 15:SX:98:ASN:OD1     | 2.31                     | 0.48              |
| 40:LA:1046:A:O2'    | 40:LA:1048:A:OP2     | 2.24                     | 0.48              |
| 40:LA:1813:A:O2'    | 40:LA:1816:A:N3      | 2.42                     | 0.48              |
| 44:LE:183:LEU:O     | 44:LE:191:LYS:NZ     | 2.47                     | 0.48              |
| 45:LF:217:LYS:O     | 45:LF:220:ARG:HB3    | 2.14                     | 0.48              |
| 47:LH:43:LEU:HD11   | 47:LH:85:ILE:HG13    | 1.94                     | 0.48              |
| 56:LQ:42[A]:ASN:OD1 | 56:LQ:125[A]:ARG:NH1 | 2.47                     | 0.48              |
| 84:Ls:63:ASP:HB2    | 84:Ls:68:LYS:H       | 1.78                     | 0.48              |
| 86:A:930:ALA:N      | 86:A:932:ALA:H       | 2.11                     | 0.48              |
| 86:A:1458:ALA:O     | 86:A:1459:ALA:C      | 2.55                     | 0.48              |
| 86:A:1668:ALA:O     | 86:A:1672:ALA:N      | 2.46                     | 0.48              |
| 86:A:2100:ALA:C     | 86:A:2215:ALA:HB1    | 2.39                     | 0.48              |
| 86:A:2272:ALA:O     | 86:A:2274:ALA:N      | 2.44                     | 0.48              |
| 9:SB:100:ASN:HD22   | 9:SB:180:ARG:HD3     | 1.79                     | 0.48              |
| 37:Sn:15:G:H22      | 37:Sn:48:C:N4        | 2.09                     | 0.48              |
| 40:LA:1580:A:H8     | 40:LA:2522:G:H21     | 1.60                     | 0.48              |
| 40:LA:3242:G:O6     | 44:LE:150:ARG:NH2    | 2.47                     | 0.48              |
| 42:LC:40:A:OP2      | 42:LC:103:G:N1       | 2.46                     | 0.48              |
| 42:LC:126:A:O2'     | 42:LC:128:U:OP2      | 2.26                     | 0.48              |
| 43:LD:45:VAL:HG22   | 43:LD:61:VAL:HG22    | 1.95                     | 0.48              |
| 86:A:1393:ALA:O     | 86:A:1395:LEU:N      | 2.45                     | 0.48              |
| 86:A:1551:ALA:O     | 86:A:1554:ALA:O      | 2.32                     | 0.48              |
| 86:A:1640:ALA:C     | 86:A:1642:ALA:N      | 2.72                     | 0.48              |
| 1:S2:748:U:O3'      | 25:Sb:122:SER:OG     | 2.32                     | 0.48              |
| 22:SI:84:LYS:HE2    | 22:SI:86:ARG:HG2     | 1.96                     | 0.48              |
| 22:SI:138:GLN:NE2   | 86:A:1302:LYS:O      | 2.31                     | 0.48              |
| 27:Sd:86:GLU:OE1    | 27:Sd:90:ARG:NH1     | 2.47                     | 0.48              |
| 30:Sf:55:THR:OG1    | 30:Sf:56:CYS:N       | 2.46                     | 0.48              |
| 38:So:67:ARG:HD2    | 38:So:143:ALA:HA     | 1.94                     | 0.48              |
| 38:So:184:LYS:HG3   | 38:So:216:ILE:HD11   | 1.95                     | 0.48              |
| 40:LA:1601:U:OP1    | 59:LT:42:ARG:NH2     | 2.42                     | 0.48              |
| 1:S2:1280:C:OP1     | 31:SM:44:ARG:NH2     | 2.46                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S2:1441:C:O2'    | 1:S2:1447:C:N4     | 2.47                     | 0.48              |
| 3:SP:156:VAL:O     | 24:Sa:65:SER:OG    | 2.26                     | 0.48              |
| 21:SH:67:GLU:HA    | 21:SH:70:VAL:HG22  | 1.96                     | 0.48              |
| 26:Sc:104:LEU:HA   | 26:Sc:123:LYS:O    | 2.14                     | 0.48              |
| 27:Sd:2:SER:OG     | 27:Sd:3:ASP:N      | 2.45                     | 0.48              |
| 40:LA:515:C:OP1    | 45:LF:343:LYS:NZ   | 2.45                     | 0.48              |
| 18:SZ:92:LYS:HZ3   | 29:Se:69:ASN:HB2   | 1.79                     | 0.48              |
| 19:SF:95:LYS:HD2   | 34:SO:59:ARG:HH22  | 1.77                     | 0.48              |
| 25:Sb:18:GLU:HG3   | 25:Sb:69:LEU:HD23  | 1.95                     | 0.48              |
| 40:LA:590:G:O2'    | 45:LF:309:ARG:NH1  | 2.46                     | 0.48              |
| 40:LA:691:A:N1     | 42:LC:28:C:O2'     | 2.40                     | 0.48              |
| 45:LF:57:GLY:HA3   | 45:LF:98:ARG:HB3   | 1.95                     | 0.48              |
| 53:LN:3:ILE:HD13   | 68:Lc:45:MET:HE3   | 1.95                     | 0.48              |
| 53:LN:170:LEU:HD21 | 68:Lc:147:LEU:HD13 | 1.96                     | 0.48              |
| 54:LO:15:VAL:HG12  | 54:LO:65:LEU:HD11  | 1.95                     | 0.48              |
| 85:Lt:203:UNK:O    | 85:Lt:205:UNK:N    | 2.47                     | 0.48              |
| 86:A:965:ALA:N     | 86:A:969:ALA:HB2   | 2.21                     | 0.48              |
| 86:A:1705:ALA:HA   | 86:A:1815:ALA:CB   | 2.43                     | 0.48              |
| 1:S2:418:G:H8      | 10:ST:59:GLN:HE21  | 1.62                     | 0.48              |
| 1:S2:1149:G:N2     | 1:S2:1766:A:OP1    | 2.46                     | 0.48              |
| 1:S2:1677:C:O3'    | 12:SV:59:ARG:NH1   | 2.47                     | 0.48              |
| 12:SV:20:GLN:NE2   | 12:SV:22:ARG:O     | 2.47                     | 0.48              |
| 21:SH:122:HIS:HE1  | 21:SH:126:ARG:HH11 | 1.62                     | 0.48              |
| 22:SI:138:GLN:HB3  | 86:A:1303:GLU:CB   | 2.40                     | 0.48              |
| 23:SJ:70:THR:OG1   | 23:SJ:72:ASN:OD1   | 2.32                     | 0.48              |
| 40:LA:727:G:OP2    | 40:LA:742:G:N2     | 2.45                     | 0.48              |
| 40:LA:799:G:H2'    | 40:LA:801:A:H62    | 1.79                     | 0.48              |
| 42:LC:151:C:OP1    | 49:LJ:60:ARG:NH2   | 2.46                     | 0.48              |
| 53:LN:157:ARG:NH2  | 68:Lc:146:GLU:OE2  | 2.47                     | 0.48              |
| 1:S2:68:A:N6       | 10:ST:132:ARG:O    | 2.34                     | 0.48              |
| 9:SB:117:THR:HG21  | 9:SB:194:LEU:HD23  | 1.96                     | 0.48              |
| 21:SH:17:LEU:HD21  | 21:SH:66:LEU:HD23  | 1.96                     | 0.48              |
| 26:Sc:132:LEU:HD23 | 26:Sc:135:LEU:HD12 | 1.94                     | 0.48              |
| 36:Sm:15:G:N2      | 36:Sm:21:A:N3      | 2.61                     | 0.48              |
| 38:So:150:LEU:HD11 | 38:So:249:TYR:HD1  | 1.79                     | 0.48              |
| 38:So:262:VAL:HG22 | 38:So:273:VAL:HG11 | 1.96                     | 0.48              |
| 40:LA:612:U:H4'    | 47:LH:21:THR:HG21  | 1.94                     | 0.48              |
| 40:LA:638:C:OP1    | 72:Lg:21:HIS:NE2   | 2.42                     | 0.48              |
| 40:LA:1546:A:N7    | 55:LP:71:ARG:NH2   | 2.58                     | 0.48              |
| 86:A:1599:ALA:CB   | 86:A:1604:ALA:H    | 2.27                     | 0.48              |
| 1:S2:1754:A:O2'    | 26:Sc:60:GLU:OE2   | 2.31                     | 0.47              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 7:SA:25:PHE:HD2    | 7:SA:37:VAL:HG11     | 1.79                     | 0.47              |
| 10:ST:223:LYS:O    | 10:ST:226:ILE:C      | 2.58                     | 0.47              |
| 38:So:37:ARG:HB2   | 38:So:214:TYR:HE1    | 1.79                     | 0.47              |
| 40:LA:664:U:H2'    | 40:LA:665:A:C8       | 2.49                     | 0.47              |
| 86:A:1138:THR:HA   | 86:A:1139:VAL:HA     | 1.69                     | 0.47              |
| 86:A:1593:ALA:HB1  | 86:A:1631:ALA:HB2    | 1.96                     | 0.47              |
| 1:S2:511:A:H5''    | 13:SW:172:VAL:HG13   | 1.95                     | 0.47              |
| 1:S2:1253:U:H5''   | 33:SN:130:VAL:HG23   | 1.96                     | 0.47              |
| 8:SS:183:VAL:HG11  | 8:SS:188:ASN:HB2     | 1.97                     | 0.47              |
| 11:SU:142:TYR:O    | 25:Sb:42:GLN:NE2     | 2.40                     | 0.47              |
| 37:Sn:75:C:OP2     | 51:LL:110:ARG:NH1    | 2.47                     | 0.47              |
| 40:LA:217:U:O2     | 66:La:103:LYS:NZ     | 2.35                     | 0.47              |
| 40:LA:1312:C:O2'   | 56:LQ:83[A]:ALA:O    | 2.32                     | 0.47              |
| 40:LA:2392:C:O2'   | 44:LE:266:ARG:NH2    | 2.47                     | 0.47              |
| 45:LF:26:PHE:CD1   | 45:LF:130:ALA:HB2    | 2.49                     | 0.47              |
| 86:A:1872:ALA:O    | 86:A:1874:ALA:N      | 2.44                     | 0.47              |
| 86:A:2104:ALA:H    | 86:A:2215:ALA:HB2    | 1.79                     | 0.47              |
| 86:A:2240:ALA:N    | 86:A:2240:ALA:CB     | 2.67                     | 0.47              |
| 86:A:2262:ALA:CB   | 86:A:2302:ALA:CB     | 2.89                     | 0.47              |
| 1:S2:4:C:OP2       | 6:SR:200:SER:OG      | 2.24                     | 0.47              |
| 1:S2:399:A:N3      | 8:SS:3:ARG:NH2       | 2.62                     | 0.47              |
| 1:S2:1785:U:H2'    | 1:S2:1786:G:H8       | 1.80                     | 0.47              |
| 11:SU:162:ILE:HA   | 11:SU:165:LYS:HE2    | 1.95                     | 0.47              |
| 40:LA:720:A:OP1    | 58:LS:72:LYS:NZ      | 2.37                     | 0.47              |
| 64:LY:6:ASP:HB3    | 64:LY:11:ALA:H       | 1.79                     | 0.47              |
| 1:S2:31:C:O2'      | 1:S2:547:U:OP1       | 2.32                     | 0.47              |
| 1:S2:59:C:O2'      | 1:S2:60:U:O4'        | 2.31                     | 0.47              |
| 9:SB:129:PRO:HA    | 9:SB:132:VAL:HG22    | 1.96                     | 0.47              |
| 40:LA:838:G:N7     | 83:Lr:4:ARG:NH2      | 2.56                     | 0.47              |
| 40:LA:1203:A:N3    | 40:LA:2855:U:O2'     | 2.46                     | 0.47              |
| 43:LD:190:ARG:HG3  | 43:LD:191:LEU:HD12   | 1.96                     | 0.47              |
| 56:LQ:27[A]:LEU:HG | 56:LQ:33[A]:ILE:HD12 | 1.96                     | 0.47              |
| 38:So:67:ARG:NH2   | 40:LA:3027:A:N3      | 2.63                     | 0.47              |
| 44:LE:313:HIS:HB2  | 44:LE:332:ARG:HG3    | 1.95                     | 0.47              |
| 45:LF:8:VAL:HG13   | 45:LF:151:VAL:HG12   | 1.97                     | 0.47              |
| 63:LX:18:PRO:HA    | 63:LX:51:ALA:HA      | 1.96                     | 0.47              |
| 67:Lb:41:ALA:HB2   | 67:Lb:77:TYR:HE1     | 1.79                     | 0.47              |
| 1:S2:207:U:O2      | 12:SV:178:ARG:NH1    | 2.47                     | 0.47              |
| 1:S2:477:A:O2'     | 32:Sg:33:ARG:NH2     | 2.48                     | 0.47              |
| 1:S2:1785:U:OP2    | 18:SZ:133:ARG:NH1    | 2.45                     | 0.47              |
| 20:SG:108:ASP:HA   | 20:SG:111:LYS:HG2    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:LA:801:A:N6    | 53:LN:19:GLN:HE22 | 2.11                     | 0.47              |
| 40:LA:910:G:O6    | 43:LD:3:ARG:NH2   | 2.48                     | 0.47              |
| 40:LA:1447:G:N7   | 57:LR:25:SER:OG   | 2.32                     | 0.47              |
| 40:LA:1621:A:N7   | 40:LA:1820:U:O4   | 2.47                     | 0.47              |
| 40:LA:1868:G:HO2' | 40:LA:2118:C:HO2' | 1.58                     | 0.47              |
| 42:LC:36:G:OP1    | 77:Ll:66:TYR:OH   | 2.27                     | 0.47              |
| 62:LW:89:LEU:HB3  | 62:LW:93:ILE:HD12 | 1.95                     | 0.47              |
| 84:Ls:37:ARG:NH2  | 84:Ls:66:THR:OG1  | 2.41                     | 0.47              |
| 1:S2:58:U:O2'     | 1:S2:451:A:N3     | 2.45                     | 0.47              |
| 1:S2:473:A:OP1    | 13:SW:44:ARG:NH1  | 2.40                     | 0.47              |
| 1:S2:1482:C:H4'   | 19:SF:77:GLN:HE22 | 1.80                     | 0.47              |
| 5:SE:44:ARG:O     | 5:SE:47:ARG:O     | 2.31                     | 0.47              |
| 8:SS:103:TYR:HB2  | 8:SS:182:TYR:HE2  | 1.79                     | 0.47              |
| 23:SJ:56:VAL:O    | 23:SJ:89:ARG:HA   | 2.14                     | 0.47              |
| 40:LA:116:A:OP2   | 76:Lk:36:ARG:NH2  | 2.41                     | 0.47              |
| 40:LA:645:A:N6    | 40:LA:2869:U:OP1  | 2.48                     | 0.47              |
| 40:LA:990:U:H4'   | 61:LV:100:LYS:HB3 | 1.97                     | 0.47              |
| 40:LA:1134:G:O2'  | 40:LA:2642:A:N3   | 2.42                     | 0.47              |
| 40:LA:1494:U:OP1  | 79:Ln:42:ARG:NH1  | 2.42                     | 0.47              |
| 40:LA:1799:A:H2'  | 40:LA:1800:A:H8   | 1.80                     | 0.47              |
| 42:LC:8:C:H2'     | 42:LC:9:A:C8      | 2.50                     | 0.47              |
| 42:LC:97:A:O2'    | 75:Lj:59:ASN:OD1  | 2.30                     | 0.47              |
| 86:A:1636:ALA:CB  | 86:A:1677:ALA:HB2 | 2.38                     | 0.47              |
| 86:A:2062:ALA:CB  | 86:A:2102:ALA:CB  | 2.89                     | 0.47              |
| 1:S2:329:G:H2'    | 1:S2:330:G:H8     | 1.80                     | 0.47              |
| 1:S2:479:C:H2'    | 1:S2:480:G:H8     | 1.80                     | 0.47              |
| 1:S2:1488:G:H3'   | 1:S2:1515:A:H61   | 1.80                     | 0.47              |
| 3:SP:84:ARG:NH1   | 3:SP:203:PHE:O    | 2.48                     | 0.47              |
| 4:SQ:149:GLN:HE22 | 4:SQ:154:SER:HB3  | 1.80                     | 0.47              |
| 12:SV:22:ARG:HE   | 12:SV:25:ARG:NH2  | 2.13                     | 0.47              |
| 12:SV:81:VAL:HG12 | 12:SV:94:ASN:HA   | 1.96                     | 0.47              |
| 34:SO:69:GLN:HB2  | 34:SO:85:TRP:CD1  | 2.50                     | 0.47              |
| 40:LA:1003:A:N1   | 40:LA:1049:C:O2'  | 2.43                     | 0.47              |
| 40:LA:1062:A:N3   | 61:LV:130:ARG:NH2 | 2.60                     | 0.47              |
| 40:LA:1150:A:O2'  | 73:Lh:21:ARG:NH1  | 2.47                     | 0.47              |
| 40:LA:2724:U:OP2  | 40:LA:2726:C:N4   | 2.48                     | 0.47              |
| 1:S2:753:A:H8     | 8:SS:187:ARG:HH22 | 1.62                     | 0.47              |
| 1:S2:1426:C:H3'   | 1:S2:1427:A:H4'   | 1.97                     | 0.47              |
| 1:S2:1541:G:N2    | 1:S2:1570:A:H62   | 2.11                     | 0.47              |
| 21:SH:14:ILE:HG21 | 52:LM:118:PRO:HD3 | 1.97                     | 0.47              |
| 26:Sc:97:ASP:OD2  | 38:So:224:ARG:NH2 | 2.48                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:218:G:O6     | 66:La:62:SER:OG    | 2.29                     | 0.47              |
| 44:LE:221:THR:O    | 44:LE:272:TYR:N    | 2.47                     | 0.47              |
| 53:LN:136:GLU:O    | 75:Lj:119:LYS:NZ   | 2.40                     | 0.47              |
| 66:La:47:ALA:O     | 66:La:122:LYS:NZ   | 2.48                     | 0.47              |
| 67:Lb:11:ALA:HB2   | 67:Lb:25:ILE:HD11  | 1.97                     | 0.47              |
| 12:SV:106:ALA:HB2  | 12:SV:165:LEU:HB2  | 1.96                     | 0.47              |
| 19:SF:95:LYS:O     | 34:SO:59:ARG:NH1   | 2.30                     | 0.47              |
| 23:SJ:22:ILE:HG22  | 23:SJ:118:VAL:HG22 | 1.97                     | 0.47              |
| 40:LA:1748:G:OP2   | 78:Lm:42:LYS:NZ    | 2.40                     | 0.47              |
| 41:LB:28:C:OP1     | 52:LM:141:ARG:NH1  | 2.48                     | 0.47              |
| 43:LD:126:LEU:HD12 | 43:LD:150:LEU:HD22 | 1.95                     | 0.47              |
| 67:Lb:114:VAL:O    | 67:Lb:118:PHE:N    | 2.47                     | 0.47              |
| 71:Lf:41:LYS:HD3   | 71:Lf:47:ASP:HA    | 1.97                     | 0.47              |
| 1:S2:246:G:N2      | 15:SX:38:ALA:O     | 2.48                     | 0.46              |
| 1:S2:863:A:OP1     | 25:Sb:57:ARG:NH2   | 2.41                     | 0.46              |
| 1:S2:1114:G:O2'    | 1:S2:1130:G:O6     | 2.31                     | 0.46              |
| 1:S2:1198:G:OP1    | 1:S2:1199:G:O2'    | 2.26                     | 0.46              |
| 1:S2:1358:G:O2'    | 22:SI:133:ASP:OD2  | 2.27                     | 0.46              |
| 34:SO:108:SER:OG   | 34:SO:128:ASP:N    | 2.48                     | 0.46              |
| 40:LA:726:G:N1     | 40:LA:743:C:OP2    | 2.44                     | 0.46              |
| 40:LA:764:U:O2'    | 40:LA:766:U:OP2    | 2.31                     | 0.46              |
| 86:A:987:ALA:HB2   | 86:A:988:ALA:CB    | 2.45                     | 0.46              |
| 86:A:1457:ALA:HB1  | 86:A:1462:ALA:HB2  | 1.97                     | 0.46              |
| 18:SZ:80:HIS:HA    | 18:SZ:113:GLY:O    | 2.15                     | 0.46              |
| 30:Sf:15:GLU:O     | 30:Sf:29:ARG:NH2   | 2.48                     | 0.46              |
| 40:LA:655:C:OP2    | 72:Lg:27:ARG:NH1   | 2.39                     | 0.46              |
| 40:LA:826:G:OP1    | 40:LA:1590:G:O2'   | 2.30                     | 0.46              |
| 40:LA:1238:C:N4    | 40:LA:1245:A:OP2   | 2.47                     | 0.46              |
| 40:LA:2556:C:H41   | 43:LD:42:ARG:HH22  | 1.62                     | 0.46              |
| 50:LK:133:THR:HG1  | 50:LK:147:SER:HG   | 1.63                     | 0.46              |
| 54:LO:60:LEU:HD13  | 60:LU:152:LEU:HD11 | 1.98                     | 0.46              |
| 86:A:2373:ALA:CB   | 86:A:2413:ALA:CB   | 2.89                     | 0.46              |
| 1:S2:56:U:OP1      | 1:S2:403:G:N1      | 2.35                     | 0.46              |
| 1:S2:1755:A:O4'    | 26:Sc:63:GLN:NE2   | 2.48                     | 0.46              |
| 3:SP:17:LEU:HD22   | 3:SP:22:THR:HG21   | 1.96                     | 0.46              |
| 5:SE:37:ALA:O      | 5:SE:42:ARG:NH1    | 2.48                     | 0.46              |
| 7:SA:154:ASP:OD1   | 7:SA:154:ASP:N     | 2.48                     | 0.46              |
| 11:SU:141:ARG:HB2  | 11:SU:149:ILE:HB   | 1.96                     | 0.46              |
| 12:SV:48:THR:OG1   | 12:SV:52:ASN:O     | 2.28                     | 0.46              |
| 40:LA:36:C:O2'     | 40:LA:808:A:N1     | 2.47                     | 0.46              |
| 40:LA:424:G:O2'    | 72:Lg:23:ASP:OD2   | 2.31                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S2:419:G:H5'     | 10:ST:72:ARG:HH21  | 1.79                     | 0.46              |
| 6:SR:236:PRO:O     | 24:Sa:33:GLN:NE2   | 2.48                     | 0.46              |
| 11:SU:49:ILE:O     | 11:SU:57:ALA:N     | 2.47                     | 0.46              |
| 21:SH:51:ASP:OD2   | 86:A:1379:ALA:HB3  | 2.15                     | 0.46              |
| 36:Sm:74:C:O2'     | 40:LA:2862:U:OP1   | 2.31                     | 0.46              |
| 40:LA:3379:C:H4'   | 44:LE:315:GLY:HA2  | 1.96                     | 0.46              |
| 55:LP:31:ARG:HG3   | 55:LP:129:TYR:OH   | 2.15                     | 0.46              |
| 55:LP:48:ALA:HB1   | 55:LP:53:TYR:HB3   | 1.97                     | 0.46              |
| 60:LU:109:ASP:OD1  | 60:LU:113:ARG:NH1  | 2.43                     | 0.46              |
| 64:LY:4:GLU:HG2    | 64:LY:30:ARG:HH11  | 1.80                     | 0.46              |
| 71:Lf:87:ASN:HD22  | 71:Lf:88:PRO:HD2   | 1.80                     | 0.46              |
| 86:A:1655:ALA:C    | 86:A:1657:ALA:H    | 2.24                     | 0.46              |
| 4:SQ:71:ALA:HB2    | 4:SQ:80:SER:HA     | 1.97                     | 0.46              |
| 13:SW:112:GLN:NE2  | 13:SW:153:GLU:OE2  | 2.48                     | 0.46              |
| 40:LA:3330:A:H4'   | 44:LE:366:GLY:HA3  | 1.97                     | 0.46              |
| 42:LC:63:G:H1      | 42:LC:97:A:N6      | 2.05                     | 0.46              |
| 43:LD:142:ASP:N    | 43:LD:142:ASP:OD1  | 2.49                     | 0.46              |
| 46:LG:126:GLU:HA   | 46:LG:196:ARG:HD2  | 1.96                     | 0.46              |
| 57:LR:29:THR:HG23  | 57:LR:119:VAL:HG11 | 1.98                     | 0.46              |
| 70:Le:25:LEU:O     | 70:Le:29:SER:OG    | 2.33                     | 0.46              |
| 86:A:1810:ALA:O    | 86:A:1814:ALA:N    | 2.49                     | 0.46              |
| 1:S2:707:A:N7      | 1:S2:731:C:N4      | 2.62                     | 0.46              |
| 1:S2:1085:G:N2     | 1:S2:1088:A:OP2    | 2.42                     | 0.46              |
| 49:LJ:228:GLU:O    | 49:LJ:232:HIS:ND1  | 2.49                     | 0.46              |
| 51:LL:54:SER:HB2   | 51:LL:135:ILE:HD11 | 1.97                     | 0.46              |
| 65:LZ:137:ASN:HB3  | 65:LZ:142:ILE:HD11 | 1.98                     | 0.46              |
| 1:S2:590:C:OP1     | 32:Sg:42:ARG:NH2   | 2.30                     | 0.46              |
| 3:SP:70:PRO:HB2    | 3:SP:94:GLY:HA3    | 1.97                     | 0.46              |
| 13:SW:89:ASP:OD1   | 13:SW:89:ASP:N     | 2.49                     | 0.46              |
| 23:SJ:28:SER:OG    | 23:SJ:29:THR:N     | 2.48                     | 0.46              |
| 34:SO:167:VAL:HG13 | 34:SO:183:LEU:HD21 | 1.96                     | 0.46              |
| 34:SO:261:LYS:NZ   | 34:SO:273:ASP:OD2  | 2.47                     | 0.46              |
| 40:LA:341:G:O2'    | 42:LC:22:U:O4      | 2.31                     | 0.46              |
| 40:LA:831:G:O2'    | 40:LA:1864:A:N3    | 2.44                     | 0.46              |
| 40:LA:1240:A:H61   | 40:LA:1244:A:H2'   | 1.81                     | 0.46              |
| 40:LA:1243:G:N2    | 40:LA:1270:A:O2'   | 2.49                     | 0.46              |
| 40:LA:3231:U:H2'   | 40:LA:3232:G:C8    | 2.51                     | 0.46              |
| 46:LG:197:SER:O    | 46:LG:202:GLY:N    | 2.48                     | 0.46              |
| 51:LL:169:LYS:NZ   | 61:LV:160:ILE:O    | 2.42                     | 0.46              |
| 73:Lh:37:THR:OG1   | 73:Lh:39:GLN:OE1   | 2.25                     | 0.46              |
| 83:Lr:75:ALA:O     | 83:Lr:78:THR:OG1   | 2.28                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 84:Ls:92:LEU:CB    | 84:Ls:134:LEU:O    | 2.63                     | 0.46              |
| 86:A:930:ALA:C     | 86:A:932:ALA:H     | 2.23                     | 0.46              |
| 86:A:2010:ALA:O    | 86:A:2014:ALA:N    | 2.49                     | 0.46              |
| 1:S2:405:C:O2'     | 10:ST:92:ARG:O     | 2.28                     | 0.46              |
| 1:S2:1489:U:O2'    | 1:S2:1492:A:N3     | 2.47                     | 0.46              |
| 1:S2:1523:G:OP2    | 1:S2:1523:G:N2     | 2.44                     | 0.46              |
| 1:S2:1665:U:O2     | 1:S2:1736:G:O6     | 2.34                     | 0.46              |
| 10:ST:3:LEU:HD13   | 10:ST:18:ILE:HG21  | 1.97                     | 0.46              |
| 18:SZ:18:ARG:HB2   | 18:SZ:29:HIS:O     | 2.16                     | 0.46              |
| 22:SI:134:ARG:HB2  | 86:A:1301:HIS:HA   | 1.34                     | 0.46              |
| 29:Se:13:LYS:O     | 29:Se:15:ARG:NH1   | 2.49                     | 0.46              |
| 40:LA:1595:U:OP2   | 74:Li:36:LYS:NZ    | 2.48                     | 0.46              |
| 40:LA:2107:A:H2    | 40:LA:3344:A:H8    | 1.63                     | 0.46              |
| 40:LA:2151:C:O2'   | 40:LA:2243:A:N1    | 2.43                     | 0.46              |
| 40:LA:2688:U:N3    | 46:LG:17:GLN:O     | 2.49                     | 0.46              |
| 40:LA:2997:G:H1    | 40:LA:3151:U:H3    | 1.64                     | 0.46              |
| 46:LG:128:GLU:O    | 46:LG:164:LYS:NZ   | 2.34                     | 0.46              |
| 84:Ls:88:ASN:HD22  | 84:Ls:138:ILE:HD11 | 1.79                     | 0.46              |
| 86:A:1872:ALA:C    | 86:A:1874:ALA:N    | 2.73                     | 0.46              |
| 1:S2:65:A:H2       | 1:S2:84:A:H62      | 1.63                     | 0.46              |
| 1:S2:472:U:O2'     | 1:S2:769:A:N3      | 2.40                     | 0.46              |
| 1:S2:1022:C:O2'    | 1:S2:1125:A:N1     | 2.42                     | 0.46              |
| 1:S2:1161:C:H1'    | 1:S2:1619:C:H42    | 1.81                     | 0.46              |
| 11:SU:166:LEU:HD12 | 11:SU:183:PHE:CG   | 2.51                     | 0.46              |
| 21:SH:140:THR:O    | 21:SH:143:ARG:NE   | 2.49                     | 0.46              |
| 29:Se:66:LYS:NZ    | 29:Se:68:TYR:OH    | 2.49                     | 0.46              |
| 30:Sf:30:SER:OG    | 30:Sf:31:TYR:N     | 2.49                     | 0.46              |
| 38:So:152:ALA:HB2  | 38:So:251:TYR:HB3  | 1.98                     | 0.46              |
| 40:LA:3299:A:H61   | 40:LA:3315:G:H1    | 1.64                     | 0.46              |
| 57:LR:47:TYR:OH    | 57:LR:57:ALA:O     | 2.33                     | 0.46              |
| 66:La:60:ARG:HG2   | 66:La:103:LYS:HD2  | 1.96                     | 0.46              |
| 68:Lc:114:GLY:O    | 68:Lc:137:LYS:NZ   | 2.49                     | 0.46              |
| 86:A:2072:ALA:C    | 86:A:2074:ALA:N    | 2.73                     | 0.46              |
| 8:SS:72:VAL:HG22   | 8:SS:90:ILE:HD13   | 1.96                     | 0.46              |
| 18:SZ:43:THR:HG23  | 18:SZ:46:MET:H     | 1.81                     | 0.46              |
| 38:So:301:LYS:HB3  | 38:So:367:SER:HA   | 1.98                     | 0.46              |
| 40:LA:221:A:O2'    | 40:LA:223:U:OP2    | 2.25                     | 0.46              |
| 40:LA:1473:G:O3'   | 59:LT:23:TRP:NE1   | 2.48                     | 0.46              |
| 40:LA:1631:C:OP2   | 67:Lb:48:ARG:NH2   | 2.36                     | 0.46              |
| 43:LD:45:VAL:O     | 43:LD:85:GLY:N     | 2.49                     | 0.46              |
| 1:S2:1316:G:OP1    | 20:SG:7:LYS:N      | 2.48                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:LA:436:A:OP2   | 40:LA:621:A:N6     | 2.36                     | 0.45              |
| 40:LA:1695:U:O2'  | 40:LA:1749:A:N1    | 2.36                     | 0.45              |
| 40:LA:2452:G:N2   | 40:LA:2494:A:C6    | 2.85                     | 0.45              |
| 63:LX:38:ALA:HB3  | 63:LX:59:MET:HB2   | 1.98                     | 0.45              |
| 1:S2:140:A:H1'    | 10:ST:184:LEU:HD11 | 1.98                     | 0.45              |
| 1:S2:968:U:OP1    | 1:S2:1033:C:O2'    | 2.34                     | 0.45              |
| 34:SO:132:LYS:HA  | 34:SO:143:THR:HA   | 1.98                     | 0.45              |
| 34:SO:175:ASP:OD2 | 34:SO:179:LYS:NZ   | 2.48                     | 0.45              |
| 40:LA:198:A:N3    | 40:LA:218:G:O2'    | 2.42                     | 0.45              |
| 41:LB:63:A:O2'    | 41:LB:65:G:O4'     | 2.35                     | 0.45              |
| 46:LG:34:LYS:O    | 46:LG:38:THR:OG1   | 2.25                     | 0.45              |
| 51:LL:77:THR:HG22 | 51:LL:82:ARG:HA    | 1.98                     | 0.45              |
| 67:Lb:88:ASP:O    | 67:Lb:121:ARG:NH1  | 2.37                     | 0.45              |
| 86:A:1415:ALA:CB  | 86:A:1427:ALA:CB   | 2.54                     | 0.45              |
| 1:S2:16:G:O6      | 6:SR:203:LYS:NZ    | 2.37                     | 0.45              |
| 1:S2:1202:A:O2'   | 1:S2:1204:A:OP2    | 2.29                     | 0.45              |
| 1:S2:1294:G:H1    | 1:S2:1303:U:H3     | 1.64                     | 0.45              |
| 1:S2:1523:G:N7    | 22:SI:64:HIS:NE2   | 2.60                     | 0.45              |
| 4:SQ:137:ILE:HD11 | 4:SQ:172:LEU:HB3   | 1.97                     | 0.45              |
| 40:LA:707:U:O2    | 40:LA:754:G:O2'    | 2.34                     | 0.45              |
| 40:LA:901:G:P     | 77:Ll:13:ASN:HD21  | 2.39                     | 0.45              |
| 40:LA:1203:A:H2'  | 40:LA:1204:A:C8    | 2.52                     | 0.45              |
| 45:LF:166:VAL:HA  | 45:LF:169:LEU:HD12 | 1.98                     | 0.45              |
| 50:LK:41:ILE:HD13 | 50:LK:71:VAL:HB    | 1.99                     | 0.45              |
| 86:A:1331:LEU:O   | 86:A:1335:ILE:N    | 2.48                     | 0.45              |
| 86:A:2321:ALA:O   | 86:A:2325:ALA:N    | 2.48                     | 0.45              |
| 1:S2:21:U:O2      | 13:SW:17:ARG:NH1   | 2.49                     | 0.45              |
| 1:S2:1288:G:OP1   | 1:S2:1624:C:O2'    | 2.34                     | 0.45              |
| 1:S2:1353:U:H3    | 1:S2:1372:U:H3     | 1.64                     | 0.45              |
| 4:SQ:33:LYS:HG3   | 4:SQ:42:ASN:HA     | 1.99                     | 0.45              |
| 38:So:8:ILE:HD11  | 38:So:39:ARG:HD2   | 1.97                     | 0.45              |
| 40:LA:743:C:O2'   | 58:LS:66:ARG:NH2   | 2.45                     | 0.45              |
| 40:LA:837:A:H3'   | 40:LA:838:G:H8     | 1.80                     | 0.45              |
| 41:LB:38:U:N3     | 41:LB:41:G:OP2     | 2.49                     | 0.45              |
| 45:LF:217:LYS:HB3 | 45:LF:220:ARG:HH21 | 1.82                     | 0.45              |
| 49:LJ:74:THR:HA   | 49:LJ:77:GLN:HG3   | 1.98                     | 0.45              |
| 50:LK:167:VAL:HB  | 50:LK:172:ILE:HG22 | 1.99                     | 0.45              |
| 60:LU:132:THR:HB  | 60:LU:144:LEU:HD13 | 1.98                     | 0.45              |
| 86:A:2272:ALA:C   | 86:A:2274:ALA:N    | 2.73                     | 0.45              |
| 15:SX:16:GLN:NE2  | 15:SX:61:THR:OG1   | 2.50                     | 0.45              |
| 17:SY:13:SER:OG   | 17:SY:14:SER:N     | 2.49                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 34:SO:33:LEU:HB3     | 34:SO:45:TRP:HB2     | 1.98                     | 0.45              |
| 40:LA:1757:A:H4'     | 62:LW:96:VAL:HG13    | 1.97                     | 0.45              |
| 40:LA:2815:G:N2      | 40:LA:2818:U:O2      | 2.46                     | 0.45              |
| 47:LH:66:THR:HB      | 47:LH:76:LEU:HD23    | 1.98                     | 0.45              |
| 49:LJ:227:ASP:OD1    | 49:LJ:227:ASP:N      | 2.45                     | 0.45              |
| 79:Ln:27:ILE:O       | 79:Ln:33:ASN:ND2     | 2.49                     | 0.45              |
| 86:A:1537:ALA:C      | 86:A:1539:ALA:N      | 2.59                     | 0.45              |
| 4:SQ:11:LYS:HE2      | 4:SQ:11:LYS:HB3      | 1.79                     | 0.45              |
| 6:SR:153:SER:OG      | 6:SR:154:LEU:N       | 2.49                     | 0.45              |
| 21:SH:51:ASP:CB      | 86:A:1378:SER:O      | 2.48                     | 0.45              |
| 56:LQ:157[A]:GLU:OE1 | 56:LQ:160[A]:ARG:NH2 | 2.45                     | 0.45              |
| 70:Le:17:VAL:HG11    | 70:Le:92:ILE:HD12    | 1.99                     | 0.45              |
| 1:S2:762:A:OP1       | 13:SW:79:ARG:NH2     | 2.49                     | 0.45              |
| 1:S2:1477:G:H2'      | 1:S2:1478:G:H8       | 1.81                     | 0.45              |
| 25:Sb:22:LYS:NZ      | 30:Sf:2:VAL:O        | 2.49                     | 0.45              |
| 40:LA:411:U:H2'      | 40:LA:412:G:H8       | 1.82                     | 0.45              |
| 40:LA:2806:U:OP1     | 84:Ls:49:THR:OG1     | 2.35                     | 0.45              |
| 40:LA:2838:A:N6      | 40:LA:2850:G:O2'     | 2.48                     | 0.45              |
| 50:LK:90:MET:HE3     | 50:LK:181:VAL:HB     | 1.97                     | 0.45              |
| 74:Li:58:ARG:HB2     | 74:Li:61:GLN:HE21    | 1.81                     | 0.45              |
| 1:S2:1109:G:H1       | 1:S2:1136:U:H3       | 1.63                     | 0.45              |
| 6:SR:139:ILE:HD12    | 6:SR:218:ILE:HB      | 1.98                     | 0.45              |
| 40:LA:655:C:H2'      | 40:LA:656:A:H8       | 1.81                     | 0.45              |
| 40:LA:3294:A:OP2     | 44:LE:126:LYS:NZ     | 2.49                     | 0.45              |
| 44:LE:92:TYR:HB2     | 44:LE:157:VAL:HB     | 1.98                     | 0.45              |
| 49:LJ:41:GLN:OE1     | 49:LJ:44:ARG:NH1     | 2.36                     | 0.45              |
| 55:LP:35:VAL:O       | 55:LP:64:VAL:HA      | 2.17                     | 0.45              |
| 86:A:2071:ALA:O      | 86:A:2074:ALA:HB2    | 2.17                     | 0.45              |
| 1:S2:29:U:H2'        | 1:S2:30:G:H8         | 1.81                     | 0.45              |
| 1:S2:1171:A:H2'      | 1:S2:1172:G:C8       | 2.52                     | 0.45              |
| 18:SZ:71:CYS:HA      | 18:SZ:74:VAL:HG12    | 1.99                     | 0.45              |
| 40:LA:2621:G:O2'     | 84:Ls:53:GLY:O       | 2.35                     | 0.45              |
| 40:LA:3192:U:H3      | 40:LA:3200:G:H1      | 1.65                     | 0.45              |
| 40:LA:3232:G:O6      | 40:LA:3255:U:O4      | 2.35                     | 0.45              |
| 62:LW:77:LYS:HG2     | 62:LW:81:LYS:HE2     | 1.99                     | 0.45              |
| 63:LX:17:LEU:HB2     | 63:LX:52:ALA:HB3     | 1.99                     | 0.45              |
| 86:A:2012:ALA:HB3    | 86:A:2024:ALA:HB2    | 1.99                     | 0.45              |
| 86:A:2271:ALA:O      | 86:A:2274:ALA:HB2    | 2.17                     | 0.45              |
| 86:A:2383:ALA:C      | 86:A:2385:ALA:N      | 2.74                     | 0.45              |
| 1:S2:190:C:N4        | 1:S2:191:C:O2        | 2.50                     | 0.45              |
| 9:SB:208:SER:HB3     | 9:SB:211:ILE:HG12    | 1.99                     | 0.45              |

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| Atom-1               | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 13:SW:18:PRO:O       | 13:SW:23:ARG:NH2      | 2.36                     | 0.45              |
| 28:SK:77:ARG:HB3     | 28:SK:81:ARG:NH1      | 2.31                     | 0.45              |
| 28:SK:89:ILE:HD12    | 28:SK:101:TYR:HD2     | 1.82                     | 0.45              |
| 40:LA:164:A:C2       | 40:LA:258:G:C2        | 3.05                     | 0.45              |
| 40:LA:439:C:O2'      | 40:LA:440:A:OP1       | 2.31                     | 0.45              |
| 40:LA:1347:U:H5''    | 45:LF:303:GLY:H       | 1.82                     | 0.45              |
| 55:LP:56:LYS:NZ      | 55:LP:145:ASP:OD2     | 2.44                     | 0.45              |
| 63:LX:13:ILE:HG12    | 63:LX:85:TRP:CD1      | 2.53                     | 0.45              |
| 70:Le:26:GLY:O       | 70:Le:30:THR:OG1      | 2.34                     | 0.45              |
| 74:Li:101:VAL:HA     | 74:Li:104:VAL:HG12    | 1.99                     | 0.45              |
| 8:SS:19:LEU:HD11     | 8:SS:108:ARG:HD2      | 1.98                     | 0.44              |
| 11:SU:91:ILE:HG12    | 11:SU:129:LEU:HD23    | 1.99                     | 0.44              |
| 40:LA:551:A:O2'      | 40:LA:552:G:O4'       | 2.34                     | 0.44              |
| 40:LA:1814:A:N3      | 40:LA:1815:U:N3       | 2.65                     | 0.44              |
| 40:LA:1925:U:O2'     | 40:LA:1927:G:N7       | 2.49                     | 0.44              |
| 42:LC:97:A:OP1       | 75:Lj:67:ARG:NH2      | 2.41                     | 0.44              |
| 45:LF:290:ILE:O      | 45:LF:296:GLN:NE2     | 2.50                     | 0.44              |
| 46:LG:79:TYR:HB2     | 46:LG:82:GLU:HG2      | 1.99                     | 0.44              |
| 55:LP:66:VAL:HG23    | 55:LP:98:LEU:HD23     | 1.99                     | 0.44              |
| 55:LP:165:THR:OG1    | 55:LP:166:ALA:N       | 2.49                     | 0.44              |
| 86:A:1162:ALA:O      | 86:A:1166:PHE:N       | 2.48                     | 0.44              |
| 86:A:1708:ALA:HB3    | 86:A:1711:ALA:CB      | 2.47                     | 0.44              |
| 1:S2:250:C:H2'       | 1:S2:251:A:H8         | 1.81                     | 0.44              |
| 1:S2:1498:G:H5''     | 22:SI:72:GLY:HA3      | 1.98                     | 0.44              |
| 18:SZ:50:ALA:HB3     | 18:SZ:53:ASP:HB2      | 1.99                     | 0.44              |
| 30:Sf:80:ARG:HD2     | 30:Sf:81:ARG:O        | 2.17                     | 0.44              |
| 48:LI:64:GLN:NE2     | 48:LI:68:ASP:OD1      | 2.50                     | 0.44              |
| 54:LO:21:VAL:HG12    | 54:LO:65:LEU:HD23     | 1.98                     | 0.44              |
| 58:LS:67:ILE:HG12    | 58:LS:81:VAL:HG11     | 1.99                     | 0.44              |
| 71:Lf:75:ILE:HG12    | 71:Lf:93:VAL:HG22     | 1.99                     | 0.44              |
| 86:A:2211:ALA:O      | 86:A:2215:ALA:HB3     | 2.16                     | 0.44              |
| 1:S2:123:G:OP1       | 8:SS:77:ARG:NH2       | 2.49                     | 0.44              |
| 1:S2:934:C:H5'       | 29:Se:95:ARG:HH21     | 1.82                     | 0.44              |
| 12:SV:12:SER:OG      | 12:SV:13:ALA:N        | 2.50                     | 0.44              |
| 40:LA:1186:G:O3'     | 60:LU:113:ARG:NH2     | 2.51                     | 0.44              |
| 56:LQ:84[A]:LEU:HD22 | 56:LQ:102[A]:LEU:HD22 | 1.99                     | 0.44              |
| 62:LW:77:LYS:HE2     | 62:LW:95:PHE:HD2      | 1.83                     | 0.44              |
| 86:A:1137:PRO:C      | 86:A:1140:ALA:H       | 2.24                     | 0.44              |
| 86:A:1540:ALA:O      | 86:A:1542:ALA:N       | 2.50                     | 0.44              |
| 86:A:1871:ALA:O      | 86:A:1874:ALA:HB2     | 2.17                     | 0.44              |
| 1:S2:371:G:O2'       | 25:Sb:88:LYS:NZ       | 2.35                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S2:512:A:O2'     | 13:SW:133:HIS:NE2  | 2.39                     | 0.44              |
| 1:S2:1144:U:O2'    | 1:S2:1301:U:O2'    | 2.34                     | 0.44              |
| 11:SU:150:GLN:HB3  | 11:SU:181:ILE:HG22 | 1.98                     | 0.44              |
| 13:SW:37:LYS:HB3   | 32:Sg:33:ARG:HB3   | 1.99                     | 0.44              |
| 29:Se:23:CYS:SG    | 29:Se:24:VAL:N     | 2.87                     | 0.44              |
| 40:LA:911:C:OP1    | 43:LD:14:SER:OG    | 2.31                     | 0.44              |
| 40:LA:2661:G:H2'   | 40:LA:2662:G:H8    | 1.83                     | 0.44              |
| 43:LD:68:LYS:HD3   | 43:LD:70:ARG:HE    | 1.82                     | 0.44              |
| 44:LE:10:ARG:NH1   | 44:LE:263:SER:O    | 2.51                     | 0.44              |
| 49:LJ:187:GLY:O    | 49:LJ:192:GLN:N    | 2.41                     | 0.44              |
| 78:Lm:43:PHE:HD2   | 78:Lm:54:LEU:HD23  | 1.83                     | 0.44              |
| 86:A:2104:ALA:H    | 86:A:2215:ALA:CB   | 2.30                     | 0.44              |
| 3:SP:54:TRP:HZ3    | 3:SP:176:LEU:HD22  | 1.81                     | 0.44              |
| 6:SR:169:LEU:HD22  | 6:SR:198:THR:HG22  | 1.98                     | 0.44              |
| 8:SS:145:ARG:HG2   | 8:SS:147:ILE:HD11  | 2.00                     | 0.44              |
| 16:SD:29:LYS:HG2   | 16:SD:100:TRP:HB3  | 1.98                     | 0.44              |
| 40:LA:651:G:O2'    | 40:LA:1435:A:OP1   | 2.34                     | 0.44              |
| 40:LA:1532:C:O2'   | 40:LA:1799:A:N3    | 2.48                     | 0.44              |
| 40:LA:3329:U:H4'   | 44:LE:308:MET:HB3  | 1.99                     | 0.44              |
| 47:LH:58:LEU:HD21  | 47:LH:64:LEU:HB2   | 2.00                     | 0.44              |
| 51:LL:42:THR:OG1   | 51:LL:43:VAL:N     | 2.50                     | 0.44              |
| 52:LM:9:MET:HE2    | 52:LM:134:PRO:HG2  | 1.99                     | 0.44              |
| 65:LZ:129:ASP:N    | 65:LZ:129:ASP:OD1  | 2.51                     | 0.44              |
| 70:Le:51:LEU:HD13  | 74:Li:91:ARG:HG2   | 2.00                     | 0.44              |
| 86:A:2104:ALA:CA   | 86:A:2215:ALA:HB2  | 2.43                     | 0.44              |
| 86:A:2323:ALA:HB3  | 86:A:2335:ALA:HB2  | 1.99                     | 0.44              |
| 86:A:2382:ALA:O    | 86:A:2385:ALA:HB2  | 2.17                     | 0.44              |
| 1:S2:74:U:O2'      | 1:S2:76:A:OP2      | 2.27                     | 0.44              |
| 1:S2:1474:G:H2'    | 1:S2:1475:A:C8     | 2.53                     | 0.44              |
| 29:Se:87:ARG:NH2   | 29:Se:92:ARG:O     | 2.50                     | 0.44              |
| 34:SO:123:ILE:HB   | 34:SO:131:ILE:HD11 | 1.99                     | 0.44              |
| 34:SO:169:ILE:HG23 | 34:SO:183:LEU:HD22 | 1.99                     | 0.44              |
| 38:So:147:LEU:HD21 | 38:So:289:ILE:HD11 | 1.99                     | 0.44              |
| 40:LA:1638:A:O2'   | 74:Li:52:GLN:NE2   | 2.50                     | 0.44              |
| 42:LC:141:C:O3'    | 55:LP:62:TYR:OH    | 2.36                     | 0.44              |
| 44:LE:63:PRO:HD2   | 44:LE:348:ARG:HH21 | 1.83                     | 0.44              |
| 45:LF:208:VAL:HA   | 45:LF:228:ALA:O    | 2.18                     | 0.44              |
| 52:LM:168:ASP:OD2  | 86:A:1562:ALA:CA   | 2.60                     | 0.44              |
| 63:LX:80:ARG:HB2   | 63:LX:99:ALA:H     | 1.82                     | 0.44              |
| 75:Lj:77:PRO:HD2   | 75:Lj:80:LEU:HD12  | 1.98                     | 0.44              |
| 79:Ln:25:GLN:HE22  | 79:Ln:28:ARG:HE    | 1.66                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:A:948:ALA:CB    | 86:A:983:ALA:HB1   | 2.27                     | 0.44              |
| 1:S2:953:G:H2'     | 1:S2:954:G:C8      | 2.53                     | 0.44              |
| 22:SI:18:TYR:HD1   | 22:SI:135:ILE:HG21 | 1.83                     | 0.44              |
| 25:Sb:6:VAL:HG23   | 25:Sb:29:PRO:HD2   | 2.00                     | 0.44              |
| 38:So:346:SER:HB2  | 38:So:361:GLU:HG3  | 2.00                     | 0.44              |
| 40:LA:129:U:H2'    | 40:LA:130:A:C8     | 2.53                     | 0.44              |
| 40:LA:627:U:H2'    | 40:LA:628:A:C8     | 2.51                     | 0.44              |
| 40:LA:3343:G:H21   | 40:LA:3362:A:H2    | 1.66                     | 0.44              |
| 86:A:1862:ALA:CB   | 86:A:1902:ALA:HA   | 2.48                     | 0.44              |
| 1:S2:1474:G:OP1    | 9:SB:109:LYS:NZ    | 2.49                     | 0.44              |
| 1:S2:1525:A:N3     | 1:S2:1589:C:O2'    | 2.38                     | 0.44              |
| 29:Se:87:ARG:HH12  | 29:Se:94:ASN:HB2   | 1.82                     | 0.44              |
| 38:So:233:PHE:HA   | 38:So:236:VAL:HG12 | 2.00                     | 0.44              |
| 86:A:2373:ALA:CB   | 86:A:2413:ALA:HA   | 2.48                     | 0.44              |
| 1:S2:924:A:O2'     | 1:S2:987:G:OP1     | 2.27                     | 0.44              |
| 1:S2:1478:G:OP1    | 22:SI:39:THR:OG1   | 2.35                     | 0.44              |
| 1:S2:1641:C:H2'    | 1:S2:1642:G:C8     | 2.52                     | 0.44              |
| 3:SP:198:MET:HE3   | 20:SG:89:SER:HA    | 1.99                     | 0.44              |
| 6:SR:80:VAL:HG12   | 6:SR:102:VAL:HG12  | 2.00                     | 0.44              |
| 20:SG:29:GLN:HB3   | 34:SO:85:TRP:CZ3   | 2.53                     | 0.44              |
| 27:Sd:57:VAL:HB    | 27:Sd:60:PHE:HE2   | 1.83                     | 0.44              |
| 40:LA:2357:A:H2'   | 40:LA:2358:A:H8    | 1.83                     | 0.44              |
| 40:LA:2597:U:O2    | 55:LP:125:SER:OG   | 2.34                     | 0.44              |
| 66:La:29:VAL:O     | 66:La:32:SER:OG    | 2.30                     | 0.44              |
| 79:Ln:27:ILE:HA    | 79:Ln:30:ARG:HG3   | 2.00                     | 0.44              |
| 86:A:1636:ALA:C    | 86:A:1638:ALA:N    | 2.73                     | 0.44              |
| 86:A:1812:ALA:HB3  | 86:A:1824:ALA:HB2  | 1.99                     | 0.44              |
| 86:A:1862:ALA:CB   | 86:A:1902:ALA:CB   | 2.89                     | 0.44              |
| 7:SA:170:THR:HA    | 7:SA:186:VAL:O     | 2.18                     | 0.43              |
| 27:Sd:51:GLU:OE1   | 27:Sd:53:ASP:N     | 2.50                     | 0.43              |
| 40:LA:90:C:OP1     | 68:Lc:59:ARG:NH1   | 2.45                     | 0.43              |
| 40:LA:1655:G:N2    | 40:LA:1801:U:O4    | 2.51                     | 0.43              |
| 40:LA:3002:C:O2'   | 44:LE:180:GLU:OE2  | 2.36                     | 0.43              |
| 40:LA:3344:A:C2    | 40:LA:3361:G:N2    | 2.76                     | 0.43              |
| 48:LI:147:LEU:HD23 | 48:LI:244:ASN:HD22 | 1.82                     | 0.43              |
| 72:Lg:19:ARG:NH1   | 72:Lg:33:ARG:HG3   | 2.33                     | 0.43              |
| 72:Lg:23:ASP:OD1   | 72:Lg:23:ASP:N     | 2.48                     | 0.43              |
| 77:LI:59:THR:HG22  | 77:LI:64:MET:HE3   | 2.00                     | 0.43              |
| 86:A:1639:ALA:HB1  | 86:A:1641:ALA:N    | 2.32                     | 0.43              |
| 1:S2:534:A:OP1     | 13:SW:168:ARG:NH2  | 2.51                     | 0.43              |
| 13:SW:159:ALA:HB3  | 13:SW:162:SER:HB3  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:SD:54:ARG:HH22  | 33:SN:127:GLY:HA3  | 1.82                     | 0.43              |
| 28:SK:103:ARG:NH2  | 28:SK:105:THR:OG1  | 2.51                     | 0.43              |
| 40:LA:705:A:O4'    | 40:LA:715:A:N6     | 2.51                     | 0.43              |
| 40:LA:873:C:H3'    | 40:LA:874:U:H4'    | 2.00                     | 0.43              |
| 71:Lf:10:ARG:HG2   | 71:Lf:108:VAL:HG23 | 2.00                     | 0.43              |
| 86:A:1657:ALA:C    | 86:A:1659:ALA:H    | 2.25                     | 0.43              |
| 1:S2:603:U:H2'     | 1:S2:604:A:H8      | 1.82                     | 0.43              |
| 1:S2:1218:G:H5''   | 1:S2:1444:A:H61    | 1.84                     | 0.43              |
| 27:Sd:12:VAL:HA    | 27:Sd:23:PHE:HB3   | 2.01                     | 0.43              |
| 40:LA:836:A:O2'    | 83:Lr:9:GLY:O      | 2.28                     | 0.43              |
| 53:LN:18:TRP:O     | 53:LN:21:ARG:C     | 2.61                     | 0.43              |
| 54:LO:45:LEU:HD21  | 54:LO:55:ARG:HE    | 1.83                     | 0.43              |
| 54:LO:98:SER:HA    | 54:LO:101:LYS:HE3  | 1.99                     | 0.43              |
| 55:LP:46:ASP:OD1   | 55:LP:46:ASP:N     | 2.51                     | 0.43              |
| 58:LS:64:VAL:HG22  | 58:LS:90:ASP:H     | 1.83                     | 0.43              |
| 58:LS:151:ARG:HE   | 58:LS:162:ALA:HB1  | 1.83                     | 0.43              |
| 86:A:2262:ALA:CB   | 86:A:2302:ALA:HA   | 2.48                     | 0.43              |
| 1:S2:323:A:OP2     | 12:SV:10:LYS:NZ    | 2.31                     | 0.43              |
| 1:S2:818:C:N4      | 1:S2:819:G:N7      | 2.66                     | 0.43              |
| 1:S2:1043:A:O2'    | 4:SQ:152:ARG:NH1   | 2.41                     | 0.43              |
| 8:SS:98:ASN:HB2    | 8:SS:114:ILE:O     | 2.19                     | 0.43              |
| 40:LA:315:C:OP2    | 76:Lk:28:TYR:OH    | 2.30                     | 0.43              |
| 42:LC:150:G:H21    | 49:LJ:59:GLN:NE2   | 2.16                     | 0.43              |
| 50:LK:21:LYS:HB3   | 50:LK:22:SER:H     | 1.66                     | 0.43              |
| 55:LP:114:ARG:NH1  | 55:LP:153:ASP:O    | 2.45                     | 0.43              |
| 64:LY:22:VAL:HG22  | 64:LY:28:ILE:HG12  | 2.00                     | 0.43              |
| 86:A:1636:ALA:HB1  | 86:A:1677:ALA:N    | 2.32                     | 0.43              |
| 1:S2:575:C:N4      | 26:Sc:65:ASN:OD1   | 2.47                     | 0.43              |
| 1:S2:859:A:O2'     | 17:SY:73:ARG:NH1   | 2.52                     | 0.43              |
| 19:SF:62:ASN:H     | 19:SF:63:ILE:HD12  | 1.84                     | 0.43              |
| 34:SO:19:TRP:HB2   | 34:SO:38:ARG:HB2   | 1.99                     | 0.43              |
| 38:So:248:LEU:HD23 | 38:So:270:ASN:HB2  | 2.00                     | 0.43              |
| 40:LA:999:G:N3     | 40:LA:1002:A:N6    | 2.67                     | 0.43              |
| 40:LA:1493:G:OP2   | 40:LA:1493:G:N2    | 2.44                     | 0.43              |
| 40:LA:1523:U:O4    | 65:LZ:75:LYS:NZ    | 2.51                     | 0.43              |
| 53:LN:90:ALA:HB1   | 53:LN:95:ILE:HB    | 2.00                     | 0.43              |
| 58:LS:145:ASN:HA   | 58:LS:150:VAL:HG21 | 2.00                     | 0.43              |
| 61:LV:36:VAL:HG23  | 61:LV:65:TYR:HA    | 2.01                     | 0.43              |
| 1:S2:843:U:H2'     | 1:S2:844:A:H8      | 1.84                     | 0.43              |
| 4:SQ:8:ARG:HD3     | 4:SQ:11:LYS:HB2    | 2.01                     | 0.43              |
| 25:Sb:75:ILE:N     | 25:Sb:126:LEU:O    | 2.44                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:SO:88:THR:HG22  | 34:SO:104:VAL:HG12 | 2.00                     | 0.43              |
| 37:Sn:27:C:H2'     | 37:Sn:28:A:H8      | 1.83                     | 0.43              |
| 40:LA:449:U:O2'    | 40:LA:450:G:N2     | 2.51                     | 0.43              |
| 40:LA:951:A:OP1    | 69:Ld:18:ARG:NH2   | 2.51                     | 0.43              |
| 40:LA:1562:C:O2'   | 40:LA:1563:C:O4'   | 2.36                     | 0.43              |
| 40:LA:2557:A:OP1   | 43:LD:69:TYR:OH    | 2.28                     | 0.43              |
| 46:LG:132:THR:HG21 | 46:LG:170:GLY:HA2  | 2.01                     | 0.43              |
| 1:S2:620:A:N3      | 1:S2:1107:G:O2'    | 2.41                     | 0.43              |
| 1:S2:1565:C:OP1    | 21:SH:41:ARG:NH1   | 2.45                     | 0.43              |
| 28:SK:78:ILE:HA    | 28:SK:81:ARG:HD2   | 2.01                     | 0.43              |
| 40:LA:1222:G:N2    | 40:LA:1285:G:O2'   | 2.48                     | 0.43              |
| 40:LA:2523:A:N6    | 49:LJ:57:ARG:HH11  | 2.17                     | 0.43              |
| 42:LC:59:A:O2'     | 65:LZ:61:LYS:NZ    | 2.52                     | 0.43              |
| 48:LI:176:TYR:CZ   | 48:LI:197:GLN:HG2  | 2.53                     | 0.43              |
| 53:LN:66:ASN:OD1   | 68:Lc:128:ARG:NH2  | 2.51                     | 0.43              |
| 84:Ls:99:PHE:HA    | 84:Ls:114:LYS:HA   | 2.01                     | 0.43              |
| 1:S2:872:G:H1'     | 30:Sf:68:GLY:H     | 1.84                     | 0.43              |
| 1:S2:1461:C:H5''   | 21:SH:143:ARG:HG2  | 2.00                     | 0.43              |
| 7:SA:40:ARG:HB2    | 7:SA:47:GLU:HG2    | 2.00                     | 0.43              |
| 7:SA:94:ARG:O      | 7:SA:97:SER:OG     | 2.36                     | 0.43              |
| 35:SL:60:GLU:OE1   | 35:SL:60:GLU:N     | 2.51                     | 0.43              |
| 40:LA:70:A:H5'     | 68:Lc:64:GLN:HE22  | 1.83                     | 0.43              |
| 40:LA:264:G:OP1    | 76:Lk:34:SER:OG    | 2.32                     | 0.43              |
| 47:LH:55:LEU:HD11  | 47:LH:66:THR:HG22  | 1.99                     | 0.43              |
| 50:LK:27:VAL:HG13  | 50:LK:82:VAL:HG21  | 2.01                     | 0.43              |
| 59:LT:115:ILE:HG13 | 59:LT:119:LEU:HD23 | 2.00                     | 0.43              |
| 77:Ll:21:ARG:NH1   | 77:Ll:41:ALA:O     | 2.51                     | 0.43              |
| 83:Lr:46:THR:OG1   | 83:Lr:57:CYS:SG    | 2.68                     | 0.43              |
| 86:A:1260:ALA:HB1  | 86:A:1264:LYS:N    | 2.33                     | 0.43              |
| 86:A:1383:ARG:CB   | 86:A:1423:THR:HA   | 2.49                     | 0.43              |
| 86:A:1583:ALA:C    | 86:A:1585:ALA:N    | 2.77                     | 0.43              |
| 1:S2:1545:A:OP2    | 21:SH:136:GLN:NE2  | 2.52                     | 0.43              |
| 28:SK:45:GLU:O     | 28:SK:49:ARG:HB2   | 2.19                     | 0.43              |
| 32:Sg:31:LYS:HA    | 32:Sg:31:LYS:HD3   | 1.71                     | 0.43              |
| 38:So:179:ASN:HB3  | 38:So:224:ARG:HD2  | 2.00                     | 0.43              |
| 40:LA:929:A:O2'    | 77:Ll:49:TRP:O     | 2.36                     | 0.43              |
| 40:LA:2445:A:N1    | 40:LA:2502:A:N6    | 2.67                     | 0.43              |
| 44:LE:220:VAL:O    | 44:LE:334:ARG:NH1  | 2.51                     | 0.43              |
| 74:Li:74:ARG:HH12  | 74:Li:85:VAL:HG21  | 1.83                     | 0.43              |
| 86:A:2062:ALA:CB   | 86:A:2102:ALA:HA   | 2.48                     | 0.43              |
| 1:S2:188:A:N6      | 1:S2:197:A:O2'     | 2.51                     | 0.43              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:S2:871:G:N2       | 30:Sf:68:GLY:O       | 2.46                     | 0.43              |
| 1:S2:1486:G:H2'     | 1:S2:1487:A:C8       | 2.54                     | 0.43              |
| 4:SQ:30:PHE:CD1     | 4:SQ:94:LYS:HG3      | 2.54                     | 0.43              |
| 7:SA:39:VAL:HA      | 7:SA:47:GLU:O        | 2.18                     | 0.43              |
| 13:SW:119:ALA:O     | 13:SW:124:HIS:ND1    | 2.52                     | 0.43              |
| 18:SZ:125:SER:OG    | 18:SZ:126:THR:N      | 2.51                     | 0.43              |
| 40:LA:921:A:N6      | 40:LA:1846:C:OP2     | 2.33                     | 0.43              |
| 40:LA:2155:G:O2'    | 43:LD:227:ARG:NH2    | 2.37                     | 0.43              |
| 45:LF:138:ARG:HH21  | 45:LF:240:PRO:HG2    | 1.83                     | 0.43              |
| 86:A:1599:ALA:HB2   | 86:A:1604:ALA:H      | 1.84                     | 0.43              |
| 1:S2:478:A:H62      | 1:S2:539:G:H22       | 1.65                     | 0.42              |
| 1:S2:966:A:H5''     | 17:SY:4:MET:HE1      | 2.00                     | 0.42              |
| 8:SS:141:THR:OG1    | 8:SS:143:ASP:OD1     | 2.26                     | 0.42              |
| 22:SI:138:GLN:NE2   | 86:A:1300:SER:C      | 2.77                     | 0.42              |
| 30:Sf:35:VAL:HA     | 30:Sf:78:SER:O       | 2.18                     | 0.42              |
| 40:LA:1131:G:O2'    | 40:LA:2373:A:N1      | 2.37                     | 0.42              |
| 40:LA:1244:A:O2'    | 40:LA:1247:U:OP1     | 2.36                     | 0.42              |
| 41:LB:46:A:OP2      | 46:LG:158:ARG:NH1    | 2.51                     | 0.42              |
| 86:A:921:ALA:O      | 86:A:925:ALA:HB2     | 2.18                     | 0.42              |
| 86:A:1222:VAL:O     | 86:A:1226:ARG:N      | 2.40                     | 0.42              |
| 1:S2:886:U:OP2      | 4:SQ:216:LYS:NZ      | 2.52                     | 0.42              |
| 28:SK:65:LEU:HB3    | 28:SK:71:ILE:HD11    | 2.00                     | 0.42              |
| 29:Se:36:ILE:O      | 29:Se:73:TYR:HB2     | 2.19                     | 0.42              |
| 40:LA:360:G:N3      | 40:LA:814:U:O2'      | 2.52                     | 0.42              |
| 40:LA:646:A:N6      | 40:LA:2371:G:H21     | 2.16                     | 0.42              |
| 40:LA:1369:A:H5''   | 68:Lc:21:ARG:HH11    | 1.83                     | 0.42              |
| 40:LA:2549:G:N2     | 40:LA:2549:G:OP2     | 2.52                     | 0.42              |
| 40:LA:3116:G:OP1    | 40:LA:3116:G:N2      | 2.51                     | 0.42              |
| 44:LE:308:MET:HE3   | 44:LE:308:MET:HB2    | 1.63                     | 0.42              |
| 55:LP:8:GLU:O       | 55:LP:12:ARG:HG3     | 2.19                     | 0.42              |
| 56:LQ:189[A]:ASP:HA | 56:LQ:192[A]:LYS:HE2 | 2.02                     | 0.42              |
| 86:A:2062:ALA:HB1   | 86:A:2102:ALA:HA     | 2.01                     | 0.42              |
| 86:A:2262:ALA:HB1   | 86:A:2302:ALA:HA     | 2.01                     | 0.42              |
| 1:S2:434:G:N1       | 1:S2:437:A:OP2       | 2.52                     | 0.42              |
| 1:S2:1388:A:OP2     | 20:SG:32:LYS:NZ      | 2.52                     | 0.42              |
| 1:S2:1542:G:N1      | 1:S2:1568:C:O2'      | 2.45                     | 0.42              |
| 6:SR:165:VAL:HG11   | 6:SR:210:THR:HG22    | 2.01                     | 0.42              |
| 7:SA:40:ARG:NH2     | 7:SA:47:GLU:OE2      | 2.52                     | 0.42              |
| 9:SB:97:LEU:O       | 9:SB:180:ARG:NH2     | 2.49                     | 0.42              |
| 12:SV:171:SER:HB2   | 12:SV:180:ASP:HB2    | 2.01                     | 0.42              |
| 16:SD:60:VAL:HG22   | 16:SD:122:VAL:HG22   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:650:C:H2'    | 40:LA:651:G:C8     | 2.53                     | 0.42              |
| 45:LF:26:PHE:HD1   | 45:LF:130:ALA:HB2  | 1.84                     | 0.42              |
| 49:LJ:78:PHE:HE2   | 49:LJ:164:VAL:HA   | 1.84                     | 0.42              |
| 49:LJ:147:LYS:O    | 49:LJ:201:THR:OG1  | 2.33                     | 0.42              |
| 86:A:1862:ALA:HB1  | 86:A:1902:ALA:HA   | 2.01                     | 0.42              |
| 1:S2:311:U:OP1     | 26:Sc:24:TRP:NE1   | 2.43                     | 0.42              |
| 3:SP:66:ALA:HB2    | 24:Sa:37:ALA:HB2   | 1.99                     | 0.42              |
| 9:SB:140:THR:HA    | 9:SB:214:LYS:HE2   | 2.01                     | 0.42              |
| 16:SD:34:THR:OG1   | 16:SD:127:GLY:O    | 2.31                     | 0.42              |
| 38:So:136:VAL:O    | 38:So:139:THR:OG1  | 2.38                     | 0.42              |
| 40:LA:695:C:OP2    | 45:LF:115:HIS:NE2  | 2.36                     | 0.42              |
| 49:LJ:83:ASP:N     | 49:LJ:83:ASP:OD1   | 2.50                     | 0.42              |
| 68:Lc:90:TYR:CZ    | 68:Lc:100:PRO:HB3  | 2.55                     | 0.42              |
| 77:Ll:54:LYS:O     | 77:Ll:58:THR:HB    | 2.19                     | 0.42              |
| 84:Ls:56:LYS:HA    | 84:Ls:75:PRO:HA    | 2.00                     | 0.42              |
| 86:A:1260:ALA:O    | 86:A:1261:TRP:C    | 2.63                     | 0.42              |
| 1:S2:66:U:O4       | 10:ST:134:GLY:N    | 2.50                     | 0.42              |
| 1:S2:780:A:C2      | 27:Sd:8:ARG:HD3    | 2.55                     | 0.42              |
| 1:S2:1217:A:C4     | 14:SC:40:LEU:HD11  | 2.54                     | 0.42              |
| 5:SE:117:GLY:HA2   | 5:SE:120:SER:HB3   | 2.02                     | 0.42              |
| 6:SR:173:PRO:O     | 6:SR:176:SER:OG    | 2.28                     | 0.42              |
| 11:SU:14:THR:OG1   | 11:SU:15:GLU:N     | 2.52                     | 0.42              |
| 38:So:44:ALA:HB3   | 38:So:134:LYS:HD3  | 2.02                     | 0.42              |
| 40:LA:341:G:H21    | 40:LA:349:A:N6     | 2.16                     | 0.42              |
| 40:LA:612:U:H2'    | 40:LA:613:G:H8     | 1.83                     | 0.42              |
| 40:LA:658:G:N2     | 45:LF:93:MET:HB2   | 2.34                     | 0.42              |
| 45:LF:311:HIS:CE1  | 48:LI:162:PRO:HG3  | 2.55                     | 0.42              |
| 47:LH:84:VAL:O     | 73:Lh:105:SER:OG   | 2.35                     | 0.42              |
| 52:LM:48:SER:HB2   | 52:LM:66:ALA:HB3   | 2.01                     | 0.42              |
| 54:LO:109:ARG:HA   | 54:LO:112:LEU:HG   | 2.01                     | 0.42              |
| 64:LY:9:SER:HA     | 64:LY:52:THR:HG23  | 2.01                     | 0.42              |
| 86:A:1657:ALA:O    | 86:A:1659:ALA:N    | 2.51                     | 0.42              |
| 1:S2:1182:U:H5     | 1:S2:1185:U:H5''   | 1.85                     | 0.42              |
| 5:SE:118:GLU:O     | 21:SH:122:HIS:N    | 2.53                     | 0.42              |
| 12:SV:159:GLN:HE22 | 12:SV:189:LEU:HD11 | 1.85                     | 0.42              |
| 1:S2:505:A:O2'     | 1:S2:507:U:OP1     | 2.31                     | 0.42              |
| 1:S2:523:G:O2'     | 1:S2:529:A:N6      | 2.52                     | 0.42              |
| 1:S2:541:A:O2'     | 1:S2:542:A:OP1     | 2.36                     | 0.42              |
| 1:S2:1187:U:H2'    | 1:S2:1188:G:H8     | 1.83                     | 0.42              |
| 9:SB:190:ILE:HA    | 9:SB:193:THR:HG22  | 2.01                     | 0.42              |
| 23:SJ:46:GLU:O     | 23:SJ:49:ASN:ND2   | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LA:1874:A:N7    | 59:LT:20:ARG:NH1   | 2.68                     | 0.42              |
| 40:LA:2516:U:OP1   | 55:LP:31:ARG:NH1   | 2.52                     | 0.42              |
| 40:LA:3369:G:N2    | 44:LE:380:MET:O    | 2.36                     | 0.42              |
| 49:LJ:152:LEU:O    | 49:LJ:197:VAL:HA   | 2.19                     | 0.42              |
| 79:Ln:23:LEU:HD11  | 79:Ln:35:ILE:HG22  | 2.02                     | 0.42              |
| 79:Ln:25:GLN:NE2   | 79:Ln:28:ARG:HE    | 2.17                     | 0.42              |
| 4:SQ:27:LYS:HB3    | 4:SQ:47:LEU:HD12   | 2.02                     | 0.42              |
| 6:SR:116:LYS:HG2   | 6:SR:127:ALA:HB3   | 2.02                     | 0.42              |
| 7:SA:225:TYR:HB2   | 34:SO:189:GLU:HA   | 2.01                     | 0.42              |
| 38:So:211:LEU:HD12 | 38:So:216:ILE:HG21 | 2.00                     | 0.42              |
| 40:LA:2149:A:N6    | 40:LA:2187:G:O2'   | 2.42                     | 0.42              |
| 59:LT:8:LYS:HD3    | 59:LT:19:LYS:HB3   | 2.02                     | 0.42              |
| 82:Lq:45:ARG:O     | 82:Lq:48:SER:OG    | 2.30                     | 0.42              |
| 86:A:1708:ALA:HB3  | 86:A:1711:ALA:HB2  | 2.01                     | 0.42              |
| 1:S2:1690:G:H2'    | 1:S2:1691:A:C8     | 2.55                     | 0.42              |
| 5:SE:95:GLY:HA2    | 5:SE:103:ASN:O     | 2.19                     | 0.42              |
| 8:SS:64:ILE:HD12   | 27:Sd:17:LEU:HB3   | 2.01                     | 0.42              |
| 19:SF:44:LEU:HD12  | 19:SF:78:VAL:HG11  | 2.02                     | 0.42              |
| 20:SG:101:ASN:ND2  | 20:SG:120:SER:OG   | 2.53                     | 0.42              |
| 29:Se:7:SER:OG     | 29:Se:7:SER:O      | 2.37                     | 0.42              |
| 40:LA:2799:A:O2'   | 68:Lc:42:ARG:NH1   | 2.53                     | 0.42              |
| 50:LK:4:ILE:H      | 60:LU:142:GLN:NE2  | 2.17                     | 0.42              |
| 58:LS:64:VAL:HA    | 58:LS:67:ILE:HD12  | 2.02                     | 0.42              |
| 77:Ll:64:MET:HB2   | 77:Ll:68:LYS:HG3   | 2.02                     | 0.42              |
| 86:A:1561:ALA:HA   | 86:A:1599:ALA:O    | 2.20                     | 0.42              |
| 86:A:2040:ALA:N    | 86:A:2040:ALA:CB   | 2.67                     | 0.42              |
| 1:S2:17:C:O2'      | 1:S2:1137:A:N1     | 2.41                     | 0.42              |
| 1:S2:1770:U:H5''   | 1:S2:1794:A:H62    | 1.84                     | 0.42              |
| 4:SQ:127:VAL:HG11  | 4:SQ:176:VAL:HG11  | 2.02                     | 0.42              |
| 8:SS:9:LEU:HB2     | 8:SS:30:ARG:HD2    | 2.02                     | 0.42              |
| 20:SG:35:CYS:HA    | 20:SG:38:ILE:HG22  | 2.01                     | 0.42              |
| 40:LA:592:A:HO2'   | 47:LH:20:LYS:NZ    | 2.17                     | 0.42              |
| 40:LA:3279:A:N6    | 73:Lh:54:ARG:HD3   | 2.35                     | 0.42              |
| 53:LN:46:ILE:HD11  | 53:LN:51:LEU:HD12  | 2.02                     | 0.42              |
| 61:LV:42:ILE:O     | 61:LV:59:GLY:N     | 2.53                     | 0.42              |
| 86:A:2373:ALA:HB1  | 86:A:2413:ALA:HA   | 2.01                     | 0.42              |
| 1:S2:351:C:OP1     | 1:S2:630:A:O2'     | 2.35                     | 0.41              |
| 6:SR:139:ILE:HG13  | 6:SR:191:ALA:HB1   | 2.02                     | 0.41              |
| 17:SY:6:SER:OG     | 17:SY:7:ALA:N      | 2.53                     | 0.41              |
| 18:SZ:81:VAL:HB    | 18:SZ:115:ILE:HG22 | 2.02                     | 0.41              |
| 25:Sb:79:PHE:HB2   | 25:Sb:125:ILE:HG22 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:SO:159:ASN:HD21 | 34:SO:167:VAL:HA   | 1.84                     | 0.41              |
| 40:LA:723:U:O2'    | 69:Ld:29:TYR:OH    | 2.36                     | 0.41              |
| 40:LA:937:G:C6     | 40:LA:2410:U:H5''  | 2.55                     | 0.41              |
| 40:LA:2241:U:O2'   | 43:LD:243:THR:N    | 2.45                     | 0.41              |
| 40:LA:2357:A:H2'   | 40:LA:2358:A:C8    | 2.55                     | 0.41              |
| 45:LF:157:GLU:HG3  | 45:LF:251:THR:HG21 | 2.02                     | 0.41              |
| 51:LL:169:LYS:HZ1  | 61:LV:159:PHE:HA   | 1.85                     | 0.41              |
| 63:LX:14:SER:O     | 63:LX:81:GLN:NE2   | 2.53                     | 0.41              |
| 1:S2:168:A:OP1     | 10:ST:137:ARG:N    | 2.50                     | 0.41              |
| 1:S2:1588:G:H1     | 1:S2:1608:U:H3     | 1.66                     | 0.41              |
| 40:LA:170:G:H2'    | 40:LA:171:G:C8     | 2.55                     | 0.41              |
| 40:LA:528:U:H3     | 40:LA:564:G:H1     | 1.68                     | 0.41              |
| 40:LA:629:U:H2'    | 40:LA:630:A:C8     | 2.55                     | 0.41              |
| 40:LA:1261:G:O2'   | 40:LA:1278:A:N1    | 2.40                     | 0.41              |
| 40:LA:1786:G:H2'   | 40:LA:1787:A:C8    | 2.55                     | 0.41              |
| 43:LD:180:LEU:HD22 | 83:Lr:18:TYR:HB3   | 2.02                     | 0.41              |
| 67:Lb:42:LEU:HD23  | 67:Lb:96:VAL:HG22  | 2.02                     | 0.41              |
| 1:S2:126:A:O2'     | 1:S2:264:G:O2'     | 2.27                     | 0.41              |
| 9:SB:57:SER:HA     | 35:SL:53:ILE:HB    | 2.03                     | 0.41              |
| 10:ST:78:THR:HG23  | 10:ST:92:ARG:HG2   | 2.02                     | 0.41              |
| 11:SU:156:SER:OG   | 11:SU:186:PRO:O    | 2.38                     | 0.41              |
| 22:SI:138:GLN:NE2  | 86:A:1300:SER:O    | 2.53                     | 0.41              |
| 40:LA:504:A:HO2'   | 45:LF:315:LYS:HZ2  | 1.58                     | 0.41              |
| 40:LA:819:U:H2'    | 40:LA:820:A:H8     | 1.85                     | 0.41              |
| 40:LA:1078:U:OP2   | 46:LG:140:ARG:NH1  | 2.48                     | 0.41              |
| 40:LA:1795:U:OP2   | 43:LD:50:HIS:NE2   | 2.53                     | 0.41              |
| 40:LA:2964:G:N2    | 40:LA:2967:A:OP2   | 2.39                     | 0.41              |
| 40:LA:3016:A:H2'   | 40:LA:3017:A:H8    | 1.85                     | 0.41              |
| 51:LL:48:LEU:O     | 51:LL:139:ARG:HA   | 2.20                     | 0.41              |
| 65:LZ:59:SER:HA    | 65:LZ:62:VAL:HG22  | 2.03                     | 0.41              |
| 69:Ld:37:PRO:HA    | 69:Ld:40:ARG:HB2   | 2.02                     | 0.41              |
| 86:A:2104:ALA:HB3  | 86:A:2215:ALA:HB2  | 1.86                     | 0.41              |
| 1:S2:1147:A:O2'    | 1:S2:1636:C:OP2    | 2.27                     | 0.41              |
| 4:SQ:119:THR:N     | 4:SQ:143:THR:OG1   | 2.50                     | 0.41              |
| 5:SE:117:GLY:O     | 5:SE:120:SER:C     | 2.64                     | 0.41              |
| 13:SW:141:VAL:HG21 | 13:SW:146:PHE:HE1  | 1.85                     | 0.41              |
| 15:SX:111:VAL:HG23 | 15:SX:139:VAL:HG21 | 2.02                     | 0.41              |
| 23:SJ:74:GLU:HG3   | 23:SJ:75:GLY:H     | 1.86                     | 0.41              |
| 40:LA:712:G:OP1    | 53:LN:174:ARG:NH1  | 2.53                     | 0.41              |
| 40:LA:874:U:OP2    | 40:LA:1907:C:O2'   | 2.37                     | 0.41              |
| 53:LN:162:ASN:N    | 53:LN:162:ASN:OD1  | 2.53                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 84:Ls:23:CYS:HB2   | 84:Ls:76:SER:HA    | 2.03                     | 0.41              |
| 1:S2:996:U:H2'     | 1:S2:997:G:H8      | 1.84                     | 0.41              |
| 6:SR:239:PRO:HA    | 6:SR:242:ILE:HD12  | 2.02                     | 0.41              |
| 12:SV:87:ASN:HB3   | 12:SV:90:LEU:HG    | 2.03                     | 0.41              |
| 16:SD:61:VAL:HG12  | 16:SD:121:VAL:HB   | 2.01                     | 0.41              |
| 16:SD:98:GLY:O     | 16:SD:101:ALA:C    | 2.64                     | 0.41              |
| 17:SY:16:ILE:H     | 25:Sb:57:ARG:HH22  | 1.68                     | 0.41              |
| 18:SZ:14:PHE:CD1   | 18:SZ:78:ALA:HB3   | 2.56                     | 0.41              |
| 40:LA:900:G:H1'    | 40:LA:1589:A:N6    | 2.36                     | 0.41              |
| 40:LA:953:G:OP1    | 69:Ld:12:GLN:NE2   | 2.45                     | 0.41              |
| 40:LA:1364:C:OP1   | 48:LI:110:ARG:NH2  | 2.45                     | 0.41              |
| 40:LA:2516:U:O2    | 40:LA:2594:C:N4    | 2.53                     | 0.41              |
| 40:LA:2836:C:H5    | 40:LA:2852:C:H42   | 1.68                     | 0.41              |
| 40:LA:3253:G:H2'   | 40:LA:3254:G:H8    | 1.85                     | 0.41              |
| 41:LB:7:G:OP1      | 46:LG:33:ARG:NH1   | 2.53                     | 0.41              |
| 46:LG:46:THR:HA    | 46:LG:47:PRO:HD3   | 1.96                     | 0.41              |
| 62:LW:17:VAL:HA    | 62:LW:103:TYR:O    | 2.21                     | 0.41              |
| 5:SE:14:THR:OG1    | 5:SE:15:HIS:N      | 2.53                     | 0.41              |
| 8:SS:207:LEU:HD22  | 8:SS:219:VAL:HG12  | 2.02                     | 0.41              |
| 34:SO:200:ASN:ND2  | 34:SO:240:VAL:O    | 2.52                     | 0.41              |
| 40:LA:95:A:C5      | 40:LA:96:G:H1'     | 2.56                     | 0.41              |
| 40:LA:417:A:H2'    | 40:LA:418:A:C8     | 2.54                     | 0.41              |
| 40:LA:655:C:H2'    | 40:LA:656:A:C8     | 2.56                     | 0.41              |
| 40:LA:669:U:H1'    | 40:LA:1110:U:H4'   | 2.01                     | 0.41              |
| 40:LA:2519:A:H2'   | 40:LA:2520:A:H8    | 1.86                     | 0.41              |
| 60:LU:115:ARG:O    | 60:LU:117:ARG:NH2  | 2.53                     | 0.41              |
| 61:LV:101:CYS:SG   | 61:LV:102:ARG:N    | 2.93                     | 0.41              |
| 69:Ld:13:THR:O     | 69:Ld:17:HIS:ND1   | 2.54                     | 0.41              |
| 74:Li:58:ARG:HB2   | 74:Li:61:GLN:NE2   | 2.36                     | 0.41              |
| 86:A:1428:ALA:HB1  | 86:A:1461:ALA:CA   | 2.38                     | 0.41              |
| 1:S2:200:A:H2'     | 1:S2:201:G:C8      | 2.55                     | 0.41              |
| 1:S2:924:A:H2'     | 1:S2:925:G:C8      | 2.56                     | 0.41              |
| 8:SS:11:ARG:NH2    | 8:SS:20:LEU:HB3    | 2.36                     | 0.41              |
| 10:ST:138:ALA:HA   | 10:ST:153:VAL:HG11 | 2.03                     | 0.41              |
| 17:SY:5:HIS:CE1    | 17:SY:121:ARG:HG3  | 2.56                     | 0.41              |
| 19:SF:79:TYR:CD1   | 19:SF:82:ARG:HD3   | 2.56                     | 0.41              |
| 22:SI:40:SER:OG    | 22:SI:41:SER:N     | 2.54                     | 0.41              |
| 38:So:166:LEU:HA   | 38:So:169:VAL:HG22 | 2.02                     | 0.41              |
| 40:LA:1203:A:H2'   | 40:LA:1204:A:H8    | 1.86                     | 0.41              |
| 44:LE:134:SER:O    | 44:LE:137:TYR:C    | 2.64                     | 0.41              |
| 44:LE:229:VAL:HG21 | 44:LE:249:VAL:HG23 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:LS:80:THR:HG23  | 58:LS:100:THR:HG23 | 2.02                     | 0.41              |
| 83:Lr:82:THR:HA    | 83:Lr:85:ARG:HG2   | 2.02                     | 0.41              |
| 86:A:930:ALA:C     | 86:A:932:ALA:N     | 2.79                     | 0.41              |
| 1:S2:406:U:H2'     | 1:S2:407:A:H8      | 1.85                     | 0.41              |
| 1:S2:590:C:H2'     | 1:S2:591:A:H8      | 1.86                     | 0.41              |
| 1:S2:1160:A:H2'    | 1:S2:1161:C:C6     | 2.56                     | 0.41              |
| 12:SV:67:TRP:HE3   | 12:SV:72:ILE:HD11  | 1.85                     | 0.41              |
| 16:SD:31:VAL:HA    | 16:SD:34:THR:HG22  | 2.03                     | 0.41              |
| 17:SY:54:LEU:HB3   | 17:SY:60:VAL:HG21  | 2.03                     | 0.41              |
| 22:SI:138:GLN:CG   | 86:A:1303:GLU:H    | 1.92                     | 0.41              |
| 27:Sd:10:ARG:HB2   | 27:Sd:24:VAL:O     | 2.21                     | 0.41              |
| 40:LA:2843:U:OP2   | 40:LA:2844:C:N4    | 2.49                     | 0.41              |
| 40:LA:3110:C:H2'   | 40:LA:3111:U:C6    | 2.56                     | 0.41              |
| 47:LH:40:LEU:O     | 47:LH:51:ARG:HA    | 2.20                     | 0.41              |
| 49:LJ:83:ASP:OD1   | 49:LJ:86:THR:OG1   | 2.28                     | 0.41              |
| 66:La:89:LYS:O     | 66:La:92:GLY:N     | 2.48                     | 0.41              |
| 67:Lb:49:TYR:CD2   | 67:Lb:133:LYS:HG3  | 2.55                     | 0.41              |
| 86:A:1561:ALA:CB   | 86:A:1600:ALA:HB2  | 2.50                     | 0.41              |
| 1:S2:757:A:O3'     | 8:SS:22:LYS:NZ     | 2.54                     | 0.41              |
| 1:S2:918:U:H4'     | 18:SZ:18:ARG:HD3   | 2.03                     | 0.41              |
| 1:S2:1171:A:H2'    | 1:S2:1172:G:H8     | 1.86                     | 0.41              |
| 1:S2:1320:U:H2'    | 3:SP:101:ARG:HH21  | 1.86                     | 0.41              |
| 1:S2:1383:G:OP1    | 23:SJ:89:ARG:NH2   | 2.53                     | 0.41              |
| 1:S2:1524:A:H2'    | 1:S2:1525:A:C8     | 2.56                     | 0.41              |
| 1:S2:1628:U:H2'    | 1:S2:1629:G:C8     | 2.56                     | 0.41              |
| 1:S2:1727:G:H2'    | 1:S2:1728:A:C8     | 2.55                     | 0.41              |
| 6:SR:157:LYS:HA    | 6:SR:169:LEU:O     | 2.21                     | 0.41              |
| 12:SV:7:SER:O      | 12:SV:18:ARG:NH1   | 2.54                     | 0.41              |
| 13:SW:132:ARG:HH21 | 13:SW:140:ILE:HD13 | 1.86                     | 0.41              |
| 18:SZ:55:SER:O     | 18:SZ:55:SER:OG    | 2.29                     | 0.41              |
| 20:SG:36:ASP:OD1   | 20:SG:37:GLU:N     | 2.54                     | 0.41              |
| 38:So:68:VAL:HG22  | 38:So:145:LEU:HB3  | 2.03                     | 0.41              |
| 40:LA:1050:U:OP2   | 61:LV:13:TYR:OH    | 2.33                     | 0.41              |
| 40:LA:1083:G:H2'   | 40:LA:1084:A:H8    | 1.85                     | 0.41              |
| 40:LA:2555:G:N7    | 74:Li:95:ILE:HD11  | 2.36                     | 0.41              |
| 40:LA:3068:U:OP2   | 59:LT:62:ARG:NH1   | 2.49                     | 0.41              |
| 40:LA:3084:C:O2'   | 40:LA:3332:U:OP1   | 2.29                     | 0.41              |
| 40:LA:3115:C:O2    | 40:LA:3117:C:N4    | 2.53                     | 0.41              |
| 40:LA:3206:C:H2'   | 54:LO:99:TRP:CZ2   | 2.56                     | 0.41              |
| 41:LB:1:G:O6       | 46:LG:262:LYS:NZ   | 2.43                     | 0.41              |
| 41:LB:4:U:H2'      | 41:LB:5:G:H8       | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:LE:86:VAL:HG22  | 44:LE:162:VAL:HG12 | 2.02                     | 0.41              |
| 47:LH:64:LEU:HD11  | 47:LH:76:LEU:HD22  | 2.02                     | 0.41              |
| 55:LP:51:LEU:O     | 55:LP:117:ASN:ND2  | 2.54                     | 0.41              |
| 57:LR:168:LEU:HD12 | 57:LR:172:GLN:HB3  | 2.02                     | 0.41              |
| 62:LW:10:LYS:O     | 62:LW:68:THR:OG1   | 2.33                     | 0.41              |
| 80:Lo:99:CYS:HB3   | 80:Lo:115:CYS:HB3  | 2.01                     | 0.41              |
| 86:A:1428:ALA:CB   | 86:A:1464:ALA:CB   | 2.99                     | 0.41              |
| 1:S2:391:A:OP2     | 12:SV:23:LYS:NZ    | 2.37                     | 0.41              |
| 1:S2:1474:G:H2'    | 1:S2:1475:A:H8     | 1.86                     | 0.41              |
| 4:SQ:210:ILE:HD12  | 4:SQ:210:ILE:HG23  | 1.83                     | 0.41              |
| 40:LA:170:G:H5''   | 75:Lj:109:ILE:HG12 | 2.01                     | 0.41              |
| 40:LA:584:G:H2'    | 40:LA:585:A:C8     | 2.56                     | 0.41              |
| 40:LA:2683:U:H2'   | 40:LA:2684:C:C6    | 2.56                     | 0.41              |
| 44:LE:260:VAL:HG11 | 44:LE:266:ARG:HH11 | 1.86                     | 0.41              |
| 44:LE:307:PRO:HA   | 44:LE:361:THR:HG22 | 2.03                     | 0.41              |
| 45:LF:35:VAL:HG21  | 45:LF:244:LEU:HD21 | 2.03                     | 0.41              |
| 55:LP:150:TRP:O    | 55:LP:156:HIS:ND1  | 2.53                     | 0.41              |
| 86:A:987:ALA:CB    | 86:A:988:ALA:CA    | 2.97                     | 0.41              |
| 1:S2:209:U:H2'     | 1:S2:210:A:H8      | 1.85                     | 0.40              |
| 1:S2:406:U:H2'     | 1:S2:407:A:C8      | 2.56                     | 0.40              |
| 1:S2:628:G:OP1     | 17:SY:124:ARG:NH1  | 2.50                     | 0.40              |
| 5:SE:118:GLU:HA    | 21:SH:122:HIS:HB2  | 2.03                     | 0.40              |
| 8:SS:44:LEU:HD12   | 8:SS:65:LEU:HD11   | 2.03                     | 0.40              |
| 10:ST:39:GLU:HB3   | 10:ST:47:GLY:H     | 1.85                     | 0.40              |
| 40:LA:1403:C:OP2   | 72:Lg:11:LYS:NZ    | 2.54                     | 0.40              |
| 40:LA:2585:G:O6    | 49:LJ:47:SER:OG    | 2.28                     | 0.40              |
| 40:LA:2883:U:H4'   | 44:LE:261:MET:HE1  | 2.02                     | 0.40              |
| 40:LA:2904:U:H2'   | 40:LA:2905:U:H6    | 1.86                     | 0.40              |
| 86:A:2104:ALA:N    | 86:A:2215:ALA:HB2  | 2.36                     | 0.40              |
| 10:ST:31:ARG:HG2   | 10:ST:101:ILE:HD13 | 2.03                     | 0.40              |
| 10:ST:77:LEU:HD12  | 10:ST:95:LYS:HB2   | 2.03                     | 0.40              |
| 35:SL:58:GLU:OE1   | 35:SL:60:GLU:N     | 2.54                     | 0.40              |
| 40:LA:1084:A:H4'   | 46:LG:44:TYR:CE2   | 2.56                     | 0.40              |
| 40:LA:1132:C:HO2'  | 40:LA:2865:U:HO2'  | 1.68                     | 0.40              |
| 40:LA:1798:A:H2'   | 40:LA:1799:A:C8    | 2.56                     | 0.40              |
| 40:LA:2184:U:OP2   | 43:LD:6:ARG:NH2    | 2.54                     | 0.40              |
| 40:LA:2366:C:H2'   | 40:LA:2367:A:H8    | 1.87                     | 0.40              |
| 40:LA:2728:G:O6    | 61:LV:87:LYS:NZ    | 2.54                     | 0.40              |
| 40:LA:3067:C:H3'   | 59:LT:62:ARG:HH12  | 1.85                     | 0.40              |
| 40:LA:3313:U:H4'   | 44:LE:173:GLN:HG3  | 2.04                     | 0.40              |
| 40:LA:3322:A:H2'   | 40:LA:3323:A:H8    | 1.86                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:LC:9:A:H2'      | 42:LC:10:A:C8       | 2.57                     | 0.40              |
| 47:LH:83:TYR:HD1   | 73:Lh:103:TYR:HB2   | 1.86                     | 0.40              |
| 48:LI:37:ASN:O     | 48:LI:41:ARG:HG2    | 2.20                     | 0.40              |
| 48:LI:156:ILE:HD12 | 48:LI:161:VAL:HG21  | 2.01                     | 0.40              |
| 58:LS:66:ARG:HD2   | 58:LS:66:ARG:HA     | 1.90                     | 0.40              |
| 63:LX:95:PHE:CD1   | 64:LY:22:VAL:HB     | 2.55                     | 0.40              |
| 84:Ls:40:LYS:HE3   | 84:Ls:40:LYS:HB2    | 1.97                     | 0.40              |
| 86:A:1333:GLN:CB   | 86:A:1345:ALA:HB2   | 2.52                     | 0.40              |
| 3:SP:2:SER:OG      | 3:SP:3:LEU:N        | 2.54                     | 0.40              |
| 3:SP:3:LEU:HD13    | 3:SP:7:PHE:HB2      | 2.04                     | 0.40              |
| 4:SQ:133:TYR:HE2   | 4:SQ:181:LEU:HD22   | 1.85                     | 0.40              |
| 15:SX:33:ARG:NH2   | 15:SX:51:GLY:O      | 2.54                     | 0.40              |
| 28:SK:48:ASP:HA    | 28:SK:51:LEU:HD12   | 2.03                     | 0.40              |
| 31:SM:12:ARG:O     | 31:SM:18:SER:OG     | 2.26                     | 0.40              |
| 34:SO:21:THR:H     | 34:SO:37:SER:HA     | 1.86                     | 0.40              |
| 40:LA:312:C:H2'    | 40:LA:313:A:H8      | 1.86                     | 0.40              |
| 45:LF:206:LEU:HD23 | 45:LF:248:VAL:HG22  | 2.03                     | 0.40              |
| 49:LJ:214:LEU:O    | 49:LJ:217:THR:OG1   | 2.30                     | 0.40              |
| 57:LR:125:GLN:O    | 57:LR:140:GLU:HA    | 2.21                     | 0.40              |
| 78:Lm:11:PHE:O     | 78:Lm:15:THR:HG23   | 2.22                     | 0.40              |
| 1:S2:916:U:H3      | 18:SZ:41:ARG:NE     | 2.20                     | 0.40              |
| 1:S2:1779:U:O4     | 81:Lp:12:ARG:NH1    | 2.51                     | 0.40              |
| 3:SP:17:LEU:HD13   | 3:SP:50:VAL:HB      | 2.04                     | 0.40              |
| 7:SA:222:VAL:HA    | 34:SO:191:ASP:O     | 2.21                     | 0.40              |
| 8:SS:206:ASP:HB3   | 8:SS:222:LEU:HD13   | 2.02                     | 0.40              |
| 11:SU:103:SER:OG   | 11:SU:104:ARG:N     | 2.50                     | 0.40              |
| 16:SD:130:THR:HG23 | 16:SD:133:LEU:H     | 1.87                     | 0.40              |
| 40:LA:110:G:OP2    | 53:LN:73:ARG:NH1    | 2.40                     | 0.40              |
| 40:LA:2116:G:OP1   | 40:LA:2118:C:N4     | 2.55                     | 0.40              |
| 40:LA:3181:C:O2'   | 56:LQ:164[A]:SER:OG | 2.37                     | 0.40              |
| 49:LJ:94:PHE:HB3   | 49:LJ:189:LEU:HD11  | 2.04                     | 0.40              |
| 49:LJ:130:TYR:HD2  | 49:LJ:204:ARG:HH21  | 1.70                     | 0.40              |
| 52:LM:40:LEU:HD12  | 52:LM:114:ILE:HD11  | 2.03                     | 0.40              |
| 80:Lo:110:CYS:SG   | 80:Lo:111:ARG:N     | 2.95                     | 0.40              |
| 86:A:1280:THR:C    | 86:A:1282:LEU:H     | 2.29                     | 0.40              |
| 1:S2:126:A:OP2     | 10:ST:197:ASN:ND2   | 2.54                     | 0.40              |
| 1:S2:1699:G:H2'    | 1:S2:1701:A:H62     | 1.87                     | 0.40              |
| 4:SQ:158:SER:HA    | 4:SQ:161:ILE:HD12   | 2.04                     | 0.40              |
| 9:SB:94:THR:HA     | 9:SB:97:LEU:HD12    | 2.04                     | 0.40              |
| 9:SB:198:LEU:HD23  | 9:SB:198:LEU:HA     | 1.98                     | 0.40              |
| 12:SV:26:LYS:HA    | 12:SV:29:LEU:HD23   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:SW:85:VAL:HG12 | 13:SW:99:LEU:HD13  | 2.04                     | 0.40              |
| 21:SH:88:ARG:O    | 21:SH:98:TYR:N     | 2.48                     | 0.40              |
| 25:Sb:94:LEU:HD21 | 25:Sb:102:VAL:HG23 | 2.04                     | 0.40              |
| 27:Sd:37:LYS:HZ3  | 27:Sd:60:PHE:HD2   | 1.70                     | 0.40              |
| 33:SN:113:LYS:NZ  | 33:SN:114:VAL:O    | 2.54                     | 0.40              |
| 52:LM:32:ARG:HD2  | 52:LM:120:ILE:HA   | 2.03                     | 0.40              |
| 69:Ld:36:ASP:HA   | 69:Ld:37:PRO:HD3   | 1.97                     | 0.40              |
| 79:Ln:16:ALA:HB1  | 79:Ln:42:ARG:HH21  | 1.86                     | 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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | SP    | 204/206 (99%) | 183 (90%) | 21 (10%) | 0        | 100         | 100 |
| 4   | SQ    | 222/232 (96%) | 201 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | SE    | 115/117 (98%) | 100 (87%) | 15 (13%) | 0        | 100         | 100 |
| 6   | SR    | 214/216 (99%) | 190 (89%) | 24 (11%) | 0        | 100         | 100 |
| 7   | SA    | 220/222 (99%) | 209 (95%) | 11 (5%)  | 0        | 100         | 100 |
| 8   | SS    | 256/258 (99%) | 229 (90%) | 27 (10%) | 0        | 100         | 100 |
| 9   | SB    | 204/206 (99%) | 189 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 10  | ST    | 226/228 (99%) | 211 (93%) | 14 (6%)  | 1 (0%)   | 30          | 64  |
| 11  | SU    | 182/184 (99%) | 163 (90%) | 19 (10%) | 0        | 100         | 100 |
| 12  | SV    | 183/198 (92%) | 167 (91%) | 16 (9%)  | 0        | 100         | 100 |
| 13  | SW    | 182/184 (99%) | 165 (91%) | 16 (9%)  | 1 (0%)   | 24          | 59  |
| 14  | SC    | 90/92 (98%)   | 79 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 15  | SX    | 140/142 (99%) | 124 (89%) | 16 (11%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 16  | SD    | 119/121 (98%)  | 91 (76%)  | 26 (22%) | 2 (2%)   | 7           | 35  |
| 17  | SY    | 148/150 (99%)  | 133 (90%) | 15 (10%) | 0        | 100         | 100 |
| 18  | SZ    | 125/127 (98%)  | 110 (88%) | 15 (12%) | 0        | 100         | 100 |
| 19  | SF    | 139/141 (99%)  | 125 (90%) | 14 (10%) | 0        | 100         | 100 |
| 20  | SG    | 117/125 (94%)  | 112 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 21  | SH    | 143/145 (99%)  | 131 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 22  | SI    | 141/143 (99%)  | 128 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 23  | SJ    | 98/100 (98%)   | 88 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 24  | Sa    | 85/87 (98%)    | 73 (86%)  | 12 (14%) | 0        | 100         | 100 |
| 25  | Sb    | 127/129 (98%)  | 113 (89%) | 14 (11%) | 0        | 100         | 100 |
| 26  | Sc    | 142/144 (99%)  | 123 (87%) | 19 (13%) | 0        | 100         | 100 |
| 27  | Sd    | 132/134 (98%)  | 124 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 28  | SK    | 80/82 (98%)    | 69 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 29  | Se    | 95/97 (98%)    | 84 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 30  | Sf    | 79/81 (98%)    | 67 (85%)  | 12 (15%) | 0        | 100         | 100 |
| 31  | SM    | 51/53 (96%)    | 48 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 32  | Sg    | 55/57 (96%)    | 43 (78%)  | 12 (22%) | 0        | 100         | 100 |
| 33  | SN    | 71/73 (97%)    | 48 (68%)  | 23 (32%) | 0        | 100         | 100 |
| 34  | SO    | 310/312 (99%)  | 268 (86%) | 42 (14%) | 0        | 100         | 100 |
| 35  | SL    | 61/63 (97%)    | 57 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 38  | So    | 341/366 (93%)  | 311 (91%) | 30 (9%)  | 0        | 100         | 100 |
| 43  | LD    | 249/251 (99%)  | 223 (90%) | 26 (10%) | 0        | 100         | 100 |
| 44  | LE    | 384/386 (100%) | 355 (92%) | 29 (8%)  | 0        | 100         | 100 |
| 45  | LF    | 359/361 (99%)  | 323 (90%) | 35 (10%) | 1 (0%)   | 36          | 69  |
| 46  | LG    | 292/294 (99%)  | 266 (91%) | 26 (9%)  | 0        | 100         | 100 |
| 47  | LH    | 163/175 (93%)  | 147 (90%) | 16 (10%) | 0        | 100         | 100 |
| 48  | LI    | 220/222 (99%)  | 203 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 49  | LJ    | 231/233 (99%)  | 208 (90%) | 23 (10%) | 0        | 100         | 100 |
| 50  | LK    | 189/191 (99%)  | 174 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 51  | LL    | 216/218 (99%)  | 189 (88%) | 27 (12%) | 0        | 100         | 100 |
| 52  | LM    | 167/169 (99%)  | 153 (92%) | 14 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 53  | LN    | 191/193 (99%) | 171 (90%) | 19 (10%) | 1 (0%)   | 24          | 59  |
| 54  | LO    | 134/136 (98%) | 121 (90%) | 13 (10%) | 0        | 100         | 100 |
| 55  | LP    | 201/203 (99%) | 181 (90%) | 19 (10%) | 1 (0%)   | 24          | 59  |
| 56  | LQ    | 195/197 (99%) | 186 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 57  | LR    | 181/183 (99%) | 168 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 58  | LS    | 183/185 (99%) | 170 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 59  | LT    | 186/188 (99%) | 178 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 60  | LU    | 169/171 (99%) | 159 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 61  | LV    | 157/159 (99%) | 143 (91%) | 14 (9%)  | 0        | 100         | 100 |
| 62  | LW    | 98/100 (98%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 63  | LX    | 134/136 (98%) | 128 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 64  | LY    | 63/65 (97%)   | 59 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 65  | LZ    | 119/121 (98%) | 110 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 66  | La    | 123/125 (98%) | 117 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 67  | Lb    | 133/135 (98%) | 117 (88%) | 16 (12%) | 0        | 100         | 100 |
| 68  | Lc    | 146/148 (99%) | 130 (89%) | 16 (11%) | 0        | 100         | 100 |
| 69  | Ld    | 56/58 (97%)   | 47 (84%)  | 9 (16%)  | 0        | 100         | 100 |
| 70  | Le    | 94/96 (98%)   | 92 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 71  | Lf    | 107/109 (98%) | 93 (87%)  | 14 (13%) | 0        | 100         | 100 |
| 72  | Lg    | 125/127 (98%) | 115 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 73  | Lh    | 104/106 (98%) | 98 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 74  | Li    | 110/112 (98%) | 105 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 75  | Lj    | 117/119 (98%) | 109 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 76  | Lk    | 97/99 (98%)   | 91 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 77  | Ll    | 79/81 (98%)   | 71 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 78  | Lm    | 75/77 (97%)   | 72 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 79  | Ln    | 48/50 (96%)   | 46 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 80  | Lo    | 50/52 (96%)   | 44 (88%)  | 6 (12%)  | 0        | 100         | 100 |
| 81  | Lp    | 23/25 (92%)   | 23 (100%) | 0        | 0        | 100         | 100 |
| 82  | Lq    | 101/103 (98%) | 93 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 83  | Lr    | 89/91 (98%)   | 87 (98%)  | 2 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 84  | Ls    | 151/154 (98%)     | 117 (78%)   | 31 (20%)   | 3 (2%)   | 6           | 32 |
| 86  | A     | 1182/1209 (98%)   | 929 (79%)   | 190 (16%)  | 63 (5%)  | 1           | 17 |
| All | All   | 12588/12828 (98%) | 11260 (90%) | 1255 (10%) | 73 (1%)  | 23          | 55 |

All (73) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 84  | Ls    | 133  | ASP  |
| 86  | A     | 1162 | ALA  |
| 86  | A     | 1163 | LEU  |
| 86  | A     | 1164 | SER  |
| 86  | A     | 1182 | PRO  |
| 86  | A     | 1341 | TYR  |
| 86  | A     | 1353 | GLN  |
| 86  | A     | 1394 | ILE  |
| 86  | A     | 1421 | PRO  |
| 86  | A     | 1442 | ALA  |
| 86  | A     | 1459 | ALA  |
| 86  | A     | 1538 | ALA  |
| 86  | A     | 1541 | ALA  |
| 86  | A     | 1561 | ALA  |
| 86  | A     | 1616 | ALA  |
| 86  | A     | 1820 | ALA  |
| 86  | A     | 1832 | ALA  |
| 86  | A     | 1839 | ALA  |
| 86  | A     | 1900 | ALA  |
| 86  | A     | 2020 | ALA  |
| 86  | A     | 2032 | ALA  |
| 86  | A     | 2039 | ALA  |
| 86  | A     | 2101 | ALA  |
| 86  | A     | 2232 | ALA  |
| 86  | A     | 2239 | ALA  |
| 86  | A     | 2300 | ALA  |
| 86  | A     | 2331 | ALA  |
| 86  | A     | 2343 | ALA  |
| 86  | A     | 2350 | ALA  |
| 86  | A     | 2411 | ALA  |
| 16  | SD    | 109  | GLU  |
| 86  | A     | 1136 | ASN  |
| 86  | A     | 1245 | VAL  |
| 86  | A     | 1249 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 86  | A     | 1257 | ASP  |
| 86  | A     | 1290 | VAL  |
| 86  | A     | 1691 | ALA  |
| 86  | A     | 1815 | ALA  |
| 86  | A     | 1873 | ALA  |
| 86  | A     | 2015 | ALA  |
| 86  | A     | 2073 | ALA  |
| 86  | A     | 2273 | ALA  |
| 86  | A     | 2326 | ALA  |
| 86  | A     | 2384 | ALA  |
| 45  | LF    | 4    | PRO  |
| 84  | Ls    | 8    | PHE  |
| 86  | A     | 1402 | ILE  |
| 86  | A     | 1454 | ALA  |
| 86  | A     | 1457 | ALA  |
| 86  | A     | 1521 | ALA  |
| 86  | A     | 1618 | ALA  |
| 86  | A     | 1707 | ALA  |
| 86  | A     | 1881 | ALA  |
| 86  | A     | 2081 | ALA  |
| 86  | A     | 2281 | ALA  |
| 86  | A     | 2392 | ALA  |
| 84  | Ls    | 98   | GLY  |
| 86  | A     | 943  | ALA  |
| 86  | A     | 1137 | PRO  |
| 86  | A     | 1277 | LEU  |
| 86  | A     | 1537 | ALA  |
| 86  | A     | 1556 | ALA  |
| 86  | A     | 1600 | ALA  |
| 86  | A     | 1637 | ALA  |
| 86  | A     | 1223 | PRO  |
| 86  | A     | 1641 | ALA  |
| 55  | LP    | 146  | ALA  |
| 86  | A     | 1236 | ILE  |
| 13  | SW    | 18   | PRO  |
| 53  | LN    | 61   | PRO  |
| 10  | ST    | 226  | ILE  |
| 16  | SD    | 127  | GLY  |
| 86  | A     | 1338 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | SP    | 170/173 (98%)  | 170 (100%) | 0        | 100         | 100 |
| 4   | SQ    | 200/205 (98%)  | 200 (100%) | 0        | 100         | 100 |
| 5   | SE    | 95/98 (97%)    | 95 (100%)  | 0        | 100         | 100 |
| 6   | SR    | 175/175 (100%) | 175 (100%) | 0        | 100         | 100 |
| 7   | SA    | 182/182 (100%) | 180 (99%)  | 2 (1%)   | 65          | 74  |
| 8   | SS    | 220/220 (100%) | 220 (100%) | 0        | 100         | 100 |
| 9   | SB    | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 10  | ST    | 189/195 (97%)  | 189 (100%) | 0        | 100         | 100 |
| 11  | SU    | 163/165 (99%)  | 163 (100%) | 0        | 100         | 100 |
| 12  | SV    | 148/159 (93%)  | 148 (100%) | 0        | 100         | 100 |
| 13  | SW    | 156/157 (99%)  | 155 (99%)  | 1 (1%)   | 78          | 80  |
| 14  | SC    | 77/85 (91%)    | 76 (99%)   | 1 (1%)   | 61          | 71  |
| 15  | SX    | 126/127 (99%)  | 125 (99%)  | 1 (1%)   | 73          | 77  |
| 16  | SD    | 88/98 (90%)    | 88 (100%)  | 0        | 100         | 100 |
| 17  | SY    | 127/127 (100%) | 126 (99%)  | 1 (1%)   | 73          | 77  |
| 18  | SZ    | 90/96 (94%)    | 90 (100%)  | 0        | 100         | 100 |
| 19  | SF    | 117/117 (100%) | 116 (99%)  | 1 (1%)   | 70          | 75  |
| 20  | SG    | 101/113 (89%)  | 101 (100%) | 0        | 100         | 100 |
| 21  | SH    | 127/128 (99%)  | 126 (99%)  | 1 (1%)   | 73          | 77  |
| 22  | SI    | 115/115 (100%) | 114 (99%)  | 1 (1%)   | 70          | 75  |
| 23  | SJ    | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 24  | Sa    | 71/74 (96%)    | 71 (100%)  | 0        | 100         | 100 |
| 25  | Sb    | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 26  | Sc    | 119/119 (100%) | 118 (99%)  | 1 (1%)   | 73          | 77  |
| 27  | Sd    | 102/112 (91%)  | 102 (100%) | 0        | 100         | 100 |
| 28  | SK    | 67/73 (92%)    | 67 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 29  | Se    | 82/83 (99%)    | 81 (99%)   | 1 (1%)   | 63          | 72  |
| 30  | Sf    | 70/70 (100%)   | 70 (100%)  | 0        | 100         | 100 |
| 31  | SM    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 32  | Sg    | 48/49 (98%)    | 48 (100%)  | 0        | 100         | 100 |
| 33  | SN    | 56/63 (89%)    | 56 (100%)  | 0        | 100         | 100 |
| 34  | SO    | 250/257 (97%)  | 250 (100%) | 0        | 100         | 100 |
| 35  | SL    | 55/56 (98%)    | 55 (100%)  | 0        | 100         | 100 |
| 38  | So    | 298/308 (97%)  | 297 (100%) | 1 (0%)   | 86          | 85  |
| 43  | LD    | 190/193 (98%)  | 190 (100%) | 0        | 100         | 100 |
| 44  | LE    | 318/322 (99%)  | 317 (100%) | 1 (0%)   | 86          | 85  |
| 45  | LF    | 288/288 (100%) | 287 (100%) | 1 (0%)   | 86          | 85  |
| 46  | LG    | 241/243 (99%)  | 241 (100%) | 0        | 100         | 100 |
| 47  | LH    | 139/154 (90%)  | 138 (99%)  | 1 (1%)   | 76          | 78  |
| 48  | LI    | 186/186 (100%) | 186 (100%) | 0        | 100         | 100 |
| 49  | LJ    | 187/191 (98%)  | 187 (100%) | 0        | 100         | 100 |
| 50  | LK    | 168/171 (98%)  | 168 (100%) | 0        | 100         | 100 |
| 51  | LL    | 185/185 (100%) | 185 (100%) | 0        | 100         | 100 |
| 52  | LM    | 145/147 (99%)  | 145 (100%) | 0        | 100         | 100 |
| 53  | LN    | 154/154 (100%) | 154 (100%) | 0        | 100         | 100 |
| 54  | LO    | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 55  | LP    | 175/175 (100%) | 174 (99%)  | 1 (1%)   | 78          | 80  |
| 56  | LQ    | 160/160 (100%) | 160 (100%) | 0        | 100         | 100 |
| 57  | LR    | 138/145 (95%)  | 138 (100%) | 0        | 100         | 100 |
| 58  | LS    | 150/150 (100%) | 149 (99%)  | 1 (1%)   | 76          | 78  |
| 59  | LT    | 152/153 (99%)  | 152 (100%) | 0        | 100         | 100 |
| 60  | LU    | 155/155 (100%) | 155 (100%) | 0        | 100         | 100 |
| 61  | LV    | 135/136 (99%)  | 135 (100%) | 0        | 100         | 100 |
| 62  | LW    | 87/87 (100%)   | 87 (100%)  | 0        | 100         | 100 |
| 63  | LX    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 64  | LY    | 54/57 (95%)    | 54 (100%)  | 0        | 100         | 100 |
| 65  | LZ    | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 66  | La    | 108/108 (100%)  | 107 (99%)   | 1 (1%)   | 70          | 75  |
| 67  | Lb    | 112/115 (97%)   | 112 (100%)  | 0        | 100         | 100 |
| 68  | Lc    | 117/118 (99%)   | 117 (100%)  | 0        | 100         | 100 |
| 69  | Ld    | 46/46 (100%)    | 46 (100%)   | 0        | 100         | 100 |
| 70  | Le    | 81/81 (100%)    | 81 (100%)   | 0        | 100         | 100 |
| 71  | Lf    | 92/96 (96%)     | 92 (100%)   | 0        | 100         | 100 |
| 72  | Lg    | 108/109 (99%)   | 108 (100%)  | 0        | 100         | 100 |
| 73  | Lh    | 90/90 (100%)    | 89 (99%)    | 1 (1%)   | 65          | 74  |
| 74  | Li    | 95/95 (100%)    | 95 (100%)   | 0        | 100         | 100 |
| 75  | Lj    | 104/104 (100%)  | 103 (99%)   | 1 (1%)   | 68          | 75  |
| 76  | Lk    | 80/81 (99%)     | 79 (99%)    | 1 (1%)   | 61          | 71  |
| 77  | Ll    | 67/67 (100%)    | 64 (96%)    | 3 (4%)   | 24          | 49  |
| 78  | Lm    | 68/68 (100%)    | 68 (100%)   | 0        | 100         | 100 |
| 79  | Ln    | 45/45 (100%)    | 45 (100%)   | 0        | 100         | 100 |
| 80  | Lo    | 45/47 (96%)     | 45 (100%)   | 0        | 100         | 100 |
| 81  | Lp    | 22/23 (96%)     | 22 (100%)   | 0        | 100         | 100 |
| 82  | Lq    | 87/88 (99%)     | 87 (100%)   | 0        | 100         | 100 |
| 83  | Lr    | 71/71 (100%)    | 70 (99%)    | 1 (1%)   | 59          | 71  |
| 84  | Ls    | 118/129 (92%)   | 117 (99%)   | 1 (1%)   | 73          | 77  |
| All | All   | 9584/9771 (98%) | 9558 (100%) | 26 (0%)  | 84          | 85  |

All (26) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | SA    | 168 | ILE  |
| 7   | SA    | 185 | LYS  |
| 13  | SW    | 39  | LYS  |
| 14  | SC    | 64  | TYR  |
| 15  | SX    | 32  | LYS  |
| 17  | SY    | 39  | LYS  |
| 19  | SF    | 107 | LYS  |
| 21  | SH    | 98  | TYR  |
| 22  | SI    | 84  | LYS  |
| 26  | Sc    | 140 | LYS  |
| 29  | Se    | 66  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | So    | 257 | VAL  |
| 44  | LE    | 104 | THR  |
| 45  | LF    | 12  | THR  |
| 47  | LH    | 156 | LYS  |
| 55  | LP    | 27  | VAL  |
| 58  | LS    | 31  | LYS  |
| 66  | La    | 74  | TYR  |
| 73  | Lh    | 20  | LYS  |
| 75  | Lj    | 107 | LYS  |
| 76  | Lk    | 4   | LYS  |
| 77  | Ll    | 11  | ARG  |
| 77  | Ll    | 19  | CYS  |
| 77  | Ll    | 22  | CYS  |
| 83  | Lr    | 45  | LYS  |
| 84  | Ls    | 102 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | SP    | 39  | ASN  |
| 3   | SP    | 140 | ASN  |
| 4   | SQ    | 40  | ASN  |
| 4   | SQ    | 74  | GLN  |
| 6   | SR    | 94  | GLN  |
| 6   | SR    | 110 | HIS  |
| 6   | SR    | 220 | ASN  |
| 8   | SS    | 69  | HIS  |
| 8   | SS    | 96  | ASN  |
| 9   | SB    | 34  | GLN  |
| 9   | SB    | 100 | ASN  |
| 9   | SB    | 186 | ASN  |
| 10  | ST    | 56  | ASN  |
| 10  | ST    | 59  | GLN  |
| 10  | ST    | 139 | ASN  |
| 10  | ST    | 197 | ASN  |
| 11  | SU    | 29  | ASN  |
| 11  | SU    | 74  | GLN  |
| 11  | SU    | 174 | ASN  |
| 12  | SV    | 20  | GLN  |
| 12  | SV    | 35  | ASN  |
| 12  | SV    | 52  | ASN  |
| 12  | SV    | 103 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | SV    | 159 | GLN  |
| 13  | SW    | 112 | GLN  |
| 13  | SW    | 176 | ASN  |
| 14  | SC    | 62  | GLN  |
| 15  | SX    | 22  | ASN  |
| 17  | SY    | 58  | HIS  |
| 17  | SY    | 105 | ASN  |
| 18  | SZ    | 12  | GLN  |
| 18  | SZ    | 24  | ASN  |
| 19  | SF    | 77  | GLN  |
| 19  | SF    | 83  | GLN  |
| 20  | SG    | 29  | GLN  |
| 20  | SG    | 74  | GLN  |
| 20  | SG    | 101 | ASN  |
| 21  | SH    | 8   | GLN  |
| 21  | SH    | 21  | ASN  |
| 21  | SH    | 71  | GLN  |
| 21  | SH    | 99  | HIS  |
| 22  | SI    | 16  | ASN  |
| 22  | SI    | 70  | GLN  |
| 22  | SI    | 101 | ASN  |
| 22  | SI    | 138 | GLN  |
| 23  | SJ    | 49  | ASN  |
| 24  | Sa    | 29  | HIS  |
| 25  | Sb    | 56  | HIS  |
| 25  | Sb    | 80  | ASN  |
| 27  | Sd    | 34  | ASN  |
| 27  | Sd    | 110 | GLN  |
| 29  | Se    | 43  | ASN  |
| 30  | Sf    | 5   | GLN  |
| 30  | Sf    | 19  | HIS  |
| 30  | Sf    | 42  | ASN  |
| 32  | Sg    | 17  | GLN  |
| 33  | SN    | 123 | ASN  |
| 33  | SN    | 135 | HIS  |
| 33  | SN    | 145 | HIS  |
| 33  | SN    | 151 | ASN  |
| 34  | SO    | 159 | ASN  |
| 34  | SO    | 308 | ASN  |
| 35  | SL    | 27  | GLN  |
| 38  | So    | 168 | ASN  |
| 38  | So    | 241 | HIS  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 38  | So    | 292   | GLN  |
| 38  | So    | 358   | HIS  |
| 43  | LD    | 47    | GLN  |
| 43  | LD    | 97    | ASN  |
| 43  | LD    | 205   | ASN  |
| 44  | LE    | 198   | HIS  |
| 44  | LE    | 279   | ASN  |
| 44  | LE    | 293   | ASN  |
| 45  | LF    | 87    | GLN  |
| 45  | LF    | 296   | GLN  |
| 45  | LF    | 316   | ASN  |
| 45  | LF    | 322   | GLN  |
| 46  | LG    | 206   | GLN  |
| 48  | LI    | 61    | ASN  |
| 48  | LI    | 64    | GLN  |
| 48  | LI    | 186   | HIS  |
| 48  | LI    | 244   | ASN  |
| 49  | LJ    | 59    | GLN  |
| 49  | LJ    | 77    | GLN  |
| 49  | LJ    | 192   | GLN  |
| 49  | LJ    | 243   | GLN  |
| 50  | LK    | 59    | ASN  |
| 50  | LK    | 149   | ASN  |
| 50  | LK    | 157   | ASN  |
| 50  | LK    | 169   | ASN  |
| 52  | LM    | 90    | GLN  |
| 53  | LN    | 19    | GLN  |
| 53  | LN    | 105   | ASN  |
| 53  | LN    | 160   | GLN  |
| 54  | LO    | 41    | GLN  |
| 55  | LP    | 117   | ASN  |
| 55  | LP    | 182   | ASN  |
| 56  | LQ    | 50[A] | ASN  |
| 57  | LR    | 55    | GLN  |
| 57  | LR    | 97    | ASN  |
| 57  | LR    | 118   | GLN  |
| 58  | LS    | 9     | GLN  |
| 58  | LS    | 23    | ASN  |
| 58  | LS    | 45    | ASN  |
| 58  | LS    | 58    | ASN  |
| 59  | LT    | 166   | ASN  |
| 60  | LU    | 49    | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 60  | LU    | 108 | GLN  |
| 60  | LU    | 138 | GLN  |
| 62  | LW    | 49  | ASN  |
| 62  | LW    | 87  | ASN  |
| 64  | LY    | 59  | HIS  |
| 66  | La    | 4   | GLN  |
| 66  | La    | 110 | HIS  |
| 67  | Lb    | 103 | GLN  |
| 67  | Lb    | 122 | HIS  |
| 67  | Lb    | 123 | GLN  |
| 67  | Lb    | 127 | ASN  |
| 68  | Lc    | 14  | HIS  |
| 68  | Lc    | 62  | HIS  |
| 68  | Lc    | 64  | GLN  |
| 69  | Ld    | 10  | HIS  |
| 70  | Le    | 11  | ASN  |
| 71  | Lf    | 87  | ASN  |
| 72  | Lg    | 6   | HIS  |
| 72  | Lg    | 13  | HIS  |
| 73  | Lh    | 26  | ASN  |
| 73  | Lh    | 42  | GLN  |
| 73  | Lh    | 88  | ASN  |
| 74  | Li    | 52  | GLN  |
| 74  | Li    | 61  | GLN  |
| 76  | Lk    | 92  | ASN  |
| 78  | Lm    | 57  | ASN  |
| 79  | Ln    | 25  | GLN  |
| 79  | Ln    | 32  | ASN  |
| 80  | Lo    | 109 | ASN  |
| 82  | Lq    | 23  | HIS  |
| 82  | Lq    | 59  | HIS  |
| 84  | Ls    | 88  | ASN  |
| 84  | Ls    | 104 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | S2    | 1768/1800 (98%) | 533 (30%)         | 52 (2%)         |
| 2   | Sl    | 5/6 (83%)       | 1 (20%)           | 0               |
| 36  | Sm    | 75/76 (98%)     | 35 (46%)          | 0               |
| 37  | Sn    | 74/75 (98%)     | 23 (31%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 40  | LA    | 3180/3394 (93%) | 717 (22%)         | 42 (1%)         |
| 41  | LB    | 120/121 (99%)   | 15 (12%)          | 1 (0%)          |
| 42  | LC    | 157/158 (99%)   | 32 (20%)          | 3 (1%)          |
| All | All   | 5379/5630 (95%) | 1356 (25%)        | 98 (1%)         |

All (1356) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 2   | A    |
| 1   | S2    | 4   | C    |
| 1   | S2    | 14  | C    |
| 1   | S2    | 25  | C    |
| 1   | S2    | 26  | A    |
| 1   | S2    | 34  | G    |
| 1   | S2    | 43  | A    |
| 1   | S2    | 45  | U    |
| 1   | S2    | 47  | A    |
| 1   | S2    | 56  | U    |
| 1   | S2    | 57  | G    |
| 1   | S2    | 62  | A    |
| 1   | S2    | 65  | A    |
| 1   | S2    | 67  | A    |
| 1   | S2    | 68  | A    |
| 1   | S2    | 69  | G    |
| 1   | S2    | 73  | U    |
| 1   | S2    | 74  | U    |
| 1   | S2    | 75  | U    |
| 1   | S2    | 76  | A    |
| 1   | S2    | 78  | A    |
| 1   | S2    | 79  | C    |
| 1   | S2    | 80  | A    |
| 1   | S2    | 81  | G    |
| 1   | S2    | 104 | A    |
| 1   | S2    | 114 | C    |
| 1   | S2    | 116 | U    |
| 1   | S2    | 121 | U    |
| 1   | S2    | 127 | G    |
| 1   | S2    | 129 | U    |
| 1   | S2    | 130 | C    |
| 1   | S2    | 131 | C    |
| 1   | S2    | 132 | U    |
| 1   | S2    | 133 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 134 | U    |
| 1   | S2    | 135 | A    |
| 1   | S2    | 136 | C    |
| 1   | S2    | 137 | U    |
| 1   | S2    | 138 | A    |
| 1   | S2    | 140 | A    |
| 1   | S2    | 141 | U    |
| 1   | S2    | 142 | G    |
| 1   | S2    | 153 | G    |
| 1   | S2    | 155 | U    |
| 1   | S2    | 156 | A    |
| 1   | S2    | 158 | U    |
| 1   | S2    | 161 | U    |
| 1   | S2    | 168 | A    |
| 1   | S2    | 171 | A    |
| 1   | S2    | 172 | C    |
| 1   | S2    | 174 | U    |
| 1   | S2    | 176 | C    |
| 1   | S2    | 178 | U    |
| 1   | S2    | 179 | A    |
| 1   | S2    | 182 | A    |
| 1   | S2    | 185 | U    |
| 1   | S2    | 186 | C    |
| 1   | S2    | 187 | G    |
| 1   | S2    | 188 | A    |
| 1   | S2    | 189 | C    |
| 1   | S2    | 191 | C    |
| 1   | S2    | 193 | U    |
| 1   | S2    | 194 | U    |
| 1   | S2    | 195 | G    |
| 1   | S2    | 201 | G    |
| 1   | S2    | 203 | U    |
| 1   | S2    | 204 | G    |
| 1   | S2    | 216 | U    |
| 1   | S2    | 217 | A    |
| 1   | S2    | 218 | A    |
| 1   | S2    | 223 | U    |
| 1   | S2    | 224 | C    |
| 1   | S2    | 225 | A    |
| 1   | S2    | 227 | U    |
| 1   | S2    | 228 | G    |
| 1   | S2    | 230 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 232 | U    |
| 1   | S2    | 233 | C    |
| 1   | S2    | 234 | G    |
| 1   | S2    | 235 | G    |
| 1   | S2    | 236 | A    |
| 1   | S2    | 238 | U    |
| 1   | S2    | 240 | U    |
| 1   | S2    | 241 | U    |
| 1   | S2    | 243 | G    |
| 1   | S2    | 246 | G    |
| 1   | S2    | 250 | C    |
| 1   | S2    | 256 | A    |
| 1   | S2    | 260 | U    |
| 1   | S2    | 261 | U    |
| 1   | S2    | 265 | A    |
| 1   | S2    | 270 | C    |
| 1   | S2    | 272 | U    |
| 1   | S2    | 274 | G    |
| 1   | S2    | 276 | C    |
| 1   | S2    | 277 | U    |
| 1   | S2    | 278 | U    |
| 1   | S2    | 279 | G    |
| 1   | S2    | 280 | U    |
| 1   | S2    | 287 | G    |
| 1   | S2    | 299 | A    |
| 1   | S2    | 313 | U    |
| 1   | S2    | 314 | C    |
| 1   | S2    | 316 | A    |
| 1   | S2    | 320 | U    |
| 1   | S2    | 321 | C    |
| 1   | S2    | 322 | G    |
| 1   | S2    | 323 | A    |
| 1   | S2    | 324 | U    |
| 1   | S2    | 330 | G    |
| 1   | S2    | 333 | A    |
| 1   | S2    | 334 | G    |
| 1   | S2    | 337 | G    |
| 1   | S2    | 338 | C    |
| 1   | S2    | 352 | A    |
| 1   | S2    | 353 | A    |
| 1   | S2    | 359 | A    |
| 1   | S2    | 360 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 361 | C    |
| 1   | S2    | 369 | A    |
| 1   | S2    | 370 | A    |
| 1   | S2    | 373 | G    |
| 1   | S2    | 378 | A    |
| 1   | S2    | 380 | U    |
| 1   | S2    | 388 | G    |
| 1   | S2    | 390 | G    |
| 1   | S2    | 400 | A    |
| 1   | S2    | 401 | A    |
| 1   | S2    | 402 | C    |
| 1   | S2    | 404 | G    |
| 1   | S2    | 406 | U    |
| 1   | S2    | 411 | C    |
| 1   | S2    | 415 | C    |
| 1   | S2    | 417 | A    |
| 1   | S2    | 419 | G    |
| 1   | S2    | 423 | G    |
| 1   | S2    | 424 | C    |
| 1   | S2    | 425 | A    |
| 1   | S2    | 426 | G    |
| 1   | S2    | 434 | G    |
| 1   | S2    | 435 | C    |
| 1   | S2    | 438 | A    |
| 1   | S2    | 439 | U    |
| 1   | S2    | 444 | C    |
| 1   | S2    | 446 | A    |
| 1   | S2    | 447 | U    |
| 1   | S2    | 448 | C    |
| 1   | S2    | 454 | U    |
| 1   | S2    | 460 | A    |
| 1   | S2    | 468 | A    |
| 1   | S2    | 482 | U    |
| 1   | S2    | 485 | A    |
| 1   | S2    | 487 | G    |
| 1   | S2    | 489 | C    |
| 1   | S2    | 491 | C    |
| 1   | S2    | 492 | A    |
| 1   | S2    | 493 | U    |
| 1   | S2    | 494 | U    |
| 1   | S2    | 495 | C    |
| 1   | S2    | 496 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 498 | G    |
| 1   | S2    | 499 | U    |
| 1   | S2    | 500 | C    |
| 1   | S2    | 502 | U    |
| 1   | S2    | 506 | A    |
| 1   | S2    | 507 | U    |
| 1   | S2    | 510 | G    |
| 1   | S2    | 511 | A    |
| 1   | S2    | 512 | A    |
| 1   | S2    | 513 | U    |
| 1   | S2    | 517 | U    |
| 1   | S2    | 518 | A    |
| 1   | S2    | 519 | C    |
| 1   | S2    | 520 | A    |
| 1   | S2    | 525 | A    |
| 1   | S2    | 527 | A    |
| 1   | S2    | 529 | A    |
| 1   | S2    | 534 | A    |
| 1   | S2    | 538 | A    |
| 1   | S2    | 539 | G    |
| 1   | S2    | 540 | G    |
| 1   | S2    | 541 | A    |
| 1   | S2    | 542 | A    |
| 1   | S2    | 543 | C    |
| 1   | S2    | 554 | C    |
| 1   | S2    | 555 | A    |
| 1   | S2    | 556 | A    |
| 1   | S2    | 557 | G    |
| 1   | S2    | 558 | U    |
| 1   | S2    | 565 | C    |
| 1   | S2    | 571 | G    |
| 1   | S2    | 572 | C    |
| 1   | S2    | 578 | U    |
| 1   | S2    | 579 | A    |
| 1   | S2    | 580 | A    |
| 1   | S2    | 594 | A    |
| 1   | S2    | 595 | G    |
| 1   | S2    | 606 | A    |
| 1   | S2    | 609 | U    |
| 1   | S2    | 610 | G    |
| 1   | S2    | 611 | U    |
| 1   | S2    | 617 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 619 | A    |
| 1   | S2    | 620 | A    |
| 1   | S2    | 623 | A    |
| 1   | S2    | 624 | G    |
| 1   | S2    | 635 | A    |
| 1   | S2    | 638 | U    |
| 1   | S2    | 639 | U    |
| 1   | S2    | 640 | U    |
| 1   | S2    | 641 | G    |
| 1   | S2    | 643 | G    |
| 1   | S2    | 645 | C    |
| 1   | S2    | 651 | G    |
| 1   | S2    | 653 | C    |
| 1   | S2    | 654 | C    |
| 1   | S2    | 655 | G    |
| 1   | S2    | 656 | G    |
| 1   | S2    | 677 | G    |
| 1   | S2    | 678 | A    |
| 1   | S2    | 680 | U    |
| 1   | S2    | 682 | C    |
| 1   | S2    | 684 | A    |
| 1   | S2    | 687 | G    |
| 1   | S2    | 693 | U    |
| 1   | S2    | 694 | U    |
| 1   | S2    | 696 | C    |
| 1   | S2    | 697 | C    |
| 1   | S2    | 698 | U    |
| 1   | S2    | 700 | C    |
| 1   | S2    | 702 | G    |
| 1   | S2    | 703 | G    |
| 1   | S2    | 704 | C    |
| 1   | S2    | 705 | U    |
| 1   | S2    | 706 | A    |
| 1   | S2    | 707 | A    |
| 1   | S2    | 708 | C    |
| 1   | S2    | 709 | C    |
| 1   | S2    | 710 | U    |
| 1   | S2    | 711 | U    |
| 1   | S2    | 712 | G    |
| 1   | S2    | 714 | G    |
| 1   | S2    | 728 | U    |
| 1   | S2    | 729 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 730 | G    |
| 1   | S2    | 732 | G    |
| 1   | S2    | 733 | A    |
| 1   | S2    | 736 | C    |
| 1   | S2    | 738 | G    |
| 1   | S2    | 739 | G    |
| 1   | S2    | 741 | C    |
| 1   | S2    | 742 | U    |
| 1   | S2    | 743 | U    |
| 1   | S2    | 744 | U    |
| 1   | S2    | 745 | U    |
| 1   | S2    | 753 | A    |
| 1   | S2    | 755 | A    |
| 1   | S2    | 756 | A    |
| 1   | S2    | 765 | G    |
| 1   | S2    | 766 | U    |
| 1   | S2    | 771 | A    |
| 1   | S2    | 774 | A    |
| 1   | S2    | 775 | G    |
| 1   | S2    | 778 | G    |
| 1   | S2    | 781 | U    |
| 1   | S2    | 782 | U    |
| 1   | S2    | 783 | G    |
| 1   | S2    | 787 | G    |
| 1   | S2    | 789 | A    |
| 1   | S2    | 794 | U    |
| 1   | S2    | 804 | A    |
| 1   | S2    | 807 | A    |
| 1   | S2    | 812 | A    |
| 1   | S2    | 813 | U    |
| 1   | S2    | 814 | A    |
| 1   | S2    | 815 | G    |
| 1   | S2    | 816 | G    |
| 1   | S2    | 818 | C    |
| 1   | S2    | 819 | G    |
| 1   | S2    | 820 | U    |
| 1   | S2    | 821 | U    |
| 1   | S2    | 823 | G    |
| 1   | S2    | 832 | U    |
| 1   | S2    | 833 | U    |
| 1   | S2    | 836 | U    |
| 1   | S2    | 837 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 839  | U    |
| 1   | S2    | 840  | U    |
| 1   | S2    | 841  | U    |
| 1   | S2    | 846  | G    |
| 1   | S2    | 851  | U    |
| 1   | S2    | 852  | C    |
| 1   | S2    | 855  | A    |
| 1   | S2    | 856  | A    |
| 1   | S2    | 857  | U    |
| 1   | S2    | 863  | A    |
| 1   | S2    | 865  | A    |
| 1   | S2    | 873  | U    |
| 1   | S2    | 876  | G    |
| 1   | S2    | 877  | G    |
| 1   | S2    | 886  | U    |
| 1   | S2    | 898  | A    |
| 1   | S2    | 899  | G    |
| 1   | S2    | 901  | G    |
| 1   | S2    | 902  | G    |
| 1   | S2    | 904  | G    |
| 1   | S2    | 912  | U    |
| 1   | S2    | 913  | G    |
| 1   | S2    | 929  | A    |
| 1   | S2    | 932  | U    |
| 1   | S2    | 933  | A    |
| 1   | S2    | 934  | C    |
| 1   | S2    | 935  | U    |
| 1   | S2    | 940  | A    |
| 1   | S2    | 945  | U    |
| 1   | S2    | 960  | U    |
| 1   | S2    | 964  | U    |
| 1   | S2    | 966  | A    |
| 1   | S2    | 970  | A    |
| 1   | S2    | 973  | A    |
| 1   | S2    | 977  | A    |
| 1   | S2    | 988  | A    |
| 1   | S2    | 989  | U    |
| 1   | S2    | 992  | A    |
| 1   | S2    | 996  | U    |
| 1   | S2    | 998  | A    |
| 1   | S2    | 1001 | A    |
| 1   | S2    | 1004 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 1024 | U    |
| 1   | S2    | 1026 | A    |
| 1   | S2    | 1028 | C    |
| 1   | S2    | 1029 | U    |
| 1   | S2    | 1032 | G    |
| 1   | S2    | 1039 | A    |
| 1   | S2    | 1040 | G    |
| 1   | S2    | 1052 | U    |
| 1   | S2    | 1053 | G    |
| 1   | S2    | 1057 | U    |
| 1   | S2    | 1058 | U    |
| 1   | S2    | 1059 | U    |
| 1   | S2    | 1060 | U    |
| 1   | S2    | 1061 | A    |
| 1   | S2    | 1062 | A    |
| 1   | S2    | 1063 | U    |
| 1   | S2    | 1074 | G    |
| 1   | S2    | 1080 | U    |
| 1   | S2    | 1081 | A    |
| 1   | S2    | 1082 | C    |
| 1   | S2    | 1092 | A    |
| 1   | S2    | 1096 | C    |
| 1   | S2    | 1099 | U    |
| 1   | S2    | 1100 | G    |
| 1   | S2    | 1109 | G    |
| 1   | S2    | 1111 | G    |
| 1   | S2    | 1113 | A    |
| 1   | S2    | 1138 | A    |
| 1   | S2    | 1156 | C    |
| 1   | S2    | 1158 | C    |
| 1   | S2    | 1160 | A    |
| 1   | S2    | 1164 | G    |
| 1   | S2    | 1167 | G    |
| 1   | S2    | 1170 | G    |
| 1   | S2    | 1183 | A    |
| 1   | S2    | 1185 | U    |
| 1   | S2    | 1186 | U    |
| 1   | S2    | 1187 | U    |
| 1   | S2    | 1191 | U    |
| 1   | S2    | 1194 | A    |
| 1   | S2    | 1196 | A    |
| 1   | S2    | 1197 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 1199 | G    |
| 1   | S2    | 1200 | G    |
| 1   | S2    | 1208 | A    |
| 1   | S2    | 1212 | G    |
| 1   | S2    | 1214 | U    |
| 1   | S2    | 1217 | A    |
| 1   | S2    | 1218 | G    |
| 1   | S2    | 1227 | A    |
| 1   | S2    | 1229 | G    |
| 1   | S2    | 1241 | G    |
| 1   | S2    | 1243 | G    |
| 1   | S2    | 1244 | A    |
| 1   | S2    | 1245 | G    |
| 1   | S2    | 1246 | C    |
| 1   | S2    | 1252 | C    |
| 1   | S2    | 1256 | A    |
| 1   | S2    | 1257 | U    |
| 1   | S2    | 1258 | U    |
| 1   | S2    | 1263 | G    |
| 1   | S2    | 1264 | G    |
| 1   | S2    | 1265 | G    |
| 1   | S2    | 1269 | U    |
| 1   | S2    | 1273 | G    |
| 1   | S2    | 1274 | C    |
| 1   | S2    | 1275 | A    |
| 1   | S2    | 1276 | U    |
| 1   | S2    | 1285 | U    |
| 1   | S2    | 1294 | G    |
| 1   | S2    | 1301 | U    |
| 1   | S2    | 1307 | U    |
| 1   | S2    | 1314 | U    |
| 1   | S2    | 1315 | U    |
| 1   | S2    | 1318 | G    |
| 1   | S2    | 1321 | A    |
| 1   | S2    | 1322 | A    |
| 1   | S2    | 1325 | A    |
| 1   | S2    | 1337 | A    |
| 1   | S2    | 1341 | A    |
| 1   | S2    | 1344 | A    |
| 1   | S2    | 1345 | A    |
| 1   | S2    | 1346 | A    |
| 1   | S2    | 1348 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 1349 | G    |
| 1   | S2    | 1354 | G    |
| 1   | S2    | 1360 | A    |
| 1   | S2    | 1361 | U    |
| 1   | S2    | 1363 | U    |
| 1   | S2    | 1367 | G    |
| 1   | S2    | 1370 | U    |
| 1   | S2    | 1371 | A    |
| 1   | S2    | 1372 | U    |
| 1   | S2    | 1373 | C    |
| 1   | S2    | 1381 | U    |
| 1   | S2    | 1382 | A    |
| 1   | S2    | 1383 | G    |
| 1   | S2    | 1385 | G    |
| 1   | S2    | 1390 | U    |
| 1   | S2    | 1398 | U    |
| 1   | S2    | 1399 | C    |
| 1   | S2    | 1400 | A    |
| 1   | S2    | 1402 | G    |
| 1   | S2    | 1414 | U    |
| 1   | S2    | 1415 | U    |
| 1   | S2    | 1421 | A    |
| 1   | S2    | 1427 | A    |
| 1   | S2    | 1431 | C    |
| 1   | S2    | 1432 | U    |
| 1   | S2    | 1433 | G    |
| 1   | S2    | 1446 | A    |
| 1   | S2    | 1447 | C    |
| 1   | S2    | 1448 | G    |
| 1   | S2    | 1457 | C    |
| 1   | S2    | 1458 | G    |
| 1   | S2    | 1459 | C    |
| 1   | S2    | 1460 | A    |
| 1   | S2    | 1469 | A    |
| 1   | S2    | 1472 | C    |
| 1   | S2    | 1473 | U    |
| 1   | S2    | 1479 | A    |
| 1   | S2    | 1482 | C    |
| 1   | S2    | 1483 | A    |
| 1   | S2    | 1488 | G    |
| 1   | S2    | 1489 | U    |
| 1   | S2    | 1490 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 1491 | U    |
| 1   | S2    | 1492 | A    |
| 1   | S2    | 1493 | A    |
| 1   | S2    | 1496 | U    |
| 1   | S2    | 1510 | U    |
| 1   | S2    | 1514 | U    |
| 1   | S2    | 1515 | A    |
| 1   | S2    | 1516 | A    |
| 1   | S2    | 1517 | U    |
| 1   | S2    | 1518 | C    |
| 1   | S2    | 1521 | G    |
| 1   | S2    | 1523 | G    |
| 1   | S2    | 1524 | A    |
| 1   | S2    | 1528 | U    |
| 1   | S2    | 1529 | C    |
| 1   | S2    | 1531 | G    |
| 1   | S2    | 1537 | C    |
| 1   | S2    | 1540 | G    |
| 1   | S2    | 1543 | A    |
| 1   | S2    | 1545 | A    |
| 1   | S2    | 1556 | A    |
| 1   | S2    | 1557 | U    |
| 1   | S2    | 1558 | U    |
| 1   | S2    | 1559 | A    |
| 1   | S2    | 1572 | G    |
| 1   | S2    | 1573 | A    |
| 1   | S2    | 1574 | G    |
| 1   | S2    | 1575 | G    |
| 1   | S2    | 1576 | A    |
| 1   | S2    | 1583 | A    |
| 1   | S2    | 1584 | G    |
| 1   | S2    | 1585 | U    |
| 1   | S2    | 1590 | G    |
| 1   | S2    | 1592 | A    |
| 1   | S2    | 1601 | G    |
| 1   | S2    | 1607 | G    |
| 1   | S2    | 1611 | A    |
| 1   | S2    | 1614 | A    |
| 1   | S2    | 1616 | G    |
| 1   | S2    | 1619 | C    |
| 1   | S2    | 1622 | G    |
| 1   | S2    | 1634 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 1637 | C    |
| 1   | S2    | 1657 | U    |
| 1   | S2    | 1658 | G    |
| 1   | S2    | 1660 | A    |
| 1   | S2    | 1673 | G    |
| 1   | S2    | 1676 | U    |
| 1   | S2    | 1682 | U    |
| 1   | S2    | 1688 | U    |
| 1   | S2    | 1689 | A    |
| 1   | S2    | 1693 | A    |
| 1   | S2    | 1700 | C    |
| 1   | S2    | 1701 | A    |
| 1   | S2    | 1702 | A    |
| 1   | S2    | 1703 | C    |
| 1   | S2    | 1709 | C    |
| 1   | S2    | 1711 | C    |
| 1   | S2    | 1715 | G    |
| 1   | S2    | 1717 | G    |
| 1   | S2    | 1736 | G    |
| 1   | S2    | 1740 | A    |
| 1   | S2    | 1755 | A    |
| 1   | S2    | 1757 | G    |
| 1   | S2    | 1760 | G    |
| 1   | S2    | 1762 | A    |
| 1   | S2    | 1766 | A    |
| 1   | S2    | 1767 | G    |
| 1   | S2    | 1769 | U    |
| 1   | S2    | 1770 | U    |
| 1   | S2    | 1780 | G    |
| 1   | S2    | 1782 | A    |
| 1   | S2    | 1783 | C    |
| 1   | S2    | 1788 | G    |
| 1   | S2    | 1792 | G    |
| 1   | S2    | 1793 | G    |
| 1   | S2    | 1794 | A    |
| 1   | S2    | 1796 | C    |
| 1   | S2    | 1799 | U    |
| 2   | Sl    | 2    | U    |
| 36  | Sm    | 3    | G    |
| 36  | Sm    | 8    | U    |
| 36  | Sm    | 10   | G    |
| 36  | Sm    | 14   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | Sm    | 15  | G    |
| 36  | Sm    | 16  | U    |
| 36  | Sm    | 19  | G    |
| 36  | Sm    | 20  | U    |
| 36  | Sm    | 21  | A    |
| 36  | Sm    | 34  | U    |
| 36  | Sm    | 35  | U    |
| 36  | Sm    | 46  | G    |
| 36  | Sm    | 47  | U    |
| 36  | Sm    | 48  | C    |
| 36  | Sm    | 49  | G    |
| 36  | Sm    | 50  | C    |
| 36  | Sm    | 51  | A    |
| 36  | Sm    | 52  | G    |
| 36  | Sm    | 53  | G    |
| 36  | Sm    | 54  | U    |
| 36  | Sm    | 55  | U    |
| 36  | Sm    | 57  | G    |
| 36  | Sm    | 58  | A    |
| 36  | Sm    | 59  | A    |
| 36  | Sm    | 60  | U    |
| 36  | Sm    | 61  | C    |
| 36  | Sm    | 62  | C    |
| 36  | Sm    | 64  | G    |
| 36  | Sm    | 65  | C    |
| 36  | Sm    | 66  | A    |
| 36  | Sm    | 67  | C    |
| 36  | Sm    | 68  | G    |
| 36  | Sm    | 69  | A    |
| 36  | Sm    | 73  | A    |
| 36  | Sm    | 74  | C    |
| 37  | Sn    | 8   | U    |
| 37  | Sn    | 9   | G    |
| 37  | Sn    | 11  | C    |
| 37  | Sn    | 14  | A    |
| 37  | Sn    | 19  | G    |
| 37  | Sn    | 20  | A    |
| 37  | Sn    | 21  | A    |
| 37  | Sn    | 25  | C    |
| 37  | Sn    | 27  | C    |
| 37  | Sn    | 36  | U    |
| 37  | Sn    | 45  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | Sn    | 46  | G    |
| 37  | Sn    | 47  | U    |
| 37  | Sn    | 48  | C    |
| 37  | Sn    | 49  | C    |
| 37  | Sn    | 54  | A    |
| 37  | Sn    | 57  | G    |
| 37  | Sn    | 59  | A    |
| 37  | Sn    | 61  | C    |
| 37  | Sn    | 63  | G    |
| 37  | Sn    | 64  | A    |
| 37  | Sn    | 66  | C    |
| 37  | Sn    | 76  | A    |
| 40  | LA    | 6   | A    |
| 40  | LA    | 11  | A    |
| 40  | LA    | 14  | U    |
| 40  | LA    | 21  | G    |
| 40  | LA    | 22  | G    |
| 40  | LA    | 26  | A    |
| 40  | LA    | 30  | G    |
| 40  | LA    | 40  | A    |
| 40  | LA    | 43  | A    |
| 40  | LA    | 44  | U    |
| 40  | LA    | 48  | A    |
| 40  | LA    | 49  | A    |
| 40  | LA    | 51  | A    |
| 40  | LA    | 59  | G    |
| 40  | LA    | 60  | A    |
| 40  | LA    | 65  | A    |
| 40  | LA    | 66  | A    |
| 40  | LA    | 73  | C    |
| 40  | LA    | 74  | G    |
| 40  | LA    | 76  | G    |
| 40  | LA    | 85  | A    |
| 40  | LA    | 89  | A    |
| 40  | LA    | 92  | G    |
| 40  | LA    | 109 | A    |
| 40  | LA    | 110 | G    |
| 40  | LA    | 111 | C    |
| 40  | LA    | 113 | C    |
| 40  | LA    | 120 | G    |
| 40  | LA    | 121 | A    |
| 40  | LA    | 122 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | LA    | 133 | U    |
| 40  | LA    | 136 | G    |
| 40  | LA    | 150 | A    |
| 40  | LA    | 156 | G    |
| 40  | LA    | 157 | A    |
| 40  | LA    | 166 | C    |
| 40  | LA    | 173 | G    |
| 40  | LA    | 187 | A    |
| 40  | LA    | 190 | U    |
| 40  | LA    | 191 | U    |
| 40  | LA    | 200 | C    |
| 40  | LA    | 206 | G    |
| 40  | LA    | 210 | U    |
| 40  | LA    | 211 | A    |
| 40  | LA    | 213 | A    |
| 40  | LA    | 218 | G    |
| 40  | LA    | 219 | A    |
| 40  | LA    | 221 | A    |
| 40  | LA    | 231 | G    |
| 40  | LA    | 236 | G    |
| 40  | LA    | 239 | G    |
| 40  | LA    | 240 | U    |
| 40  | LA    | 243 | G    |
| 40  | LA    | 249 | U    |
| 40  | LA    | 252 | U    |
| 40  | LA    | 258 | G    |
| 40  | LA    | 263 | C    |
| 40  | LA    | 269 | G    |
| 40  | LA    | 282 | G    |
| 40  | LA    | 283 | G    |
| 40  | LA    | 286 | U    |
| 40  | LA    | 295 | A    |
| 40  | LA    | 298 | U    |
| 40  | LA    | 315 | C    |
| 40  | LA    | 323 | A    |
| 40  | LA    | 329 | U    |
| 40  | LA    | 330 | G    |
| 40  | LA    | 334 | A    |
| 40  | LA    | 338 | A    |
| 40  | LA    | 339 | C    |
| 40  | LA    | 346 | C    |
| 40  | LA    | 350 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | LA    | 351 | A    |
| 40  | LA    | 376 | G    |
| 40  | LA    | 385 | A    |
| 40  | LA    | 390 | G    |
| 40  | LA    | 395 | A    |
| 40  | LA    | 397 | A    |
| 40  | LA    | 399 | A    |
| 40  | LA    | 401 | U    |
| 40  | LA    | 402 | A    |
| 40  | LA    | 403 | C    |
| 40  | LA    | 421 | G    |
| 40  | LA    | 422 | A    |
| 40  | LA    | 438 | A    |
| 40  | LA    | 440 | A    |
| 40  | LA    | 441 | U    |
| 40  | LA    | 442 | G    |
| 40  | LA    | 443 | G    |
| 40  | LA    | 445 | G    |
| 40  | LA    | 446 | U    |
| 40  | LA    | 447 | U    |
| 40  | LA    | 448 | U    |
| 40  | LA    | 449 | U    |
| 40  | LA    | 450 | G    |
| 40  | LA    | 487 | U    |
| 40  | LA    | 488 | U    |
| 40  | LA    | 489 | U    |
| 40  | LA    | 490 | C    |
| 40  | LA    | 491 | A    |
| 40  | LA    | 492 | C    |
| 40  | LA    | 494 | G    |
| 40  | LA    | 498 | A    |
| 40  | LA    | 510 | G    |
| 40  | LA    | 515 | C    |
| 40  | LA    | 517 | G    |
| 40  | LA    | 520 | U    |
| 40  | LA    | 521 | A    |
| 40  | LA    | 535 | G    |
| 40  | LA    | 543 | C    |
| 40  | LA    | 544 | C    |
| 40  | LA    | 545 | U    |
| 40  | LA    | 546 | C    |
| 40  | LA    | 547 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | LA    | 552 | G    |
| 40  | LA    | 555 | U    |
| 40  | LA    | 557 | A    |
| 40  | LA    | 559 | A    |
| 40  | LA    | 568 | G    |
| 40  | LA    | 578 | A    |
| 40  | LA    | 579 | G    |
| 40  | LA    | 597 | G    |
| 40  | LA    | 600 | G    |
| 40  | LA    | 603 | A    |
| 40  | LA    | 604 | G    |
| 40  | LA    | 609 | G    |
| 40  | LA    | 610 | G    |
| 40  | LA    | 611 | A    |
| 40  | LA    | 612 | U    |
| 40  | LA    | 619 | A    |
| 40  | LA    | 620 | U    |
| 40  | LA    | 621 | A    |
| 40  | LA    | 625 | G    |
| 40  | LA    | 637 | C    |
| 40  | LA    | 638 | C    |
| 40  | LA    | 642 | U    |
| 40  | LA    | 649 | A    |
| 40  | LA    | 650 | C    |
| 40  | LA    | 660 | A    |
| 40  | LA    | 667 | C    |
| 40  | LA    | 677 | A    |
| 40  | LA    | 681 | U    |
| 40  | LA    | 691 | A    |
| 40  | LA    | 699 | A    |
| 40  | LA    | 705 | A    |
| 40  | LA    | 712 | G    |
| 40  | LA    | 716 | A    |
| 40  | LA    | 720 | A    |
| 40  | LA    | 726 | G    |
| 40  | LA    | 737 | G    |
| 40  | LA    | 742 | G    |
| 40  | LA    | 758 | C    |
| 40  | LA    | 763 | G    |
| 40  | LA    | 764 | U    |
| 40  | LA    | 765 | C    |
| 40  | LA    | 766 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | LA    | 767 | U    |
| 40  | LA    | 771 | A    |
| 40  | LA    | 774 | G    |
| 40  | LA    | 776 | U    |
| 40  | LA    | 777 | U    |
| 40  | LA    | 780 | A    |
| 40  | LA    | 781 | G    |
| 40  | LA    | 785 | G    |
| 40  | LA    | 786 | A    |
| 40  | LA    | 806 | A    |
| 40  | LA    | 808 | A    |
| 40  | LA    | 817 | A    |
| 40  | LA    | 830 | A    |
| 40  | LA    | 832 | G    |
| 40  | LA    | 848 | A    |
| 40  | LA    | 849 | C    |
| 40  | LA    | 850 | U    |
| 40  | LA    | 851 | C    |
| 40  | LA    | 861 | C    |
| 40  | LA    | 865 | U    |
| 40  | LA    | 868 | C    |
| 40  | LA    | 871 | U    |
| 40  | LA    | 874 | U    |
| 40  | LA    | 879 | U    |
| 40  | LA    | 894 | G    |
| 40  | LA    | 895 | A    |
| 40  | LA    | 896 | A    |
| 40  | LA    | 899 | U    |
| 40  | LA    | 906 | A    |
| 40  | LA    | 907 | G    |
| 40  | LA    | 908 | G    |
| 40  | LA    | 914 | A    |
| 40  | LA    | 916 | G    |
| 40  | LA    | 917 | A    |
| 40  | LA    | 921 | A    |
| 40  | LA    | 923 | C    |
| 40  | LA    | 932 | U    |
| 40  | LA    | 934 | G    |
| 40  | LA    | 937 | G    |
| 40  | LA    | 944 | C    |
| 40  | LA    | 959 | C    |
| 40  | LA    | 960 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 971  | G    |
| 40  | LA    | 974  | G    |
| 40  | LA    | 981  | U    |
| 40  | LA    | 982  | C    |
| 40  | LA    | 991  | G    |
| 40  | LA    | 1002 | A    |
| 40  | LA    | 1012 | G    |
| 40  | LA    | 1015 | U    |
| 40  | LA    | 1018 | G    |
| 40  | LA    | 1020 | G    |
| 40  | LA    | 1021 | G    |
| 40  | LA    | 1024 | G    |
| 40  | LA    | 1026 | A    |
| 40  | LA    | 1028 | U    |
| 40  | LA    | 1029 | G    |
| 40  | LA    | 1040 | A    |
| 40  | LA    | 1041 | U    |
| 40  | LA    | 1045 | C    |
| 40  | LA    | 1047 | A    |
| 40  | LA    | 1049 | C    |
| 40  | LA    | 1064 | A    |
| 40  | LA    | 1065 | A    |
| 40  | LA    | 1072 | G    |
| 40  | LA    | 1081 | U    |
| 40  | LA    | 1093 | A    |
| 40  | LA    | 1094 | U    |
| 40  | LA    | 1095 | U    |
| 40  | LA    | 1096 | U    |
| 40  | LA    | 1097 | G    |
| 40  | LA    | 1098 | A    |
| 40  | LA    | 1103 | A    |
| 40  | LA    | 1104 | G    |
| 40  | LA    | 1117 | G    |
| 40  | LA    | 1118 | C    |
| 40  | LA    | 1128 | U    |
| 40  | LA    | 1131 | G    |
| 40  | LA    | 1144 | U    |
| 40  | LA    | 1145 | G    |
| 40  | LA    | 1148 | G    |
| 40  | LA    | 1153 | A    |
| 40  | LA    | 1158 | A    |
| 40  | LA    | 1159 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 1177 | G    |
| 40  | LA    | 1178 | G    |
| 40  | LA    | 1180 | A    |
| 40  | LA    | 1181 | U    |
| 40  | LA    | 1182 | A    |
| 40  | LA    | 1190 | A    |
| 40  | LA    | 1192 | C    |
| 40  | LA    | 1193 | A    |
| 40  | LA    | 1196 | C    |
| 40  | LA    | 1197 | A    |
| 40  | LA    | 1201 | C    |
| 40  | LA    | 1202 | A    |
| 40  | LA    | 1206 | G    |
| 40  | LA    | 1208 | U    |
| 40  | LA    | 1217 | A    |
| 40  | LA    | 1218 | U    |
| 40  | LA    | 1222 | G    |
| 40  | LA    | 1223 | A    |
| 40  | LA    | 1227 | C    |
| 40  | LA    | 1229 | G    |
| 40  | LA    | 1234 | G    |
| 40  | LA    | 1236 | G    |
| 40  | LA    | 1237 | G    |
| 40  | LA    | 1238 | C    |
| 40  | LA    | 1239 | C    |
| 40  | LA    | 1240 | A    |
| 40  | LA    | 1241 | U    |
| 40  | LA    | 1242 | G    |
| 40  | LA    | 1243 | G    |
| 40  | LA    | 1244 | A    |
| 40  | LA    | 1245 | A    |
| 40  | LA    | 1246 | G    |
| 40  | LA    | 1248 | C    |
| 40  | LA    | 1251 | A    |
| 40  | LA    | 1253 | U    |
| 40  | LA    | 1258 | U    |
| 40  | LA    | 1262 | G    |
| 40  | LA    | 1263 | A    |
| 40  | LA    | 1264 | G    |
| 40  | LA    | 1266 | G    |
| 40  | LA    | 1267 | U    |
| 40  | LA    | 1269 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 1270 | A    |
| 40  | LA    | 1271 | A    |
| 40  | LA    | 1272 | C    |
| 40  | LA    | 1278 | A    |
| 40  | LA    | 1279 | C    |
| 40  | LA    | 1280 | C    |
| 40  | LA    | 1282 | G    |
| 40  | LA    | 1285 | G    |
| 40  | LA    | 1286 | A    |
| 40  | LA    | 1287 | A    |
| 40  | LA    | 1295 | G    |
| 40  | LA    | 1307 | G    |
| 40  | LA    | 1308 | A    |
| 40  | LA    | 1309 | U    |
| 40  | LA    | 1313 | G    |
| 40  | LA    | 1316 | C    |
| 40  | LA    | 1318 | A    |
| 40  | LA    | 1325 | U    |
| 40  | LA    | 1330 | A    |
| 40  | LA    | 1345 | G    |
| 40  | LA    | 1348 | U    |
| 40  | LA    | 1349 | G    |
| 40  | LA    | 1351 | U    |
| 40  | LA    | 1352 | A    |
| 40  | LA    | 1354 | G    |
| 40  | LA    | 1355 | A    |
| 40  | LA    | 1356 | U    |
| 40  | LA    | 1357 | G    |
| 40  | LA    | 1386 | A    |
| 40  | LA    | 1392 | G    |
| 40  | LA    | 1399 | A    |
| 40  | LA    | 1400 | G    |
| 40  | LA    | 1418 | A    |
| 40  | LA    | 1419 | A    |
| 40  | LA    | 1421 | G    |
| 40  | LA    | 1429 | G    |
| 40  | LA    | 1430 | U    |
| 40  | LA    | 1431 | G    |
| 40  | LA    | 1434 | G    |
| 40  | LA    | 1437 | C    |
| 40  | LA    | 1442 | U    |
| 40  | LA    | 1443 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 1446 | A    |
| 40  | LA    | 1450 | G    |
| 40  | LA    | 1455 | U    |
| 40  | LA    | 1481 | A    |
| 40  | LA    | 1482 | A    |
| 40  | LA    | 1483 | G    |
| 40  | LA    | 1484 | U    |
| 40  | LA    | 1487 | G    |
| 40  | LA    | 1488 | G    |
| 40  | LA    | 1503 | A    |
| 40  | LA    | 1508 | C    |
| 40  | LA    | 1511 | U    |
| 40  | LA    | 1523 | U    |
| 40  | LA    | 1528 | G    |
| 40  | LA    | 1533 | U    |
| 40  | LA    | 1536 | G    |
| 40  | LA    | 1542 | G    |
| 40  | LA    | 1549 | U    |
| 40  | LA    | 1555 | U    |
| 40  | LA    | 1556 | C    |
| 40  | LA    | 1557 | A    |
| 40  | LA    | 1559 | A    |
| 40  | LA    | 1560 | G    |
| 40  | LA    | 1562 | C    |
| 40  | LA    | 1563 | C    |
| 40  | LA    | 1565 | G    |
| 40  | LA    | 1566 | A    |
| 40  | LA    | 1567 | U    |
| 40  | LA    | 1568 | U    |
| 40  | LA    | 1569 | U    |
| 40  | LA    | 1572 | U    |
| 40  | LA    | 1573 | G    |
| 40  | LA    | 1574 | C    |
| 40  | LA    | 1575 | A    |
| 40  | LA    | 1576 | G    |
| 40  | LA    | 1580 | A    |
| 40  | LA    | 1581 | C    |
| 40  | LA    | 1582 | C    |
| 40  | LA    | 1583 | A    |
| 40  | LA    | 1587 | A    |
| 40  | LA    | 1588 | A    |
| 40  | LA    | 1589 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 1590 | G    |
| 40  | LA    | 1602 | A    |
| 40  | LA    | 1605 | A    |
| 40  | LA    | 1621 | A    |
| 40  | LA    | 1629 | U    |
| 40  | LA    | 1632 | A    |
| 40  | LA    | 1639 | C    |
| 40  | LA    | 1642 | A    |
| 40  | LA    | 1643 | A    |
| 40  | LA    | 1645 | U    |
| 40  | LA    | 1658 | G    |
| 40  | LA    | 1677 | G    |
| 40  | LA    | 1683 | A    |
| 40  | LA    | 1687 | U    |
| 40  | LA    | 1688 | U    |
| 40  | LA    | 1696 | A    |
| 40  | LA    | 1704 | A    |
| 40  | LA    | 1705 | U    |
| 40  | LA    | 1715 | A    |
| 40  | LA    | 1716 | U    |
| 40  | LA    | 1717 | U    |
| 40  | LA    | 1722 | U    |
| 40  | LA    | 1724 | U    |
| 40  | LA    | 1725 | C    |
| 40  | LA    | 1750 | A    |
| 40  | LA    | 1751 | G    |
| 40  | LA    | 1756 | C    |
| 40  | LA    | 1760 | A    |
| 40  | LA    | 1765 | U    |
| 40  | LA    | 1766 | G    |
| 40  | LA    | 1770 | G    |
| 40  | LA    | 1775 | G    |
| 40  | LA    | 1780 | G    |
| 40  | LA    | 1788 | C    |
| 40  | LA    | 1796 | G    |
| 40  | LA    | 1797 | A    |
| 40  | LA    | 1814 | A    |
| 40  | LA    | 1816 | A    |
| 40  | LA    | 1817 | G    |
| 40  | LA    | 1819 | U    |
| 40  | LA    | 1820 | U    |
| 40  | LA    | 1821 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 1822 | C    |
| 40  | LA    | 1839 | A    |
| 40  | LA    | 1840 | U    |
| 40  | LA    | 1841 | A    |
| 40  | LA    | 1842 | A    |
| 40  | LA    | 1846 | C    |
| 40  | LA    | 1849 | C    |
| 40  | LA    | 1850 | A    |
| 40  | LA    | 1866 | C    |
| 40  | LA    | 1867 | A    |
| 40  | LA    | 1874 | A    |
| 40  | LA    | 1880 | U    |
| 40  | LA    | 1881 | A    |
| 40  | LA    | 1893 | A    |
| 40  | LA    | 1897 | G    |
| 40  | LA    | 1906 | G    |
| 40  | LA    | 1908 | A    |
| 40  | LA    | 1930 | A    |
| 40  | LA    | 1935 | G    |
| 40  | LA    | 1943 | C    |
| 40  | LA    | 1951 | C    |
| 40  | LA    | 1952 | G    |
| 40  | LA    | 1953 | G    |
| 40  | LA    | 1954 | G    |
| 40  | LA    | 2101 | C    |
| 40  | LA    | 2102 | U    |
| 40  | LA    | 2111 | G    |
| 40  | LA    | 2112 | U    |
| 40  | LA    | 2113 | A    |
| 40  | LA    | 2121 | G    |
| 40  | LA    | 2122 | G    |
| 40  | LA    | 2131 | A    |
| 40  | LA    | 2139 | A    |
| 40  | LA    | 2149 | A    |
| 40  | LA    | 2158 | A    |
| 40  | LA    | 2169 | G    |
| 40  | LA    | 2170 | U    |
| 40  | LA    | 2187 | G    |
| 40  | LA    | 2188 | A    |
| 40  | LA    | 2201 | G    |
| 40  | LA    | 2205 | U    |
| 40  | LA    | 2206 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 2207 | A    |
| 40  | LA    | 2209 | U    |
| 40  | LA    | 2223 | A    |
| 40  | LA    | 2232 | A    |
| 40  | LA    | 2244 | A    |
| 40  | LA    | 2249 | G    |
| 40  | LA    | 2250 | G    |
| 40  | LA    | 2252 | A    |
| 40  | LA    | 2256 | A    |
| 40  | LA    | 2262 | A    |
| 40  | LA    | 2272 | G    |
| 40  | LA    | 2273 | G    |
| 40  | LA    | 2274 | U    |
| 40  | LA    | 2279 | A    |
| 40  | LA    | 2280 | A    |
| 40  | LA    | 2281 | A    |
| 40  | LA    | 2282 | U    |
| 40  | LA    | 2284 | C    |
| 40  | LA    | 2285 | C    |
| 40  | LA    | 2288 | G    |
| 40  | LA    | 2299 | A    |
| 40  | LA    | 2306 | C    |
| 40  | LA    | 2307 | G    |
| 40  | LA    | 2308 | C    |
| 40  | LA    | 2309 | A    |
| 40  | LA    | 2310 | U    |
| 40  | LA    | 2313 | A    |
| 40  | LA    | 2314 | U    |
| 40  | LA    | 2315 | G    |
| 40  | LA    | 2335 | G    |
| 40  | LA    | 2336 | U    |
| 40  | LA    | 2347 | U    |
| 40  | LA    | 2364 | G    |
| 40  | LA    | 2372 | A    |
| 40  | LA    | 2373 | A    |
| 40  | LA    | 2374 | C    |
| 40  | LA    | 2375 | G    |
| 40  | LA    | 2385 | G    |
| 40  | LA    | 2388 | U    |
| 40  | LA    | 2393 | G    |
| 40  | LA    | 2394 | G    |
| 40  | LA    | 2397 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 2402 | A    |
| 40  | LA    | 2403 | G    |
| 40  | LA    | 2404 | A    |
| 40  | LA    | 2411 | U    |
| 40  | LA    | 2412 | G    |
| 40  | LA    | 2419 | A    |
| 40  | LA    | 2422 | C    |
| 40  | LA    | 2434 | U    |
| 40  | LA    | 2435 | G    |
| 40  | LA    | 2437 | G    |
| 40  | LA    | 2438 | A    |
| 40  | LA    | 2439 | A    |
| 40  | LA    | 2440 | G    |
| 40  | LA    | 2446 | U    |
| 40  | LA    | 2451 | G    |
| 40  | LA    | 2452 | G    |
| 40  | LA    | 2493 | U    |
| 40  | LA    | 2496 | C    |
| 40  | LA    | 2498 | U    |
| 40  | LA    | 2501 | U    |
| 40  | LA    | 2502 | A    |
| 40  | LA    | 2503 | G    |
| 40  | LA    | 2507 | C    |
| 40  | LA    | 2514 | U    |
| 40  | LA    | 2515 | A    |
| 40  | LA    | 2522 | G    |
| 40  | LA    | 2523 | A    |
| 40  | LA    | 2524 | A    |
| 40  | LA    | 2525 | G    |
| 40  | LA    | 2526 | C    |
| 40  | LA    | 2531 | C    |
| 40  | LA    | 2532 | U    |
| 40  | LA    | 2537 | U    |
| 40  | LA    | 2538 | U    |
| 40  | LA    | 2539 | C    |
| 40  | LA    | 2540 | A    |
| 40  | LA    | 2541 | U    |
| 40  | LA    | 2542 | U    |
| 40  | LA    | 2543 | U    |
| 40  | LA    | 2546 | C    |
| 40  | LA    | 2549 | G    |
| 40  | LA    | 2552 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 2554 | A    |
| 40  | LA    | 2561 | A    |
| 40  | LA    | 2569 | A    |
| 40  | LA    | 2570 | U    |
| 40  | LA    | 2571 | U    |
| 40  | LA    | 2572 | C    |
| 40  | LA    | 2573 | G    |
| 40  | LA    | 2576 | G    |
| 40  | LA    | 2585 | G    |
| 40  | LA    | 2589 | G    |
| 40  | LA    | 2593 | A    |
| 40  | LA    | 2594 | C    |
| 40  | LA    | 2595 | A    |
| 40  | LA    | 2606 | G    |
| 40  | LA    | 2607 | G    |
| 40  | LA    | 2614 | G    |
| 40  | LA    | 2626 | A    |
| 40  | LA    | 2629 | U    |
| 40  | LA    | 2636 | A    |
| 40  | LA    | 2648 | G    |
| 40  | LA    | 2652 | U    |
| 40  | LA    | 2656 | A    |
| 40  | LA    | 2672 | G    |
| 40  | LA    | 2674 | A    |
| 40  | LA    | 2677 | G    |
| 40  | LA    | 2689 | A    |
| 40  | LA    | 2691 | A    |
| 40  | LA    | 2694 | A    |
| 40  | LA    | 2696 | A    |
| 40  | LA    | 2703 | A    |
| 40  | LA    | 2704 | A    |
| 40  | LA    | 2714 | G    |
| 40  | LA    | 2719 | U    |
| 40  | LA    | 2728 | G    |
| 40  | LA    | 2748 | A    |
| 40  | LA    | 2749 | G    |
| 40  | LA    | 2752 | U    |
| 40  | LA    | 2753 | G    |
| 40  | LA    | 2755 | C    |
| 40  | LA    | 2777 | G    |
| 40  | LA    | 2778 | G    |
| 40  | LA    | 2796 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 2800 | G    |
| 40  | LA    | 2801 | A    |
| 40  | LA    | 2802 | A    |
| 40  | LA    | 2803 | A    |
| 40  | LA    | 2804 | A    |
| 40  | LA    | 2805 | G    |
| 40  | LA    | 2810 | C    |
| 40  | LA    | 2817 | A    |
| 40  | LA    | 2818 | U    |
| 40  | LA    | 2821 | C    |
| 40  | LA    | 2842 | U    |
| 40  | LA    | 2844 | C    |
| 40  | LA    | 2845 | A    |
| 40  | LA    | 2847 | A    |
| 40  | LA    | 2849 | C    |
| 40  | LA    | 2856 | G    |
| 40  | LA    | 2861 | U    |
| 40  | LA    | 2867 | C    |
| 40  | LA    | 2871 | G    |
| 40  | LA    | 2872 | A    |
| 40  | LA    | 2873 | U    |
| 40  | LA    | 2875 | U    |
| 40  | LA    | 2876 | C    |
| 40  | LA    | 2887 | A    |
| 40  | LA    | 2894 | C    |
| 40  | LA    | 2899 | C    |
| 40  | LA    | 2910 | A    |
| 40  | LA    | 2916 | U    |
| 40  | LA    | 2918 | G    |
| 40  | LA    | 2923 | U    |
| 40  | LA    | 2928 | C    |
| 40  | LA    | 2933 | A    |
| 40  | LA    | 2935 | U    |
| 40  | LA    | 2936 | A    |
| 40  | LA    | 2941 | A    |
| 40  | LA    | 2942 | C    |
| 40  | LA    | 2947 | G    |
| 40  | LA    | 2954 | U    |
| 40  | LA    | 2955 | U    |
| 40  | LA    | 2957 | G    |
| 40  | LA    | 2971 | A    |
| 40  | LA    | 2983 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 2990 | G    |
| 40  | LA    | 2996 | U    |
| 40  | LA    | 2997 | G    |
| 40  | LA    | 3003 | G    |
| 40  | LA    | 3012 | A    |
| 40  | LA    | 3030 | G    |
| 40  | LA    | 3055 | U    |
| 40  | LA    | 3056 | U    |
| 40  | LA    | 3058 | U    |
| 40  | LA    | 3059 | G    |
| 40  | LA    | 3078 | U    |
| 40  | LA    | 3079 | U    |
| 40  | LA    | 3080 | G    |
| 40  | LA    | 3086 | A    |
| 40  | LA    | 3092 | C    |
| 40  | LA    | 3101 | G    |
| 40  | LA    | 3104 | U    |
| 40  | LA    | 3115 | C    |
| 40  | LA    | 3116 | G    |
| 40  | LA    | 3118 | C    |
| 40  | LA    | 3119 | U    |
| 40  | LA    | 3122 | A    |
| 40  | LA    | 3129 | A    |
| 40  | LA    | 3130 | A    |
| 40  | LA    | 3131 | U    |
| 40  | LA    | 3142 | A    |
| 40  | LA    | 3143 | C    |
| 40  | LA    | 3151 | U    |
| 40  | LA    | 3154 | C    |
| 40  | LA    | 3155 | U    |
| 40  | LA    | 3156 | U    |
| 40  | LA    | 3157 | U    |
| 40  | LA    | 3158 | G    |
| 40  | LA    | 3165 | A    |
| 40  | LA    | 3170 | A    |
| 40  | LA    | 3172 | A    |
| 40  | LA    | 3173 | G    |
| 40  | LA    | 3174 | A    |
| 40  | LA    | 3175 | U    |
| 40  | LA    | 3176 | G    |
| 40  | LA    | 3180 | A    |
| 40  | LA    | 3181 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 3187 | A    |
| 40  | LA    | 3196 | U    |
| 40  | LA    | 3199 | G    |
| 40  | LA    | 3207 | U    |
| 40  | LA    | 3209 | A    |
| 40  | LA    | 3210 | A    |
| 40  | LA    | 3216 | G    |
| 40  | LA    | 3217 | C    |
| 40  | LA    | 3218 | A    |
| 40  | LA    | 3219 | G    |
| 40  | LA    | 3222 | U    |
| 40  | LA    | 3229 | G    |
| 40  | LA    | 3242 | G    |
| 40  | LA    | 3243 | A    |
| 40  | LA    | 3244 | A    |
| 40  | LA    | 3245 | A    |
| 40  | LA    | 3247 | G    |
| 40  | LA    | 3259 | U    |
| 40  | LA    | 3260 | G    |
| 40  | LA    | 3263 | G    |
| 40  | LA    | 3270 | U    |
| 40  | LA    | 3273 | A    |
| 40  | LA    | 3276 | G    |
| 40  | LA    | 3277 | U    |
| 40  | LA    | 3281 | U    |
| 40  | LA    | 3286 | G    |
| 40  | LA    | 3287 | U    |
| 40  | LA    | 3288 | G    |
| 40  | LA    | 3289 | G    |
| 40  | LA    | 3294 | A    |
| 40  | LA    | 3295 | A    |
| 40  | LA    | 3304 | U    |
| 40  | LA    | 3313 | U    |
| 40  | LA    | 3316 | A    |
| 40  | LA    | 3318 | G    |
| 40  | LA    | 3319 | U    |
| 40  | LA    | 3320 | A    |
| 40  | LA    | 3334 | U    |
| 40  | LA    | 3341 | U    |
| 40  | LA    | 3345 | G    |
| 40  | LA    | 3346 | U    |
| 40  | LA    | 3347 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 3351 | U    |
| 40  | LA    | 3352 | U    |
| 40  | LA    | 3353 | G    |
| 40  | LA    | 3354 | U    |
| 40  | LA    | 3355 | U    |
| 40  | LA    | 3356 | G    |
| 40  | LA    | 3368 | U    |
| 40  | LA    | 3369 | G    |
| 40  | LA    | 3378 | C    |
| 40  | LA    | 3381 | U    |
| 40  | LA    | 3382 | U    |
| 40  | LA    | 3386 | G    |
| 40  | LA    | 3389 | U    |
| 40  | LA    | 3390 | G    |
| 40  | LA    | 3396 | U    |
| 41  | LB    | 7    | G    |
| 41  | LB    | 10   | C    |
| 41  | LB    | 17   | A    |
| 41  | LB    | 22   | A    |
| 41  | LB    | 35   | C    |
| 41  | LB    | 52   | G    |
| 41  | LB    | 53   | U    |
| 41  | LB    | 54   | U    |
| 41  | LB    | 65   | G    |
| 41  | LB    | 74   | C    |
| 41  | LB    | 76   | A    |
| 41  | LB    | 99   | G    |
| 41  | LB    | 102  | A    |
| 41  | LB    | 112  | G    |
| 41  | LB    | 121  | U    |
| 42  | LC    | 16   | G    |
| 42  | LC    | 25   | G    |
| 42  | LC    | 34   | U    |
| 42  | LC    | 35   | C    |
| 42  | LC    | 38   | U    |
| 42  | LC    | 59   | A    |
| 42  | LC    | 62   | C    |
| 42  | LC    | 63   | G    |
| 42  | LC    | 80   | A    |
| 42  | LC    | 81   | U    |
| 42  | LC    | 82   | U    |
| 42  | LC    | 83   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | LC    | 84  | C    |
| 42  | LC    | 85  | G    |
| 42  | LC    | 86  | U    |
| 42  | LC    | 87  | G    |
| 42  | LC    | 90  | U    |
| 42  | LC    | 95  | G    |
| 42  | LC    | 97  | A    |
| 42  | LC    | 99  | C    |
| 42  | LC    | 104 | A    |
| 42  | LC    | 106 | C    |
| 42  | LC    | 111 | A    |
| 42  | LC    | 112 | U    |
| 42  | LC    | 113 | U    |
| 42  | LC    | 125 | U    |
| 42  | LC    | 126 | A    |
| 42  | LC    | 138 | A    |
| 42  | LC    | 148 | G    |
| 42  | LC    | 152 | G    |
| 42  | LC    | 157 | U    |
| 42  | LC    | 158 | U    |

All (98) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S2    | 68  | A    |
| 1   | S2    | 77  | U    |
| 1   | S2    | 139 | C    |
| 1   | S2    | 141 | U    |
| 1   | S2    | 215 | A    |
| 1   | S2    | 224 | C    |
| 1   | S2    | 237 | C    |
| 1   | S2    | 278 | U    |
| 1   | S2    | 313 | U    |
| 1   | S2    | 322 | G    |
| 1   | S2    | 352 | A    |
| 1   | S2    | 387 | A    |
| 1   | S2    | 400 | A    |
| 1   | S2    | 447 | U    |
| 1   | S2    | 511 | A    |
| 1   | S2    | 518 | A    |
| 1   | S2    | 539 | G    |
| 1   | S2    | 541 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S2    | 555  | A    |
| 1   | S2    | 609  | U    |
| 1   | S2    | 639  | U    |
| 1   | S2    | 640  | U    |
| 1   | S2    | 705  | U    |
| 1   | S2    | 711  | U    |
| 1   | S2    | 740  | A    |
| 1   | S2    | 755  | A    |
| 1   | S2    | 803  | A    |
| 1   | S2    | 819  | G    |
| 1   | S2    | 912  | U    |
| 1   | S2    | 928  | U    |
| 1   | S2    | 1023 | A    |
| 1   | S2    | 1207 | C    |
| 1   | S2    | 1226 | A    |
| 1   | S2    | 1245 | G    |
| 1   | S2    | 1251 | U    |
| 1   | S2    | 1256 | A    |
| 1   | S2    | 1273 | G    |
| 1   | S2    | 1274 | C    |
| 1   | S2    | 1314 | U    |
| 1   | S2    | 1344 | A    |
| 1   | S2    | 1348 | A    |
| 1   | S2    | 1382 | A    |
| 1   | S2    | 1399 | C    |
| 1   | S2    | 1430 | U    |
| 1   | S2    | 1471 | A    |
| 1   | S2    | 1556 | A    |
| 1   | S2    | 1557 | U    |
| 1   | S2    | 1573 | A    |
| 1   | S2    | 1584 | G    |
| 1   | S2    | 1633 | A    |
| 1   | S2    | 1636 | C    |
| 1   | S2    | 1700 | C    |
| 40  | LA    | 13   | A    |
| 40  | LA    | 282  | G    |
| 40  | LA    | 439  | C    |
| 40  | LA    | 637  | C    |
| 40  | LA    | 763  | G    |
| 40  | LA    | 849  | C    |
| 40  | LA    | 873  | C    |
| 40  | LA    | 896  | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 40  | LA    | 916  | G    |
| 40  | LA    | 993  | G    |
| 40  | LA    | 1064 | A    |
| 40  | LA    | 1097 | G    |
| 40  | LA    | 1271 | A    |
| 40  | LA    | 1307 | G    |
| 40  | LA    | 1355 | A    |
| 40  | LA    | 1562 | C    |
| 40  | LA    | 1572 | U    |
| 40  | LA    | 1582 | C    |
| 40  | LA    | 1716 | U    |
| 40  | LA    | 1815 | U    |
| 40  | LA    | 1820 | U    |
| 40  | LA    | 2112 | U    |
| 40  | LA    | 2231 | C    |
| 40  | LA    | 2445 | A    |
| 40  | LA    | 2500 | A    |
| 40  | LA    | 2501 | U    |
| 40  | LA    | 2502 | A    |
| 40  | LA    | 2513 | U    |
| 40  | LA    | 2514 | U    |
| 40  | LA    | 2525 | G    |
| 40  | LA    | 2537 | U    |
| 40  | LA    | 2538 | U    |
| 40  | LA    | 2541 | U    |
| 40  | LA    | 3055 | U    |
| 40  | LA    | 3078 | U    |
| 40  | LA    | 3121 | U    |
| 40  | LA    | 3218 | A    |
| 40  | LA    | 3228 | C    |
| 40  | LA    | 3269 | U    |
| 40  | LA    | 3275 | U    |
| 40  | LA    | 3319 | U    |
| 40  | LA    | 3350 | C    |
| 41  | LB    | 52   | G    |
| 42  | LC    | 82   | U    |
| 42  | LC    | 85   | G    |
| 42  | LC    | 125  | 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 |
| 84  | 5CT  | Ls    | 51  | 84   | 13,14,15     | 2.37 | 1 (7%)   | 8,15,17     | 2.18 | 3 (37%)  |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 84  | 5CT  | Ls    | 51  | 84   | 1/1/2/4 | 5/13/14/16 | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 84  | Ls    | 51  | 5CT  | O1-C2 | -8.40 | 1.18        | 1.43     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 84  | Ls    | 51  | 5CT  | O1-C2-C3 | 3.83  | 119.57      | 109.35   |
| 84  | Ls    | 51  | 5CT  | O1-C2-C1 | 3.52  | 120.84      | 109.29   |
| 84  | Ls    | 51  | 5CT  | C1-NZ-CE | -2.74 | 107.41      | 113.38   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 84  | Ls    | 51  | 5CT  | C2   |

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 84  | Ls    | 51  | 5CT  | C2-C1-NZ-CE |
| 84  | Ls    | 51  | 5CT  | NZ-C1-C2-C3 |
| 84  | Ls    | 51  | 5CT  | O1-C2-C3-C4 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 84  | Ls    | 51  | 5CT  | C2-C3-C4-N1 |
| 84  | Ls    | 51  | 5CT  | CE-CD-CG-CB |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 84  | Ls    | 51  | 5CT  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 |
|-----|-------|------------------|
| 86  | A     | 13               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1104:ALA  | C      | 1124:GLY  | N      | 40.36        |
| 1     | A     | 997:ALA   | C      | 1019:ALA  | N      | 35.44        |
| 1     | A     | 1917:ALA  | C      | 2000:ALA  | N      | 14.67        |
| 1     | A     | 1044:ALA  | C      | 1055:ALA  | N      | 12.76        |
| 1     | A     | 1074:ALA  | C      | 1084:ALA  | N      | 11.98        |
| 1     | A     | 2117:ALA  | C      | 2200:ALA  | N      | 11.35        |
| 1     | A     | 2317:ALA  | C      | 2320:ALA  | N      | 6.51         |
| 1     | A     | 1438:LEU  | C      | 1441:ALA  | N      | 5.15         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1722:ALA  | C      | 1800:ALA  | N      | 4.52         |
| 1     | A     | 987:ALA   | C      | 988:ALA   | N      | 3.81         |
| 1     | A     | 1241:THR  | C      | 1242:GLY  | N      | 3.62         |
| 1     | A     | 1486:ALA  | C      | 1487:ALA  | N      | 3.09         |
| 1     | A     | 1221:ALA  | C      | 1222:VAL  | N      | 2.08         |

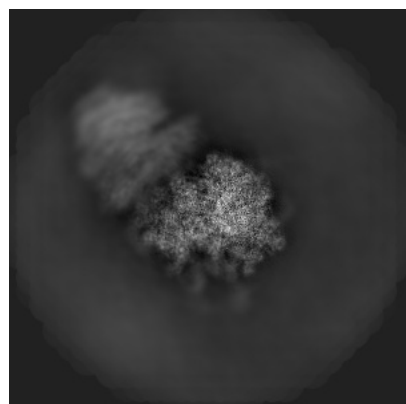
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12534. These allow visual inspection of the internal detail of the map and identification of artifacts.

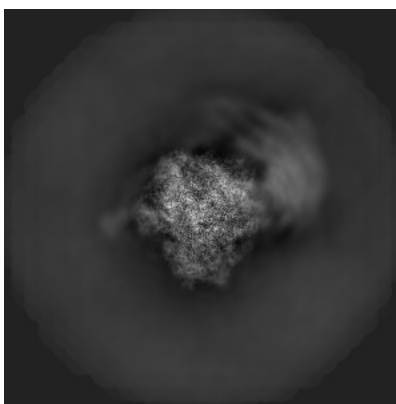
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

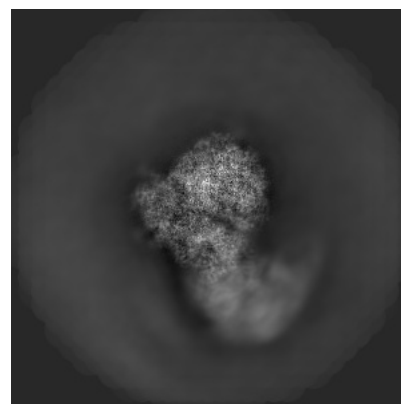
#### 6.1.1 Primary map



X

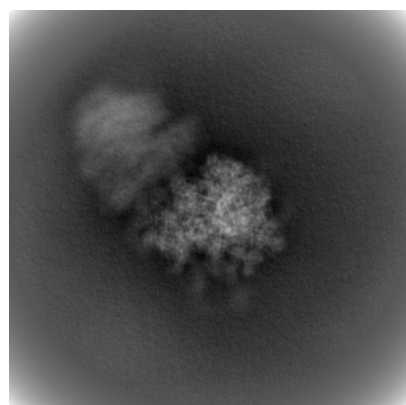


Y

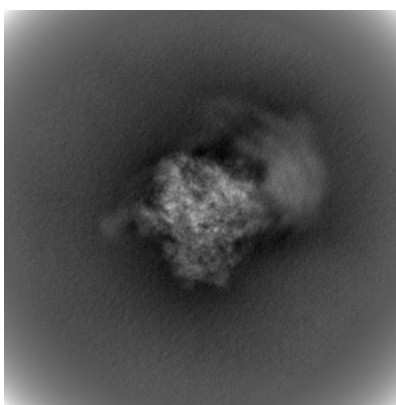


Z

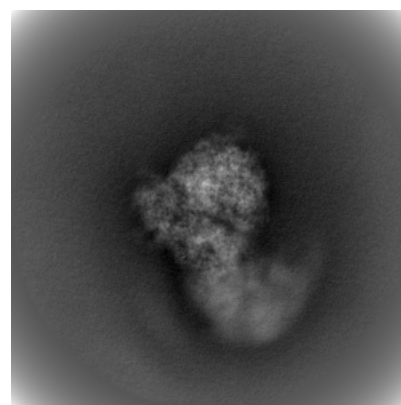
#### 6.1.2 Raw map



X



Y

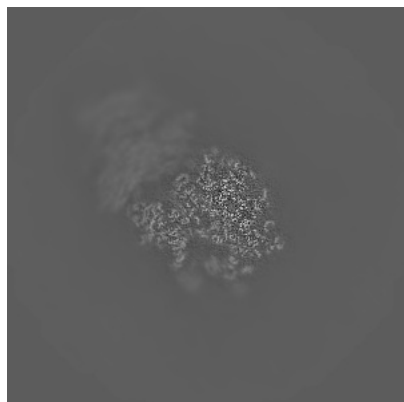


Z

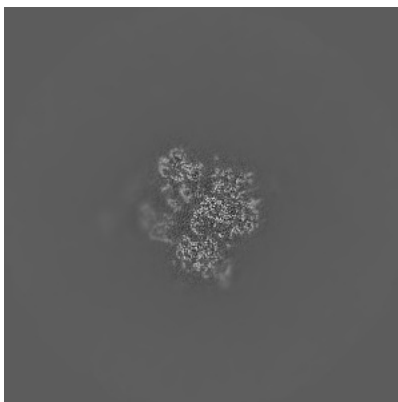
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

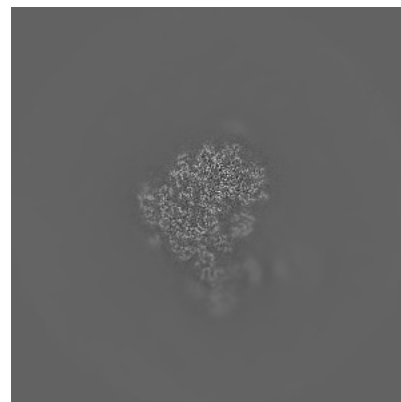
### 6.2.1 Primary map



X Index: 350

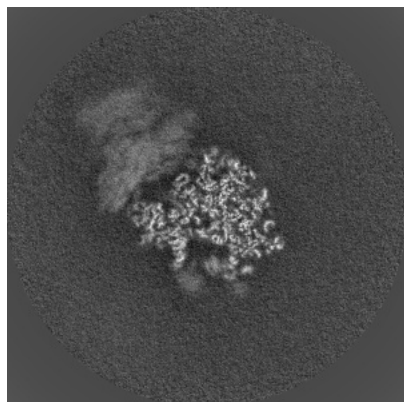


Y Index: 350

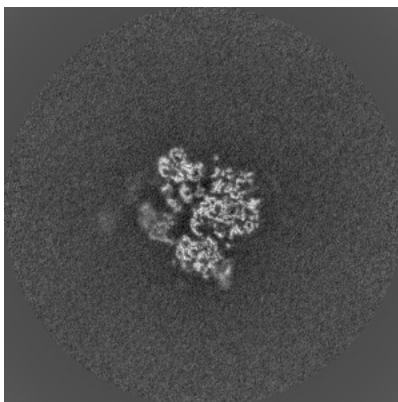


Z Index: 350

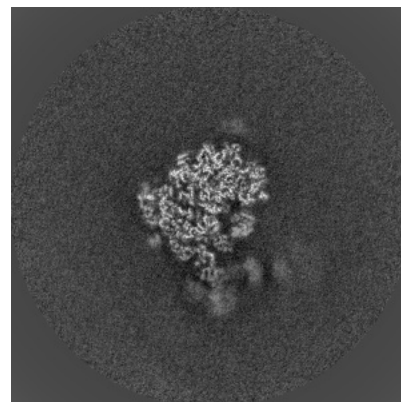
### 6.2.2 Raw map



X Index: 350



Y Index: 350

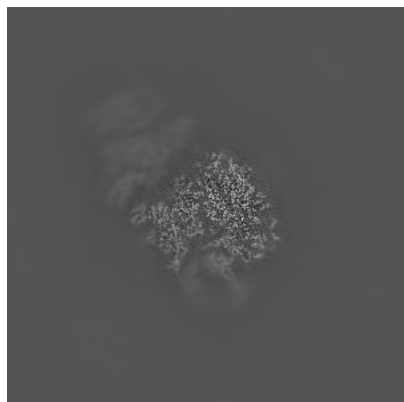


Z Index: 350

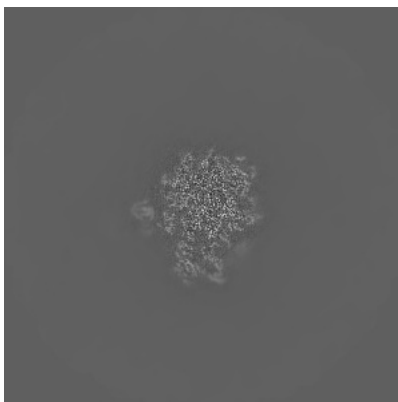
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 338

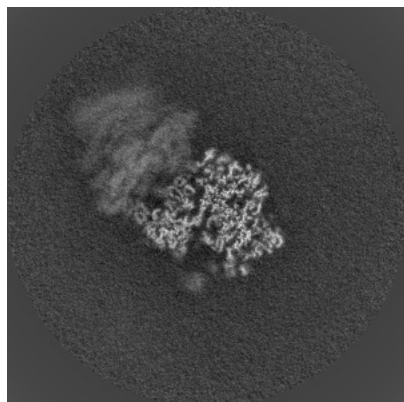


Y Index: 381

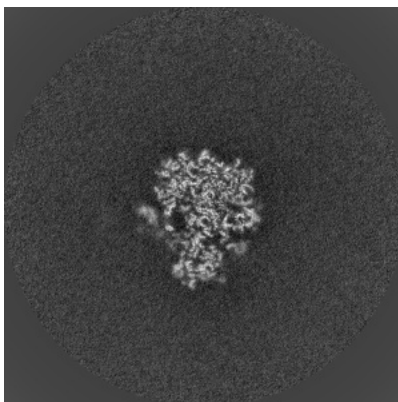


Z Index: 356

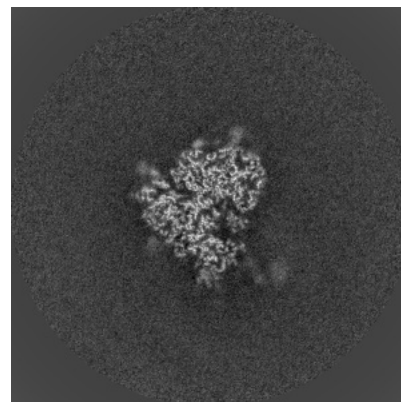
### 6.3.2 Raw map



X Index: 360



Y Index: 369

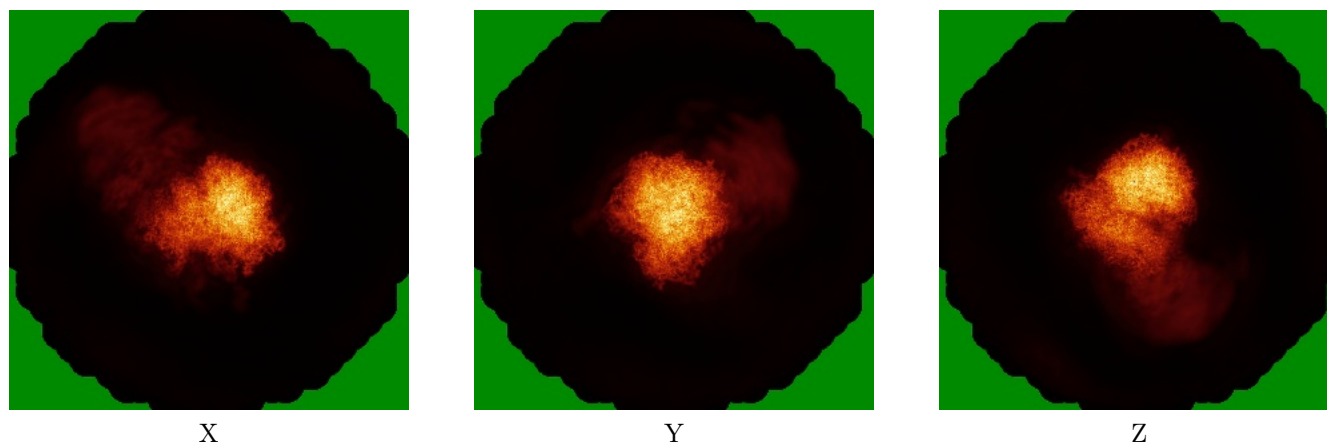


Z Index: 334

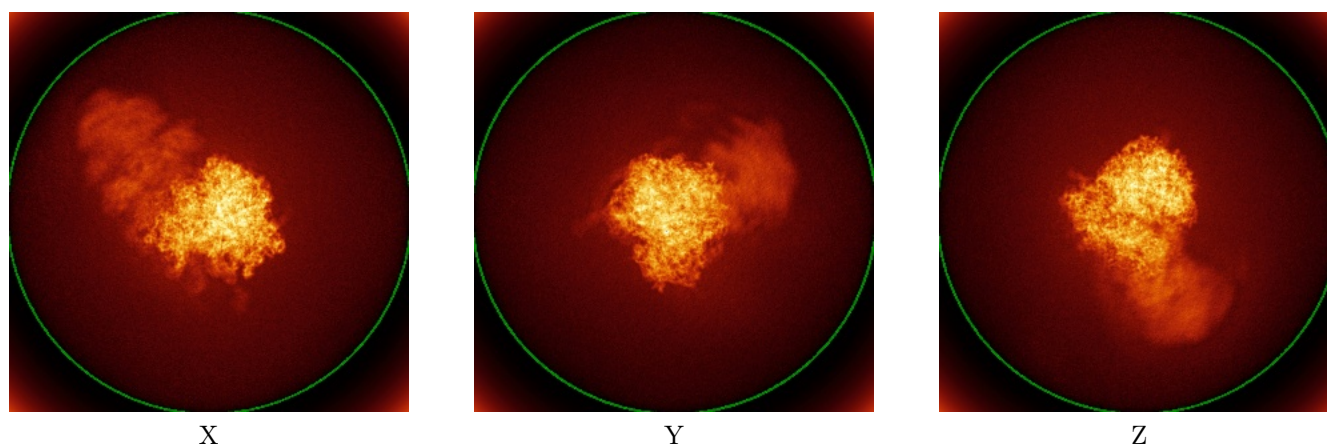
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

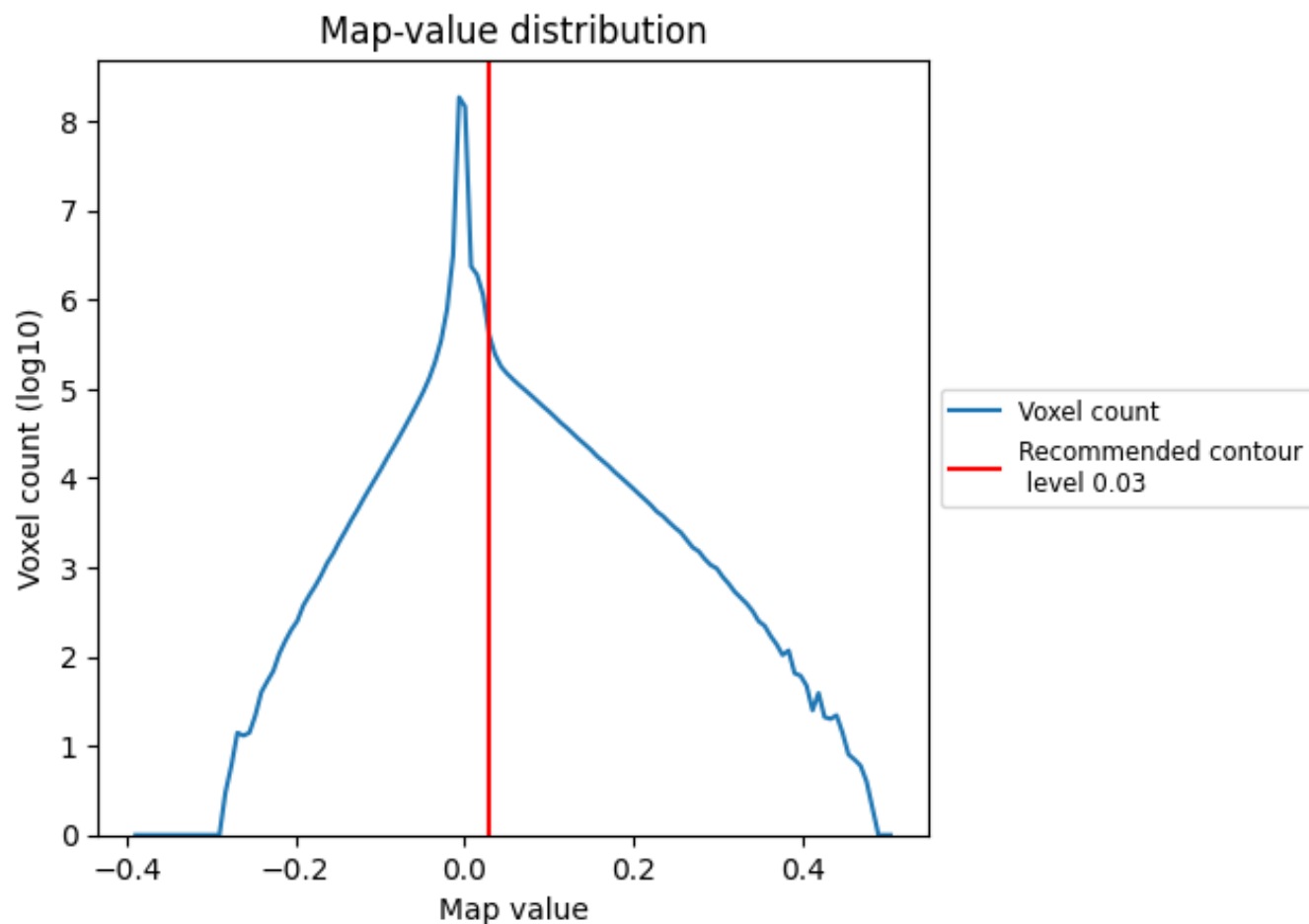
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

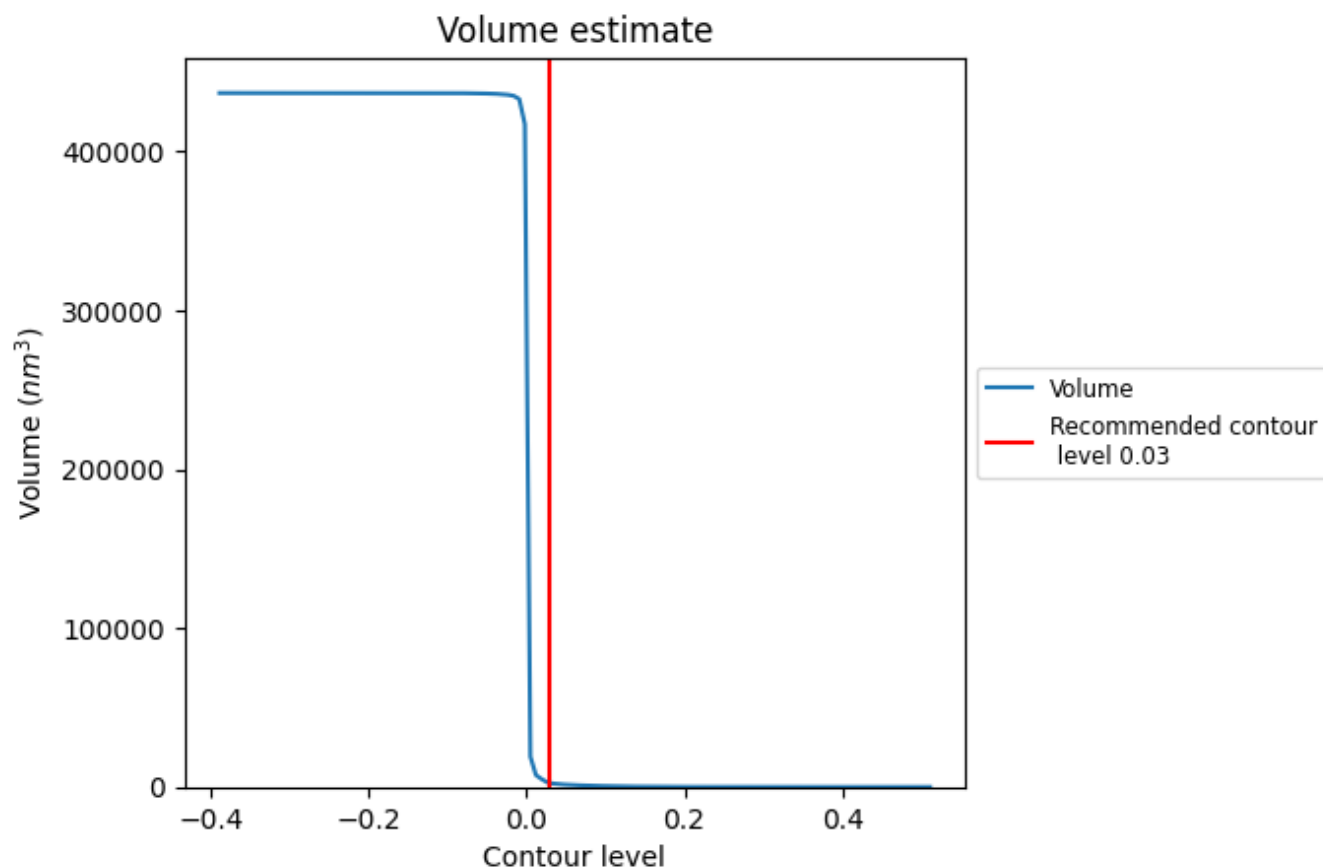
This section contains the results of statistical analysis of the map.

### 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.

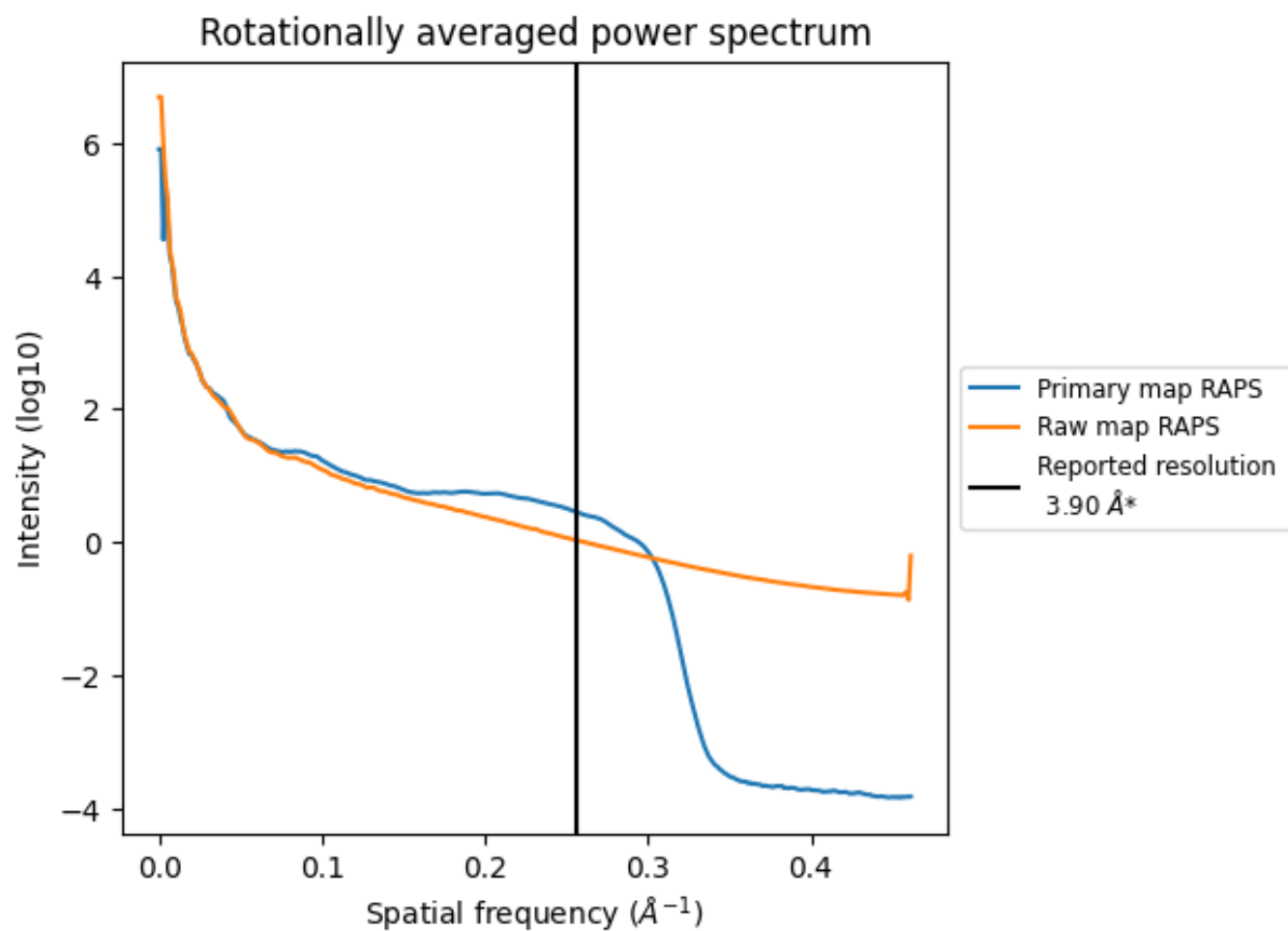
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2499  $\text{nm}^3$ ; this corresponds to an approximate mass of 2257 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 ⓘ

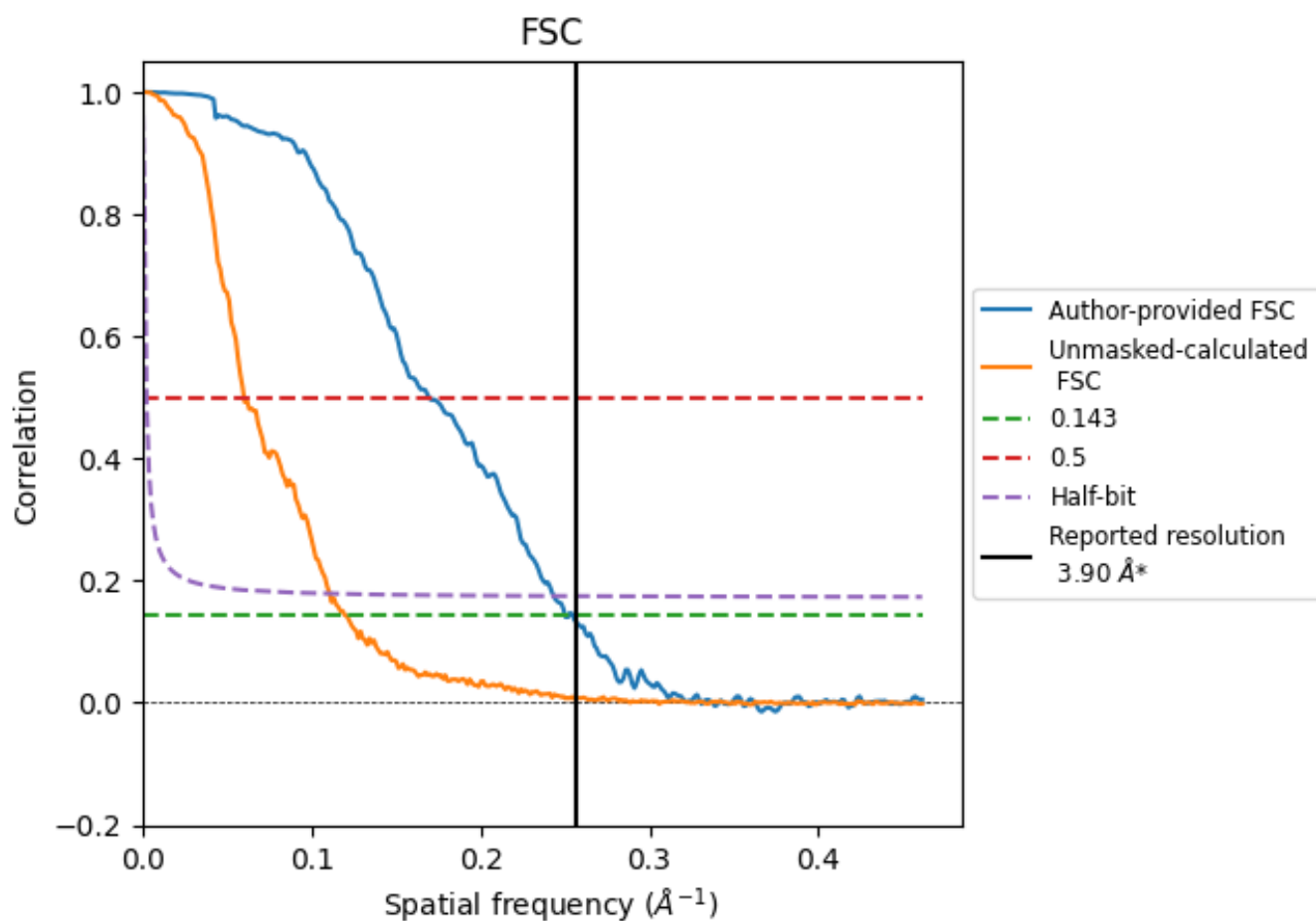


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.90                               | -     | -        |
| Author-provided FSC curve | 4.00                               | 5.90  | 4.11     |
| Unmasked-calculated*      | 8.33                               | 16.61 | 9.03     |

\*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 8.33 differs from the reported value 3.9 by more than 10 %

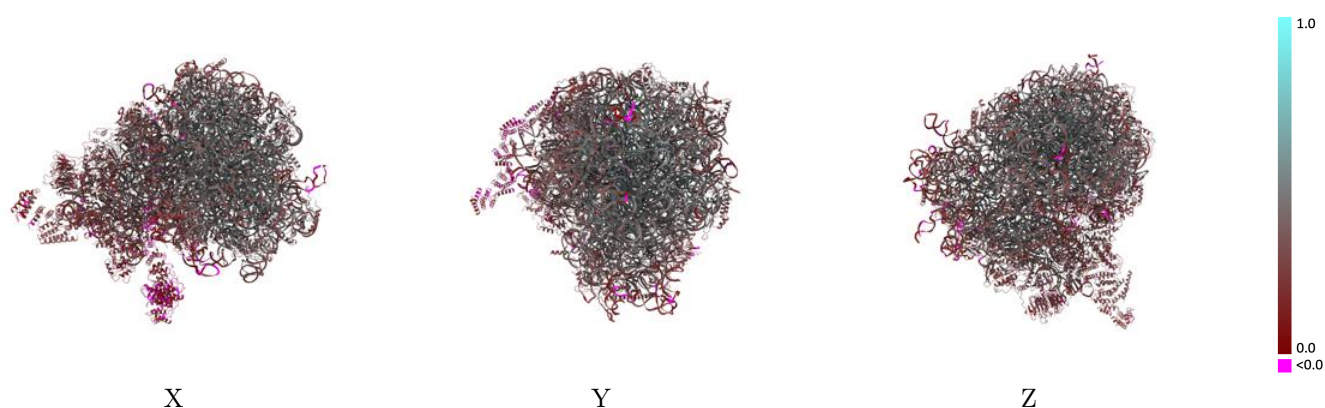
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12534 and PDB model 7NRC. Per-residue inclusion information can be found in section 3 on page 20.

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

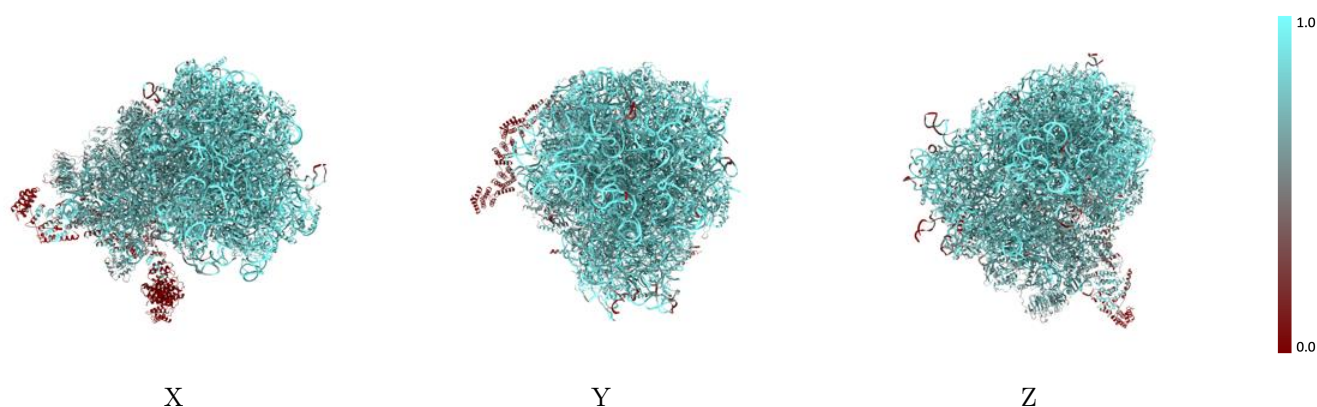
This section was not generated.

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



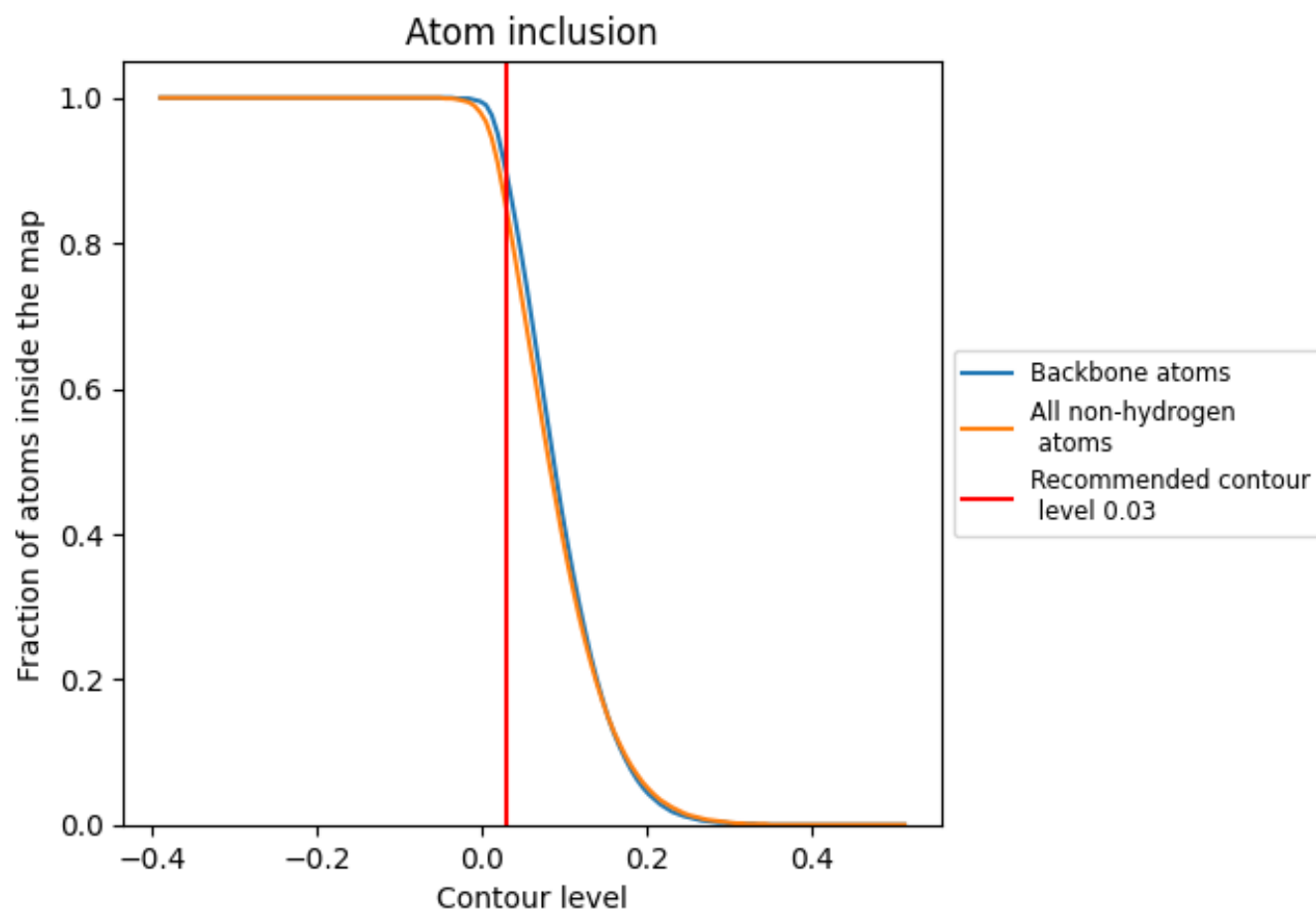
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8450   |  0.3780   |
| A     |  0.2820   |  0.1550   |
| LA    |  0.9450   |  0.4340   |
| LB    |  0.9490   |  0.3610   |
| LC    |  0.9520   |  0.4520   |
| LD    |  0.8640   |  0.4660   |
| LE    |  0.8640   |  0.4320   |
| LF    |  0.8480   |  0.4070   |
| LG    |  0.7670   |  0.2890   |
| LH    |  0.8260   |  0.3730   |
| LI    |  0.8670   |  0.4010   |
| LJ    |  0.8090   |  0.3590   |
| LK    |  0.8110   |  0.3720   |
| LL    |  0.7860   |  0.3500   |
| LM    |  0.6150  |  0.1650  |
| LN    |  0.8410 |  0.3960 |
| LO    |  0.8610 |  0.3760 |
| LP    |  0.8800 |  0.4560 |
| LQ    |  0.8740 |  0.4510 |
| LR    |  0.8630 |  0.4320 |
| LS    |  0.8550 |  0.4130 |
| LT    |  0.7830 |  0.3720 |
| LU    |  0.8390 |  0.4170 |
| LV    |  0.8430 |  0.4050 |
| LW    |  0.7860 |  0.3220 |
| LX    |  0.8210 |  0.4320 |
| LY    |  0.8500 |  0.4500 |
| LZ    |  0.8320 |  0.4090 |
| La    |  0.8350 |  0.3670 |
| Lb    |  0.8310 |  0.3800 |
| Lc    |  0.8660 |  0.4240 |
| Ld    |  0.8520 |  0.3950 |
| Le    |  0.8040 |  0.3710 |
| Lf    |  0.8120 |  0.4100 |
| Lg    |  0.8670 |  0.4440 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Lh    |  0.8840   |  0.4680   |
| Li    |  0.8060   |  0.4110   |
| Lj    |  0.8220   |  0.3790   |
| Lk    |  0.8090   |  0.3610   |
| Ll    |  0.8950   |  0.4670   |
| Lm    |  0.7860   |  0.3300   |
| Ln    |  0.8750   |  0.4410   |
| Lo    |  0.8260   |  0.3990   |
| Lp    |  0.8030   |  0.4130   |
| Lq    |  0.8350   |  0.4320   |
| Lr    |  0.8280   |  0.4270   |
| Ls    |  0.6430   |  0.3290   |
| Lt    |  0.8380   |  0.2970   |
| S2    |  0.9020   |  0.3700   |
| SA    |  0.6950   |  0.3000   |
| SB    |  0.6820   |  0.2860   |
| SC    |  0.6760   |  0.2400   |
| SD    |  0.5780  |  0.1730  |
| SE    |  0.7390 |  0.2740 |
| SF    |  0.7310 |  0.3150 |
| SG    |  0.6800 |  0.2890 |
| SH    |  0.7010 |  0.2750 |
| SI    |  0.6770 |  0.2650 |
| SJ    |  0.7050 |  0.2900 |
| SK    |  0.6080 |  0.2620 |
| SL    |  0.6960 |  0.3260 |
| SM    |  0.7850 |  0.3670 |
| SN    |  0.5750 |  0.1420 |
| SO    |  0.6180 |  0.2390 |
| SP    |  0.7100 |  0.3030 |
| SQ    |  0.6700 |  0.3000 |
| SR    |  0.7780 |  0.3720 |
| SS    |  0.7970 |  0.3580 |
| ST    |  0.7680 |  0.3090 |
| SU    |  0.6480 |  0.2620 |
| SV    |  0.8290 |  0.3660 |
| SW    |  0.7500 |  0.3100 |
| SX    |  0.7890 |  0.3990 |
| SY    |  0.7630 |  0.3580 |
| SZ    |  0.7420 |  0.3590 |
| Sa    |  0.7410 |  0.3490 |
| Sb    |  0.8140 |  0.3970 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Sc    |  0.8090 |  0.4200 |
| Sd    |  0.7740 |  0.3140 |
| Se    |  0.8140 |  0.3980 |
| Sf    |  0.7390 |  0.3380 |
| Sg    |  0.7490 |  0.3190 |
| Sl    |  0.9470 |  0.4400 |
| Sm    |  0.8870 |  0.3140 |
| Sn    |  0.8950 |  0.3330 |
| So    |  0.5370 |  0.2640 |
| Sp    |  0.7580 |  0.2700 |