



## Full wwPDB EM Validation Report ⓘ

May 4, 2026 – 07:09 PM JST

PDB ID : 9KDT / pdb\_00009kdt  
EMDB ID : EMD-62285  
Title : Cryo-EM structure of 80S ribosome  
Authors : Lu, Y.; Wang, X.; Qin, Y.; Cao, Y.  
Deposited on : 2024-11-04  
Resolution : 2.63 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:

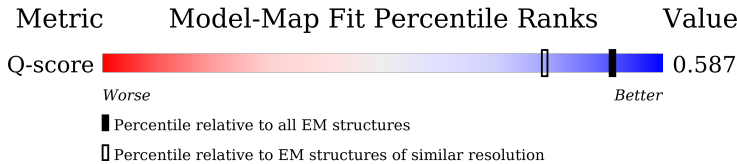
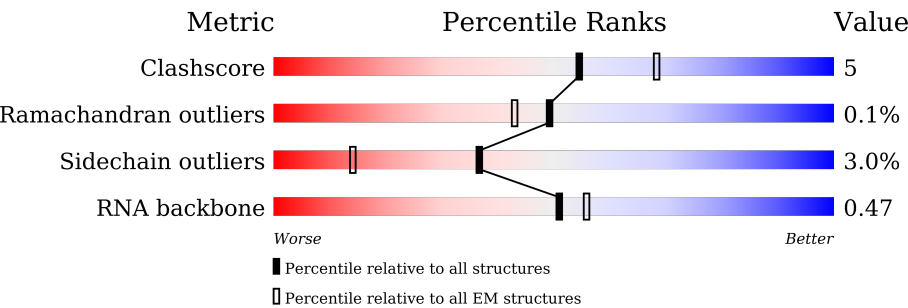
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.63 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.



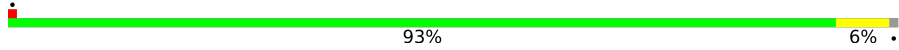

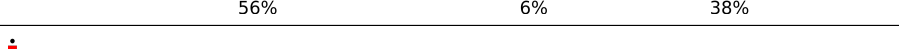
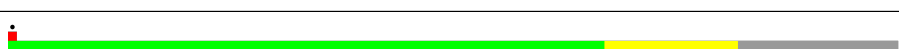



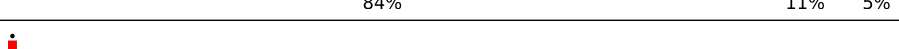



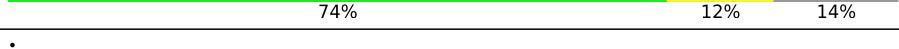

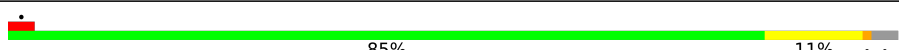


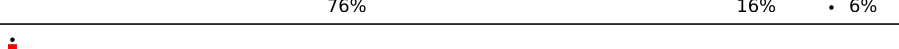







| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| RNA backbone          | 8273                        | 3508                        | -  |
| Q-score               | -                           | 25397                       | 8888 ( 2.13 - 3.13 )                                     |

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   | L5    | 4731   | <div><div></div><div>49%</div><div>18%</div><div>5%</div><div>28%</div></div> |
| 2   | L7    | 120    | <div><div></div><div>82%</div><div>14%</div><div></div></div>                 |
| 3   | L8    | 158    | <div><div></div><div>63%</div><div>28%</div><div></div></div>                 |

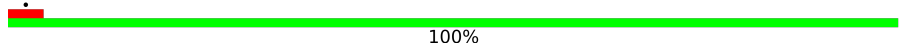
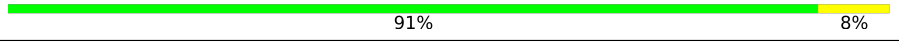
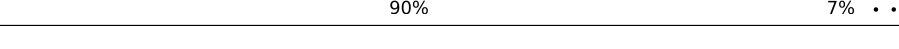
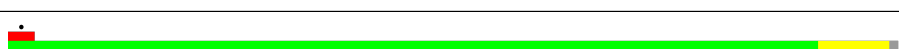

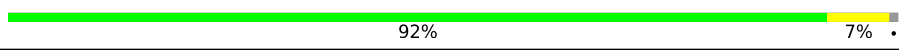

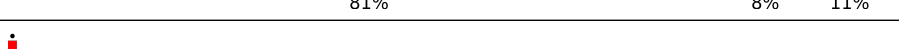



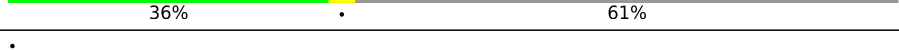

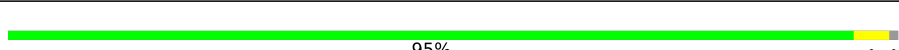


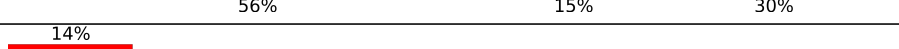







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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | La    | 148    |    |
| 5   | LA    | 257    |    |
| 6   | Lb    | 160    |    |
| 7   | LB    | 403    |    |
| 8   | Lc    | 115    |    |
| 9   | LC    | 419    |    |
| 10  | Ld    | 125    |    |
| 11  | LD    | 297    |    |
| 12  | Le    | 135    |    |
| 13  | LE    | 296    |   |
| 14  | Lf    | 110    |  |
| 15  | LF    | 270    |  |
| 16  | Lg    | 117    |  |
| 17  | LG    | 266    |  |
| 18  | Lh    | 123    |  |
| 19  | LH    | 190    |  |
| 20  | Li    | 105    |  |
| 21  | LI    | 214    |  |
| 22  | Lj    | 97     |  |
| 23  | LJ    | 178    |  |
| 24  | Lk    | 70     |  |
| 25  | Ll    | 51     |  |
| 26  | LL    | 211    |  |
| 27  | Lm    | 128    |  |
| 28  | LM    | 217    |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 29  | Ln    | 25     |  100%                   |
| 30  | LN    | 204    |  91% 8%                 |
| 31  | Lo    | 106    |  90% 7% . .             |
| 32  | LO    | 203    |  89% 9% .               |
| 33  | Lp    | 92     |  91% 8% .               |
| 34  | LP    | 184    |  77% 6% . 16%           |
| 35  | LQ    | 188    |  92% 7% .               |
| 36  | Lr    | 137    |  82% 7% . 9%            |
| 37  | LR    | 196    |  81% 8% 11%             |
| 38  | LS    | 176    |  87% 13% .             |
| 39  | LT    | 160    |  87% 12% .            |
| 40  | LU    | 128    |  60% 17% . 22%        |
| 41  | LV    | 140    |  86% 7% 7%            |
| 42  | LW    | 157    |  36% . 61%            |
| 43  | LX    | 156    |  69% 6% . 24%         |
| 44  | LY    | 145    |  81% 10% 9%           |
| 45  | LZ    | 136    |  95% . .              |
| 46  | S2    | 1870   |  9% 44% 30% 12% . 13% |
| 47  | Sa    | 115    |  75% 11% 14%          |
| 48  | SA    | 295    |  56% 15% 30%          |
| 49  | Sb    | 84     |  14% 82% 13% . .      |
| 50  | SB    | 264    |  72% 8% 19%           |
| 51  | Sc    | 69     |  6% 67% 12% 22%       |
| 52  | SC    | 293    |  64% 9% 27%           |
| 53  | Sd    | 56     |  18% 68% 27% . .      |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | SD    | 243    |                  |
| 55  | Se    | 133    |                  |
| 56  | SE    | 263    |                  |
| 57  | SF    | 204    |                  |
| 58  | Sg    | 317    |                  |
| 59  | SG    | 249    |                  |
| 60  | SH    | 194    |                  |
| 61  | SI    | 208    |                  |
| 62  | SJ    | 194    |                  |
| 63  | SK    | 165    |                  |
| 64  | SL    | 158    |                  |
| 65  | SN    | 151    |                  |
| 66  | SO    | 151    |                  |
| 67  | SP    | 145    |                  |
| 68  | SQ    | 146    |                  |
| 69  | SR    | 135    |                  |
| 70  | SS    | 152    |                  |
| 71  | ST    | 145    |                  |
| 72  | SU    | 119    |                  |
| 73  | SV    | 83     |                  |
| 74  | SW    | 130    |                  |
| 75  | Sx    | 10     |                  |
| 76  | SX    | 143    |                  |
| 77  | SY    | 133    |                  |
| 78  | SZ    | 125    |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 79  | S6    | 75     | <div><div></div><div>48%</div><div>43%</div><div>48%</div><div>9%</div></div> |
| 79  | S7    | 75     | <div><div></div><div>40%</div><div>45%</div><div>15%</div></div>              |
| 80  | Z     | 24     | <div><div></div><div>79%</div><div>63%</div><div>38%</div></div>              |

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 204155 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 Mus musculus 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | L5    | 3399     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 72884 | 32460 | 13325 | 23701 | 3398 |         |       |

- Molecule 2 is a RNA chain called Mus musculus 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2   | L7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 3 is a RNA chain called Mus musculus 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | L8    | 151      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3210  | 1433 | 567 | 1060 | 150 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1164  | 736 | 239 | 185 | 4 |         |       |

- Molecule 5 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | LA    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

- Molecule 6 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | Lb    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 807   | 505 | 174 | 124 | 4 |         |       |

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | LB    | 397      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3202  | 2039 | 603 | 546 | 14 |         |       |

- Molecule 8 is a protein called Large ribosomal subunit protein eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | Lc    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 732   | 465 | 130 | 131 | 6 |         |       |

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | LC    | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2857  | 1797 | 571 | 474 | 15 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein eL31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | Ld    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 896   | 566 | 172 | 156 | 2 |         |       |

- Molecule 11 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | LD    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2389  | 1509 | 441 | 425 | 14 |         |       |

- Molecule 12 is a protein called Large ribosomal subunit protein eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | Le    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | LE    | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1743  | 1115 | 332 | 292 | 4 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein eL33.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 143 | 4 |         |       |

- Molecule 15 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | LF    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1771  | 1139 | 337 | 287 | 8 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein eL34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Lg    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 873   | 546 | 180 | 141 | 6 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein eL8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | LG    | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1848  | 1179 | 354 | 311 | 4 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 643 | 204 | 167 | 1 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1519  | 956 | 284 | 273 | 6 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein eL36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 21 is a protein called Large ribosomal subunit protein uL16-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | LI    | 201      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1631  | 1037 | 316 | 267 | 11 |         |       |

- Molecule 22 is a protein called Large ribosomal subunit protein eL37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | Lj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | LJ    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1340  | 848 | 250 | 236 | 6 |         |       |

- Molecule 24 is a protein called Large ribosomal subunit protein eL38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 24  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 568   | 365 | 103 | 99 | 1 |         |       |

- Molecule 25 is a protein called Large ribosomal subunit protein eL39-like.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 279 | 93 | 64 | 2 |         |       |

- Molecule 26 is a protein called Large ribosomal subunit protein eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | LL    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1667  | 1043 | 343 | 277 | 4 |         |       |

- Molecule 27 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | Lm    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 260 | 88 | 65 | 6 |         |       |

- Molecule 28 is a protein called Large ribosomal subunit protein eL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1125  | 721 | 218 | 179 | 7 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein eS32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | Ln    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 30 is a protein called Large ribosomal subunit protein eL15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 31 is a protein called Large ribosomal subunit protein eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Lo    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 528 | 172 | 136 | 6 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | LO    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1640  | 1055 | 320 | 259 | 6 |         |       |

- Molecule 33 is a protein called Large ribosomal subunit protein eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | LP    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1251  | 782 | 243 | 217 | 9 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein eL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1515  | 948 | 314 | 249 | 4 |         |       |

- Molecule 36 is a protein called Large ribosomal subunit protein eL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Lr    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 994   | 616 | 206 | 167 | 5 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein eL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | LR    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1457  | 901 | 316 | 231 | 9 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein eL20.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 38  | LS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1451  | 924 | 283 | 234 | 10 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | LT    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1307  | 829 | 253 | 218 | 7 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | LU    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 523 | 143 | 149 | 2 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | LV    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 973   | 615 | 183 | 170 | 5 |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein eL24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | LW    | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 519   | 332 | 101 | 83 | 3 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | LX    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 618 | 181 | 167 | 1 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | LY    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 692 | 223 | 184 | 3 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein eL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 46 is a RNA chain called Mus musculus 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 46  | S2    | 1628     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 34749 | 15516 | 6241 | 11365 | 1627 |         |       |

- Molecule 47 is a protein called Small ribosomal subunit protein eS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Sa    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 48 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | SA    | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1636  | 1042 | 288 | 298 | 8 |         |       |

- Molecule 49 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 50 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | SB    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1729  | 1098 | 309 | 308 | 14 |         |       |

- Molecule 51 is a protein called Small ribosomal subunit protein eS28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | Sc    | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 416   | 257 | 80 | 77 | 2 |         |       |

- Molecule 52 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | SC    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1665  | 1080 | 285 | 291 | 9 |         |       |

- Molecule 53 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | Sd    | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 284 | 93 | 73 | 5 |         |       |

- Molecule 54 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | SD    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1626  | 1036 | 296 | 287 | 7 |         |       |

- Molecule 55 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | Se    | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 384   | 234 | 86 | 63 | 1 |         |       |

- Molecule 56 is a protein called Small ribosomal subunit protein eS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | SE    | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2050  | 1311 | 381 | 350 | 8 |         |       |

- Molecule 57 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SF    | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1416  | 888 | 262 | 259 | 7 |         |       |

- Molecule 58 is a protein called Small ribosomal subunit protein RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | Sg    | 276      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2148  | 1357 | 378 | 401 | 12 |         |       |

- Molecule 59 is a protein called Small ribosomal subunit protein eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59  | SG    | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1645  | 1029 | 330 | 280 | 6 |         |       |

- Molecule 60 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | SH    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1449  | 924 | 266 | 258 | 1 |         |       |

- Molecule 61 is a protein called Small ribosomal subunit protein eS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SI    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1499  | 943 | 293 | 258 | 5 |         |       |

- Molecule 62 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | SJ    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 743 | 230 | 187 | 2 |         |       |

- Molecule 63 is a protein called Small ribosomal subunit protein eS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | SK    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 760   | 495 | 135 | 124 | 6 |         |       |

- Molecule 64 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | SL    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1110  | 708 | 207 | 189 | 6 |         |       |

- Molecule 65 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 66 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | SO    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 612 | 197 | 187 | 6 |         |       |

- Molecule 67 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | SP    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 625 | 183 | 166 | 7 |         |       |

- Molecule 68 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | SQ    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1109  | 704 | 210 | 192 | 3 |         |       |

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | SR    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 668 | 198 | 194 | 4 |         |       |

- Molecule 70 is a protein called Small ribosomal subunit protein uS13.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SS    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1157  | 728 | 231 | 197 | 1 |         |       |

- Molecule 71 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | ST    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 681 | 212 | 195 | 2 |         |       |

- Molecule 72 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | SU    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 471 | 142 | 136 | 4 |         |       |

- Molecule 73 is a protein called Small ribosomal subunit protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | SV    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 619   | 379 | 116 | 119 | 5 |         |       |

- Molecule 74 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 75 is a RNA chain called RNA (5'-R(P\*AP\*UP\*CP\*AP\*UP\*GP\*AP\*AP\*GP\*U)-3').

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 75  | Sx    | 10       | Total | C  | N  | O  | P  | 0       | 0     |
|     |       |          | 214   | 96 | 39 | 69 | 10 |         |       |

- Molecule 76 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | SX    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 682 | 214 | 181 | 3 |         |       |

- Molecule 77 is a protein called Small ribosomal subunit protein eS24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | SY    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 565 | 173 | 149 | 4 |         |       |

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | SZ    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 574   | 368 | 104 | 101 | 1 |         |       |

- Molecule 79 is a RNA chain called P/P, E/E tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 79  | S6    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |
| 79  | S7    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 80 is a protein called Nascent peptide.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 80  | Z     | 24       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 119   | 71 | 24 | 24 |         |       |

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 81  | L5    | 94       | Total | Mg | 0       |
|     |       |          | 94    | 94 |         |
| 81  | L7    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 81  | LN    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 81  | LP    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 82  | Lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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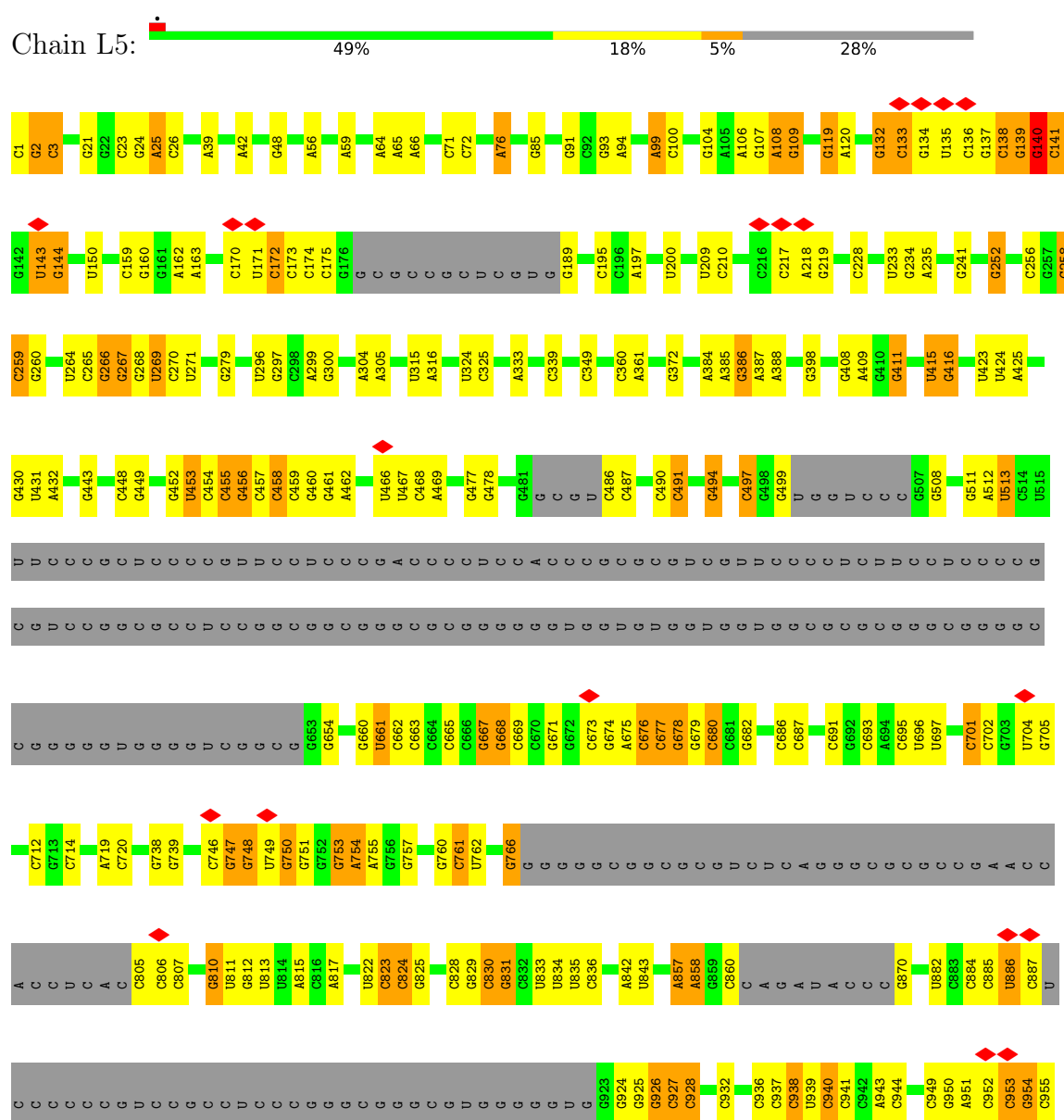
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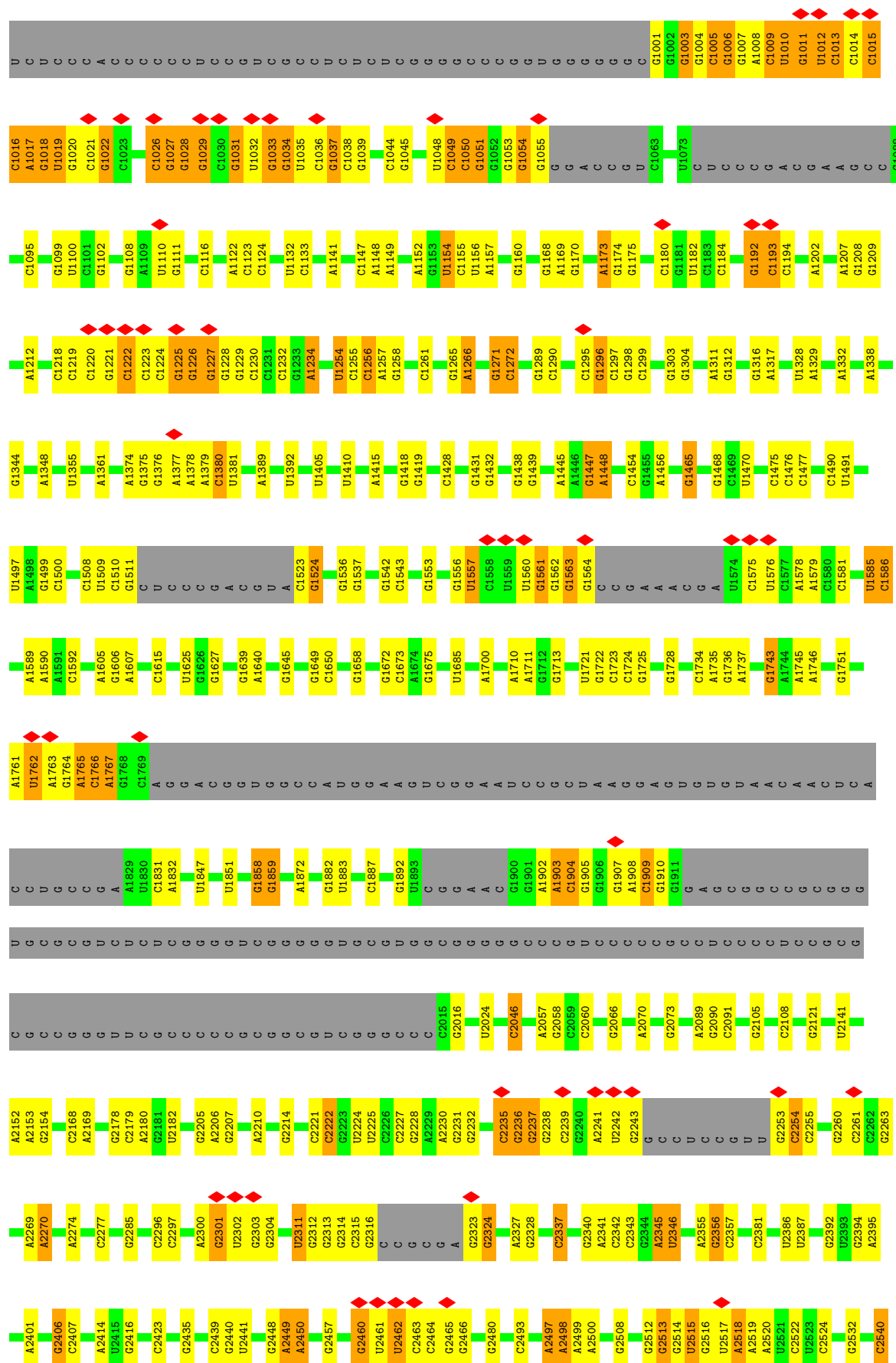
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 82  | Lm    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 82  | Lp    | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

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

- Molecule 1: Mus musculus 28S ribosomal RNA

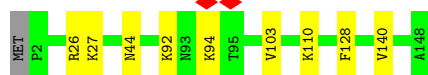






WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

Chain La:  93% 6% .



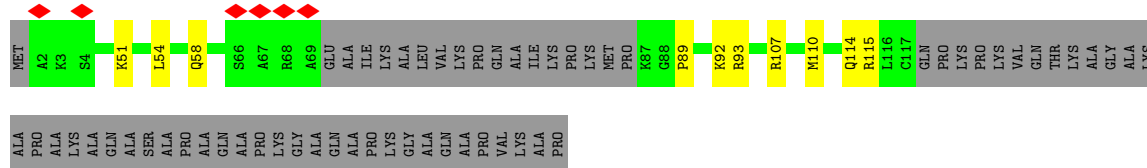
- Molecule 5: Large ribosomal subunit protein uL2

Chain LA:  89% 7% .



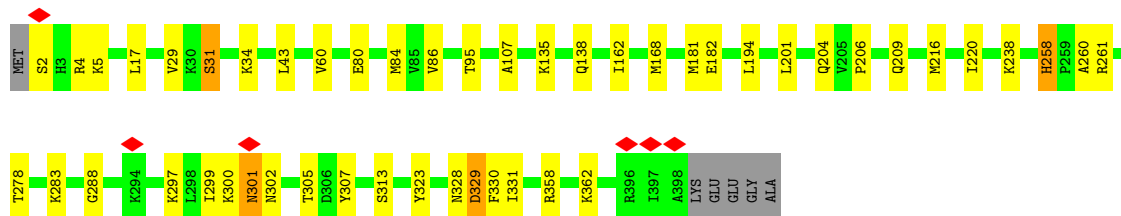
- Molecule 6: Large ribosomal subunit protein eL29

Chain Lb:  56% 6% 38%



- Molecule 7: Large ribosomal subunit protein uL3

Chain LB:  86% 11% ..




- Molecule 8: Large ribosomal subunit protein eL30

Chain Lc:  67% 15% 18%



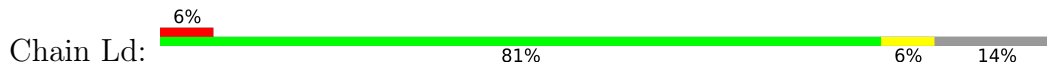
- Molecule 9: Large ribosomal subunit protein uL4

Chain LC:  76% 9% 15%

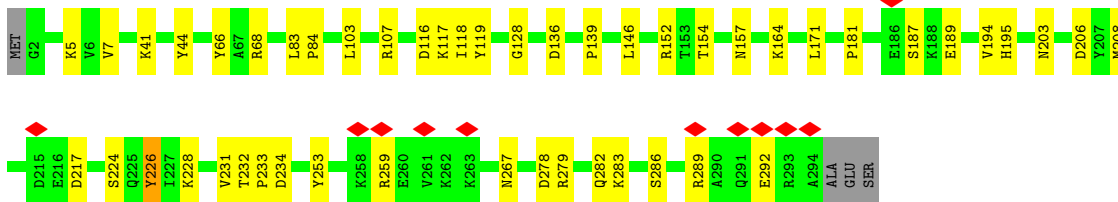
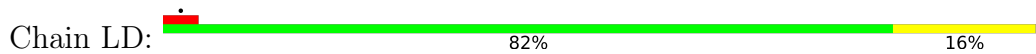




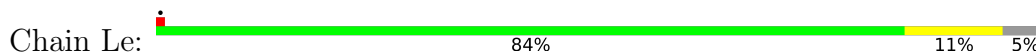
- Molecule 10: Large ribosomal subunit protein eL31



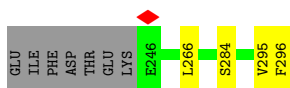
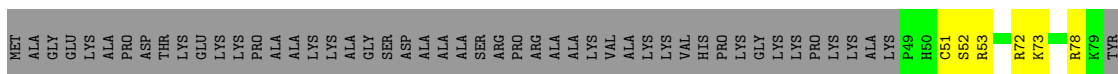
- Molecule 11: Large ribosomal subunit protein uL18



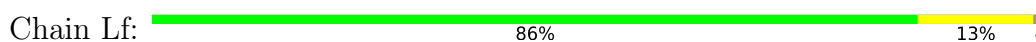
- Molecule 12: Large ribosomal subunit protein eL32



- Molecule 13: Large ribosomal subunit protein eL6




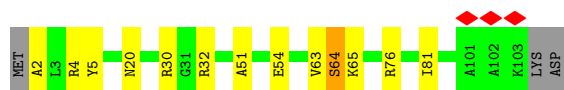
- Molecule 14: Large ribosomal subunit protein eL33






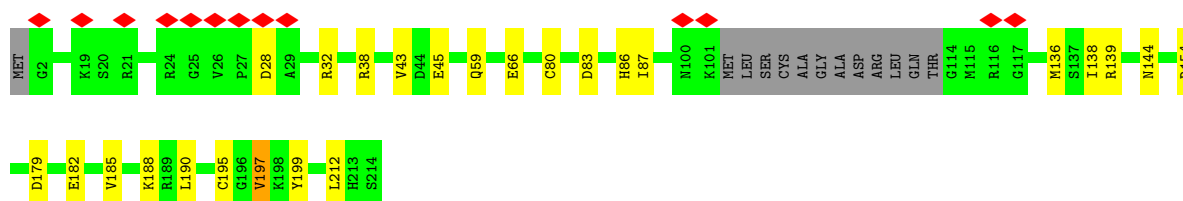
- Molecule 20: Large ribosomal subunit protein eL36

Chain Li:  85% 11% ..




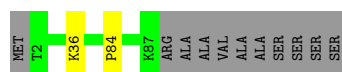
- Molecule 21: Large ribosomal subunit protein uL16-like

Chain LI:  6% 82% 11% 6%




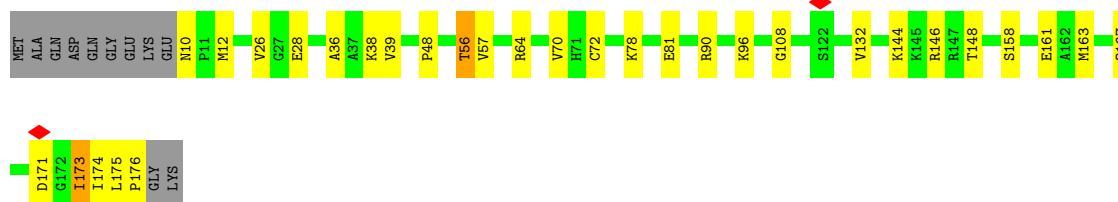
- Molecule 22: Large ribosomal subunit protein eL37

Chain Lj:  87% 11%



- Molecule 23: Large ribosomal subunit protein uL5

Chain LJ:  76% 16% 6%



- Molecule 24: Large ribosomal subunit protein eL38

Chain Lk:  86% 10% ..

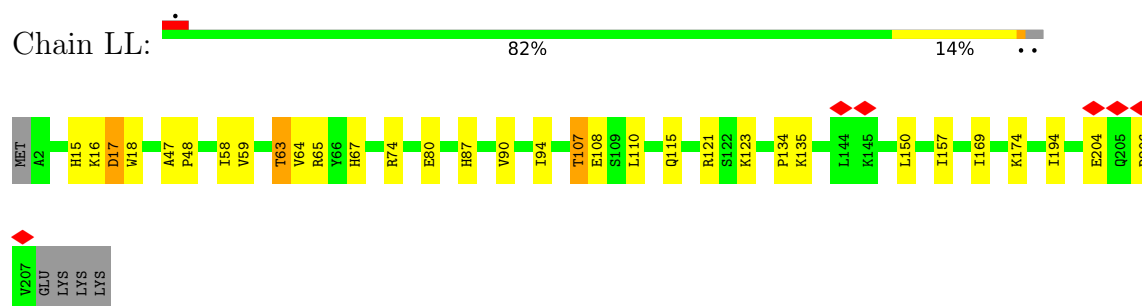


- Molecule 25: Large ribosomal subunit protein eL39-like

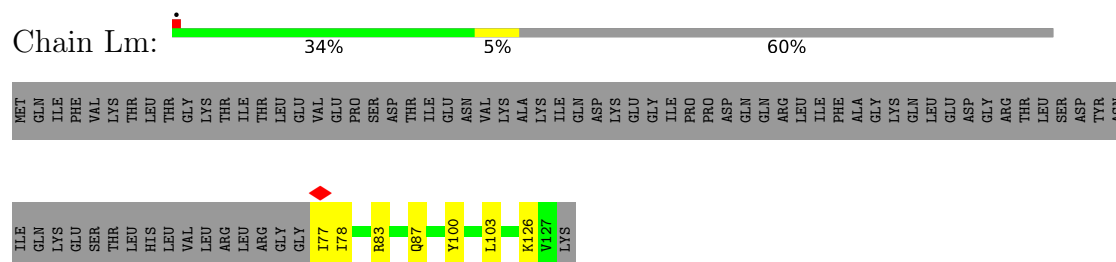
Chain Ll:  94% ..



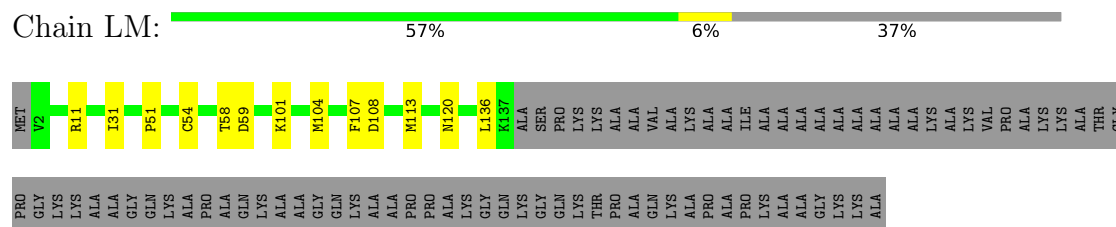
- Molecule 26: Large ribosomal subunit protein eL13



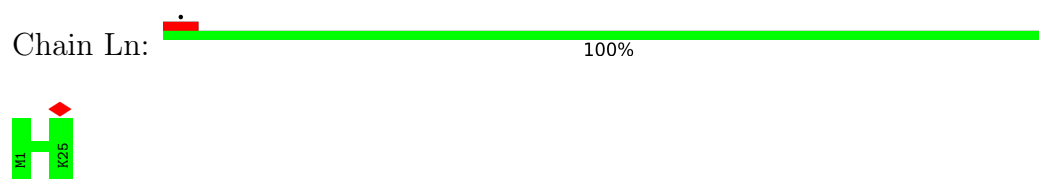
- Molecule 27: Ubiquitin-ribosomal protein eL40 fusion protein



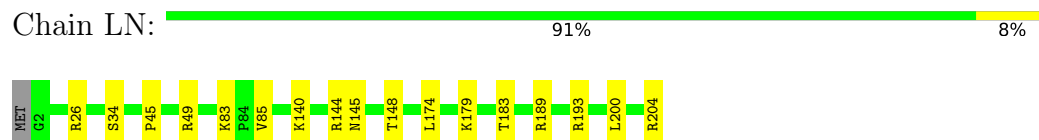
- Molecule 28: Large ribosomal subunit protein eL14



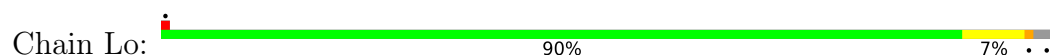
- Molecule 29: Small ribosomal subunit protein eS32

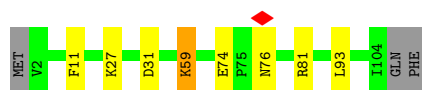


- Molecule 30: Large ribosomal subunit protein eL15



- Molecule 31: Large ribosomal subunit protein eL42





- Molecule 32: Large ribosomal subunit protein uL13

Chain LO: 89% 9%



- Molecule 33: Large ribosomal subunit protein eL43

Chain Lp: 91% 8%



- Molecule 34: Large ribosomal subunit protein uL22

Chain LP: 77% 6% 16%



- Molecule 35: Large ribosomal subunit protein eL18

Chain LQ: 92% 7%



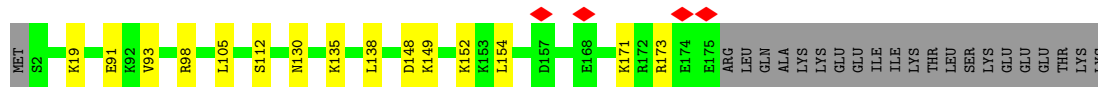
- Molecule 36: Large ribosomal subunit protein eL28

Chain Lr: 82% 7% 9%



- Molecule 37: Large ribosomal subunit protein eL19

Chain LR: 81% 8% 11%



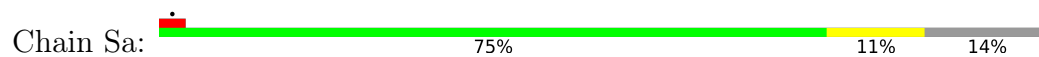
- Molecule 38: Large ribosomal subunit protein eL20



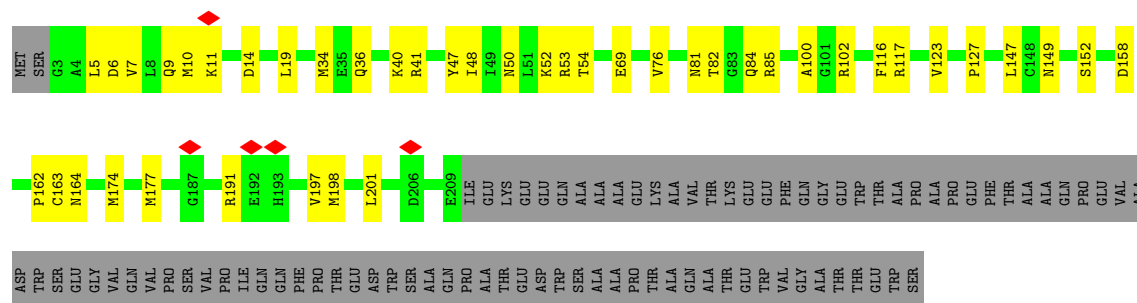




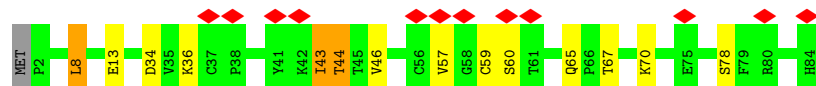
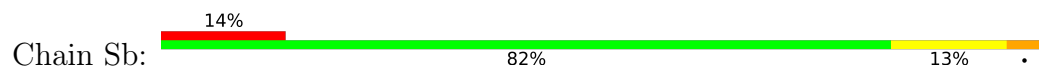




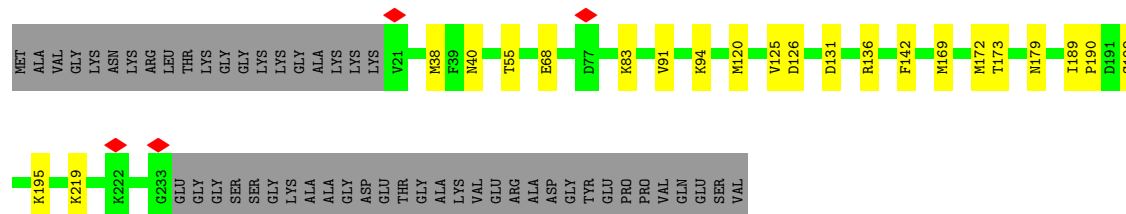
• Molecule 48: Small ribosomal subunit protein uS2



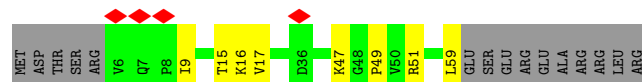
• Molecule 49: Small ribosomal subunit protein eS27



• Molecule 50: Small ribosomal subunit protein eS1



• Molecule 51: Small ribosomal subunit protein eS28




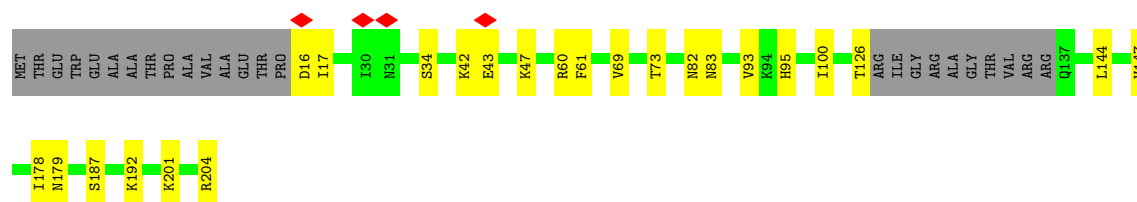
• Molecule 52: Small ribosomal subunit protein uS5





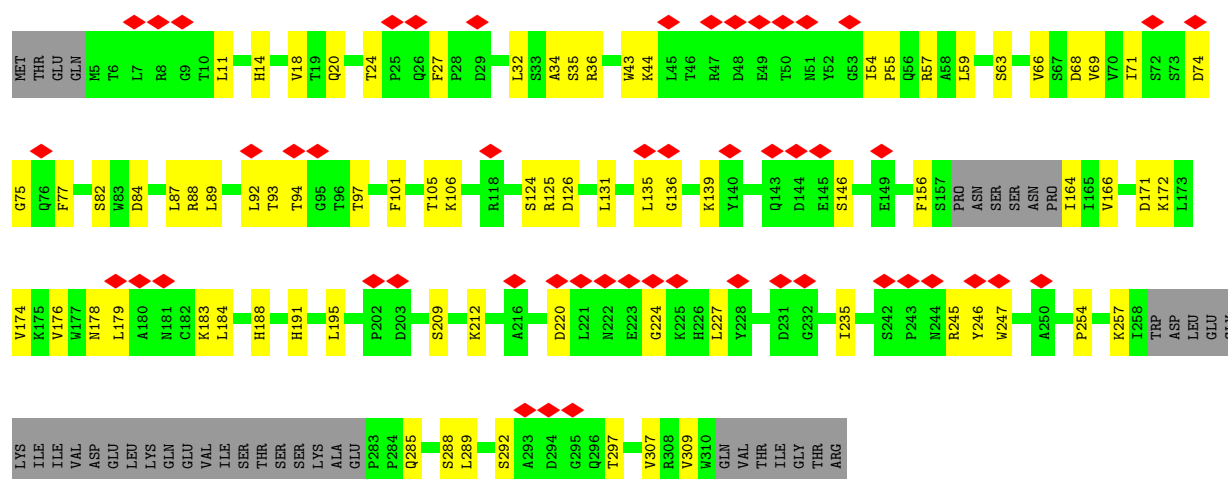
- Molecule 57: Small ribosomal subunit protein uS7

Chain SF: 



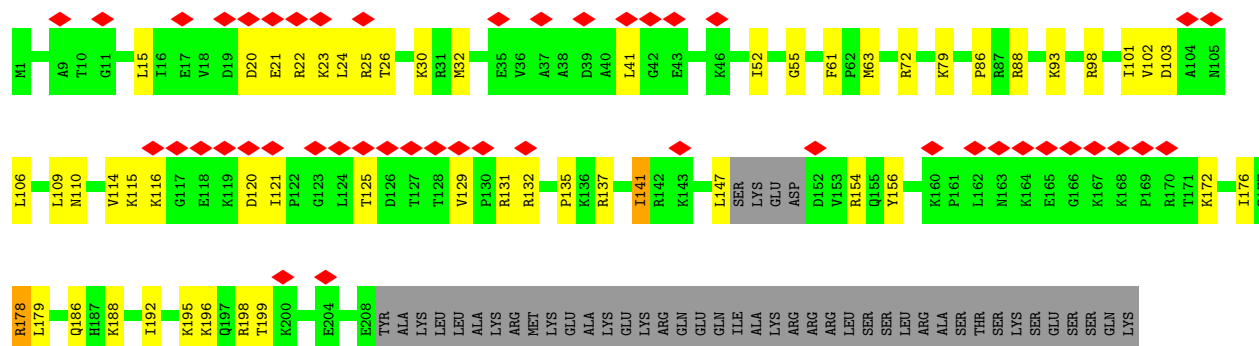
- Molecule 58: Small ribosomal subunit protein RACK1

Chain Sg: 



- Molecule 59: Small ribosomal subunit protein eS6

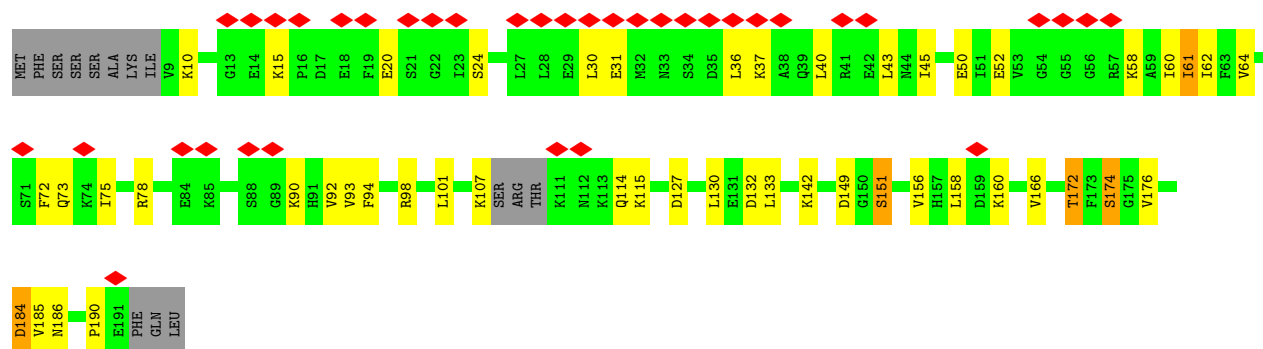
Chain SG: 



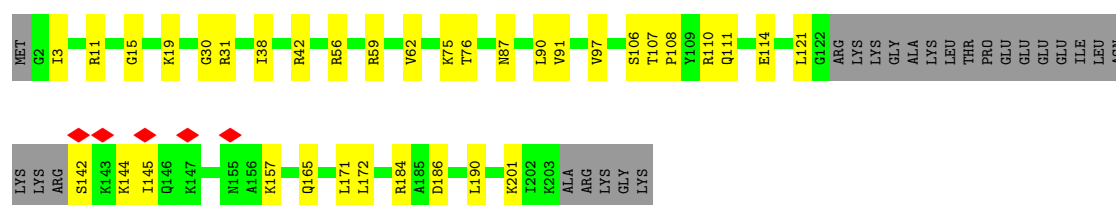
- Molecule 60: Small ribosomal subunit protein eS7

Chain SH: 

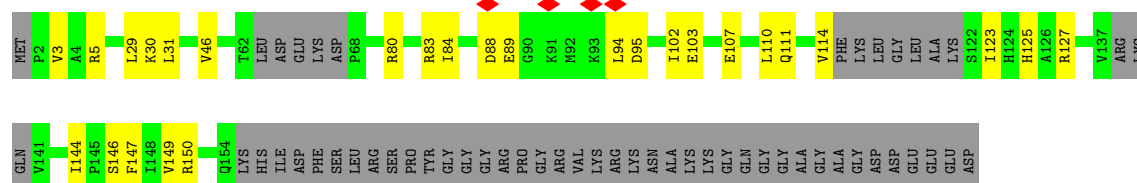




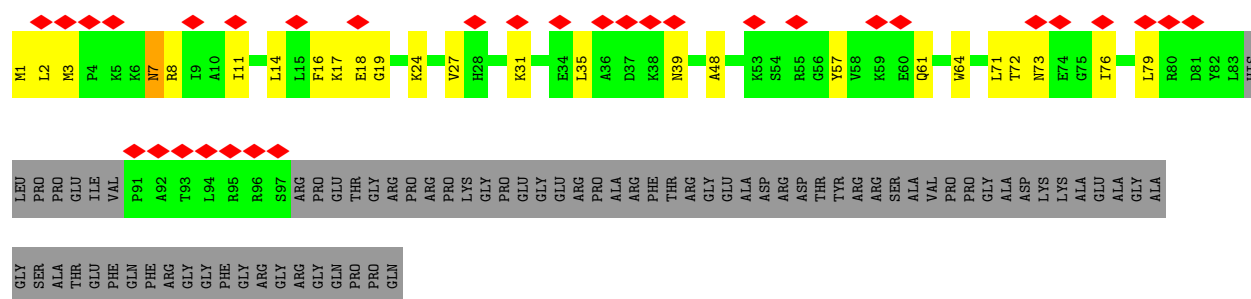
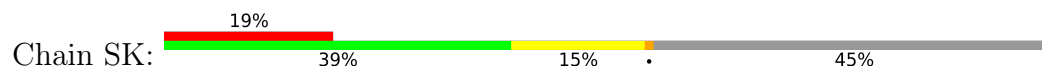
- Molecule 61: Small ribosomal subunit protein eS8



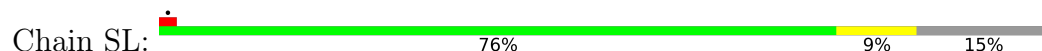
- Molecule 62: Small ribosomal subunit protein uS4



- Molecule 63: Small ribosomal subunit protein eS10



- Molecule 64: Small ribosomal subunit protein uS17

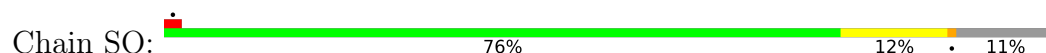




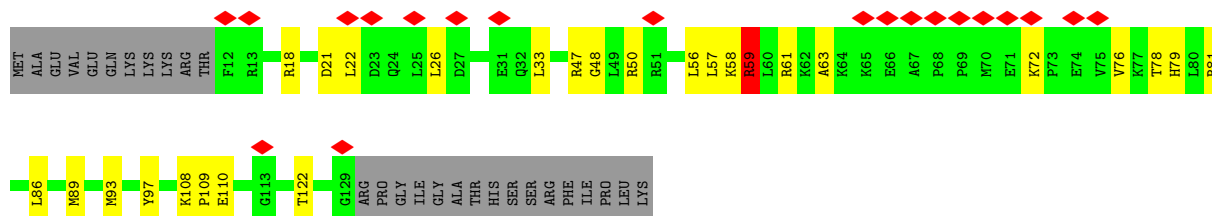
- Molecule 65: Small ribosomal subunit protein uS15



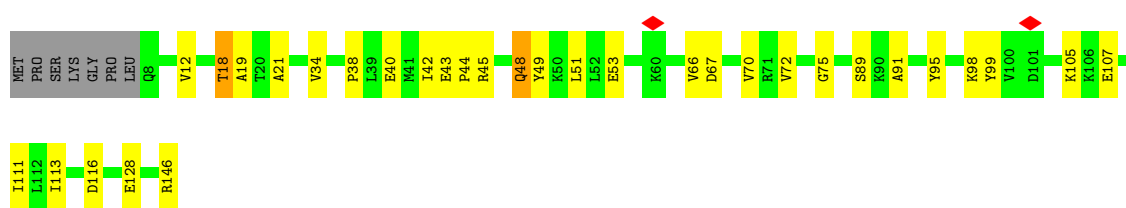
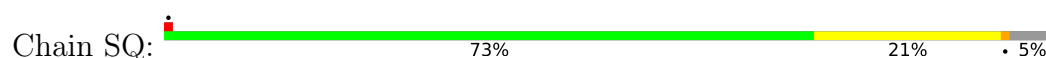
- Molecule 66: Small ribosomal subunit protein uS11



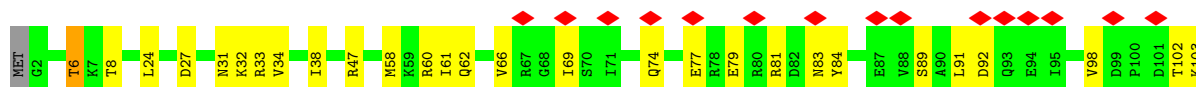
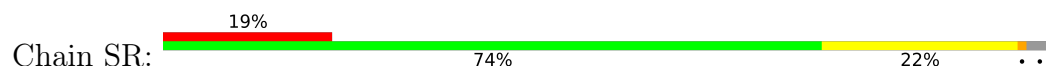
- Molecule 67: Small ribosomal subunit protein uS19

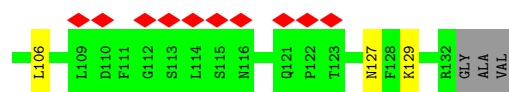


- Molecule 68: Small ribosomal subunit protein uS9

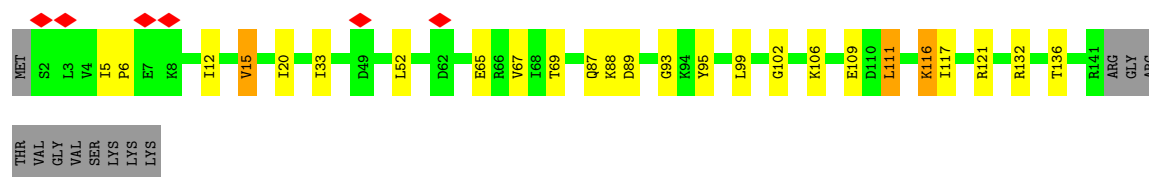
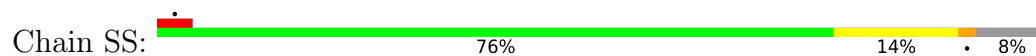


- Molecule 69: Small ribosomal subunit protein eS17

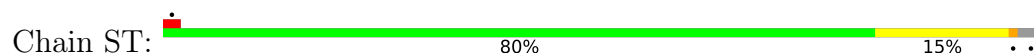




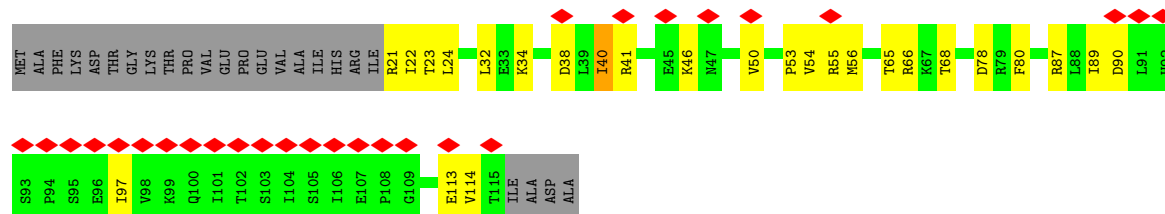
- Molecule 70: Small ribosomal subunit protein uS13



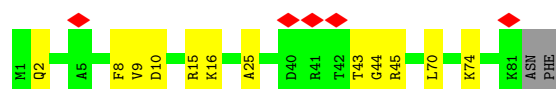
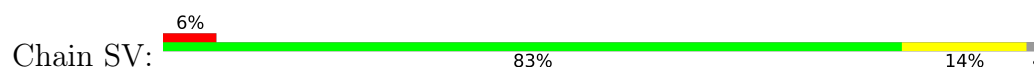
- Molecule 71: Small ribosomal subunit protein eS19



- Molecule 72: Small ribosomal subunit protein uS10



- Molecule 73: Small ribosomal subunit protein eS21

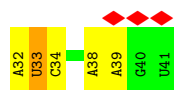


- Molecule 74: Small ribosomal subunit protein uS8

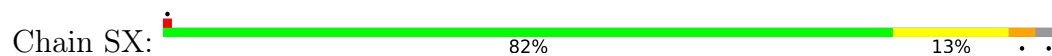


- Molecule 75: RNA (5'-R(P\*AP\*UP\*CP\*AP\*UP\*GP\*AP\*AP\*GP\*U)-3')

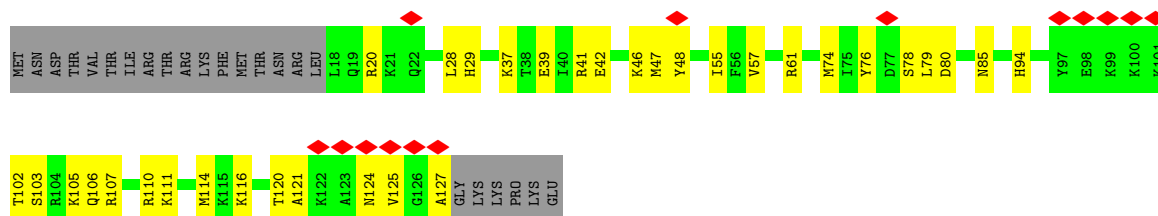




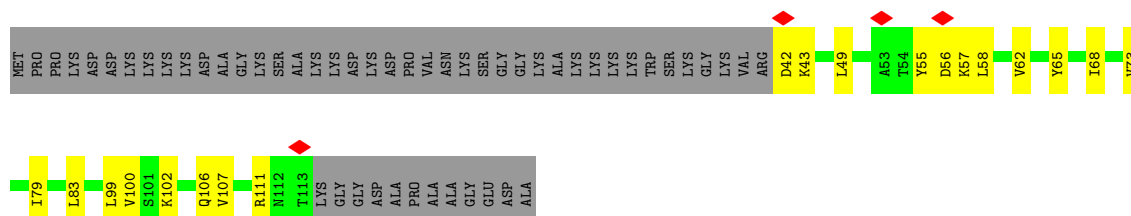
- Molecule 76: Small ribosomal subunit protein uS12



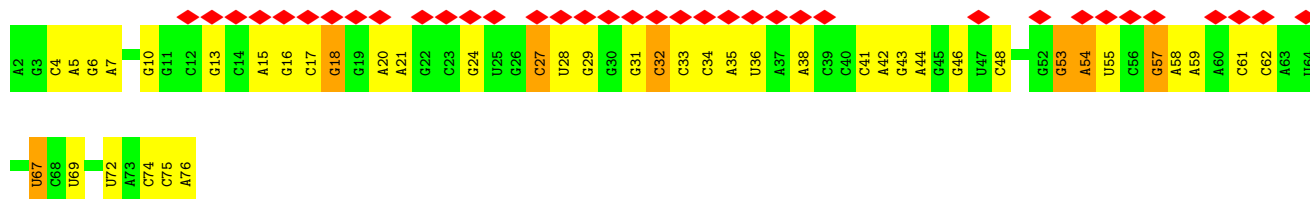
- Molecule 77: Small ribosomal subunit protein eS24



- Molecule 78: Small ribosomal subunit protein eS25

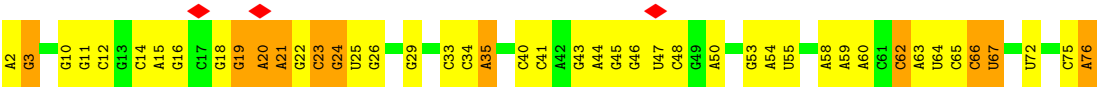


- Molecule 79: P/P, E/E tRNA

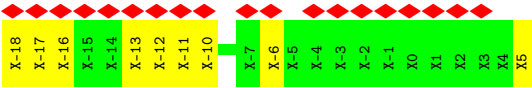
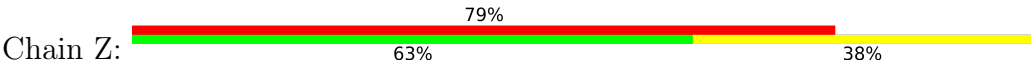


- Molecule 79: P/P, E/E tRNA





• Molecule 80: Nascent peptide





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 217714                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2600                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 9.612                                   | Depositor |
| Minimum map value                    | -4.282                                  | Depositor |
| Average map value                    | -0.006                                  | Depositor |
| Map value standard deviation         | 0.230                                   | Depositor |
| Recommended contour level            | 0.8                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 616.0, 616.0, 616.0                     | wwPDB     |
| Map dimensions                       | 560, 560, 560                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.1, 1.1, 1.1                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$      |
| 1   | L5    | 0.15         | 0/81527       | 0.34        | 21/127149 (0.0%) |
| 2   | L7    | 0.11         | 0/2858        | 0.28        | 0/4455           |
| 3   | L8    | 0.12         | 0/3584        | 0.29        | 0/5582           |
| 4   | La    | 0.19         | 0/1193        | 0.39        | 0/1593           |
| 5   | LA    | 0.15         | 0/1936        | 0.42        | 0/2596           |
| 6   | Lb    | 0.24         | 0/821         | 0.41        | 0/1082           |
| 7   | LB    | 0.21         | 1/3269 (0.0%) | 0.44        | 0/4375           |
| 8   | Lc    | 0.30         | 0/742         | 0.53        | 0/996            |
| 9   | LC    | 0.22         | 0/2911        | 0.42        | 0/3907           |
| 10  | Ld    | 0.19         | 0/911         | 0.41        | 0/1227           |
| 11  | LD    | 0.23         | 0/2435        | 0.46        | 0/3260           |
| 12  | Le    | 0.20         | 0/1071        | 0.38        | 0/1429           |
| 13  | LE    | 0.18         | 0/1775        | 0.39        | 0/2381           |
| 14  | Lf    | 0.17         | 0/895         | 0.39        | 0/1198           |
| 15  | LF    | 0.26         | 0/1805        | 0.44        | 0/2408           |
| 16  | Lg    | 0.18         | 0/883         | 0.36        | 0/1178           |
| 17  | LG    | 0.30         | 0/1880        | 0.48        | 0/2531           |
| 18  | Lh    | 0.31         | 0/1023        | 0.44        | 0/1350           |
| 19  | LH    | 0.22         | 0/1537        | 0.44        | 0/2065           |
| 20  | Li    | 0.25         | 0/843         | 0.42        | 0/1115           |
| 21  | LI    | 0.25         | 0/1669        | 0.43        | 0/2227           |
| 22  | Lj    | 0.19         | 0/720         | 0.38        | 0/952            |
| 23  | LJ    | 0.25         | 0/1363        | 0.49        | 2/1824 (0.1%)    |
| 24  | Lk    | 0.22         | 0/574         | 0.43        | 0/760            |
| 25  | Ll    | 0.19         | 0/448         | 0.33        | 0/592            |
| 26  | LL    | 0.38         | 2/1698 (0.1%) | 0.62        | 3/2274 (0.1%)    |
| 27  | Lm    | 0.21         | 0/425         | 0.41        | 0/564            |
| 28  | LM    | 0.29         | 0/1146        | 0.51        | 0/1531           |
| 29  | Ln    | 0.34         | 0/240         | 0.45        | 0/305            |
| 30  | LN    | 0.21         | 0/1746        | 0.44        | 0/2338           |
| 31  | Lo    | 0.18         | 0/855         | 0.40        | 0/1128           |
| 32  | LO    | 0.36         | 0/1670        | 0.59        | 2/2232 (0.1%)    |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 33  | Lp    | 0.23         | 0/718          | 0.41        | 0/953           |
| 34  | LP    | 0.25         | 0/1277         | 0.46        | 0/1712          |
| 35  | LQ    | 0.21         | 0/1539         | 0.40        | 0/2053          |
| 36  | Lr    | 0.34         | 0/1009         | 0.56        | 3/1353 (0.2%)   |
| 37  | LR    | 0.31         | 0/1473         | 0.47        | 0/1947          |
| 38  | LS    | 0.47         | 4/1491 (0.3%)  | 0.58        | 0/2000          |
| 39  | LT    | 0.16         | 0/1335         | 0.37        | 0/1781          |
| 40  | LU    | 0.25         | 0/831          | 0.52        | 0/1115          |
| 41  | LV    | 0.14         | 0/987          | 0.38        | 0/1324          |
| 42  | LW    | 0.20         | 0/532          | 0.42        | 0/708           |
| 43  | LX    | 0.19         | 0/984          | 0.40        | 0/1323          |
| 44  | LY    | 0.23         | 0/1119         | 0.41        | 0/1488          |
| 45  | LZ    | 0.20         | 0/1130         | 0.39        | 0/1507          |
| 46  | S2    | 0.21         | 2/38859 (0.0%) | 0.45        | 55/60556 (0.1%) |
| 47  | Sa    | 0.64         | 2/805 (0.2%)   | 0.63        | 2/1079 (0.2%)   |
| 48  | SA    | 0.24         | 0/1673         | 0.48        | 0/2275          |
| 49  | Sb    | 0.15         | 0/665          | 0.42        | 0/891           |
| 50  | SB    | 0.20         | 0/1756         | 0.41        | 0/2350          |
| 51  | Sc    | 0.18         | 0/418          | 0.47        | 0/562           |
| 52  | SC    | 0.21         | 0/1701         | 0.46        | 0/2300          |
| 53  | Sd    | 0.18         | 0/466          | 0.36        | 0/618           |
| 54  | SD    | 0.27         | 0/1651         | 0.53        | 0/2219          |
| 55  | Se    | 0.17         | 0/386          | 0.41        | 0/504           |
| 56  | SE    | 0.20         | 0/2092         | 0.48        | 0/2816          |
| 57  | SF    | 0.27         | 0/1436         | 0.47        | 0/1930          |
| 58  | Sg    | 0.19         | 0/2199         | 0.52        | 0/2989          |
| 59  | SG    | 0.21         | 0/1666         | 0.40        | 0/2222          |
| 60  | SH    | 0.23         | 0/1470         | 0.47        | 0/1968          |
| 61  | SI    | 0.18         | 0/1526         | 0.41        | 0/2038          |
| 62  | SJ    | 0.24         | 0/1178         | 0.45        | 0/1574          |
| 63  | SK    | 0.19         | 0/780          | 0.43        | 0/1046          |
| 64  | SL    | 0.13         | 0/1130         | 0.34        | 0/1514          |
| 65  | SN    | 0.32         | 0/1232         | 0.43        | 0/1656          |
| 66  | SO    | 0.23         | 0/1015         | 0.46        | 0/1361          |
| 67  | SP    | 0.33         | 0/1000         | 0.69        | 5/1335 (0.4%)   |
| 68  | SQ    | 0.22         | 0/1126         | 0.49        | 0/1506          |
| 69  | SR    | 0.26         | 0/1078         | 0.49        | 0/1447          |
| 70  | SS    | 0.18         | 0/1175         | 0.34        | 0/1575          |
| 71  | ST    | 0.25         | 0/1108         | 0.41        | 0/1486          |
| 72  | SU    | 0.25         | 0/762          | 0.51        | 0/1023          |
| 73  | SV    | 0.18         | 0/625          | 0.40        | 0/836           |
| 74  | SW    | 0.24         | 0/1051         | 0.44        | 0/1406          |
| 75  | Sx    | 0.09         | 0/239          | 0.25        | 0/370           |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 76  | SX    | 0.21         | 0/1097           | 0.46        | 0/1464           |
| 77  | SY    | 0.27         | 0/907            | 0.57        | 0/1204           |
| 78  | SZ    | 0.22         | 0/580            | 0.48        | 0/780            |
| 79  | S6    | 0.19         | 0/1795           | 0.39        | 1/2798 (0.0%)    |
| 79  | S7    | 0.13         | 0/1795           | 0.31        | 0/2798           |
| All | All   | 0.20         | 11/219320 (0.0%) | 0.41        | 94/322364 (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 |
|-----|-------|---------------------|---------------------|
| 56  | SE    | 0                   | 1                   |
| 60  | SH    | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 47  | Sa    | 98  | PRO  | CA-C  | 15.29 | 1.60        | 1.51     |
| 38  | LS    | 167 | PHE  | C-O   | -7.07 | 1.15        | 1.24     |
| 47  | Sa    | 97  | PRO  | CA-C  | 6.83  | 1.56        | 1.52     |
| 38  | LS    | 164 | LYS  | C-O   | -6.57 | 1.17        | 1.24     |
| 46  | S2    | 485 | A    | O3'-P | -6.55 | 1.51        | 1.61     |
| 7   | LB    | 301 | ASN  | CA-C  | -6.09 | 1.44        | 1.52     |
| 26  | LL    | 18  | TRP  | C-O   | -5.85 | 1.16        | 1.24     |
| 38  | LS    | 166 | ARG  | C-O   | -5.65 | 1.17        | 1.24     |
| 38  | LS    | 163 | HIS  | C-O   | -5.43 | 1.16        | 1.24     |
| 26  | LL    | 15  | HIS  | C-O   | -5.10 | 1.17        | 1.24     |
| 46  | S2    | 594 | C    | O3'-P | 5.01  | 1.68        | 1.61     |

All (94) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 46  | S2    | 593 | C    | C4'-C3'-O3' | 13.58  | 133.37      | 113.00   |
| 46  | S2    | 482 | C    | C2'-C3'-O3' | -13.56 | 93.36       | 113.70   |
| 26  | LL    | 16  | LYS  | CB-CA-C     | -12.30 | 92.19       | 111.74   |
| 46  | S2    | 492 | C    | C4'-C3'-O3' | 12.02  | 131.03      | 113.00   |
| 47  | Sa    | 98  | PRO  | O-C-N       | 11.96  | 126.81      | 121.31   |
| 46  | S2    | 115 | U    | C2'-C3'-O3' | -11.08 | 92.89       | 109.50   |
| 32  | LO    | 186 | GLU  | CB-CA-C     | -11.04 | 94.17       | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | S2    | 483  | G    | C2'-C3'-O3' | 10.52 | 129.48      | 113.70   |
| 46  | S2    | 495  | C    | C1'-C2'-O2' | 10.38 | 127.36      | 111.80   |
| 46  | S2    | 484  | C    | N1-C1'-C2'  | 9.63  | 126.45      | 112.00   |
| 46  | S2    | 594  | C    | C4'-C3'-O3' | -9.60 | 95.00       | 109.40   |
| 46  | S2    | 483  | G    | C4'-C3'-C2' | -9.50 | 93.10       | 102.60   |
| 46  | S2    | 539  | U    | C2'-C3'-O3' | -9.50 | 99.46       | 113.70   |
| 46  | S2    | 508  | G    | C1'-C2'-O2' | 9.30  | 122.35      | 108.40   |
| 46  | S2    | 482  | C    | C4'-C3'-O3' | 9.23  | 126.85      | 113.00   |
| 46  | S2    | 483  | G    | O4'-C4'-C3' | -8.82 | 95.18       | 104.00   |
| 46  | S2    | 115  | U    | C4'-C3'-O3' | 8.77  | 122.55      | 109.40   |
| 46  | S2    | 116  | U    | C1'-C2'-O2' | 8.70  | 124.84      | 111.80   |
| 46  | S2    | 538  | C    | N1-C1'-C2'  | 8.43  | 124.64      | 112.00   |
| 46  | S2    | 485  | A    | C4'-C3'-O3' | 8.28  | 125.42      | 113.00   |
| 46  | S2    | 1297 | U    | C2'-C3'-O3' | -8.12 | 97.32       | 109.50   |
| 46  | S2    | 486  | A    | C2'-C3'-O3' | 8.05  | 125.78      | 113.70   |
| 46  | S2    | 508  | G    | C2'-C3'-O3' | -7.87 | 101.90      | 113.70   |
| 46  | S2    | 1414 | G    | C4'-C3'-C2' | -7.71 | 94.89       | 102.60   |
| 46  | S2    | 591  | A    | C4'-C3'-O3' | 7.64  | 124.46      | 113.00   |
| 1   | L5    | 3410 | G    | C4'-C3'-O3' | 7.50  | 120.65      | 109.40   |
| 46  | S2    | 539  | U    | C3'-C2'-O2' | -7.50 | 99.45       | 110.70   |
| 46  | S2    | 483  | G    | C4'-C3'-O3' | 7.45  | 124.18      | 113.00   |
| 1   | L5    | 4549 | G    | C4'-C3'-O3' | 7.39  | 120.49      | 109.40   |
| 46  | S2    | 1426 | G    | C4'-C3'-C2' | -7.38 | 95.22       | 102.60   |
| 1   | L5    | 455  | C    | C4'-C3'-O3' | 7.27  | 120.31      | 109.40   |
| 46  | S2    | 1308 | U    | C2'-C3'-O3' | 7.17  | 120.26      | 109.50   |
| 47  | Sa    | 97   | PRO  | O-C-N       | 7.15  | 124.51      | 121.15   |
| 26  | LL    | 17   | ASP  | N-CA-C      | 7.11  | 121.33      | 111.74   |
| 46  | S2    | 508  | G    | C4'-C3'-O3' | 7.11  | 123.66      | 113.00   |
| 1   | L5    | 3716 | G    | C2'-C3'-O3' | -6.99 | 103.21      | 113.70   |
| 46  | S2    | 117  | C    | C4'-C3'-O3' | -6.96 | 102.57      | 113.00   |
| 67  | SP    | 59   | ARG  | CB-CG-CD    | 6.95  | 127.28      | 111.30   |
| 1   | L5    | 3427 | U    | C1'-C2'-O2' | 6.94  | 118.81      | 108.40   |
| 46  | S2    | 492  | C    | C2'-C3'-O3' | -6.86 | 103.41      | 113.70   |
| 46  | S2    | 116  | U    | O4'-C1'-C2' | -6.61 | 99.19       | 105.80   |
| 46  | S2    | 1414 | G    | C2'-C3'-O3' | 6.57  | 123.56      | 113.70   |
| 46  | S2    | 482  | C    | C3'-C2'-O2' | -6.57 | 100.85      | 110.70   |
| 79  | S6    | 72   | U    | C2'-C3'-O3' | -6.50 | 103.95      | 113.70   |
| 1   | L5    | 3717 | U    | C2'-C3'-O3' | -6.46 | 99.80       | 109.50   |
| 1   | L5    | 456  | G    | C4'-C3'-C2' | -6.44 | 96.16       | 102.60   |
| 46  | S2    | 594  | C    | C2'-C3'-O3' | 6.42  | 119.13      | 109.50   |
| 1   | L5    | 453  | U    | P-O3'-C3'   | 6.42  | 129.82      | 120.20   |
| 46  | S2    | 485  | A    | C1'-C2'-O2' | 6.29  | 117.83      | 108.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | S2    | 1454 | C    | N1-C1'-C2'  | 6.24  | 121.35      | 112.00   |
| 32  | LO    | 186  | GLU  | CA-C-O      | -6.21 | 114.89      | 122.41   |
| 1   | L5    | 458  | C    | C2'-C3'-O3' | 6.21  | 123.02      | 113.70   |
| 1   | L5    | 456  | G    | C4'-C3'-O3' | 6.21  | 118.71      | 109.40   |
| 46  | S2    | 593  | C    | C4'-C3'-C2' | -6.18 | 96.42       | 102.60   |
| 46  | S2    | 1543 | C    | C2'-C3'-O3' | -6.12 | 104.53      | 113.70   |
| 46  | S2    | 483  | G    | O4'-C1'-N9  | 6.09  | 117.63      | 108.50   |
| 1   | L5    | 456  | G    | C1'-C2'-O2' | 5.99  | 120.79      | 111.80   |
| 46  | S2    | 593  | C    | O4'-C4'-C3' | -5.96 | 98.04       | 104.00   |
| 1   | L5    | 3410 | G    | N9-C1'-C2'  | -5.95 | 105.08      | 114.00   |
| 46  | S2    | 509  | A    | C3'-C2'-O2' | 5.80  | 119.40      | 110.70   |
| 46  | S2    | 510  | G    | C2'-C3'-O3' | -5.80 | 105.00      | 113.70   |
| 1   | L5    | 140  | G    | C4'-C3'-O3' | -5.76 | 104.35      | 113.00   |
| 36  | Lr    | 123  | PRO  | N-CA-CB     | -5.75 | 97.21       | 103.25   |
| 67  | SP    | 56   | LEU  | N-CA-C      | -5.74 | 105.00      | 112.23   |
| 23  | LJ    | 57   | VAL  | CA-C-N      | 5.72  | 132.47      | 121.54   |
| 23  | LJ    | 57   | VAL  | C-N-CA      | 5.72  | 132.47      | 121.54   |
| 46  | S2    | 493  | C    | C1'-C2'-O2' | 5.68  | 120.31      | 111.80   |
| 46  | S2    | 508  | G    | C3'-C2'-O2' | -5.67 | 102.19      | 110.70   |
| 46  | S2    | 495  | C    | C4'-C3'-O3' | 5.65  | 117.88      | 109.40   |
| 1   | L5    | 3413 | A    | C4'-C3'-O3' | 5.60  | 121.40      | 113.00   |
| 36  | Lr    | 121  | GLN  | CB-CA-C     | -5.54 | 103.64      | 112.05   |
| 46  | S2    | 1454 | C    | C4'-C3'-O3' | -5.46 | 104.81      | 113.00   |
| 1   | L5    | 4551 | C    | O4'-C1'-C2' | -5.44 | 100.36      | 105.80   |
| 26  | LL    | 16   | LYS  | CA-C-O      | -5.42 | 111.72      | 122.23   |
| 46  | S2    | 485  | A    | C2'-C3'-O3' | 5.37  | 121.75      | 113.70   |
| 1   | L5    | 3427 | U    | N1-C1'-C2'  | -5.36 | 103.96      | 112.00   |
| 46  | S2    | 357  | C    | N1-C1'-C2'  | 5.35  | 120.02      | 112.00   |
| 46  | S2    | 491  | C    | C2'-C3'-O3' | -5.34 | 105.69      | 113.70   |
| 1   | L5    | 3427 | U    | C4'-C3'-O3' | 5.33  | 121.00      | 113.00   |
| 46  | S2    | 483  | G    | C3'-C2'-C1' | -5.33 | 95.97       | 101.30   |
| 46  | S2    | 1297 | U    | C4'-C3'-O3' | 5.32  | 117.38      | 109.40   |
| 1   | L5    | 455  | C    | C2'-C3'-O3' | -5.26 | 101.61      | 109.50   |
| 1   | L5    | 3717 | U    | C1'-C2'-O2' | 5.26  | 119.68      | 111.80   |
| 67  | SP    | 59   | ARG  | CB-CA-C     | 5.20  | 121.18      | 110.31   |
| 46  | S2    | 512  | U    | C2'-C3'-O3' | 5.20  | 121.50      | 113.70   |
| 1   | L5    | 4550 | G    | C1'-O4'-C4' | -5.19 | 104.71      | 109.90   |
| 36  | Lr    | 121  | GLN  | CA-C-O      | -5.16 | 116.31      | 122.13   |
| 46  | S2    | 117  | C    | C2'-C3'-O3' | 5.15  | 121.42      | 113.70   |
| 46  | S2    | 1752 | C    | C3'-C2'-O2' | 5.14  | 118.41      | 110.70   |
| 67  | SP    | 63   | ALA  | CA-C-N      | -5.08 | 113.08      | 120.29   |
| 67  | SP    | 63   | ALA  | C-N-CA      | -5.08 | 113.08      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | S2    | 594  | C    | C5'-C4'-C3' | 5.06  | 122.78      | 115.20   |
| 46  | S2    | 1598 | C    | C4'-C3'-O3' | -5.03 | 105.46      | 113.00   |
| 1   | L5    | 3427 | U    | O4'-C1'-C2' | -5.02 | 102.58      | 107.60   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 56  | SE    | 18  | TRP  | Peptide |
| 60  | SH    | 15  | LYS  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | L5    | 72884 | 0        | 36803    | 455     | 0            |
| 2   | L7    | 2558  | 0        | 1296     | 13      | 0            |
| 3   | L8    | 3210  | 0        | 1630     | 25      | 0            |
| 4   | La    | 1164  | 0        | 1213     | 5       | 0            |
| 5   | LA    | 1898  | 0        | 1993     | 11      | 0            |
| 6   | Lb    | 807   | 0        | 875      | 7       | 0            |
| 7   | LB    | 3202  | 0        | 3347     | 32      | 0            |
| 8   | Lc    | 732   | 0        | 769      | 9       | 0            |
| 9   | LC    | 2857  | 0        | 3030     | 29      | 0            |
| 10  | Ld    | 896   | 0        | 941      | 2       | 0            |
| 11  | LD    | 2389  | 0        | 2420     | 28      | 0            |
| 12  | Le    | 1053  | 0        | 1147     | 7       | 0            |
| 13  | LE    | 1743  | 0        | 1880     | 16      | 0            |
| 14  | Lf    | 876   | 0        | 912      | 9       | 0            |
| 15  | LF    | 1771  | 0        | 1886     | 16      | 0            |
| 16  | Lg    | 873   | 0        | 961      | 4       | 0            |
| 17  | LG    | 1848  | 0        | 1981     | 21      | 0            |
| 18  | Lh    | 1015  | 0        | 1156     | 11      | 0            |
| 19  | LH    | 1519  | 0        | 1603     | 17      | 0            |
| 20  | Li    | 832   | 0        | 917      | 9       | 0            |
| 21  | LI    | 1631  | 0        | 1682     | 13      | 0            |
| 22  | Lj    | 705   | 0        | 737      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | LJ    | 1340  | 0        | 1377     | 15      | 0            |
| 24  | Lk    | 568   | 0        | 635      | 6       | 0            |
| 25  | Ll    | 438   | 0        | 474      | 1       | 0            |
| 26  | LL    | 1667  | 0        | 1771     | 15      | 0            |
| 27  | Lm    | 419   | 0        | 452      | 4       | 0            |
| 28  | LM    | 1125  | 0        | 1202     | 8       | 0            |
| 29  | Ln    | 239   | 0        | 289      | 0       | 0            |
| 30  | LN    | 1701  | 0        | 1749     | 10      | 0            |
| 31  | Lo    | 842   | 0        | 916      | 6       | 0            |
| 32  | LO    | 1640  | 0        | 1792     | 13      | 0            |
| 33  | Lp    | 708   | 0        | 756      | 3       | 0            |
| 34  | LP    | 1251  | 0        | 1282     | 7       | 0            |
| 35  | LQ    | 1515  | 0        | 1639     | 10      | 0            |
| 36  | Lr    | 994   | 0        | 1057     | 5       | 0            |
| 37  | LR    | 1457  | 0        | 1601     | 8       | 0            |
| 38  | LS    | 1451  | 0        | 1488     | 7       | 0            |
| 39  | LT    | 1307  | 0        | 1380     | 15      | 0            |
| 40  | LU    | 817   | 0        | 839      | 14      | 0            |
| 41  | LV    | 973   | 0        | 1034     | 7       | 0            |
| 42  | LW    | 519   | 0        | 533      | 4       | 0            |
| 43  | LX    | 967   | 0        | 1040     | 6       | 0            |
| 44  | LY    | 1102  | 0        | 1189     | 8       | 0            |
| 45  | LZ    | 1107  | 0        | 1182     | 4       | 0            |
| 46  | S2    | 34749 | 0        | 17548    | 459     | 0            |
| 47  | Sa    | 792   | 0        | 845      | 7       | 0            |
| 48  | SA    | 1636  | 0        | 1641     | 27      | 0            |
| 49  | Sb    | 651   | 0        | 672      | 5       | 0            |
| 50  | SB    | 1729  | 0        | 1803     | 13      | 0            |
| 51  | Sc    | 416   | 0        | 445      | 5       | 0            |
| 52  | SC    | 1665  | 0        | 1753     | 17      | 0            |
| 53  | Sd    | 455   | 0        | 449      | 12      | 0            |
| 54  | SD    | 1626  | 0        | 1714     | 26      | 0            |
| 55  | Se    | 384   | 0        | 422      | 6       | 0            |
| 56  | SE    | 2050  | 0        | 2156     | 38      | 0            |
| 57  | SF    | 1416  | 0        | 1458     | 20      | 0            |
| 58  | Sg    | 2148  | 0        | 2108     | 47      | 0            |
| 59  | SG    | 1645  | 0        | 1780     | 39      | 0            |
| 60  | SH    | 1449  | 0        | 1539     | 29      | 0            |
| 61  | SI    | 1499  | 0        | 1561     | 19      | 0            |
| 62  | SJ    | 1162  | 0        | 1252     | 22      | 0            |
| 63  | SK    | 760   | 0        | 783      | 18      | 0            |
| 64  | SL    | 1110  | 0        | 1165     | 9       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 65  | SN    | 1208   | 0        | 1294     | 6       | 0            |
| 66  | SO    | 1002   | 0        | 1023     | 10      | 0            |
| 67  | SP    | 981    | 0        | 1026     | 19      | 0            |
| 68  | SQ    | 1109   | 0        | 1174     | 16      | 0            |
| 69  | SR    | 1064   | 0        | 1118     | 21      | 0            |
| 70  | SS    | 1157   | 0        | 1213     | 14      | 0            |
| 71  | ST    | 1090   | 0        | 1116     | 16      | 0            |
| 72  | SU    | 753    | 0        | 815      | 21      | 0            |
| 73  | SV    | 619    | 0        | 620      | 7       | 0            |
| 74  | SW    | 1034   | 0        | 1080     | 11      | 0            |
| 75  | Sx    | 214    | 0        | 108      | 5       | 0            |
| 76  | SX    | 1080   | 0        | 1147     | 16      | 0            |
| 77  | SY    | 891    | 0        | 948      | 28      | 0            |
| 78  | SZ    | 574    | 0        | 627      | 19      | 0            |
| 79  | S6    | 1604   | 0        | 816      | 17      | 0            |
| 79  | S7    | 1604   | 0        | 816      | 20      | 0            |
| 80  | Z     | 119    | 0        | 36       | 9       | 0            |
| 81  | L5    | 94     | 0        | 0        | 0       | 0            |
| 81  | L7    | 1      | 0        | 0        | 0       | 0            |
| 81  | LN    | 1      | 0        | 0        | 0       | 0            |
| 81  | LP    | 1      | 0        | 0        | 0       | 0            |
| 82  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 82  | Lm    | 1      | 0        | 0        | 0       | 0            |
| 82  | Lp    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 204155 | 0        | 150927   | 1780    | 0            |

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

All (1780) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:S2:1720:A:H62  | 46:S2:1815:G:N2    | 1.36                     | 1.22              |
| 46:S2:1720:A:N6   | 46:S2:1815:G:H21   | 1.41                     | 1.17              |
| 46:S2:159:A:C2    | 46:S2:468:G:N2     | 2.26                     | 1.01              |
| 79:S7:76:A:O3'    | 80:Z:5:UNK:C       | 2.08                     | 1.01              |
| 46:S2:1744:G:H21  | 46:S2:1792:A:H62   | 1.15                     | 0.94              |
| 54:SD:194:PRO:HG3 | 54:SD:198:ILE:HG22 | 1.57                     | 0.85              |
| 46:S2:1749:G:H1   | 46:S2:1787:U:H3    | 1.20                     | 0.85              |
| 26:LL:63:THR:HG22 | 26:LL:65:ARG:H     | 1.41                     | 0.85              |
| 59:SG:98:ARG:NH2  | 59:SG:101:ILE:O    | 2.09                     | 0.85              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 75:Sx:38:A:H2'   | 75:Sx:39:A:H8      | 1.44                     | 0.82              |
| 46:S2:1272:C:H42 | 46:S2:1513:C:H42   | 1.25                     | 0.81              |
| 58:Sg:87:LEU:HB2 | 58:Sg:101:PHE:HB2  | 1.63                     | 0.81              |
| 46:S2:159:A:H2   | 46:S2:468:G:N2     | 1.78                     | 0.81              |
| 46:S2:1262:C:O2  | 53:Sd:10:HIS:NE2   | 2.14                     | 0.81              |
| 1:L5:1013:C:OP1  | 1:L5:1015:C:N4     | 2.13                     | 0.81              |
| 48:SA:163:CYS:O  | 48:SA:164:ASN:ND2  | 2.10                     | 0.80              |
| 46:S2:1421:G:H1' | 46:S2:1422:A:H4'   | 1.64                     | 0.80              |
| 46:S2:1442:U:N3  | 46:S2:1445:U:O4    | 2.13                     | 0.79              |
| 9:LC:71:ARG:HH21 | 80:Z:-6:UNK:CB     | 1.95                     | 0.79              |
| 46:S2:225:C:HO2' | 46:S2:226:A:H8     | 1.32                     | 0.78              |
| 46:S2:536:G:H2'  | 46:S2:538:C:H1'    | 1.65                     | 0.78              |
| 46:S2:516:G:H5'' | 46:S2:517:A:H5'    | 1.64                     | 0.78              |
| 46:S2:534:A:H2'  | 46:S2:535:G:C8     | 2.18                     | 0.77              |
| 1:L5:2656:G:N2   | 1:L5:3255:C:N3     | 2.32                     | 0.77              |
| 40:LU:48:LYS:HG2 | 40:LU:53:ALA:HB2   | 1.65                     | 0.77              |
| 46:S2:527:A:HO2' | 62:SJ:125:HIS:HD1  | 1.32                     | 0.77              |
| 1:L5:3408:G:H21  | 1:L5:3432:A:H8     | 1.33                     | 0.76              |
| 46:S2:145:G:H2'  | 46:S2:146:G:C8     | 2.20                     | 0.76              |
| 69:SR:24:LEU:HB2 | 69:SR:58:MET:HE3   | 1.67                     | 0.76              |
| 72:SU:55:ARG:HG3 | 72:SU:87:ARG:NH2   | 2.01                     | 0.76              |
| 24:Lk:5:ILE:HD11 | 24:Lk:43:TYR:HB3   | 1.67                     | 0.76              |
| 40:LU:20:LYS:HB3 | 40:LU:73:THR:HG22  | 1.68                     | 0.76              |
| 46:S2:57:U:H3    | 46:S2:88:G:H22     | 1.32                     | 0.75              |
| 46:S2:435:G:H21  | 46:S2:474:A:H2     | 1.34                     | 0.75              |
| 1:L5:858:A:H3'   | 1:L5:870:G:H22     | 1.52                     | 0.74              |
| 46:S2:83:A:N1    | 46:S2:150:A:O2'    | 2.20                     | 0.74              |
| 46:S2:1744:G:N2  | 46:S2:1792:A:H62   | 1.86                     | 0.74              |
| 1:L5:497:C:H42   | 1:L5:665:C:H42     | 1.34                     | 0.74              |
| 8:Lc:20:LEU:HD23 | 8:Lc:101:ASP:HB3   | 1.69                     | 0.74              |
| 1:L5:3298:U:OP2  | 1:L5:3303:A:N6     | 2.21                     | 0.73              |
| 7:LB:216:MET:HE2 | 7:LB:283:LYS:HD3   | 1.70                     | 0.73              |
| 66:SO:57:THR:H   | 66:SO:60:MET:HE2   | 1.51                     | 0.73              |
| 46:S2:1522:C:OP2 | 70:SS:136:THR:OG1  | 2.06                     | 0.73              |
| 60:SH:31:GLU:HA  | 60:SH:37:LYS:HD2   | 1.71                     | 0.73              |
| 46:S2:95:G:H1    | 46:S2:435:G:H22    | 1.36                     | 0.72              |
| 1:L5:4399:G:H1   | 1:L5:4603:A:H62    | 1.34                     | 0.72              |
| 46:S2:1366:G:N2  | 46:S2:1463:U:O4    | 2.22                     | 0.72              |
| 80:Z:-17:UNK:O   | 80:Z:-16:UNK:C     | 2.37                     | 0.72              |
| 69:SR:79:GLU:OE1 | 69:SR:83:ASN:ND2   | 2.23                     | 0.72              |
| 46:S2:820:G:H4'  | 56:SE:255:ARG:HH22 | 1.52                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:1557:U:H3     | 1:L5:1579:A:H61    | 1.37                     | 0.71              |
| 46:S2:889:U:H4'    | 46:S2:890:U:H5'    | 1.72                     | 0.71              |
| 79:S6:7:A:H62      | 79:S6:67:U:H3      | 1.38                     | 0.71              |
| 46:S2:165:G:H1'    | 59:SG:110:ASN:HD22 | 1.56                     | 0.71              |
| 1:L5:189:G:H22     | 1:L5:252:G:H22     | 1.38                     | 0.71              |
| 46:S2:1753:C:H4'   | 46:S2:1783:G:H22   | 1.56                     | 0.70              |
| 72:SU:55:ARG:HG3   | 72:SU:87:ARG:HH21  | 1.54                     | 0.70              |
| 15:LF:127:VAL:HG13 | 15:LF:158:VAL:HG12 | 1.72                     | 0.70              |
| 46:S2:537:A:H3'    | 46:S2:538:C:H4'    | 1.72                     | 0.70              |
| 1:L5:4323:C:O2'    | 1:L5:4325:A:OP2    | 2.08                     | 0.70              |
| 46:S2:41:G:H22     | 46:S2:481:G:N2     | 1.89                     | 0.70              |
| 46:S2:1753:C:H3'   | 46:S2:1754:C:H4'   | 1.74                     | 0.70              |
| 48:SA:34:MET:HE1   | 48:SA:162:PRO:HB3  | 1.74                     | 0.70              |
| 1:L5:1009:C:H42    | 1:L5:1017:A:H61    | 1.39                     | 0.70              |
| 17:LG:162:ASP:HB2  | 17:LG:163:PRO:HD3  | 1.74                     | 0.70              |
| 1:L5:4560:C:H2'    | 1:L5:4561:G:C8     | 2.26                     | 0.70              |
| 77:SY:37:LYS:NZ    | 77:SY:57:VAL:O     | 2.25                     | 0.69              |
| 1:L5:761:C:H5      | 1:L5:810:G:H1      | 1.39                     | 0.69              |
| 1:L5:3374:A:H2'    | 1:L5:3375:A:C8     | 2.28                     | 0.69              |
| 56:SE:45:ILE:HG13  | 56:SE:61:VAL:HG11  | 1.75                     | 0.69              |
| 46:S2:482:C:H4'    | 46:S2:483:G:H5'    | 1.74                     | 0.69              |
| 68:SQ:42:ILE:HD11  | 68:SQ:51:LEU:HD21  | 1.73                     | 0.69              |
| 1:L5:2237:G:N2     | 1:L5:2238:G:O6     | 2.26                     | 0.68              |
| 46:S2:1268:C:OP1   | 46:S2:1269:C:N4    | 2.27                     | 0.68              |
| 21:LI:80:CYS:SG    | 21:LI:144:ASN:ND2  | 2.66                     | 0.68              |
| 1:L5:1743:G:N2     | 1:L5:4087:C:OP1    | 2.23                     | 0.68              |
| 46:S2:896:G:H2'    | 46:S2:897:U:H4'    | 1.76                     | 0.68              |
| 46:S2:1601:G:H4'   | 78:SZ:43:LYS:HE2   | 1.75                     | 0.68              |
| 8:Lc:26:LYS:HD2    | 8:Lc:98:ASP:HB3    | 1.75                     | 0.68              |
| 46:S2:514:G:H3'    | 46:S2:515:U:H6     | 1.59                     | 0.68              |
| 54:SD:62:LYS:O     | 54:SD:67:ARG:NH2   | 2.26                     | 0.68              |
| 46:S2:1489:C:O2'   | 46:S2:1491:G:OP2   | 2.11                     | 0.68              |
| 58:Sg:57:ARG:HD2   | 58:Sg:94:THR:HA    | 1.75                     | 0.68              |
| 1:L5:766:G:H22     | 1:L5:805:C:H42     | 1.42                     | 0.68              |
| 56:SE:87:MET:HE2   | 56:SE:123:LEU:HB2  | 1.76                     | 0.68              |
| 58:Sg:24:THR:HB    | 58:Sg:71:ILE:HG21  | 1.76                     | 0.68              |
| 46:S2:1229:A:H2'   | 46:S2:1230:G:C8    | 2.29                     | 0.67              |
| 19:LH:51:LYS:HD2   | 19:LH:51:LYS:H     | 1.59                     | 0.67              |
| 52:SC:92:GLU:OE1   | 52:SC:92:GLU:N     | 2.24                     | 0.67              |
| 1:L5:508:G:H1      | 1:L5:661:U:H3      | 1.40                     | 0.67              |
| 1:L5:1470:U:OP2    | 4:La:26:ARG:NH2    | 2.27                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:L5:4640:G:H2'   | 1:L5:4641:G:C8     | 2.30                     | 0.67              |
| 46:S2:1553:G:N2   | 53:Sd:32:ARG:O     | 2.28                     | 0.66              |
| 23:LJ:96:LYS:HE2  | 23:LJ:163:MET:HE1  | 1.78                     | 0.66              |
| 46:S2:833:G:H22   | 46:S2:842:G:H22    | 1.44                     | 0.66              |
| 46:S2:1417:C:H42  | 46:S2:1425:G:H1    | 1.42                     | 0.66              |
| 58:Sg:57:ARG:HG3  | 58:Sg:59:LEU:HD23  | 1.77                     | 0.66              |
| 46:S2:1270:G:H1   | 46:S2:1515:G:H1    | 1.42                     | 0.66              |
| 69:SR:98:VAL:HG13 | 69:SR:102:THR:HG23 | 1.77                     | 0.66              |
| 46:S2:1673:U:OP1  | 68:SQ:18:THR:OG1   | 2.14                     | 0.66              |
| 64:SL:48:LYS:NZ   | 64:SL:52:GLU:OE1   | 2.29                     | 0.65              |
| 46:S2:63:U:O2'    | 46:S2:170:A:N3     | 2.27                     | 0.65              |
| 46:S2:126:G:N7    | 46:S2:180:G:N2     | 2.45                     | 0.65              |
| 1:L5:4553:G:H2'   | 1:L5:4554:G:C8     | 2.31                     | 0.65              |
| 1:L5:4664:A:H2    | 1:L5:4681:G:H21    | 1.42                     | 0.65              |
| 46:S2:54:A:OP2    | 46:S2:452:G:N2     | 2.29                     | 0.65              |
| 54:SD:31:GLU:N    | 54:SD:31:GLU:OE2   | 2.30                     | 0.65              |
| 1:L5:4573:G:N2    | 1:L5:4573:G:OP2    | 2.27                     | 0.65              |
| 9:LC:56:GLU:CD    | 9:LC:56:GLU:H      | 2.05                     | 0.65              |
| 19:LH:15:ASN:HD21 | 19:LH:81:ILE:HG12  | 1.61                     | 0.65              |
| 1:L5:719:A:H2'    | 1:L5:720:C:C6      | 2.32                     | 0.65              |
| 46:S2:1723:G:O6   | 46:S2:1813:U:O2    | 2.14                     | 0.64              |
| 57:SF:42:LYS:HE2  | 57:SF:42:LYS:HA    | 1.79                     | 0.64              |
| 1:L5:1338:A:H62   | 1:L5:1465:G:H1     | 1.44                     | 0.64              |
| 46:S2:914:A:N6    | 60:SH:98:ARG:O     | 2.24                     | 0.64              |
| 46:S2:435:G:O2'   | 46:S2:474:A:N6     | 2.20                     | 0.64              |
| 1:L5:3326:G:H21   | 1:L5:3329:G:N2     | 1.96                     | 0.64              |
| 46:S2:1745:G:O2'  | 46:S2:1791:A:N6    | 2.30                     | 0.64              |
| 7:LB:300:LYS:HD3  | 7:LB:301:ASN:N     | 2.13                     | 0.64              |
| 46:S2:982:A:H2'   | 46:S2:983:G:C8     | 2.32                     | 0.64              |
| 1:L5:386:G:O2'    | 1:L5:411:G:O6      | 2.11                     | 0.64              |
| 46:S2:168:C:OP1   | 59:SG:131:ARG:NH2  | 2.29                     | 0.64              |
| 46:S2:530:A:N6    | 46:S2:558:U:O4     | 2.31                     | 0.64              |
| 77:SY:42:GLU:O    | 77:SY:46:LYS:NZ    | 2.31                     | 0.64              |
| 46:S2:353:U:O2    | 64:SL:71:ARG:NH1   | 2.30                     | 0.64              |
| 21:LI:28:ASP:OD2  | 21:LI:32:ARG:NH1   | 2.31                     | 0.63              |
| 46:S2:1241:A:O2'  | 46:S2:1242:A:OP1   | 2.15                     | 0.63              |
| 46:S2:833:G:H22   | 46:S2:842:G:N2     | 1.96                     | 0.63              |
| 52:SC:161:SER:O   | 52:SC:161:SER:OG   | 2.16                     | 0.63              |
| 46:S2:830:C:O3'   | 46:S2:846:G:N2     | 2.31                     | 0.63              |
| 6:Lb:93:ARG:HH11  | 6:Lb:93:ARG:HG2    | 1.63                     | 0.63              |
| 1:L5:1170:G:OP1   | 35:LQ:108:ARG:NH2  | 2.28                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:S2:477:A:H4'   | 46:S2:488:U:H2'    | 1.81                     | 0.63              |
| 46:S2:1611:G:OP1  | 70:SS:121:ARG:NH1  | 2.31                     | 0.63              |
| 60:SH:149:ASP:OD1 | 60:SH:151:SER:OG   | 2.17                     | 0.63              |
| 21:LI:87:ILE:HD13 | 21:LI:138:ILE:HG12 | 1.80                     | 0.63              |
| 44:LY:2:LYS:NZ    | 44:LY:7:VAL:O      | 2.31                     | 0.63              |
| 55:Se:116:PHE:HE2 | 62:SJ:30:LYS:HD2   | 1.64                     | 0.63              |
| 46:S2:1753:C:H5'  | 46:S2:1754:C:H1'   | 1.80                     | 0.63              |
| 61:SI:62:VAL:HG11 | 61:SI:75:LYS:HE3   | 1.81                     | 0.63              |
| 58:Sg:212:LYS:HB3 | 58:Sg:235:ILE:HD12 | 1.81                     | 0.63              |
| 1:L5:171:U:OP2    | 1:L5:172:C:N4      | 2.32                     | 0.62              |
| 1:L5:939:U:H3     | 1:L5:1050:C:H41    | 1.47                     | 0.62              |
| 40:LU:75:GLU:N    | 40:LU:75:GLU:OE2   | 2.32                     | 0.62              |
| 77:SY:102:THR:OG1 | 77:SY:106:GLN:NE2  | 2.32                     | 0.62              |
| 1:L5:1380:C:H2'   | 1:L5:1381:U:C6     | 2.33                     | 0.62              |
| 78:SZ:65:TYR:HA   | 78:SZ:111:ARG:HH21 | 1.63                     | 0.62              |
| 1:L5:138:C:H2'    | 1:L5:139:G:H8      | 1.63                     | 0.62              |
| 46:S2:47:G:H1     | 46:S2:479:G:H22    | 1.47                     | 0.62              |
| 48:SA:14:ASP:HB2  | 48:SA:177:MET:HE1  | 1.82                     | 0.62              |
| 46:S2:144:U:OP1   | 59:SG:178:ARG:NH1  | 2.32                     | 0.62              |
| 79:S6:31:G:H2'    | 79:S6:32:C:H6      | 1.63                     | 0.62              |
| 1:L5:2565:G:N1    | 1:L5:2568:C:OP2    | 2.28                     | 0.62              |
| 46:S2:1276:G:H5'  | 46:S2:1277:A:H5'   | 1.81                     | 0.62              |
| 57:SF:73:THR:HG22 | 57:SF:93:VAL:HG21  | 1.82                     | 0.62              |
| 46:S2:523:A:OP1   | 62:SJ:146:SER:OG   | 2.14                     | 0.62              |
| 54:SD:42:THR:HG22 | 54:SD:44:THR:H     | 1.65                     | 0.62              |
| 46:S2:47:G:H22    | 46:S2:479:G:N2     | 1.97                     | 0.61              |
| 46:S2:819:A:OP1   | 62:SJ:80:ARG:NH2   | 2.33                     | 0.61              |
| 1:L5:119:G:N2     | 17:LG:105:GLU:OE1  | 2.32                     | 0.61              |
| 1:L5:1296:G:O6    | 20:Li:4:ARG:NH1    | 2.30                     | 0.61              |
| 48:SA:36:GLN:O    | 48:SA:53:ARG:NH1   | 2.33                     | 0.61              |
| 2:L7:3:C:H2'      | 2:L7:4:U:C6        | 2.35                     | 0.61              |
| 26:LL:58:ILE:HG12 | 26:LL:157:ILE:HG12 | 1.81                     | 0.61              |
| 46:S2:1555:C:O2   | 63:SK:24:LYS:NZ    | 2.33                     | 0.61              |
| 1:L5:3873:A:OP2   | 39:LT:2:THR:OG1    | 2.18                     | 0.61              |
| 20:Li:20:ASN:HB2  | 26:LL:107:THR:HG22 | 1.81                     | 0.61              |
| 20:Li:30:ARG:O    | 20:Li:32:ARG:NH1   | 2.34                     | 0.61              |
| 46:S2:1274:C:O2'  | 46:S2:1276:G:OP1   | 2.18                     | 0.61              |
| 80:Z:-13:UNK:O    | 80:Z:-12:UNK:CB    | 2.48                     | 0.61              |
| 7:LB:220:ILE:HG12 | 7:LB:278:THR:HG23  | 1.82                     | 0.61              |
| 28:LM:101:LYS:HB2 | 32:LO:200:GLY:HA3  | 1.83                     | 0.61              |
| 79:S7:76:A:C3'    | 80:Z:5:UNK:C       | 2.78                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:4544:G:H2'    | 1:L5:4545:G:C8     | 2.36                     | 0.61              |
| 46:S2:58:C:O2'     | 46:S2:59:U:O5'     | 2.19                     | 0.61              |
| 1:L5:3269:C:H1'    | 1:L5:4664:A:C8     | 2.36                     | 0.60              |
| 46:S2:311:C:O2'    | 46:S2:341:C:O4'    | 2.18                     | 0.60              |
| 67:SP:48:GLY:O     | 67:SP:50:ARG:NH1   | 2.33                     | 0.60              |
| 53:Sd:12:ARG:HB3   | 53:Sd:18:SER:HB3   | 1.83                     | 0.60              |
| 64:SL:12:LYS:HG3   | 64:SL:18:GLN:HE21  | 1.66                     | 0.60              |
| 1:L5:3913:U:H2'    | 1:L5:3914:C:C6     | 2.36                     | 0.60              |
| 1:L5:1012:U:HO2'   | 1:L5:1015:C:H42    | 1.47                     | 0.60              |
| 1:L5:1013:C:O2'    | 1:L5:1016:C:N4     | 2.32                     | 0.60              |
| 20:Li:2:ALA:N      | 20:Li:5:TYR:HH     | 1.99                     | 0.60              |
| 46:S2:800:U:OP2    | 46:S2:868:G:N2     | 2.32                     | 0.60              |
| 1:L5:415:U:O2'     | 1:L5:416:G:OP1     | 2.18                     | 0.60              |
| 15:LF:120:ILE:O    | 15:LF:120:ILE:HD12 | 2.01                     | 0.60              |
| 63:SK:1:MET:HE2    | 63:SK:1:MET:HA     | 1.82                     | 0.60              |
| 1:L5:4548:C:O2'    | 1:L5:4549:G:H2'    | 2.02                     | 0.60              |
| 74:SW:28:ARG:HB3   | 74:SW:29:PRO:HD3   | 1.83                     | 0.60              |
| 39:LT:143:THR:HG23 | 39:LT:145:GLY:H    | 1.67                     | 0.60              |
| 40:LU:62:THR:OG1   | 40:LU:73:THR:OG1   | 2.19                     | 0.60              |
| 47:Sa:90:GLU:OE2   | 47:Sa:90:GLU:N     | 2.29                     | 0.60              |
| 51:Sc:9:ILE:HD12   | 51:Sc:59:LEU:HD22  | 1.84                     | 0.60              |
| 1:L5:2499:A:H2'    | 1:L5:2500:A:C8     | 2.36                     | 0.60              |
| 1:L5:3374:A:OP2    | 1:L5:3392:G:N2     | 2.35                     | 0.60              |
| 46:S2:171:A:H2'    | 46:S2:173:A:C8     | 2.37                     | 0.60              |
| 60:SH:184:ASP:OD1  | 60:SH:184:ASP:N    | 2.32                     | 0.60              |
| 1:L5:189:G:N2      | 1:L5:252:G:H22     | 2.00                     | 0.59              |
| 1:L5:828:C:H3'     | 1:L5:829:G:H21     | 1.66                     | 0.59              |
| 28:LM:58:THR:HG22  | 28:LM:59:ASP:H     | 1.67                     | 0.59              |
| 1:L5:1168:G:N7     | 35:LQ:104:ARG:NH2  | 2.49                     | 0.59              |
| 13:LE:149:ARG:NH2  | 13:LE:199:GLN:O    | 2.35                     | 0.59              |
| 46:S2:1537:G:H2'   | 46:S2:1538:A:C8    | 2.37                     | 0.59              |
| 1:L5:3606:A:H62    | 1:L5:3715:C:H42    | 1.50                     | 0.59              |
| 1:L5:3904:A:H5''   | 23:LJ:108:GLY:HA3  | 1.83                     | 0.59              |
| 46:S2:1093:G:H4'   | 74:SW:2:VAL:HG13   | 1.85                     | 0.59              |
| 39:LT:111:GLU:O    | 39:LT:115:LYS:HG2  | 2.02                     | 0.59              |
| 58:Sg:20:GLN:NE2   | 58:Sg:68:ASP:HB2   | 2.17                     | 0.59              |
| 1:L5:753:G:O2'     | 1:L5:754:A:OP1     | 2.19                     | 0.59              |
| 17:LG:187:LYS:HG2  | 17:LG:198:THR:HB   | 1.85                     | 0.59              |
| 46:S2:800:U:H2'    | 46:S2:801:U:C6     | 2.37                     | 0.59              |
| 59:SG:188:LYS:O    | 59:SG:192:ILE:HD12 | 2.03                     | 0.59              |
| 76:SX:24:ASP:OD1   | 76:SX:24:ASP:N     | 2.31                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:2513:G:H21    | 1:L5:2518:A:H62    | 1.49                     | 0.59              |
| 1:L5:4161:C:H5''   | 41:LV:43:LYS:HE3   | 1.84                     | 0.59              |
| 38:LS:15:ARG:HB3   | 38:LS:27:LEU:HD23  | 1.84                     | 0.59              |
| 46:S2:473:C:O2'    | 46:S2:475:G:OP2    | 2.20                     | 0.59              |
| 76:SX:77:ASN:O     | 76:SX:77:ASN:ND2   | 2.33                     | 0.59              |
| 1:L5:2221:C:HO2'   | 1:L5:2222:C:H6     | 1.49                     | 0.59              |
| 68:SQ:21:ALA:HB2   | 68:SQ:72:VAL:HG23  | 1.85                     | 0.59              |
| 32:LO:3:GLU:HG3    | 32:LO:31:ARG:HH22  | 1.68                     | 0.59              |
| 46:S2:66:G:N2      | 46:S2:68:A:O4'     | 2.35                     | 0.59              |
| 46:S2:1728:G:O2'   | 46:S2:1729:U:H5'   | 2.02                     | 0.59              |
| 79:S7:29:G:H22     | 79:S7:41:C:H5      | 1.51                     | 0.59              |
| 1:L5:189:G:H1      | 1:L5:252:G:H1      | 1.50                     | 0.59              |
| 1:L5:4615:A:H2'    | 1:L5:4616:A:H8     | 1.68                     | 0.59              |
| 46:S2:965:A:H2'    | 46:S2:966:U:H6     | 1.67                     | 0.59              |
| 68:SQ:45:ARG:HG3   | 68:SQ:48:GLN:HG3   | 1.84                     | 0.59              |
| 46:S2:118:C:O2'    | 46:S2:119:U:OP1    | 2.20                     | 0.58              |
| 69:SR:69:ILE:HD11  | 69:SR:74:GLN:HB3   | 1.85                     | 0.58              |
| 79:S7:76:A:O3'     | 80:Z:5:UNK:CA      | 2.50                     | 0.58              |
| 1:L5:499:G:H1      | 1:L5:663:C:H5      | 1.51                     | 0.58              |
| 11:LD:41:LYS:HE3   | 39:LT:93:ILE:HD13  | 1.85                     | 0.58              |
| 19:LH:140:GLN:HG3  | 19:LH:141:LYS:H    | 1.69                     | 0.58              |
| 46:S2:799:G:N2     | 60:SH:107:LYS:O    | 2.36                     | 0.58              |
| 46:S2:943:G:H2'    | 46:S2:944:U:C6     | 2.38                     | 0.58              |
| 1:L5:932:C:H5''    | 1:L5:1049:C:H2'    | 1.84                     | 0.58              |
| 55:Se:110:MET:SD   | 55:Se:114:ARG:NH2  | 2.77                     | 0.58              |
| 46:S2:1269:C:H1'   | 46:S2:1270:G:H5''  | 1.84                     | 0.58              |
| 1:L5:3374:A:H2'    | 1:L5:3375:A:H8     | 1.66                     | 0.58              |
| 46:S2:71:G:H2'     | 46:S2:72:C:H4'     | 1.85                     | 0.58              |
| 46:S2:483:G:OP2    | 46:S2:484:C:H5''   | 2.02                     | 0.58              |
| 46:S2:558:U:O2'    | 46:S2:559:G:H5'    | 2.04                     | 0.58              |
| 1:L5:2328:G:OP2    | 45:LZ:67:LYS:NZ    | 2.36                     | 0.58              |
| 46:S2:1777:G:H5'   | 46:S2:1778:G:N7    | 2.19                     | 0.58              |
| 48:SA:197:VAL:HG23 | 48:SA:201:LEU:HD13 | 1.86                     | 0.58              |
| 1:L5:1012:U:HO2'   | 1:L5:1015:C:N4     | 2.01                     | 0.58              |
| 1:L5:1745:A:H2'    | 1:L5:1746:A:C8     | 2.39                     | 0.58              |
| 46:S2:67:C:OP2     | 46:S2:68:A:N6      | 2.35                     | 0.58              |
| 46:S2:1276:G:O4'   | 46:S2:1507:A:N6    | 2.36                     | 0.58              |
| 46:S2:525:U:H3     | 46:S2:595:A:H2     | 1.51                     | 0.58              |
| 46:S2:538:C:H42    | 46:S2:547:G:H1     | 1.52                     | 0.58              |
| 9:LC:303:ARG:O     | 35:LQ:38:ARG:NH2   | 2.32                     | 0.57              |
| 26:LL:80:GLU:HG3   | 26:LL:110:LEU:HD12 | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:SY:121:ALA:HB1  | 77:SY:125:VAL:HG23 | 1.86                     | 0.57              |
| 46:S2:1260:A:N6    | 46:S2:1520:U:OP1   | 2.33                     | 0.57              |
| 50:SB:189:ILE:HB   | 50:SB:190:PRO:HD3  | 1.85                     | 0.57              |
| 1:L5:2314:G:H1     | 1:L5:2324:G:H22    | 1.52                     | 0.57              |
| 1:L5:4190:C:H2'    | 1:L5:4191:G:C8     | 2.39                     | 0.57              |
| 15:LF:184:ILE:HB   | 15:LF:189:ILE:HD12 | 1.86                     | 0.57              |
| 46:S2:172:U:P      | 46:S2:316:C:H5'    | 2.44                     | 0.57              |
| 46:S2:1270:G:N2    | 46:S2:1515:G:H22   | 2.02                     | 0.57              |
| 46:S2:1571:G:N7    | 71:ST:97:LYS:NZ    | 2.52                     | 0.57              |
| 1:L5:4615:A:H2'    | 1:L5:4616:A:C8     | 2.39                     | 0.57              |
| 5:LA:28:ARG:HG3    | 5:LA:123:ARG:HH11  | 1.69                     | 0.57              |
| 8:Lc:34:THR:HG23   | 8:Lc:95:ALA:HB2    | 1.84                     | 0.57              |
| 46:S2:875:G:H2'    | 46:S2:876:A:H8     | 1.70                     | 0.57              |
| 46:S2:1229:A:H2'   | 46:S2:1230:G:H8    | 1.70                     | 0.57              |
| 58:Sg:257:LYS:HA   | 58:Sg:257:LYS:HE3  | 1.85                     | 0.57              |
| 26:LL:47:ALA:HB3   | 26:LL:48:PRO:HD3   | 1.86                     | 0.57              |
| 31:Lo:59:LYS:HE2   | 31:Lo:59:LYS:HA    | 1.87                     | 0.57              |
| 1:L5:1123:C:H2'    | 1:L5:1124:C:C6     | 2.39                     | 0.57              |
| 1:L5:4233:U:O2'    | 7:LB:182:GLU:OE2   | 2.19                     | 0.57              |
| 37:LR:105:LEU:HD13 | 37:LR:135:LYS:HE3  | 1.85                     | 0.57              |
| 46:S2:1297:U:N3    | 67:SP:59:ARG:HB2   | 2.19                     | 0.57              |
| 70:SS:102:GLY:O    | 70:SS:106:LYS:HG2  | 2.04                     | 0.57              |
| 1:L5:3420:A:HO2'   | 1:L5:3421:U:H6     | 1.51                     | 0.57              |
| 46:S2:480:C:H3'    | 46:S2:481:G:H8     | 1.70                     | 0.57              |
| 46:S2:483:G:H4'    | 76:SX:76:LYS:HD3   | 1.87                     | 0.57              |
| 46:S2:1309:U:H2'   | 46:S2:1310:C:C6    | 2.39                     | 0.57              |
| 58:Sg:156:PHE:HE1  | 58:Sg:179:LEU:HD21 | 1.68                     | 0.57              |
| 66:SO:34:PHE:HB3   | 66:SO:41:PHE:HB2   | 1.86                     | 0.57              |
| 1:L5:3480:G:OP2    | 1:L5:3480:G:N2     | 2.22                     | 0.57              |
| 46:S2:47:G:H22     | 46:S2:479:G:H22    | 1.53                     | 0.57              |
| 46:S2:92:A:H62     | 46:S2:445:G:H8     | 1.52                     | 0.57              |
| 1:L5:477:G:H2'     | 1:L5:478:G:H8      | 1.70                     | 0.57              |
| 2:L7:34:C:O2       | 11:LD:203:ASN:ND2  | 2.37                     | 0.57              |
| 46:S2:1476:G:O2'   | 46:S2:1477:A:OP1   | 2.22                     | 0.57              |
| 61:SI:11:ARG:NH1   | 61:SI:15:GLY:O     | 2.35                     | 0.57              |
| 1:L5:1374:A:H2'    | 1:L5:1375:G:C8     | 2.40                     | 0.57              |
| 1:L5:2239:C:H42    | 1:L5:2254:C:H42    | 1.53                     | 0.57              |
| 46:S2:146:G:H2'    | 46:S2:147:A:C8     | 2.40                     | 0.57              |
| 46:S2:152:U:O4'    | 59:SG:132:ARG:NH2  | 2.38                     | 0.57              |
| 46:S2:95:G:O6      | 46:S2:435:G:N1     | 2.30                     | 0.56              |
| 46:S2:554:U:H2'    | 46:S2:555:A:H2'    | 1.87                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:L5:2205:G:H2'   | 1:L5:2206:A:C8     | 2.40                     | 0.56              |
| 1:L5:3716:G:O2'   | 1:L5:3717:U:H5'    | 2.05                     | 0.56              |
| 1:L5:3892:A:H2'   | 1:L5:3893:G:C8     | 2.39                     | 0.56              |
| 46:S2:1316:U:H2'  | 46:S2:1317:C:C6    | 2.40                     | 0.56              |
| 56:SE:35:PRO:HD2  | 56:SE:83:PRO:HG2   | 1.86                     | 0.56              |
| 58:Sg:220:ASP:HB2 | 58:Sg:224:GLY:H    | 1.69                     | 0.56              |
| 1:L5:4171:A:H5''  | 1:L5:4173:G:H4'    | 1.87                     | 0.56              |
| 3:L8:75:G:OP2     | 44:LY:74:TYR:OH    | 2.23                     | 0.56              |
| 46:S2:1589:A:H2'  | 46:S2:1590:A:C8    | 2.41                     | 0.56              |
| 59:SG:135:PRO:HG2 | 59:SG:141:ILE:HG22 | 1.87                     | 0.56              |
| 65:SN:87:ASP:OD1  | 65:SN:87:ASP:N     | 2.38                     | 0.56              |
| 79:S6:41:C:H2'    | 79:S6:42:A:H8      | 1.70                     | 0.56              |
| 46:S2:161:U:H5''  | 77:SY:116:LYS:HD3  | 1.87                     | 0.56              |
| 1:L5:4552:C:H2'   | 1:L5:4553:G:H4'    | 1.86                     | 0.56              |
| 46:S2:62:G:H2'    | 46:S2:62:G:N3      | 2.21                     | 0.56              |
| 46:S2:1620:A:OP1  | 67:SP:47:ARG:NE    | 2.38                     | 0.56              |
| 46:S2:1781:G:H3'  | 46:S2:1782:A:H4'   | 1.87                     | 0.56              |
| 59:SG:55:GLY:N    | 59:SG:63:MET:HG3   | 2.21                     | 0.56              |
| 77:SY:41:ARG:NH1  | 77:SY:57:VAL:HG22  | 2.20                     | 0.56              |
| 1:L5:1859:G:H5''  | 32:LO:128:ARG:HH21 | 1.71                     | 0.56              |
| 23:LJ:158:SER:OG  | 23:LJ:161:GLU:OE1  | 2.24                     | 0.56              |
| 46:S2:1537:G:H2'  | 46:S2:1538:A:H8    | 1.69                     | 0.56              |
| 46:S2:1719:G:C2   | 46:S2:1816:A:N6    | 2.73                     | 0.56              |
| 63:SK:3:MET:HE1   | 63:SK:48:ALA:HB2   | 1.87                     | 0.56              |
| 1:L5:461:G:H2'    | 1:L5:462:A:C8      | 2.40                     | 0.56              |
| 46:S2:558:U:H2'   | 46:S2:559:G:C8     | 2.40                     | 0.56              |
| 46:S2:1268:C:HO2' | 46:S2:1270:G:H8    | 1.54                     | 0.56              |
| 61:SI:106:SER:HB3 | 61:SI:171:LEU:HG   | 1.87                     | 0.56              |
| 69:SR:58:MET:HA   | 69:SR:61:ILE:HG22  | 1.87                     | 0.56              |
| 1:L5:830:C:H4'    | 1:L5:831:G:O5'     | 2.05                     | 0.56              |
| 1:L5:1005:C:O2'   | 1:L5:1006:G:O5'    | 2.24                     | 0.56              |
| 1:L5:4395:A:O2'   | 1:L5:4397:G:OP1    | 2.22                     | 0.56              |
| 1:L5:4594:U:HO2'  | 14:Lf:2:SER:N      | 2.02                     | 0.56              |
| 32:LO:166:MET:HE2 | 32:LO:166:MET:HA   | 1.88                     | 0.56              |
| 46:S2:1719:G:N2   | 46:S2:1816:A:H62   | 2.04                     | 0.56              |
| 7:LB:80:GLU:OE1   | 7:LB:323:TYR:OH    | 2.18                     | 0.56              |
| 17:LG:77:PRO:HG2  | 17:LG:80:ILE:HD12  | 1.87                     | 0.56              |
| 1:L5:667:G:O2'    | 1:L5:668:G:H8      | 1.89                     | 0.56              |
| 1:L5:2460:G:O2'   | 1:L5:2462:U:O4'    | 2.23                     | 0.56              |
| 1:L5:3530:G:H2'   | 1:L5:3531:G:C8     | 2.40                     | 0.56              |
| 3:L8:1:C:H3'      | 3:L8:2:G:H21       | 1.69                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:Lf:33:VAL:HG13  | 14:Lf:38:GLU:HB2   | 1.88                     | 0.56              |
| 27:Lm:77:ILE:HG22  | 27:Lm:78:ILE:H     | 1.70                     | 0.56              |
| 30:LN:45:PRO:O     | 30:LN:49:ARG:HG3   | 2.06                     | 0.56              |
| 46:S2:1270:G:H2'   | 46:S2:1270:G:N3    | 2.20                     | 0.56              |
| 2:L7:3:C:H2'       | 2:L7:4:U:H6        | 1.69                     | 0.55              |
| 46:S2:594:C:O3'    | 46:S2:595:A:H4'    | 2.06                     | 0.55              |
| 78:SZ:102:LYS:HA   | 78:SZ:107:VAL:HG12 | 1.88                     | 0.55              |
| 80:Z:-11:UNK:O     | 80:Z:-10:UNK:CB    | 2.53                     | 0.55              |
| 46:S2:311:C:H2'    | 46:S2:312:C:C6     | 2.42                     | 0.55              |
| 46:S2:820:G:H1     | 46:S2:830:C:H5     | 1.54                     | 0.55              |
| 72:SU:21:ARG:HG3   | 72:SU:90:ASP:HB3   | 1.87                     | 0.55              |
| 1:L5:494:G:H1      | 1:L5:668:G:H1      | 1.55                     | 0.55              |
| 1:L5:1265:G:H5'    | 1:L5:1266:A:OP1    | 2.07                     | 0.55              |
| 1:L5:2406:G:N2     | 33:Lp:59:SER:O     | 2.40                     | 0.55              |
| 32:LO:113:ASP:OD1  | 32:LO:113:ASP:N    | 2.33                     | 0.55              |
| 46:S2:66:G:H3'     | 46:S2:68:A:H62     | 1.71                     | 0.55              |
| 59:SG:102:VAL:HG21 | 59:SG:109:LEU:HD21 | 1.88                     | 0.55              |
| 1:L5:831:G:N2      | 1:L5:836:C:H2'     | 2.22                     | 0.55              |
| 1:L5:1332:A:OP1    | 4:La:27:LYS:NZ     | 2.40                     | 0.55              |
| 45:LZ:35:ASP:N     | 45:LZ:35:ASP:OD1   | 2.40                     | 0.55              |
| 46:S2:176:U:H3     | 46:S2:314:A:H62    | 1.54                     | 0.55              |
| 77:SY:120:THR:O    | 77:SY:124:ASN:HB2  | 2.07                     | 0.55              |
| 1:L5:1132:U:H2'    | 1:L5:1133:C:C6     | 2.42                     | 0.55              |
| 1:L5:2024:U:OP1    | 36:Lr:37:SER:OG    | 2.21                     | 0.55              |
| 44:LY:37:GLU:H     | 44:LY:37:GLU:CD    | 2.14                     | 0.55              |
| 46:S2:902:G:H2'    | 46:S2:903:G:C5     | 2.41                     | 0.55              |
| 46:S2:1744:G:H21   | 46:S2:1792:A:N6    | 1.96                     | 0.55              |
| 1:L5:511:G:O2'     | 1:L5:513:U:OP2     | 2.20                     | 0.55              |
| 38:LS:99:ASP:OD1   | 38:LS:100:LEU:N    | 2.39                     | 0.55              |
| 46:S2:1378:U:H3'   | 48:SA:102:ARG:HH12 | 1.71                     | 0.55              |
| 59:SG:196:LYS:O    | 59:SG:199:THR:HG22 | 2.05                     | 0.55              |
| 1:L5:3913:U:H2'    | 1:L5:3914:C:H6     | 1.71                     | 0.55              |
| 9:LC:144:ILE:HG13  | 9:LC:144:ILE:O     | 2.05                     | 0.55              |
| 46:S2:50:A:OP2     | 46:S2:473:C:N4     | 2.40                     | 0.55              |
| 46:S2:532:A:N1     | 46:S2:554:U:N3     | 2.45                     | 0.55              |
| 57:SF:17:ILE:HG22  | 57:SF:17:ILE:O     | 2.06                     | 0.55              |
| 72:SU:32:LEU:HD22  | 72:SU:87:ARG:HG3   | 1.89                     | 0.55              |
| 1:L5:299:A:H2'     | 1:L5:300:G:H8      | 1.72                     | 0.55              |
| 19:LH:117:PHE:O    | 19:LH:120:GLU:HG3  | 2.07                     | 0.55              |
| 46:S2:493:C:H5     | 46:S2:507:G:H4'    | 1.72                     | 0.55              |
| 46:S2:1014:U:OP1   | 46:S2:1130:G:O2'   | 2.23                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:1280:C:H2'   | 46:S2:1281:G:C8    | 2.42                     | 0.55              |
| 60:SH:61:ILE:HG22  | 60:SH:93:VAL:HB    | 1.89                     | 0.55              |
| 1:L5:3927:A:H2'    | 1:L5:3928:G:C8     | 2.42                     | 0.55              |
| 12:Le:91:CYS:O     | 12:Le:93:LYS:N     | 2.40                     | 0.55              |
| 46:S2:66:G:P       | 46:S2:82:G:H22     | 2.30                     | 0.55              |
| 46:S2:368:U:H4'    | 46:S2:372:A:C8     | 2.42                     | 0.55              |
| 67:SP:81:ARG:NH1   | 67:SP:97:TYR:O     | 2.38                     | 0.55              |
| 1:L5:3826:G:H2'    | 1:L5:3827:U:C6     | 2.42                     | 0.55              |
| 1:L5:4199:A:N7     | 5:LA:215:ASN:ND2   | 2.55                     | 0.55              |
| 46:S2:158:A:H5'    | 46:S2:465:A:C6     | 2.42                     | 0.55              |
| 77:SY:103:SER:OG   | 77:SY:106:GLN:OE1  | 2.20                     | 0.55              |
| 1:L5:140:G:H2'     | 1:L5:141:C:C6      | 2.42                     | 0.54              |
| 1:L5:477:G:H2'     | 1:L5:478:G:C8      | 2.43                     | 0.54              |
| 46:S2:482:C:C4'    | 46:S2:483:G:H5'    | 2.37                     | 0.54              |
| 46:S2:564:G:H2'    | 46:S2:565:A:C8     | 2.41                     | 0.54              |
| 67:SP:108:LYS:HD2  | 67:SP:109:PRO:HD2  | 1.89                     | 0.54              |
| 69:SR:34:VAL:O     | 69:SR:38:ILE:HG12  | 2.07                     | 0.54              |
| 14:Lf:106:TYR:HB2  | 14:Lf:107:PRO:HD3  | 1.89                     | 0.54              |
| 46:S2:480:C:H3'    | 46:S2:481:G:C8     | 2.42                     | 0.54              |
| 46:S2:1389:A:H61   | 54:SD:161:GLY:HA3  | 1.70                     | 0.54              |
| 1:L5:416:G:OP1     | 1:L5:2066:G:N2     | 2.40                     | 0.54              |
| 3:L8:8:U:H2'       | 3:L8:9:A:C8        | 2.41                     | 0.54              |
| 46:S2:92:A:OP1     | 56:SE:3:ARG:NH2    | 2.39                     | 0.54              |
| 60:SH:133:LEU:HD11 | 60:SH:176:VAL:HG13 | 1.89                     | 0.54              |
| 1:L5:424:U:H2'     | 1:L5:425:A:H8      | 1.72                     | 0.54              |
| 1:L5:4190:C:H2'    | 1:L5:4191:G:H8     | 1.71                     | 0.54              |
| 46:S2:929:G:H2'    | 46:S2:930:G:C8     | 2.43                     | 0.54              |
| 60:SH:62:ILE:HD12  | 60:SH:94:PHE:HE1   | 1.72                     | 0.54              |
| 69:SR:127:ASN:OD1  | 69:SR:127:ASN:N    | 2.41                     | 0.54              |
| 71:ST:104:LEU:HD22 | 71:ST:121:ARG:HG3  | 1.88                     | 0.54              |
| 46:S2:456:A:H2'    | 46:S2:457:C:H6     | 1.72                     | 0.54              |
| 67:SP:86:LEU:H     | 67:SP:89:MET:HE2   | 1.73                     | 0.54              |
| 1:L5:1009:C:H42    | 1:L5:1017:A:N6     | 2.05                     | 0.54              |
| 23:LJ:173:ILE:HD11 | 23:LJ:175:LEU:HD12 | 1.89                     | 0.54              |
| 46:S2:294:C:O2'    | 46:S2:295:U:H3'    | 2.07                     | 0.54              |
| 46:S2:833:G:H1     | 46:S2:842:G:H1     | 1.55                     | 0.54              |
| 46:S2:1422:A:H2'   | 46:S2:1423:G:H8    | 1.72                     | 0.54              |
| 54:SD:65:ARG:NH1   | 54:SD:68:GLU:OE1   | 2.40                     | 0.54              |
| 77:SY:41:ARG:HH21  | 77:SY:94:HIS:CE1   | 2.26                     | 0.54              |
| 78:SZ:79:ILE:HG23  | 78:SZ:83:LEU:HD23  | 1.89                     | 0.54              |
| 1:L5:3393:A:H2'    | 1:L5:3394:A:C8     | 2.43                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LX:87:MET:HE1   | 43:LX:155:ILE:HD12 | 1.88                     | 0.54              |
| 46:S2:863:A:C8     | 74:SW:107:SER:HA   | 2.42                     | 0.54              |
| 1:L5:93:G:H2'      | 1:L5:94:A:C8       | 2.42                     | 0.54              |
| 1:L5:189:G:H22     | 1:L5:252:G:H1      | 1.55                     | 0.54              |
| 1:L5:1148:A:H2'    | 1:L5:1149:A:C8     | 2.43                     | 0.54              |
| 1:L5:1377:A:H61    | 46:S2:1029:A:H2    | 1.54                     | 0.54              |
| 2:L7:53:U:OP1      | 23:LJ:10:ASN:ND2   | 2.37                     | 0.54              |
| 13:LE:100:VAL:HG12 | 13:LE:115:VAL:HB   | 1.90                     | 0.54              |
| 45:LZ:76:ASN:OD1   | 45:LZ:77:TYR:N     | 2.41                     | 0.54              |
| 46:S2:107:A:H2'    | 46:S2:108:G:C8     | 2.43                     | 0.54              |
| 3:L8:8:U:H2'       | 3:L8:9:A:H8        | 1.73                     | 0.54              |
| 1:L5:2655:G:N2     | 1:L5:3256:A:N3     | 2.57                     | 0.53              |
| 48:SA:198:MET:SD   | 69:SR:89:SER:OG    | 2.61                     | 0.53              |
| 53:Sd:26:ASN:ND2   | 53:Sd:39:CYS:SG    | 2.81                     | 0.53              |
| 54:SD:39:VAL:HG12  | 54:SD:39:VAL:O     | 2.08                     | 0.53              |
| 58:Sg:54:ILE:HG13  | 58:Sg:55:PRO:HD2   | 1.89                     | 0.53              |
| 68:SQ:66:VAL:HG12  | 68:SQ:67:ASP:H     | 1.72                     | 0.53              |
| 17:LG:160:ASP:OD1  | 17:LG:160:ASP:N    | 2.40                     | 0.53              |
| 46:S2:589:G:OP2    | 46:S2:589:G:N2     | 2.34                     | 0.53              |
| 46:S2:1420:C:H2'   | 46:S2:1421:G:C5    | 2.44                     | 0.53              |
| 11:LD:226:TYR:O    | 11:LD:228:LYS:N    | 2.42                     | 0.53              |
| 15:LF:247:THR:HG22 | 15:LF:253:GLY:HA3  | 1.90                     | 0.53              |
| 46:S2:1601:G:H5'   | 78:SZ:43:LYS:HG2   | 1.90                     | 0.53              |
| 57:SF:95:HIS:CG    | 78:SZ:106:GLN:HE21 | 2.26                     | 0.53              |
| 60:SH:73:GLN:NE2   | 60:SH:132:ASP:OD1  | 2.41                     | 0.53              |
| 63:SK:3:MET:HE2    | 63:SK:8:ARG:HA     | 1.91                     | 0.53              |
| 71:ST:40:ALA:HB3   | 71:ST:43:LYS:HG2   | 1.91                     | 0.53              |
| 77:SY:61:ARG:HG2   | 77:SY:61:ARG:HH11  | 1.72                     | 0.53              |
| 1:L5:1122:A:H2'    | 1:L5:1123:C:C6     | 2.43                     | 0.53              |
| 1:L5:3528:A:H2'    | 1:L5:3529:A:C8     | 2.44                     | 0.53              |
| 49:Sb:67:THR:OG1   | 49:Sb:70:LYS:O     | 2.26                     | 0.53              |
| 77:SY:78:SER:OG    | 77:SY:80:ASP:OD1   | 2.23                     | 0.53              |
| 1:L5:162:A:H2'     | 1:L5:163:A:C8      | 2.43                     | 0.53              |
| 39:LT:124:THR:OG1  | 39:LT:125:TRP:N    | 2.42                     | 0.53              |
| 46:S2:221:U:H1'    | 61:SI:184:ARG:HD2  | 1.90                     | 0.53              |
| 46:S2:1244:U:OP2   | 46:S2:1519:C:O2'   | 2.21                     | 0.53              |
| 60:SH:50:GLU:HG3   | 60:SH:60:ILE:HG22  | 1.90                     | 0.53              |
| 75:Sx:33:U:H2'     | 75:Sx:34:C:C6      | 2.43                     | 0.53              |
| 1:L5:468:C:N3      | 13:LE:113:ARG:NH2  | 2.54                     | 0.53              |
| 1:L5:1523:C:H2'    | 1:L5:1524:G:C8     | 2.44                     | 0.53              |
| 5:LA:180:LEU:HD21  | 33:Lp:22:LEU:HB3   | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:LH:91:LYS:HG2   | 19:LH:145:ILE:HD13 | 1.90                     | 0.53              |
| 23:LJ:174:ILE:HG22 | 23:LJ:176:PRO:HD2  | 1.90                     | 0.53              |
| 46:S2:527:A:O2'    | 62:SJ:125:HIS:ND1  | 2.25                     | 0.53              |
| 60:SH:78:ARG:H     | 60:SH:78:ARG:NE    | 2.06                     | 0.53              |
| 1:L5:1031:G:H2'    | 1:L5:1033:G:C8     | 2.44                     | 0.53              |
| 1:L5:2499:A:H2'    | 1:L5:2500:A:H8     | 1.74                     | 0.53              |
| 46:S2:1159:G:O3'   | 74:SW:76:SER:OG    | 2.21                     | 0.53              |
| 67:SP:108:LYS:HD2  | 67:SP:109:PRO:CD   | 2.38                     | 0.53              |
| 79:S7:65:C:O2'     | 79:S7:66:C:H5'     | 2.09                     | 0.53              |
| 1:L5:1154:U:H2'    | 1:L5:1155:C:C6     | 2.43                     | 0.53              |
| 1:L5:4556:A:H4'    | 7:LB:95:THR:HG22   | 1.91                     | 0.53              |
| 18:Lh:80:PRO:HD2   | 18:Lh:83:LEU:HD12  | 1.91                     | 0.53              |
| 55:Se:116:PHE:CE2  | 62:SJ:30:LYS:HD2   | 2.44                     | 0.53              |
| 63:SK:14:LEU:HD11  | 63:SK:35:LEU:HD11  | 1.91                     | 0.53              |
| 1:L5:1476:C:H2'    | 1:L5:1477:C:C6     | 2.44                     | 0.53              |
| 1:L5:2277:C:O2     | 1:L5:2394:G:N2     | 2.41                     | 0.53              |
| 40:LU:18:VAL:HG22  | 40:LU:20:LYS:HE3   | 1.90                     | 0.53              |
| 46:S2:994:G:N7     | 47:Sa:15:ARG:NH1   | 2.57                     | 0.53              |
| 46:S2:1145:A:H5'   | 46:S2:1356:C:H41   | 1.74                     | 0.53              |
| 46:S2:1736:A:H2    | 46:S2:1800:G:H21   | 1.57                     | 0.53              |
| 59:SG:176:ILE:HD11 | 59:SG:179:LEU:HD22 | 1.91                     | 0.53              |
| 62:SJ:83:ARG:HE    | 62:SJ:150:ARG:HD3  | 1.74                     | 0.53              |
| 46:S2:526:A:C2     | 46:S2:591:A:C6     | 2.96                     | 0.53              |
| 46:S2:1145:A:H2'   | 46:S2:1146:A:C8    | 2.44                     | 0.53              |
| 46:S2:1320:U:H3'   | 46:S2:1321:G:O4'   | 2.08                     | 0.53              |
| 67:SP:18:ARG:HH11  | 70:SS:88:LYS:HG2   | 1.73                     | 0.53              |
| 75:Sx:33:U:H2'     | 75:Sx:34:C:H6      | 1.74                     | 0.53              |
| 60:SH:172:THR:O    | 60:SH:176:VAL:HG12 | 2.09                     | 0.52              |
| 69:SR:6:THR:HG22   | 69:SR:8:THR:H      | 1.73                     | 0.52              |
| 1:L5:1218:C:H2'    | 1:L5:1219:C:C6     | 2.44                     | 0.52              |
| 1:L5:2656:G:H1     | 1:L5:3254:G:H1     | 1.56                     | 0.52              |
| 17:LG:58:PRO:HD2   | 17:LG:61:ILE:HD12  | 1.91                     | 0.52              |
| 1:L5:1736:G:H2'    | 1:L5:1737:A:C8     | 2.45                     | 0.52              |
| 7:LB:299:ILE:HG23  | 7:LB:313:SER:HB3   | 1.90                     | 0.52              |
| 11:LD:116:ASP:OD1  | 11:LD:116:ASP:N    | 2.38                     | 0.52              |
| 34:LP:122:ALA:HB3  | 34:LP:143:PRO:HB2  | 1.90                     | 0.52              |
| 46:S2:39:A:OP1     | 62:SJ:5:ARG:NH1    | 2.42                     | 0.52              |
| 77:SY:76:TYR:OH    | 77:SY:85:ASN:O     | 2.27                     | 0.52              |
| 1:L5:385:A:OP2     | 44:LY:89:LYS:NZ    | 2.40                     | 0.52              |
| 1:L5:1710:A:H2'    | 1:L5:1711:A:C8     | 2.44                     | 0.52              |
| 1:L5:3313:A:H2'    | 1:L5:3314:U:H6     | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:4247:U:H2'    | 1:L5:4248:G:H8     | 1.73                     | 0.52              |
| 1:L5:4425:U:H3     | 1:L5:4509:G:H1     | 1.55                     | 0.52              |
| 67:SP:72:LYS:HG2   | 67:SP:93:MET:HE2   | 1.91                     | 0.52              |
| 77:SY:102:THR:HG23 | 77:SY:107:ARG:HH11 | 1.73                     | 0.52              |
| 1:L5:4154:U:OP1    | 7:LB:2:SER:N       | 2.42                     | 0.52              |
| 46:S2:1355:G:N2    | 46:S2:1358:A:OP2   | 2.34                     | 0.52              |
| 53:Sd:33:LYS:O     | 53:Sd:36:LEU:HD12  | 2.09                     | 0.52              |
| 54:SD:41:VAL:HG12  | 54:SD:47:GLU:H     | 1.73                     | 0.52              |
| 1:L5:1605:A:H5''   | 1:L5:1606:G:H5'    | 1.92                     | 0.52              |
| 14:Lf:106:TYR:O    | 14:Lf:108:SER:N    | 2.43                     | 0.52              |
| 43:LX:84:GLU:CD    | 43:LX:84:GLU:H     | 2.17                     | 0.52              |
| 43:LX:111:GLN:O    | 43:LX:115:LYS:HE2  | 2.10                     | 0.52              |
| 46:S2:126:G:H8     | 59:SG:195:LYS:HD3  | 1.73                     | 0.52              |
| 46:S2:1275:G:H21   | 63:SK:27:VAL:HG12  | 1.75                     | 0.52              |
| 46:S2:1720:A:N6    | 46:S2:1815:G:N2    | 2.21                     | 0.52              |
| 48:SA:76:VAL:HG12  | 48:SA:123:VAL:HB   | 1.92                     | 0.52              |
| 58:Sg:88:ARG:NH2   | 58:Sg:97:THR:OG1   | 2.43                     | 0.52              |
| 1:L5:4550:G:H2'    | 1:L5:4551:C:C6     | 2.45                     | 0.52              |
| 37:LR:105:LEU:HD23 | 37:LR:138:LEU:HD23 | 1.92                     | 0.52              |
| 46:S2:72:C:O2'     | 46:S2:74:G:N2      | 2.34                     | 0.52              |
| 46:S2:126:G:OP1    | 59:SG:198:ARG:NH1  | 2.42                     | 0.52              |
| 79:S7:66:C:HO2'    | 79:S7:67:U:H6      | 1.57                     | 0.52              |
| 1:L5:189:G:H22     | 1:L5:252:G:N2      | 2.06                     | 0.52              |
| 1:L5:432:A:C2      | 1:L5:3524:A:H4'    | 2.44                     | 0.52              |
| 1:L5:761:C:H2'     | 1:L5:762:U:H6      | 1.75                     | 0.52              |
| 1:L5:4559:G:O2'    | 1:L5:4560:C:O4'    | 2.23                     | 0.52              |
| 46:S2:16:G:H2'     | 46:S2:17:C:C6      | 2.45                     | 0.52              |
| 46:S2:96:C:O2'     | 46:S2:97:U:O5'     | 2.25                     | 0.52              |
| 46:S2:925:G:H5'    | 65:SN:4:MET:HE3    | 1.91                     | 0.52              |
| 69:SR:83:ASN:OD1   | 69:SR:84:TYR:N     | 2.42                     | 0.52              |
| 77:SY:28:LEU:O     | 77:SY:29:HIS:ND1   | 2.43                     | 0.52              |
| 1:L5:76:A:OP2      | 26:LL:74:ARG:NH1   | 2.43                     | 0.52              |
| 1:L5:270:C:H2'     | 1:L5:271:U:O2      | 2.10                     | 0.52              |
| 1:L5:747:G:O2'     | 1:L5:748:G:H8      | 1.93                     | 0.52              |
| 1:L5:936:C:N4      | 1:L5:1054:G:O6     | 2.43                     | 0.52              |
| 1:L5:1254:U:O4     | 1:L5:1909:C:N3     | 2.43                     | 0.52              |
| 58:Sg:82:SER:OG    | 58:Sg:84:ASP:OD1   | 2.27                     | 0.52              |
| 69:SR:60:ARG:HG3   | 69:SR:66:VAL:HG21  | 1.92                     | 0.52              |
| 1:L5:2394:G:H2'    | 1:L5:2395:A:C8     | 2.45                     | 0.52              |
| 11:LD:128:GLY:O    | 11:LD:164:LYS:NZ   | 2.43                     | 0.52              |
| 40:LU:105:ASN:OD1  | 40:LU:109:SER:OG   | 2.27                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L5:1562:G:H3'   | 1:L5:1563:G:H8    | 1.74                     | 0.51              |
| 1:L5:2253:G:H2'   | 1:L5:2254:C:C6    | 2.45                     | 0.51              |
| 1:L5:3413:A:N1    | 1:L5:3425:U:H5    | 2.08                     | 0.51              |
| 4:La:110:LYS:HG3  | 4:La:128:PHE:HB2  | 1.92                     | 0.51              |
| 46:S2:456:A:O2'   | 46:S2:1736:A:H8   | 1.91                     | 0.51              |
| 79:S6:18:G:O2'    | 79:S6:57:G:N2     | 2.43                     | 0.51              |
| 1:L5:4352:U:H1'   | 1:L5:4353:A:H5'   | 1.91                     | 0.51              |
| 7:LB:358:ARG:HG3  | 7:LB:358:ARG:HH11 | 1.76                     | 0.51              |
| 13:LE:103:THR:OG1 | 13:LE:104:VAL:N   | 2.43                     | 0.51              |
| 34:LP:93:HIS:N    | 34:LP:93:HIS:ND1  | 2.58                     | 0.51              |
| 46:S2:526:A:N1    | 46:S2:591:A:C5    | 2.79                     | 0.51              |
| 46:S2:820:G:H4'   | 56:SE:255:ARG:NH2 | 2.23                     | 0.51              |
| 46:S2:1280:C:H2'  | 46:S2:1281:G:H8   | 1.75                     | 0.51              |
| 76:SX:68:LYS:HB3  | 76:SX:91:LEU:HD22 | 1.92                     | 0.51              |
| 79:S7:62:C:H2'    | 79:S7:63:A:C8     | 2.46                     | 0.51              |
| 1:L5:927:C:O2'    | 1:L5:928:C:OP1    | 2.28                     | 0.51              |
| 52:SC:266:TYR:O   | 52:SC:270:THR:OG1 | 2.22                     | 0.51              |
| 54:SD:27:ARG:HG3  | 63:SK:61:GLN:HE21 | 1.75                     | 0.51              |
| 58:Sg:171:ASP:O   | 58:Sg:172:LYS:HG2 | 2.10                     | 0.51              |
| 58:Sg:191:HIS:HE2 | 58:Sg:209:SER:HG  | 1.56                     | 0.51              |
| 62:SJ:88:ASP:OD1  | 62:SJ:89:GLU:N    | 2.44                     | 0.51              |
| 71:ST:42:HIS:CE1  | 71:ST:43:LYS:HE3  | 2.46                     | 0.51              |
| 79:S6:53:G:O2'    | 79:S6:54:A:OP1    | 2.27                     | 0.51              |
| 1:L5:1380:C:H2'   | 1:L5:1381:U:H6    | 1.74                     | 0.51              |
| 1:L5:4585:G:O2'   | 1:L5:4587:A:N7    | 2.40                     | 0.51              |
| 46:S2:872:U:H5'   | 65:SN:76:LYS:HE3  | 1.93                     | 0.51              |
| 46:S2:1297:U:C4   | 67:SP:59:ARG:HB2  | 2.45                     | 0.51              |
| 61:SI:76:THR:HG22 | 61:SI:108:PRO:HG2 | 1.92                     | 0.51              |
| 17:LG:165:GLU:OE2 | 30:LN:26:ARG:NH2  | 2.28                     | 0.51              |
| 46:S2:641:A:H2'   | 46:S2:642:A:C8    | 2.46                     | 0.51              |
| 60:SH:10:LYS:HD2  | 60:SH:45:ILE:HG12 | 1.92                     | 0.51              |
| 72:SU:90:ASP:OD1  | 72:SU:90:ASP:N    | 2.41                     | 0.51              |
| 1:L5:753:G:H2'    | 1:L5:754:A:C8     | 2.45                     | 0.51              |
| 11:LD:119:TYR:OH  | 11:LD:139:PRO:O   | 2.26                     | 0.51              |
| 46:S2:1268:C:O2'  | 46:S2:1270:G:H8   | 1.93                     | 0.51              |
| 46:S2:1784:C:H4'  | 46:S2:1785:G:O5'  | 2.10                     | 0.51              |
| 52:SC:85:SER:OG   | 73:SV:25:ALA:O    | 2.29                     | 0.51              |
| 1:L5:955:C:O2'    | 1:L5:1028:G:N1    | 2.41                     | 0.51              |
| 1:L5:3984:G:H3'   | 1:L5:3985:C:H5'   | 1.92                     | 0.51              |
| 63:SK:3:MET:SD    | 63:SK:8:ARG:HD3   | 2.51                     | 0.51              |
| 78:SZ:99:LEU:HD22 | 78:SZ:100:VAL:H   | 1.75                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:1418:G:H2'    | 1:L5:1419:G:C8     | 2.46                     | 0.51              |
| 1:L5:3389:A:H2'    | 1:L5:3390:A:C8     | 2.46                     | 0.51              |
| 1:L5:3892:A:H2'    | 1:L5:3893:G:H8     | 1.76                     | 0.51              |
| 34:LP:94:MET:HG2   | 34:LP:148:MET:SD   | 2.51                     | 0.51              |
| 46:S2:456:A:H2'    | 46:S2:457:C:C6     | 2.46                     | 0.51              |
| 46:S2:515:U:H2'    | 46:S2:516:G:C8     | 2.46                     | 0.51              |
| 46:S2:1514:C:H2'   | 46:S2:1515:G:C8    | 2.46                     | 0.51              |
| 49:Sb:59:CYS:SG    | 49:Sb:60:SER:N     | 2.84                     | 0.51              |
| 71:ST:64:LEU:HD21  | 71:ST:121:ARG:HB2  | 1.93                     | 0.51              |
| 1:L5:1010:U:H4'    | 11:LD:279:ARG:HH11 | 1.76                     | 0.51              |
| 1:L5:3326:G:H21    | 1:L5:3329:G:H21    | 1.57                     | 0.51              |
| 1:L5:3927:A:H2'    | 1:L5:3928:G:H8     | 1.76                     | 0.51              |
| 11:LD:152:ARG:O    | 11:LD:157:ASN:ND2  | 2.44                     | 0.51              |
| 43:LX:153:ILE:HG22 | 43:LX:155:ILE:HG23 | 1.93                     | 0.51              |
| 61:SI:165:GLN:HB2  | 61:SI:171:LEU:HD23 | 1.92                     | 0.51              |
| 79:S7:10:G:H21     | 79:S7:45:G:H3'     | 1.75                     | 0.51              |
| 79:S7:16:G:H2'     | 79:S7:20:A:H61     | 1.75                     | 0.51              |
| 1:L5:490:C:H2'     | 1:L5:491:C:C6      | 2.46                     | 0.51              |
| 1:L5:1192:G:H5''   | 1:L5:1193:C:OP2    | 2.11                     | 0.51              |
| 1:L5:2327:A:H62    | 1:L5:2515:U:H5     | 1.58                     | 0.51              |
| 1:L5:4651:U:H2'    | 1:L5:4652:C:C6     | 2.45                     | 0.51              |
| 7:LB:302:ASN:HB2   | 7:LB:313:SER:HA    | 1.93                     | 0.51              |
| 11:LD:41:LYS:HB2   | 39:LT:68:THR:O     | 2.10                     | 0.51              |
| 14:Lf:21:GLN:NE2   | 14:Lf:23:GLU:OE2   | 2.43                     | 0.51              |
| 48:SA:19:LEU:HD11  | 69:SR:106:LEU:HD11 | 1.93                     | 0.51              |
| 48:SA:85:ARG:NH2   | 69:SR:81:ARG:O     | 2.41                     | 0.51              |
| 50:SB:169:MET:O    | 50:SB:173:THR:HG22 | 2.11                     | 0.51              |
| 50:SB:192:SER:HA   | 50:SB:195:LYS:HG3  | 1.91                     | 0.51              |
| 58:Sg:124:SER:OG   | 58:Sg:126:ASP:OD1  | 2.16                     | 0.51              |
| 1:L5:1011:G:N2     | 11:LD:283:LYS:O    | 2.44                     | 0.50              |
| 2:L7:117:G:OP1     | 11:LD:253:TYR:OH   | 2.22                     | 0.50              |
| 46:S2:28:U:H2'     | 46:S2:29:G:H8      | 1.76                     | 0.50              |
| 1:L5:316:A:N1      | 1:L5:4013:U:H5     | 2.09                     | 0.50              |
| 1:L5:424:U:H2'     | 1:L5:425:A:C8      | 2.46                     | 0.50              |
| 1:L5:4111:C:H2'    | 1:L5:4112:U:C6     | 2.46                     | 0.50              |
| 2:L7:23:A:N3       | 2:L7:118:C:O2'     | 2.43                     | 0.50              |
| 46:S2:1115:U:O2'   | 46:S2:1116:U:O5'   | 2.24                     | 0.50              |
| 72:SU:24:LEU:HB2   | 72:SU:87:ARG:HB2   | 1.93                     | 0.50              |
| 1:L5:1012:U:O2'    | 1:L5:1013:C:OP1    | 2.27                     | 0.50              |
| 1:L5:1222:C:O2'    | 1:L5:1226:G:N3     | 2.43                     | 0.50              |
| 3:L8:141:C:H2'     | 3:L8:142:U:C6      | 2.47                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:LY:10:ASP:HB3  | 44:LY:13:LYS:HB2   | 1.93                     | 0.50              |
| 46:S2:796:A:O2'   | 46:S2:797:G:O4'    | 2.22                     | 0.50              |
| 56:SE:36:HIS:CE1  | 56:SE:85:GLY:HA3   | 2.46                     | 0.50              |
| 63:SK:16:PHE:HD2  | 63:SK:79:LEU:HD23  | 1.76                     | 0.50              |
| 1:L5:1011:G:O2'   | 1:L5:1012:U:H5'    | 2.12                     | 0.50              |
| 1:L5:3904:A:H4'   | 1:L5:3905:C:OP1    | 2.10                     | 0.50              |
| 27:Lm:83:ARG:O    | 27:Lm:87:GLN:HG3   | 2.11                     | 0.50              |
| 32:LO:121:PRO:HA  | 32:LO:124:LEU:HD12 | 1.93                     | 0.50              |
| 46:S2:492:C:H1'   | 46:S2:511:G:N2     | 2.26                     | 0.50              |
| 72:SU:54:VAL:HG12 | 72:SU:56:MET:HE3   | 1.94                     | 0.50              |
| 1:L5:678:G:H2'    | 1:L5:679:G:C8      | 2.47                     | 0.50              |
| 46:S2:47:G:N2     | 46:S2:479:G:H22    | 2.10                     | 0.50              |
| 46:S2:1410:A:H2'  | 46:S2:1411:C:O4'   | 2.11                     | 0.50              |
| 1:L5:937:C:H2'    | 1:L5:938:C:H5'     | 1.93                     | 0.50              |
| 2:L7:110:G:H2'    | 2:L7:111:C:C6      | 2.47                     | 0.50              |
| 46:S2:80:G:H2'    | 46:S2:81:U:C6      | 2.47                     | 0.50              |
| 46:S2:516:G:H5''  | 46:S2:517:A:H3'    | 1.93                     | 0.50              |
| 46:S2:629:A:O2'   | 46:S2:630:A:OP1    | 2.28                     | 0.50              |
| 62:SJ:103:GLU:O   | 62:SJ:107:GLU:HG2  | 2.11                     | 0.50              |
| 73:SV:43:THR:HB   | 73:SV:45:ARG:HG3   | 1.92                     | 0.50              |
| 1:L5:3802:C:H2'   | 1:L5:3803:G:C8     | 2.47                     | 0.50              |
| 46:S2:315:U:H2'   | 46:S2:316:C:C6     | 2.47                     | 0.50              |
| 56:SE:15:PRO:HD2  | 56:SE:18:TRP:CZ2   | 2.47                     | 0.50              |
| 1:L5:823:C:O2'    | 1:L5:824:C:OP1     | 2.28                     | 0.50              |
| 1:L5:831:G:H8     | 1:L5:831:G:OP1     | 1.94                     | 0.50              |
| 1:L5:4422:G:OP1   | 32:LO:168:TYR:OH   | 2.29                     | 0.50              |
| 13:LE:107:ASP:O   | 13:LE:108:LYS:HG2  | 2.11                     | 0.50              |
| 15:LF:170:LYS:O   | 15:LF:174:GLU:HG2  | 2.11                     | 0.50              |
| 16:Lg:41:ALA:O    | 16:Lg:52:ARG:NH1   | 2.37                     | 0.50              |
| 41:LV:99:GLU:HG3  | 42:LW:21:TYR:OH    | 2.12                     | 0.50              |
| 46:S2:1296:A:H2   | 46:S2:1306:C:H42   | 1.60                     | 0.50              |
| 46:S2:1729:U:O2'  | 46:S2:1730:U:O4'   | 2.29                     | 0.50              |
| 72:SU:46:LYS:HE3  | 72:SU:97:ILE:HD11  | 1.93                     | 0.50              |
| 5:LA:118:GLU:OE2  | 5:LA:156:LYS:NZ    | 2.45                     | 0.50              |
| 1:L5:884:C:H2'    | 1:L5:885:C:C6      | 2.47                     | 0.49              |
| 1:L5:1858:G:H4'   | 1:L5:1859:G:OP2    | 2.12                     | 0.49              |
| 6:Lb:89:PRO:HD2   | 6:Lb:92:LYS:HB2    | 1.94                     | 0.49              |
| 46:S2:50:A:H5''   | 46:S2:51:U:OP2     | 2.12                     | 0.49              |
| 46:S2:538:C:O2    | 46:S2:538:C:H2'    | 2.12                     | 0.49              |
| 52:SC:166:ARG:HG2 | 52:SC:181:PRO:HG3  | 1.94                     | 0.49              |
| 71:ST:108:GLU:OE2 | 71:ST:121:ARG:NH1  | 2.45                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S6:28:U:H2'     | 79:S6:29:G:C8      | 2.46                     | 0.49              |
| 1:L5:1561:G:H2'    | 1:L5:1562:G:O4'    | 2.12                     | 0.49              |
| 6:Lb:54:LEU:O      | 6:Lb:58:GLN:HG3    | 2.12                     | 0.49              |
| 26:LL:87:HIS:HB3   | 26:LL:90:VAL:HG23  | 1.93                     | 0.49              |
| 46:S2:1315:U:H5''  | 46:S2:1316:U:H5    | 1.77                     | 0.49              |
| 1:L5:1147:C:H2'    | 1:L5:1148:A:H8     | 1.75                     | 0.49              |
| 55:Se:86:VAL:O     | 55:Se:90:THR:HG23  | 2.13                     | 0.49              |
| 58:Sg:292:SER:O    | 58:Sg:292:SER:OG   | 2.27                     | 0.49              |
| 76:SX:107:ARG:HG3  | 76:SX:112:VAL:HG22 | 1.93                     | 0.49              |
| 1:L5:4054:G:H2'    | 1:L5:4055:C:H6     | 1.78                     | 0.49              |
| 2:L7:52:C:O2'      | 2:L7:53:U:OP1      | 2.29                     | 0.49              |
| 30:LN:174:LEU:HD23 | 30:LN:183:THR:HG21 | 1.94                     | 0.49              |
| 46:S2:81:U:H2'     | 46:S2:82:G:O4'     | 2.12                     | 0.49              |
| 48:SA:174:MET:HA   | 48:SA:177:MET:HB2  | 1.95                     | 0.49              |
| 68:SQ:19:ALA:HB2   | 68:SQ:75:GLY:HA3   | 1.94                     | 0.49              |
| 77:SY:39:GLU:O     | 77:SY:42:GLU:HG2   | 2.12                     | 0.49              |
| 1:L5:886:U:O4      | 1:L5:887:C:N4      | 2.46                     | 0.49              |
| 1:L5:3595:G:N2     | 1:L5:3824:C:OP2    | 2.46                     | 0.49              |
| 2:L7:4:U:H2'       | 2:L7:5:A:H8        | 1.77                     | 0.49              |
| 46:S2:862:A:O2'    | 46:S2:863:A:OP2    | 2.26                     | 0.49              |
| 46:S2:1458:U:H2'   | 46:S2:1459:G:H8    | 1.78                     | 0.49              |
| 48:SA:40:LYS:O     | 48:SA:48:ILE:HG12  | 2.12                     | 0.49              |
| 48:SA:84:GLN:HG2   | 48:SA:100:ALA:HB1  | 1.94                     | 0.49              |
| 56:SE:57:THR:HB    | 56:SE:60:GLU:HG3   | 1.94                     | 0.49              |
| 56:SE:125:LYS:O    | 56:SE:142:HIS:N    | 2.45                     | 0.49              |
| 63:SK:19:GLY:HA2   | 63:SK:71:LEU:HD12  | 1.94                     | 0.49              |
| 78:SZ:56:ASP:OD1   | 78:SZ:57:LYS:N     | 2.46                     | 0.49              |
| 1:L5:940:C:H2'     | 1:L5:941:C:H6      | 1.77                     | 0.49              |
| 1:L5:951:A:H2      | 1:L5:1034:G:H22    | 1.60                     | 0.49              |
| 1:L5:2313:G:H2'    | 1:L5:2314:G:C8     | 2.48                     | 0.49              |
| 18:Lh:95:LEU:HG    | 18:Lh:99:GLU:HB3   | 1.95                     | 0.49              |
| 46:S2:539:U:O2     | 46:S2:547:G:N2     | 2.46                     | 0.49              |
| 56:SE:175:PHE:HE2  | 56:SE:222:LEU:HD11 | 1.78                     | 0.49              |
| 24:Lk:40:ARG:NH1   | 24:Lk:41:TYR:OH    | 2.46                     | 0.49              |
| 46:S2:1210:A:O2'   | 47:Sa:85:ARG:NH1   | 2.45                     | 0.49              |
| 79:S7:63:A:H2'     | 79:S7:64:U:C6      | 2.48                     | 0.49              |
| 1:L5:304:A:OP1     | 20:Li:76:ARG:NH1   | 2.45                     | 0.49              |
| 1:L5:1497:U:OP1    | 4:La:44:ASN:ND2    | 2.45                     | 0.49              |
| 1:L5:3379:G:H2'    | 1:L5:3380:A:H8     | 1.77                     | 0.49              |
| 1:L5:3580:A:H2'    | 1:L5:3581:C:C6     | 2.48                     | 0.49              |
| 1:L5:4393:G:H1'    | 1:L5:4396:G:H5''   | 1.93                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:LE:53:ARG:O     | 13:LE:72:ARG:NH1  | 2.45                     | 0.49              |
| 46:S2:1668:U:H2'   | 46:S2:1669:U:C6   | 2.48                     | 0.49              |
| 55:Se:105:ARG:HD3  | 62:SJ:127:ARG:HG2 | 1.94                     | 0.49              |
| 1:L5:267:G:H2'     | 1:L5:268:G:H8     | 1.77                     | 0.49              |
| 1:L5:940:C:H2'     | 1:L5:941:C:C6     | 2.48                     | 0.49              |
| 1:L5:4152:G:C2     | 1:L5:4182:G:H1'   | 2.48                     | 0.49              |
| 1:L5:4652:C:H2'    | 1:L5:4653:G:O4'   | 2.13                     | 0.49              |
| 8:Lc:47:ILE:HD12   | 8:Lc:94:LEU:HD22  | 1.95                     | 0.49              |
| 46:S2:220:U:C4     | 46:S2:221:U:C5    | 3.01                     | 0.49              |
| 46:S2:988:A:OP1    | 47:Sa:32:LYS:NZ   | 2.46                     | 0.49              |
| 77:SY:47:MET:SD    | 77:SY:48:TYR:HB2  | 2.53                     | 0.49              |
| 1:L5:139:G:H2'     | 1:L5:140:G:O4'    | 2.13                     | 0.49              |
| 46:S2:946:U:H2'    | 46:S2:947:U:C6    | 2.48                     | 0.49              |
| 54:SD:32:ASP:N     | 54:SD:32:ASP:OD1  | 2.45                     | 0.49              |
| 67:SP:108:LYS:NZ   | 67:SP:109:PRO:HG2 | 2.28                     | 0.49              |
| 1:L5:468:C:H2'     | 1:L5:469:A:H8     | 1.77                     | 0.48              |
| 5:LA:226:ARG:HG3   | 5:LA:228:ASP:H    | 1.78                     | 0.48              |
| 10:Ld:32:ARG:HB3   | 10:Ld:48:GLU:HG3  | 1.95                     | 0.48              |
| 46:S2:1299:G:H4'   | 67:SP:78:THR:HA   | 1.95                     | 0.48              |
| 73:SV:2:GLN:HE21   | 73:SV:8:PHE:HE1   | 1.60                     | 0.48              |
| 1:L5:925:G:H2'     | 1:L5:926:G:H5'    | 1.94                     | 0.48              |
| 1:L5:1026:C:H2'    | 1:L5:1027:G:H8    | 1.77                     | 0.48              |
| 1:L5:2168:C:H2'    | 1:L5:2169:A:H8    | 1.78                     | 0.48              |
| 1:L5:4073:U:H5''   | 1:L5:4074:C:H5    | 1.78                     | 0.48              |
| 11:LD:206:ASP:N    | 11:LD:206:ASP:OD1 | 2.43                     | 0.48              |
| 46:S2:501:A:H3'    | 46:S2:502:C:H6    | 1.78                     | 0.48              |
| 50:SB:125:VAL:HG22 | 50:SB:172:MET:HE3 | 1.95                     | 0.48              |
| 72:SU:38:ASP:OD1   | 72:SU:41:ARG:NH2  | 2.26                     | 0.48              |
| 72:SU:46:LYS:HB2   | 72:SU:46:LYS:HE2  | 1.64                     | 0.48              |
| 7:LB:300:LYS:C     | 7:LB:302:ASN:H    | 2.20                     | 0.48              |
| 38:LS:69:GLU:OE1   | 38:LS:101:THR:HA  | 2.12                     | 0.48              |
| 46:S2:145:G:H2'    | 46:S2:146:G:H8    | 1.74                     | 0.48              |
| 46:S2:225:C:O2'    | 46:S2:226:A:H8    | 1.91                     | 0.48              |
| 64:SL:104:LYS:O    | 76:SX:11:ARG:NH2  | 2.36                     | 0.48              |
| 65:SN:115:LEU:O    | 65:SN:119:GLU:HG3 | 2.14                     | 0.48              |
| 66:SO:103:ASN:HB3  | 66:SO:142:ARG:HD3 | 1.96                     | 0.48              |
| 9:LC:150:LEU:HB3   | 9:LC:151:PRO:HD3  | 1.95                     | 0.48              |
| 35:LQ:122:THR:OG1  | 35:LQ:125:GLN:OE1 | 2.28                     | 0.48              |
| 46:S2:97:U:H4'     | 46:S2:98:C:OP2    | 2.13                     | 0.48              |
| 46:S2:833:G:N2     | 46:S2:842:G:H22   | 2.11                     | 0.48              |
| 46:S2:893:U:O2'    | 46:S2:894:U:O5'   | 2.30                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:1258:G:H1     | 1:L5:1904:C:H42    | 1.60                     | 0.48              |
| 1:L5:2356:G:H2'    | 1:L5:2357:C:C6     | 2.49                     | 0.48              |
| 1:L5:4024:G:O2'    | 1:L5:4025:U:OP2    | 2.27                     | 0.48              |
| 7:LB:206:PRO:HG2   | 7:LB:209:GLN:HG3   | 1.96                     | 0.48              |
| 28:LM:104:MET:HG2  | 28:LM:108:ASP:HB2  | 1.94                     | 0.48              |
| 46:S2:86:C:O2      | 46:S2:86:C:H2'     | 2.11                     | 0.48              |
| 46:S2:111:A:O2'    | 46:S2:112:U:H5'    | 2.14                     | 0.48              |
| 46:S2:599:G:O2'    | 46:S2:600:A:OP1    | 2.30                     | 0.48              |
| 46:S2:1476:G:HO2'  | 46:S2:1477:A:P     | 2.35                     | 0.48              |
| 64:SL:59:LYS:HG2   | 64:SL:134:LEU:HD22 | 1.94                     | 0.48              |
| 1:L5:3568:C:H2'    | 1:L5:3569:U:H6     | 1.79                     | 0.48              |
| 7:LB:297:LYS:HE3   | 7:LB:297:LYS:HB3   | 1.73                     | 0.48              |
| 43:LX:148:ASP:OD1  | 43:LX:148:ASP:N    | 2.46                     | 0.48              |
| 46:S2:1302:A:H2'   | 46:S2:1303:G:H4'   | 1.95                     | 0.48              |
| 46:S2:1448:G:H2'   | 46:S2:1449:A:C8    | 2.49                     | 0.48              |
| 46:S2:1736:A:H3'   | 46:S2:1737:G:H8    | 1.79                     | 0.48              |
| 54:SD:38:GLU:OE2   | 54:SD:39:VAL:N     | 2.47                     | 0.48              |
| 77:SY:78:SER:OG    | 77:SY:79:LEU:N     | 2.46                     | 0.48              |
| 1:L5:2:G:H2'       | 1:L5:3:C:C6        | 2.49                     | 0.48              |
| 1:L5:138:C:H2'     | 1:L5:139:G:C8      | 2.45                     | 0.48              |
| 1:L5:1005:C:O2'    | 1:L5:1006:G:N3     | 2.41                     | 0.48              |
| 1:L5:2091:C:OP2    | 9:LC:195:LYS:NZ    | 2.47                     | 0.48              |
| 19:LH:15:ASN:OD1   | 19:LH:15:ASN:N     | 2.44                     | 0.48              |
| 46:S2:514:G:H5''   | 46:S2:515:U:H5     | 1.79                     | 0.48              |
| 46:S2:1407:G:H22   | 46:S2:1440:A:H2    | 1.61                     | 0.48              |
| 59:SG:147:LEU:HD21 | 59:SG:156:TYR:CZ   | 2.48                     | 0.48              |
| 9:LC:134:PRO:O     | 9:LC:138:MET:HG2   | 2.13                     | 0.48              |
| 11:LD:83:LEU:N     | 11:LD:84:PRO:HD2   | 2.28                     | 0.48              |
| 46:S2:91:A:N1      | 59:SG:88:ARG:HD3   | 2.29                     | 0.48              |
| 46:S2:514:G:H2'    | 46:S2:514:G:N3     | 2.29                     | 0.48              |
| 46:S2:1680:A:H2'   | 57:SF:60:ARG:HD2   | 1.96                     | 0.48              |
| 58:Sg:183:LYS:HG3  | 58:Sg:184:LEU:H    | 1.77                     | 0.48              |
| 68:SQ:38:PRO:HB2   | 68:SQ:40:GLU:HG3   | 1.96                     | 0.48              |
| 1:L5:1008:A:H3'    | 1:L5:1009:C:H5''   | 1.95                     | 0.48              |
| 1:L5:1589:A:H2'    | 1:L5:1592:C:C5     | 2.48                     | 0.48              |
| 23:LJ:36:ALA:O     | 23:LJ:39:VAL:HG22  | 2.14                     | 0.48              |
| 46:S2:493:C:C5     | 46:S2:507:G:H4'    | 2.48                     | 0.48              |
| 46:S2:1228:G:C2    | 46:S2:1229:A:C8    | 3.02                     | 0.48              |
| 46:S2:1323:G:OP2   | 46:S2:1323:G:N2    | 2.38                     | 0.48              |
| 58:Sg:11:LEU:HB2   | 58:Sg:307:VAL:HB   | 1.96                     | 0.48              |
| 58:Sg:288:SER:O    | 58:Sg:289:LEU:HD23 | 2.13                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:761:C:H2'     | 1:L5:762:U:C6      | 2.49                     | 0.48              |
| 32:LO:194:GLU:HA   | 32:LO:194:GLU:OE2  | 2.14                     | 0.48              |
| 38:LS:147:ASP:HB3  | 38:LS:150:ILE:HB   | 1.95                     | 0.48              |
| 46:S2:12:U:H2'     | 46:S2:13:C:C6      | 2.49                     | 0.48              |
| 46:S2:849:U:H2'    | 46:S2:850:A:H8     | 1.79                     | 0.48              |
| 51:Sc:49:PRO:HG2   | 57:SF:144:LEU:HD23 | 1.96                     | 0.48              |
| 1:L5:2345:A:H2'    | 1:L5:2346:U:H6     | 1.77                     | 0.47              |
| 1:L5:2598:A:O2'    | 1:L5:4284:G:H4'    | 2.12                     | 0.47              |
| 1:L5:3745:G:H2'    | 1:L5:3746:G:C8     | 2.49                     | 0.47              |
| 30:LN:189:ARG:HH21 | 30:LN:193:ARG:HD3  | 1.79                     | 0.47              |
| 46:S2:41:G:H1      | 46:S2:481:G:H1     | 1.62                     | 0.47              |
| 46:S2:994:G:OP1    | 46:S2:1132:G:N2    | 2.41                     | 0.47              |
| 46:S2:1276:G:H4'   | 46:S2:1277:A:C8    | 2.49                     | 0.47              |
| 70:SS:15:VAL:HB    | 70:SS:20:ILE:HD13  | 1.96                     | 0.47              |
| 1:L5:1562:G:H22    | 1:L5:1576:U:H3     | 1.62                     | 0.47              |
| 1:L5:2656:G:H3'    | 1:L5:2657:G:N2     | 2.29                     | 0.47              |
| 46:S2:953:G:H2'    | 46:S2:954:C:C6     | 2.49                     | 0.47              |
| 46:S2:1276:G:OP2   | 46:S2:1509:A:N6    | 2.48                     | 0.47              |
| 46:S2:1567:G:N7    | 71:ST:101:ARG:NH2  | 2.55                     | 0.47              |
| 46:S2:1737:G:H2'   | 46:S2:1738:G:H8    | 1.78                     | 0.47              |
| 47:Sa:90:GLU:H     | 47:Sa:90:GLU:CD    | 2.17                     | 0.47              |
| 58:Sg:227:LEU:HD23 | 58:Sg:227:LEU:HA   | 1.76                     | 0.47              |
| 59:SG:21:GLU:HA    | 59:SG:24:LEU:HD12  | 1.97                     | 0.47              |
| 66:SO:97:LEU:HD11  | 66:SO:112:ALA:HB1  | 1.96                     | 0.47              |
| 1:L5:662:C:H2'     | 1:L5:663:C:O2      | 2.14                     | 0.47              |
| 1:L5:943:A:H2'     | 1:L5:944:C:C6      | 2.49                     | 0.47              |
| 1:L5:1050:C:H2'    | 1:L5:1051:G:C8     | 2.49                     | 0.47              |
| 1:L5:1173:A:O2'    | 1:L5:1175:G:O6     | 2.19                     | 0.47              |
| 1:L5:1219:C:H2'    | 1:L5:1220:C:C6     | 2.50                     | 0.47              |
| 1:L5:1225:G:N3     | 1:L5:1304:G:O2'    | 2.47                     | 0.47              |
| 1:L5:1255:C:N3     | 1:L5:1256:C:N4     | 2.62                     | 0.47              |
| 1:L5:3518:A:H2'    | 1:L5:3519:A:C8     | 2.49                     | 0.47              |
| 27:Lm:77:ILE:HG22  | 27:Lm:78:ILE:HG13  | 1.95                     | 0.47              |
| 46:S2:34:U:O2'     | 46:S2:35:C:OP1     | 2.32                     | 0.47              |
| 58:Sg:32:LEU:HD21  | 58:Sg:71:ILE:HD12  | 1.95                     | 0.47              |
| 68:SQ:12:VAL:HG21  | 68:SQ:91:ALA:HA    | 1.96                     | 0.47              |
| 1:L5:747:G:O2'     | 1:L5:748:G:O5'     | 2.28                     | 0.47              |
| 1:L5:1542:G:H2'    | 1:L5:1543:C:C6     | 2.49                     | 0.47              |
| 1:L5:1585:U:H2'    | 1:L5:1586:C:O2     | 2.15                     | 0.47              |
| 39:LT:103:ASP:OD1  | 39:LT:104:SER:N    | 2.47                     | 0.47              |
| 54:SD:23:GLU:HG2   | 63:SK:64:TRP:CD1   | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:Sg:106:LYS:HB3  | 58:Sg:125:ARG:HB3  | 1.96                     | 0.47              |
| 63:SK:31:LYS:HD2   | 63:SK:39:ASN:HA    | 1.95                     | 0.47              |
| 1:L5:2235:C:C4     | 1:L5:2236:G:H1'    | 2.49                     | 0.47              |
| 1:L5:2296:C:H2'    | 1:L5:2297:C:C6     | 2.50                     | 0.47              |
| 1:L5:3309:A:H2'    | 1:L5:3310:A:C8     | 2.48                     | 0.47              |
| 3:L8:92:U:H2'      | 3:L8:93:C:O4'      | 2.14                     | 0.47              |
| 46:S2:341:C:H2'    | 46:S2:342:C:O4'    | 2.14                     | 0.47              |
| 46:S2:1477:A:H4'   | 46:S2:1478:U:H5''  | 1.97                     | 0.47              |
| 54:SD:85:GLU:OE1   | 54:SD:85:GLU:N     | 2.47                     | 0.47              |
| 62:SJ:46:VAL:HG13  | 62:SJ:102:ILE:HD11 | 1.96                     | 0.47              |
| 75:Sx:38:A:H2'     | 75:Sx:39:A:C8      | 2.35                     | 0.47              |
| 1:L5:416:G:O2'     | 3:L8:16:G:N2       | 2.32                     | 0.47              |
| 1:L5:811:U:H2'     | 1:L5:812:G:O4'     | 2.14                     | 0.47              |
| 1:L5:4618:C:H2'    | 1:L5:4619:A:H8     | 1.79                     | 0.47              |
| 46:S2:381:G:P      | 61:SI:56:ARG:HH22  | 2.37                     | 0.47              |
| 46:S2:455:U:H2'    | 46:S2:456:A:C8     | 2.50                     | 0.47              |
| 46:S2:455:U:H2'    | 46:S2:456:A:H8     | 1.79                     | 0.47              |
| 46:S2:1737:G:H2'   | 46:S2:1738:G:C8    | 2.49                     | 0.47              |
| 46:S2:1799:C:H2'   | 46:S2:1800:G:O4'   | 2.14                     | 0.47              |
| 58:Sg:191:HIS:CD2  | 58:Sg:195:LEU:HD21 | 2.49                     | 0.47              |
| 65:SN:39:LYS:NZ    | 65:SN:39:LYS:HB3   | 2.30                     | 0.47              |
| 1:L5:2168:C:H2'    | 1:L5:2169:A:C8     | 2.50                     | 0.47              |
| 1:L5:3518:A:H2'    | 1:L5:3519:A:H8     | 1.80                     | 0.47              |
| 1:L5:3567:C:H2'    | 1:L5:3568:C:C6     | 2.49                     | 0.47              |
| 1:L5:3587:U:H3     | 1:L5:3833:G:H1     | 1.60                     | 0.47              |
| 1:L5:4254:U:H2'    | 1:L5:4255:A:H8     | 1.80                     | 0.47              |
| 2:L7:4:U:H2'       | 2:L7:5:A:C8        | 2.50                     | 0.47              |
| 11:LD:208:MET:HB3  | 11:LD:233:PRO:HG3  | 1.97                     | 0.47              |
| 32:LO:105:LEU:HD22 | 32:LO:109:PRO:HG2  | 1.96                     | 0.47              |
| 46:S2:120:U:H3     | 56:SE:34:GLY:HA2   | 1.79                     | 0.47              |
| 46:S2:448:A:H4'    | 56:SE:3:ARG:HG2    | 1.96                     | 0.47              |
| 46:S2:1266:A:N3    | 46:S2:1266:A:H2'   | 2.29                     | 0.47              |
| 46:S2:1277:A:C4    | 46:S2:1324:U:H1'   | 2.50                     | 0.47              |
| 46:S2:1753:C:H4'   | 46:S2:1783:G:N2    | 2.28                     | 0.47              |
| 52:SC:106:VAL:HG22 | 52:SC:128:VAL:HG22 | 1.97                     | 0.47              |
| 59:SG:21:GLU:OE1   | 59:SG:21:GLU:N     | 2.47                     | 0.47              |
| 78:SZ:55:TYR:O     | 78:SZ:55:TYR:HD1   | 1.97                     | 0.47              |
| 79:S7:15:A:H2'     | 79:S7:16:G:O4'     | 2.14                     | 0.47              |
| 1:L5:829:G:C2'     | 1:L5:830:C:H5'     | 2.45                     | 0.47              |
| 1:L5:1745:A:H2'    | 1:L5:1746:A:H8     | 1.79                     | 0.47              |
| 1:L5:2498:A:H2'    | 1:L5:2499:A:C8     | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:LC:317:ASN:HD22  | 9:LC:320:LYS:HD3   | 1.79                     | 0.47              |
| 13:LE:138:LYS:HD3  | 13:LE:138:LYS:N    | 2.30                     | 0.47              |
| 46:S2:315:U:H2'    | 46:S2:316:C:C5     | 2.50                     | 0.47              |
| 46:S2:944:U:O2'    | 66:SO:135:ILE:O    | 2.33                     | 0.47              |
| 46:S2:1279:A:N6    | 46:S2:1321:G:H22   | 2.13                     | 0.47              |
| 54:SD:127:MET:HE3  | 54:SD:127:MET:HB3  | 1.81                     | 0.47              |
| 67:SP:21:ASP:OD1   | 67:SP:22:LEU:N     | 2.45                     | 0.47              |
| 74:SW:76:SER:HB3   | 74:SW:77:PRO:HD3   | 1.96                     | 0.47              |
| 1:L5:468:C:H2'     | 1:L5:469:A:C8      | 2.50                     | 0.47              |
| 1:L5:3313:A:H2'    | 1:L5:3314:U:C6     | 2.50                     | 0.47              |
| 1:L5:3904:A:O2'    | 1:L5:3905:C:O2     | 2.24                     | 0.47              |
| 1:L5:4526:G:OP2    | 28:LM:120:ASN:ND2  | 2.43                     | 0.47              |
| 18:Lh:8:ASP:O      | 18:Lh:12:LYS:NZ    | 2.44                     | 0.47              |
| 21:LI:182:GLU:O    | 21:LI:185:VAL:HG12 | 2.15                     | 0.47              |
| 23:LJ:38:LYS:HE3   | 23:LJ:38:LYS:HB3   | 1.71                     | 0.47              |
| 46:S2:172:U:O4'    | 46:S2:315:U:O2'    | 2.33                     | 0.47              |
| 46:S2:844:C:OP1    | 56:SE:240:ARG:NH1  | 2.48                     | 0.47              |
| 48:SA:5:LEU:O      | 48:SA:9:GLN:NE2    | 2.33                     | 0.47              |
| 58:Sg:92:LEU:HD23  | 58:Sg:93:THR:H     | 1.80                     | 0.47              |
| 1:L5:174:C:H2'     | 1:L5:175:C:C6      | 2.50                     | 0.47              |
| 1:L5:1476:C:H2'    | 1:L5:1477:C:H6     | 1.79                     | 0.47              |
| 21:LI:190:LEU:HD23 | 21:LI:199:TYR:HA   | 1.97                     | 0.47              |
| 40:LU:101:ARG:O    | 40:LU:112:LEU:HA   | 2.15                     | 0.47              |
| 48:SA:163:CYS:C    | 48:SA:164:ASN:HD22 | 2.16                     | 0.47              |
| 1:L5:324:U:H2'     | 1:L5:325:C:C6      | 2.50                     | 0.46              |
| 1:L5:4612:C:H2'    | 1:L5:4613:U:C6     | 2.50                     | 0.46              |
| 9:LC:163:LYS:HB2   | 9:LC:166:GLU:HG3   | 1.97                     | 0.46              |
| 46:S2:1099:C:H2'   | 46:S2:1100:G:C8    | 2.49                     | 0.46              |
| 46:S2:1319:G:H2'   | 46:S2:1320:U:C6    | 2.50                     | 0.46              |
| 66:SO:27:VAL:H     | 66:SO:91:THR:HG22  | 1.77                     | 0.46              |
| 1:L5:132:G:H3'     | 1:L5:133:C:H4'     | 1.97                     | 0.46              |
| 1:L5:3567:C:H2'    | 1:L5:3568:C:H6     | 1.79                     | 0.46              |
| 1:L5:3996:U:O2'    | 31:Lo:31:ASP:OD2   | 2.31                     | 0.46              |
| 1:L5:4427:C:H5     | 1:L5:4428:C:H5     | 1.63                     | 0.46              |
| 23:LJ:12:MET:HE2   | 23:LJ:12:MET:HA    | 1.98                     | 0.46              |
| 41:LV:30:ASP:N     | 41:LV:30:ASP:OD1   | 2.47                     | 0.46              |
| 46:S2:58:C:N4      | 46:S2:62:G:O6      | 2.47                     | 0.46              |
| 46:S2:126:G:C8     | 59:SG:195:LYS:HB3  | 2.50                     | 0.46              |
| 70:SS:111:LEU:HA   | 70:SS:111:LEU:HD13 | 1.72                     | 0.46              |
| 1:L5:1010:U:H3     | 1:L5:1013:C:HO2'   | 1.61                     | 0.46              |
| 1:L5:4247:U:H2'    | 1:L5:4248:G:C8     | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:LT:107:LYS:HE3  | 39:LT:107:LYS:HB3  | 1.78                     | 0.46              |
| 46:S2:219:A:C5     | 46:S2:220:U:C4     | 3.03                     | 0.46              |
| 46:S2:619:C:H41    | 76:SX:67:ARG:HH22  | 1.63                     | 0.46              |
| 46:S2:1398:U:C2    | 46:S2:1443:U:H5'   | 2.50                     | 0.46              |
| 48:SA:158:ASP:N    | 48:SA:158:ASP:OD1  | 2.47                     | 0.46              |
| 57:SF:47:LYS:NZ    | 68:SQ:116:ASP:OD1  | 2.41                     | 0.46              |
| 1:L5:297:G:OP1     | 30:LN:179:LYS:HD3  | 2.14                     | 0.46              |
| 1:L5:299:A:H2'     | 1:L5:300:G:C8      | 2.50                     | 0.46              |
| 1:L5:738:G:OP2     | 15:LF:98:ARG:NE    | 2.46                     | 0.46              |
| 1:L5:4676:G:H1'    | 1:L5:4677:C:C6     | 2.51                     | 0.46              |
| 46:S2:126:G:C8     | 59:SG:195:LYS:HD3  | 2.49                     | 0.46              |
| 46:S2:833:G:H1     | 46:S2:842:G:H22    | 1.63                     | 0.46              |
| 46:S2:858:U:H2'    | 46:S2:859:A:C8     | 2.50                     | 0.46              |
| 46:S2:1417:C:N3    | 46:S2:1425:G:N2    | 2.55                     | 0.46              |
| 52:SC:77:SER:OG    | 52:SC:79:GLU:HG2   | 2.16                     | 0.46              |
| 52:SC:257:LYS:O    | 73:SV:16:LYS:NZ    | 2.35                     | 0.46              |
| 60:SH:127:ASP:OD1  | 60:SH:142:LYS:NZ   | 2.49                     | 0.46              |
| 72:SU:40:ILE:HD12  | 72:SU:53:PRO:HD3   | 1.98                     | 0.46              |
| 76:SX:128:VAL:HG23 | 76:SX:129:SER:H    | 1.80                     | 0.46              |
| 77:SY:110:ARG:HD3  | 77:SY:127:ALA:HB3  | 1.97                     | 0.46              |
| 1:L5:460:G:H2'     | 1:L5:461:G:C8      | 2.50                     | 0.46              |
| 1:L5:2316:G:H21    | 1:L5:2323:G:H1     | 1.64                     | 0.46              |
| 11:LD:103:LEU:O    | 11:LD:107:ARG:HG2  | 2.15                     | 0.46              |
| 46:S2:1278:C:C4    | 46:S2:1279:A:C8    | 3.04                     | 0.46              |
| 58:Sg:77:PHE:HB3   | 58:Sg:89:LEU:HD11  | 1.97                     | 0.46              |
| 74:SW:80:ASP:OD1   | 74:SW:80:ASP:N     | 2.39                     | 0.46              |
| 1:L5:1562:G:H3'    | 1:L5:1563:G:C8     | 2.51                     | 0.46              |
| 18:Lh:122:LYS:O    | 26:LL:123:LYS:HD2  | 2.16                     | 0.46              |
| 42:LW:25:ASP:OD1   | 42:LW:27:LYS:HG3   | 2.15                     | 0.46              |
| 46:S2:488:U:H4'    | 46:S2:490:A:H8     | 1.81                     | 0.46              |
| 46:S2:829:G:N2     | 46:S2:831:A:O2'    | 2.48                     | 0.46              |
| 46:S2:1140:C:H2'   | 46:S2:1141:G:O4'   | 2.16                     | 0.46              |
| 46:S2:1204:G:H2'   | 46:S2:1205:A:C8    | 2.51                     | 0.46              |
| 46:S2:1297:U:O4'   | 67:SP:59:ARG:HD2   | 2.15                     | 0.46              |
| 46:S2:1458:U:H2'   | 46:S2:1459:G:C8    | 2.51                     | 0.46              |
| 54:SD:38:GLU:OE2   | 54:SD:40:ARG:N     | 2.49                     | 0.46              |
| 57:SF:42:LYS:HG3   | 57:SF:43:GLU:OE1   | 2.15                     | 0.46              |
| 1:L5:1902:A:H2'    | 1:L5:1903:A:C8     | 2.51                     | 0.46              |
| 1:L5:4418:A:N1     | 19:LH:60:TRP:HB2   | 2.31                     | 0.46              |
| 8:Lc:20:LEU:HD23   | 8:Lc:101:ASP:CB    | 2.41                     | 0.46              |
| 11:LD:231:VAL:O    | 11:LD:231:VAL:HG12 | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:LE:53:ARG:HH11  | 13:LE:73:LYS:HG2   | 1.80                     | 0.46              |
| 18:Lh:103:LYS:NZ   | 18:Lh:111:GLU:OE1  | 2.49                     | 0.46              |
| 30:LN:200:LEU:HD22 | 30:LN:204:ARG:HD3  | 1.96                     | 0.46              |
| 41:LV:97:TYR:OH    | 42:LW:37:GLU:OE2   | 2.16                     | 0.46              |
| 46:S2:28:U:H2'     | 46:S2:29:G:C8      | 2.50                     | 0.46              |
| 46:S2:53:C:H2'     | 46:S2:54:A:H8      | 1.79                     | 0.46              |
| 46:S2:795:A:H2'    | 46:S2:796:A:C8     | 2.51                     | 0.46              |
| 51:Sc:47:LYS:NZ    | 57:SF:126:THR:OG1  | 2.31                     | 0.46              |
| 53:Sd:3:HIS:O      | 53:Sd:6:LEU:N      | 2.49                     | 0.46              |
| 59:SG:120:ASP:HB3  | 59:SG:125:THR:HG21 | 1.98                     | 0.46              |
| 60:SH:43:LEU:HB3   | 60:SH:72:PHE:CE2   | 2.51                     | 0.46              |
| 77:SY:107:ARG:HH11 | 77:SY:107:ARG:HB2  | 1.80                     | 0.46              |
| 1:L5:1003:G:H3'    | 1:L5:1004:G:H8     | 1.80                     | 0.46              |
| 7:LB:86:VAL:HG12   | 7:LB:201:LEU:HD12  | 1.97                     | 0.46              |
| 7:LB:288:GLY:HA3   | 7:LB:330:PHE:CE1   | 2.50                     | 0.46              |
| 12:Le:12:ILE:HD12  | 12:Le:66:THR:HG23  | 1.98                     | 0.46              |
| 19:LH:140:GLN:HB3  | 19:LH:143:GLU:HG2  | 1.98                     | 0.46              |
| 43:LX:114:LYS:HE3  | 43:LX:114:LYS:HB3  | 1.70                     | 0.46              |
| 46:S2:1713:A:H2'   | 46:S2:1714:C:C6    | 2.50                     | 0.46              |
| 56:SE:44:LEU:HD23  | 56:SE:44:LEU:HA    | 1.84                     | 0.46              |
| 1:L5:1355:U:H3     | 1:L5:1432:G:H1     | 1.62                     | 0.46              |
| 40:LU:66:SER:O     | 40:LU:66:SER:OG    | 2.30                     | 0.46              |
| 46:S2:61:A:N6      | 46:S2:503:C:OP2    | 2.49                     | 0.46              |
| 46:S2:96:C:H42     | 46:S2:434:A:H61    | 1.64                     | 0.46              |
| 46:S2:526:A:C2     | 46:S2:591:A:N6     | 2.84                     | 0.46              |
| 46:S2:832:G:H2'    | 46:S2:833:G:H8     | 1.81                     | 0.46              |
| 57:SF:100:ILE:HG23 | 57:SF:178:ILE:HD11 | 1.97                     | 0.46              |
| 1:L5:2091:C:C5     | 9:LC:191:ALA:HB2   | 2.50                     | 0.46              |
| 1:L5:4549:G:H1'    | 1:L5:4550:G:H1'    | 1.98                     | 0.46              |
| 7:LB:329:ASP:OD1   | 7:LB:329:ASP:N     | 2.47                     | 0.46              |
| 19:LH:59:LYS:HA    | 19:LH:59:LYS:HD2   | 1.65                     | 0.46              |
| 23:LJ:56:THR:HG22  | 23:LJ:64:ARG:H     | 1.80                     | 0.46              |
| 76:SX:61:GLN:HB3   | 76:SX:62:PRO:HD3   | 1.97                     | 0.46              |
| 1:L5:1509:U:H2'    | 1:L5:1510:C:C6     | 2.51                     | 0.45              |
| 1:L5:3841:U:H2'    | 1:L5:3842:U:C6     | 2.51                     | 0.45              |
| 1:L5:4112:U:H2'    | 1:L5:4113:U:C6     | 2.50                     | 0.45              |
| 1:L5:4171:A:OP2    | 7:LB:258:HIS:HB2   | 2.16                     | 0.45              |
| 40:LU:49:VAL:HG12  | 40:LU:50:ASN:H     | 1.81                     | 0.45              |
| 46:S2:102:A:OP1    | 61:SI:19:LYS:HD3   | 2.16                     | 0.45              |
| 46:S2:369:U:H2'    | 46:S2:370:C:C5     | 2.51                     | 0.45              |
| 46:S2:508:G:N7     | 56:SE:27:PHE:HE2   | 2.13                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:SE:72:ILE:HB   | 56:SE:77:ARG:HG3   | 1.98                     | 0.45              |
| 58:Sg:44:LYS:HB3  | 58:Sg:54:ILE:HG22  | 1.99                     | 0.45              |
| 59:SG:20:ASP:HB3  | 59:SG:22:ARG:HG2   | 1.98                     | 0.45              |
| 61:SI:87:ASN:HB3  | 61:SI:90:LEU:HG    | 1.97                     | 0.45              |
| 79:S6:43:G:H2'    | 79:S6:44:A:C8      | 2.51                     | 0.45              |
| 1:L5:828:C:H3'    | 1:L5:829:G:N2      | 2.30                     | 0.45              |
| 1:L5:1182:U:O2'   | 1:L5:1184:C:OP2    | 2.33                     | 0.45              |
| 1:L5:3308:A:H5'   | 5:LA:199:VAL:HG12  | 1.98                     | 0.45              |
| 1:L5:4290:G:H2'   | 1:L5:4291:U:C6     | 2.52                     | 0.45              |
| 7:LB:300:LYS:C    | 7:LB:302:ASN:N     | 2.74                     | 0.45              |
| 10:Ld:64:ILE:HG23 | 10:Ld:68:LEU:HD23  | 1.97                     | 0.45              |
| 15:LF:81:LYS:HE2  | 15:LF:81:LYS:HB3   | 1.86                     | 0.45              |
| 46:S2:1554:C:H41  | 54:SD:76:ARG:HH22  | 1.63                     | 0.45              |
| 46:S2:1582:C:H5'' | 46:S2:1583:C:H5    | 1.81                     | 0.45              |
| 58:Sg:172:LYS:HE2 | 58:Sg:172:LYS:HB3  | 1.84                     | 0.45              |
| 62:SJ:95:ASP:OD1  | 62:SJ:95:ASP:N     | 2.49                     | 0.45              |
| 80:Z:-18:UNK:O    | 80:Z:-17:UNK:CB    | 2.64                     | 0.45              |
| 1:L5:1431:G:H1'   | 1:L5:2270:A:N6     | 2.31                     | 0.45              |
| 1:L5:2311:U:H3    | 1:L5:2518:A:H2     | 1.63                     | 0.45              |
| 1:L5:3368:A:H1'   | 46:S2:971:G:C4     | 2.52                     | 0.45              |
| 3:L8:6:C:H2'      | 3:L8:7:U:H6        | 1.82                     | 0.45              |
| 7:LB:107:ALA:HB2  | 7:LB:201:LEU:HG    | 1.98                     | 0.45              |
| 9:LC:294:LYS:HE2  | 9:LC:294:LYS:HB3   | 1.60                     | 0.45              |
| 13:LE:138:LYS:HD3 | 13:LE:138:LYS:H    | 1.82                     | 0.45              |
| 15:LF:204:PHE:CD1 | 15:LF:222:ARG:HD2  | 2.51                     | 0.45              |
| 19:LH:151:ILE:O   | 19:LH:155:SER:OG   | 2.29                     | 0.45              |
| 46:S2:619:C:H41   | 76:SH:67:ARG:NH2   | 2.13                     | 0.45              |
| 46:S2:869:G:C5    | 60:SH:115:LYS:HG3  | 2.51                     | 0.45              |
| 46:S2:923:A:OP1   | 74:SW:28:ARG:NH2   | 2.47                     | 0.45              |
| 48:SA:34:MET:HE2  | 48:SA:149:ASN:O    | 2.17                     | 0.45              |
| 54:SD:135:GLU:HG3 | 54:SD:153:VAL:HG22 | 1.98                     | 0.45              |
| 60:SH:60:ILE:HD11 | 60:SH:92:VAL:HG22  | 1.97                     | 0.45              |
| 1:L5:676:C:H5'    | 9:LC:6:PRO:HB3     | 1.97                     | 0.45              |
| 1:L5:1009:C:N4    | 1:L5:1017:A:H61    | 2.11                     | 0.45              |
| 1:L5:2342:C:OP1   | 1:L5:2522:C:O2'    | 2.33                     | 0.45              |
| 44:LY:54:GLU:HB2  | 44:LY:108:ARG:HB3  | 1.98                     | 0.45              |
| 45:LZ:29:ILE:HG13 | 45:LZ:40:HIS:NE2   | 2.31                     | 0.45              |
| 46:S2:539:U:H2'   | 46:S2:540:C:O4'    | 2.15                     | 0.45              |
| 46:S2:675:C:H2'   | 46:S2:676:U:C6     | 2.51                     | 0.45              |
| 46:S2:1546:A:H2'  | 46:S2:1547:G:C8    | 2.51                     | 0.45              |
| 58:Sg:74:ASP:OD1  | 58:Sg:74:ASP:N     | 2.50                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:1010:U:N3     | 1:L5:1013:C:O2'    | 2.49                     | 0.45              |
| 1:L5:1157:A:OP1    | 30:LN:204:ARG:HD2  | 2.17                     | 0.45              |
| 1:L5:1377:A:P      | 1:L5:1377:A:H8     | 2.39                     | 0.45              |
| 24:Lk:19:ASP:OD1   | 24:Lk:19:ASP:N     | 2.48                     | 0.45              |
| 33:Lp:38:THR:HA    | 33:Lp:45:THR:HA    | 1.98                     | 0.45              |
| 37:LR:154:LEU:HD12 | 37:LR:154:LEU:HA   | 1.83                     | 0.45              |
| 41:LV:48:ARG:HG2   | 41:LV:48:ARG:HH11  | 1.80                     | 0.45              |
| 46:S2:1270:G:H22   | 46:S2:1515:G:N2    | 2.15                     | 0.45              |
| 46:S2:1407:G:H2'   | 46:S2:1408:U:C6    | 2.52                     | 0.45              |
| 46:S2:1532:A:H2'   | 46:S2:1533:C:C6    | 2.51                     | 0.45              |
| 51:Sc:16:LYS:H     | 51:Sc:16:LYS:HD3   | 1.82                     | 0.45              |
| 66:SO:75:MET:HE3   | 66:SO:75:MET:HB2   | 1.77                     | 0.45              |
| 1:L5:754:A:H2'     | 1:L5:755:A:C8      | 2.52                     | 0.45              |
| 1:L5:2224:U:H4'    | 1:L5:2225:U:H5'    | 1.98                     | 0.45              |
| 1:L5:2406:G:C6     | 16:Lg:50:PRO:HG3   | 2.51                     | 0.45              |
| 1:L5:3712:C:H2'    | 1:L5:3713:A:C5     | 2.51                     | 0.45              |
| 3:L8:128:C:H2'     | 3:L8:129:C:C6      | 2.51                     | 0.45              |
| 7:LB:135:LYS:O     | 7:LB:138:GLN:NE2   | 2.49                     | 0.45              |
| 7:LB:300:LYS:O     | 7:LB:302:ASN:N     | 2.49                     | 0.45              |
| 21:LI:188:LYS:HB3  | 21:LI:212:LEU:HD11 | 1.98                     | 0.45              |
| 46:S2:126:G:C2     | 46:S2:181:A:H4'    | 2.51                     | 0.45              |
| 46:S2:149:A:C8     | 46:S2:170:A:C8     | 3.05                     | 0.45              |
| 46:S2:1209:A:OP2   | 46:S2:1836:A:O2'   | 2.31                     | 0.45              |
| 46:S2:1719:G:O4'   | 46:S2:1817:G:N2    | 2.49                     | 0.45              |
| 52:SC:211:LYS:HE3  | 52:SC:211:LYS:HB2  | 1.64                     | 0.45              |
| 57:SF:204:ARG:HD2  | 57:SF:204:ARG:HA   | 1.73                     | 0.45              |
| 78:SZ:58:LEU:O     | 78:SZ:62:VAL:HG12  | 2.16                     | 0.45              |
| 1:L5:679:G:H2'     | 1:L5:680:C:C6      | 2.51                     | 0.45              |
| 1:L5:1147:C:H2'    | 1:L5:1148:A:C8     | 2.51                     | 0.45              |
| 1:L5:1447:G:H5'    | 1:L5:1448:A:OP1    | 2.17                     | 0.45              |
| 1:L5:2301:G:N2     | 3:L8:126:C:OP1     | 2.37                     | 0.45              |
| 21:LI:38:ARG:HD3   | 21:LI:83:ASP:HB3   | 1.98                     | 0.45              |
| 40:LU:65:ARG:HD2   | 40:LU:67:LYS:H     | 1.80                     | 0.45              |
| 46:S2:320:C:N4     | 59:SG:186:GLN:OE1  | 2.50                     | 0.45              |
| 46:S2:964:A:H2'    | 46:S2:965:A:C8     | 2.51                     | 0.45              |
| 46:S2:997:A:H2'    | 46:S2:998:A:C8     | 2.52                     | 0.45              |
| 46:S2:1165:G:O2'   | 46:S2:1166:G:H5'   | 2.16                     | 0.45              |
| 46:S2:1379:A:H4'   | 46:S2:1380:A:O5'   | 2.17                     | 0.45              |
| 48:SA:41:ARG:HD3   | 48:SA:47:TYR:CZ    | 2.52                     | 0.45              |
| 58:Sg:212:LYS:HE3  | 58:Sg:212:LYS:HB2  | 1.75                     | 0.45              |
| 60:SH:158:LEU:HD23 | 60:SH:158:LEU:HA   | 1.85                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:ST:113:VAL:HG12 | 71:ST:123:LEU:HD12 | 1.99                     | 0.45              |
| 79:S6:4:C:H2'      | 79:S6:5:A:H8       | 1.82                     | 0.45              |
| 1:L5:2497:A:H2'    | 1:L5:2498:A:C8     | 2.51                     | 0.45              |
| 1:L5:2569:A:H2'    | 1:L5:2570:G:C8     | 2.52                     | 0.45              |
| 1:L5:3577:U:H2'    | 1:L5:3578:U:C6     | 2.52                     | 0.45              |
| 1:L5:3603:G:H1     | 1:L5:3718:U:H3     | 1.65                     | 0.45              |
| 9:LC:25:PRO:HG2    | 9:LC:28:PHE:HE2    | 1.82                     | 0.45              |
| 18:Lh:74:LYS:HE2   | 18:Lh:74:LYS:HB2   | 1.69                     | 0.45              |
| 37:LR:171:LYS:HD3  | 37:LR:171:LYS:HA   | 1.73                     | 0.45              |
| 46:S2:39:A:N6      | 46:S2:516:G:H1'    | 2.32                     | 0.45              |
| 46:S2:1279:A:H61   | 46:S2:1321:G:H1    | 1.65                     | 0.45              |
| 46:S2:1294:A:H2'   | 46:S2:1295:G:C8    | 2.52                     | 0.45              |
| 46:S2:1399:G:H1'   | 58:Sg:63:SER:HB2   | 1.98                     | 0.45              |
| 48:SA:127:PRO:HG2  | 48:SA:152:SER:HB2  | 1.98                     | 0.45              |
| 60:SH:58:LYS:HB2   | 60:SH:90:LYS:HD3   | 1.98                     | 0.45              |
| 63:SK:17:LYS:HD3   | 63:SK:18:GLU:HG3   | 1.98                     | 0.45              |
| 70:SS:6:PRO:HD3    | 78:SZ:49:LEU:HD23  | 1.99                     | 0.45              |
| 72:SU:32:LEU:CD2   | 72:SU:87:ARG:HG3   | 2.46                     | 0.45              |
| 77:SY:110:ARG:HD2  | 77:SY:114:MET:HG2  | 1.98                     | 0.45              |
| 1:L5:2221:C:O2'    | 1:L5:2222:C:H6     | 1.99                     | 0.45              |
| 1:L5:3430:U:H2'    | 1:L5:3432:A:H2     | 1.81                     | 0.45              |
| 11:LD:66:TYR:CE2   | 11:LD:68:ARG:HD3   | 2.52                     | 0.45              |
| 11:LD:181:PRO:HD2  | 11:LD:195:HIS:ND1  | 2.31                     | 0.45              |
| 17:LG:205:THR:HG22 | 17:LG:206:GLN:H    | 1.81                     | 0.45              |
| 46:S2:54:A:H2'     | 46:S2:54:A:N3      | 2.32                     | 0.45              |
| 46:S2:158:A:H2'    | 46:S2:159:A:O4'    | 2.17                     | 0.45              |
| 46:S2:171:A:OP1    | 59:SG:137:ARG:NH1  | 2.36                     | 0.45              |
| 46:S2:530:A:N6     | 46:S2:557:U:O4     | 2.49                     | 0.45              |
| 46:S2:795:A:O2'    | 46:S2:796:A:O4'    | 2.27                     | 0.45              |
| 61:SI:172:LEU:HD13 | 61:SI:190:LEU:HD12 | 1.99                     | 0.45              |
| 62:SJ:31:LEU:HD21  | 62:SJ:103:GLU:OE2  | 2.17                     | 0.45              |
| 72:SU:34:LYS:HE3   | 72:SU:34:LYS:HB3   | 1.54                     | 0.45              |
| 78:SZ:62:VAL:HA    | 78:SZ:65:TYR:CZ    | 2.51                     | 0.45              |
| 79:S6:32:C:H42     | 79:S6:38:A:N6      | 2.15                     | 0.45              |
| 79:S6:41:C:H2'     | 79:S6:42:A:C8      | 2.50                     | 0.45              |
| 1:L5:425:A:N1      | 3:L8:8:U:H5        | 2.13                     | 0.45              |
| 1:L5:1376:G:O2'    | 1:L5:1377:A:N7     | 2.45                     | 0.45              |
| 1:L5:3341:G:H2'    | 1:L5:3342:C:C6     | 2.51                     | 0.45              |
| 1:L5:3522:A:H2'    | 1:L5:3523:C:H6     | 1.82                     | 0.45              |
| 13:LE:78:ARG:HA    | 13:LE:78:ARG:HD2   | 1.73                     | 0.45              |
| 23:LJ:144:LYS:O    | 23:LJ:148:THR:OG1  | 2.35                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:Lo:74:GLU:OE1   | 31:Lo:76:ASN:N     | 2.49                     | 0.45              |
| 46:S2:926:G:H1     | 46:S2:1018:U:H3    | 1.65                     | 0.45              |
| 46:S2:1682:U:H2'   | 46:S2:1683:C:C6    | 2.52                     | 0.45              |
| 46:S2:1720:A:N6    | 46:S2:1815:G:C2    | 2.82                     | 0.45              |
| 68:SQ:43:GLU:HB3   | 68:SQ:44:PRO:HD2   | 1.98                     | 0.45              |
| 72:SU:40:ILE:HG23  | 72:SU:50:VAL:HG21  | 1.98                     | 0.45              |
| 1:L5:1148:A:H2'    | 1:L5:1149:A:H8     | 1.80                     | 0.44              |
| 1:L5:1523:C:H5''   | 1:L5:1524:G:N7     | 2.32                     | 0.44              |
| 9:LC:138:MET:HE3   | 9:LC:138:MET:HB3   | 1.86                     | 0.44              |
| 13:LE:191:ARG:HA   | 13:LE:191:ARG:HD2  | 1.72                     | 0.44              |
| 17:LG:114:LEU:HD23 | 17:LG:114:LEU:HA   | 1.81                     | 0.44              |
| 23:LJ:26:VAL:O     | 23:LJ:28:GLU:N     | 2.45                     | 0.44              |
| 31:Lo:11:PHE:O     | 31:Lo:81:ARG:NH1   | 2.40                     | 0.44              |
| 32:LO:187:LYS:HB2  | 32:LO:187:LYS:HE2  | 1.42                     | 0.44              |
| 44:LY:34:LEU:HD21  | 44:LY:47:MET:HB2   | 1.98                     | 0.44              |
| 46:S2:375:G:H2'    | 46:S2:376:U:C6     | 2.52                     | 0.44              |
| 46:S2:1731:U:H2'   | 46:S2:1732:A:O4'   | 2.16                     | 0.44              |
| 54:SD:158:ILE:HG13 | 54:SD:164:VAL:HG22 | 1.98                     | 0.44              |
| 56:SE:125:LYS:HZ3  | 56:SE:157:ASN:HA   | 1.82                     | 0.44              |
| 57:SF:179:ASN:HB3  | 57:SF:187:SER:HB3  | 1.99                     | 0.44              |
| 58:Sg:166:VAL:HG12 | 58:Sg:176:VAL:HG22 | 1.99                     | 0.44              |
| 67:SP:48:GLY:C     | 67:SP:50:ARG:HH12  | 2.24                     | 0.44              |
| 67:SP:110:GLU:OE1  | 70:SS:116:LYS:NZ   | 2.39                     | 0.44              |
| 72:SU:40:ILE:HD11  | 72:SU:89:ILE:HG12  | 1.98                     | 0.44              |
| 78:SZ:49:LEU:H     | 78:SZ:83:LEU:HD22  | 1.82                     | 0.44              |
| 1:L5:162:A:H2'     | 1:L5:163:A:H8      | 1.82                     | 0.44              |
| 1:L5:4175:G:O2'    | 1:L5:4178:C:OP2    | 2.30                     | 0.44              |
| 1:L5:4510:U:H2'    | 1:L5:4511:C:C6     | 2.52                     | 0.44              |
| 7:LB:238:LYS:HE2   | 7:LB:238:LYS:HB2   | 1.75                     | 0.44              |
| 11:LD:136:ASP:OD1  | 11:LD:136:ASP:N    | 2.50                     | 0.44              |
| 11:LD:232:THR:O    | 11:LD:234:ASP:N    | 2.38                     | 0.44              |
| 12:Le:81:ASN:OD1   | 12:Le:84:GLU:HG3   | 2.17                     | 0.44              |
| 18:Lh:52:LYS:HA    | 18:Lh:52:LYS:HD3   | 1.74                     | 0.44              |
| 21:LI:66:GLU:HA    | 21:LI:66:GLU:OE2   | 2.17                     | 0.44              |
| 46:S2:455:U:OP1    | 59:SG:93:LYS:HA    | 2.16                     | 0.44              |
| 46:S2:1464:U:H5''  | 46:S2:1465:C:C5    | 2.52                     | 0.44              |
| 58:Sg:245:ARG:HG2  | 58:Sg:246:TYR:H    | 1.82                     | 0.44              |
| 79:S7:15:A:C2      | 79:S7:22:G:C4      | 3.05                     | 0.44              |
| 1:L5:4637:U:O2'    | 1:L5:4638:C:H5''   | 2.17                     | 0.44              |
| 3:L8:144:U:H2'     | 3:L8:145:C:C6      | 2.52                     | 0.44              |
| 23:LJ:48:PRO:HB2   | 23:LJ:70:VAL:HG22  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:LR:98:ARG:NH2   | 37:LR:130:ASN:OD1 | 2.41                     | 0.44              |
| 46:S2:38:A:N1      | 46:S2:516:G:H2'   | 2.32                     | 0.44              |
| 46:S2:473:C:OP1    | 46:S2:475:G:N2    | 2.51                     | 0.44              |
| 46:S2:1300:A:O2'   | 46:S2:1302:A:OP1  | 2.25                     | 0.44              |
| 46:S2:1448:G:H2'   | 46:S2:1449:A:H8   | 1.82                     | 0.44              |
| 46:S2:1659:G:OP2   | 46:S2:1661:C:N4   | 2.50                     | 0.44              |
| 50:SB:40:ASN:OD1   | 50:SB:40:ASN:N    | 2.49                     | 0.44              |
| 1:L5:460:G:H2'     | 1:L5:461:G:H8     | 1.81                     | 0.44              |
| 1:L5:1675:G:O2'    | 1:L5:3872:A:N3    | 2.39                     | 0.44              |
| 1:L5:2450:A:H5''   | 24:Lk:26:LYS:HE3  | 1.99                     | 0.44              |
| 1:L5:3287:A:N1     | 1:L5:3488:U:H5    | 2.16                     | 0.44              |
| 1:L5:3408:G:N2     | 1:L5:3432:A:H8    | 2.07                     | 0.44              |
| 26:LL:121:ARG:HH11 | 26:LL:121:ARG:HG3 | 1.83                     | 0.44              |
| 46:S2:551:C:H2'    | 46:S2:552:U:C6    | 2.52                     | 0.44              |
| 46:S2:1729:U:C2    | 46:S2:1730:U:C2   | 3.06                     | 0.44              |
| 56:SE:188:ASN:HB3  | 56:SE:191:ARG:HD3 | 2.00                     | 0.44              |
| 60:SH:20:GLU:HB3   | 60:SH:24:SER:HB3  | 2.00                     | 0.44              |
| 79:S7:23:C:H2'     | 79:S7:24:G:C8     | 2.52                     | 0.44              |
| 1:L5:423:U:H2'     | 1:L5:424:U:C6     | 2.53                     | 0.44              |
| 1:L5:2439:C:H2'    | 1:L5:2440:G:O4'   | 2.18                     | 0.44              |
| 1:L5:4544:G:H2'    | 1:L5:4545:G:H8    | 1.81                     | 0.44              |
| 19:LH:59:LYS:HE3   | 19:LH:66:GLU:HB3  | 2.00                     | 0.44              |
| 46:S2:515:U:H2'    | 46:S2:516:G:H8    | 1.82                     | 0.44              |
| 46:S2:615:C:OP2    | 46:S2:627:G:O2'   | 2.27                     | 0.44              |
| 54:SD:175:VAL:HG13 | 54:SD:182:LEU:HB2 | 1.99                     | 0.44              |
| 58:Sg:35:SER:OG    | 58:Sg:36:ARG:N    | 2.49                     | 0.44              |
| 58:Sg:254:PRO:HA   | 58:Sg:285:GLN:HA  | 2.00                     | 0.44              |
| 59:SG:22:ARG:HA    | 59:SG:25:ARG:NH1  | 2.32                     | 0.44              |
| 69:SR:74:GLN:HA    | 69:SR:77:GLU:HG2  | 1.98                     | 0.44              |
| 74:SW:9:ASP:OD1    | 74:SW:9:ASP:N     | 2.47                     | 0.44              |
| 1:L5:3267:A:H2'    | 1:L5:3268:A:C8    | 2.52                     | 0.44              |
| 1:L5:3926:A:H2'    | 1:L5:3927:A:C8    | 2.53                     | 0.44              |
| 9:LC:71:ARG:NH2    | 80:Z:-6:UNK:CB    | 2.73                     | 0.44              |
| 24:Lk:55:LYS:O     | 24:Lk:59:SER:OG   | 2.31                     | 0.44              |
| 46:S2:375:G:H1'    | 64:SL:83:GLN:HE21 | 1.83                     | 0.44              |
| 46:S2:805:U:H2'    | 46:S2:806:U:C6    | 2.52                     | 0.44              |
| 58:Sg:164:ILE:HD12 | 58:Sg:164:ILE:HA  | 1.85                     | 0.44              |
| 58:Sg:257:LYS:HA   | 58:Sg:257:LYS:CE  | 2.47                     | 0.44              |
| 79:S6:31:G:H2'     | 79:S6:32:C:C6     | 2.49                     | 0.44              |
| 1:L5:143:U:H2'     | 1:L5:144:G:H5''   | 1.98                     | 0.44              |
| 1:L5:701:C:H2'     | 1:L5:702:C:C6     | 2.52                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:L8:5:U:H2'      | 3:L8:6:C:H6        | 1.82                     | 0.44              |
| 19:LH:93:ARG:HD2  | 19:LH:143:GLU:HB3  | 1.98                     | 0.44              |
| 21:LI:136:MET:HE2 | 21:LI:136:MET:HB2  | 1.85                     | 0.44              |
| 46:S2:887:A:H61   | 46:S2:902:G:H1'    | 1.82                     | 0.44              |
| 46:S2:1290:U:H2'  | 46:S2:1291:G:C8    | 2.53                     | 0.44              |
| 50:SB:131:ASP:OD1 | 50:SB:131:ASP:N    | 2.48                     | 0.44              |
| 58:Sg:212:LYS:HA  | 58:Sg:235:ILE:HA   | 1.98                     | 0.44              |
| 60:SH:75:ILE:C    | 60:SH:78:ARG:HH21  | 2.25                     | 0.44              |
| 64:SL:49:GLU:OE1  | 64:SL:49:GLU:N     | 2.44                     | 0.44              |
| 68:SQ:107:GLU:O   | 68:SQ:111:ILE:HD12 | 2.18                     | 0.44              |
| 77:SY:111:LYS:O   | 77:SY:114:MET:HB2  | 2.17                     | 0.44              |
| 1:L5:1207:A:H2'   | 1:L5:1208:G:C8     | 2.53                     | 0.44              |
| 1:L5:3379:G:H2'   | 1:L5:3380:A:C8     | 2.53                     | 0.44              |
| 1:L5:3393:A:H2'   | 1:L5:3394:A:H8     | 1.82                     | 0.44              |
| 1:L5:4560:C:H2'   | 1:L5:4561:G:H8     | 1.81                     | 0.44              |
| 2:L7:111:C:H2'    | 2:L7:112:U:O4'     | 2.18                     | 0.44              |
| 6:Lb:107:ARG:HD2  | 15:LF:63:THR:HG22  | 2.00                     | 0.44              |
| 17:LG:44:ASP:N    | 17:LG:44:ASP:OD1   | 2.51                     | 0.44              |
| 34:LP:36:ILE:HA   | 34:LP:39:MET:HE3   | 2.00                     | 0.44              |
| 44:LY:69:LYS:H    | 44:LY:83:GLU:HG2   | 1.82                     | 0.44              |
| 46:S2:484:C:H5    | 76:SX:45:SER:HG    | 1.65                     | 0.44              |
| 46:S2:1241:A:O2'  | 46:S2:1242:A:P     | 2.75                     | 0.44              |
| 66:SO:98:ARG:HG2  | 66:SO:99:ALA:N     | 2.33                     | 0.44              |
| 68:SQ:146:ARG:NH1 | 79:S7:33:C:OP2     | 2.42                     | 0.44              |
| 76:SX:77:ASN:HD22 | 76:SX:79:LYS:HD2   | 1.83                     | 0.44              |
| 78:SZ:65:TYR:CE1  | 78:SZ:68:ILE:HG22  | 2.53                     | 0.44              |
| 79:S6:4:C:H2'     | 79:S6:5:A:C8       | 2.52                     | 0.44              |
| 1:L5:1156:U:H2'   | 1:L5:1157:A:C8     | 2.53                     | 0.44              |
| 1:L5:4237:A:H2'   | 1:L5:4238:U:O4'    | 2.18                     | 0.44              |
| 31:Lo:27:LYS:HB3  | 31:Lo:27:LYS:HE2   | 1.62                     | 0.44              |
| 34:LP:94:MET:HE3  | 34:LP:94:MET:HB2   | 1.76                     | 0.44              |
| 35:LQ:10:ASP:N    | 35:LQ:10:ASP:OD1   | 2.51                     | 0.44              |
| 40:LU:39:PHE:CE1  | 40:LU:43:LEU:HD21  | 2.53                     | 0.44              |
| 46:S2:488:U:H4'   | 46:S2:490:A:C8     | 2.53                     | 0.44              |
| 46:S2:514:G:H3'   | 46:S2:515:U:C6     | 2.46                     | 0.44              |
| 46:S2:834:C:H3'   | 46:S2:835:C:H4'    | 1.99                     | 0.44              |
| 46:S2:845:U:H2'   | 46:S2:846:G:C8     | 2.53                     | 0.44              |
| 46:S2:1798:U:H2'  | 46:S2:1799:C:C6    | 2.52                     | 0.44              |
| 56:SE:171:ASP:OD1 | 56:SE:171:ASP:N    | 2.51                     | 0.44              |
| 57:SF:69:VAL:O    | 57:SF:73:THR:HG23  | 2.18                     | 0.44              |
| 58:Sg:11:LEU:HB3  | 58:Sg:43:TRP:CH2   | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:SI:110:ARG:O    | 61:SI:114:GLU:HG2  | 2.17                     | 0.44              |
| 61:SI:144:LYS:HE3  | 61:SI:144:LYS:HB3  | 1.79                     | 0.44              |
| 68:SQ:95:TYR:C     | 68:SQ:95:TYR:CD1   | 2.96                     | 0.44              |
| 71:ST:102:ARG:HA   | 71:ST:102:ARG:HD3  | 1.70                     | 0.44              |
| 79:S7:25:U:C2      | 79:S7:26:G:C8      | 3.06                     | 0.44              |
| 1:L5:23:C:H2'      | 1:L5:24:G:O4'      | 2.17                     | 0.43              |
| 1:L5:106:A:H2'     | 1:L5:107:G:O4'     | 2.18                     | 0.43              |
| 1:L5:2314:G:H22    | 1:L5:2324:G:N2     | 2.16                     | 0.43              |
| 1:L5:3430:U:C2'    | 1:L5:3432:A:H2     | 2.31                     | 0.43              |
| 1:L5:3907:G:H2'    | 1:L5:3907:G:N3     | 2.33                     | 0.43              |
| 1:L5:4125:G:O2'    | 27:Lm:100:TYR:O    | 2.36                     | 0.43              |
| 14:Lf:36:ARG:NH1   | 14:Lf:79:GLY:O     | 2.43                     | 0.43              |
| 14:Lf:63:LYS:HA    | 14:Lf:63:LYS:HD3   | 1.66                     | 0.43              |
| 46:S2:172:U:H5'    | 46:S2:315:U:O3'    | 2.18                     | 0.43              |
| 46:S2:678:G:H21    | 46:S2:1029:A:H62   | 1.66                     | 0.43              |
| 46:S2:1556:U:N3    | 53:Sd:19:ARG:HA    | 2.33                     | 0.43              |
| 46:S2:1652:A:O2'   | 57:SF:83:ASN:OD1   | 2.26                     | 0.43              |
| 50:SB:126:ASP:OD2  | 50:SB:136:ARG:NH1  | 2.51                     | 0.43              |
| 50:SB:219:LYS:HD2  | 50:SB:219:LYS:HA   | 1.87                     | 0.43              |
| 54:SD:39:VAL:O     | 54:SD:41:VAL:HG13  | 2.17                     | 0.43              |
| 59:SG:61:PHE:HD2   | 59:SG:72:ARG:HD3   | 1.83                     | 0.43              |
| 63:SK:73:ASN:O     | 63:SK:76:ILE:HG22  | 2.18                     | 0.43              |
| 73:SV:9:VAL:HG13   | 73:SV:9:VAL:O      | 2.18                     | 0.43              |
| 78:SZ:42:ASP:N     | 78:SZ:42:ASP:OD1   | 2.50                     | 0.43              |
| 1:L5:1034:G:H2'    | 1:L5:1035:U:C6     | 2.53                     | 0.43              |
| 1:L5:1882:G:H2'    | 1:L5:1883:U:C6     | 2.53                     | 0.43              |
| 1:L5:3537:G:H2'    | 1:L5:3538:G:C8     | 2.53                     | 0.43              |
| 1:L5:3739:C:H2'    | 1:L5:3740:G:C8     | 2.53                     | 0.43              |
| 9:LC:3:CYS:SG      | 9:LC:4:ALA:N       | 2.91                     | 0.43              |
| 17:LG:175:ARG:HE   | 17:LG:175:ARG:HB3  | 1.57                     | 0.43              |
| 46:S2:532:A:N6     | 46:S2:553:G:O6     | 2.50                     | 0.43              |
| 60:SH:130:LEU:HD21 | 60:SH:156:VAL:HG21 | 1.99                     | 0.43              |
| 62:SJ:83:ARG:HH21  | 62:SJ:150:ARG:NH1  | 2.16                     | 0.43              |
| 1:L5:2449:A:OP1    | 24:Lk:35:LYS:NZ    | 2.51                     | 0.43              |
| 1:L5:4070:C:H2'    | 1:L5:4071:G:O4'    | 2.19                     | 0.43              |
| 3:L8:40:A:H2'      | 3:L8:41:A:C8       | 2.52                     | 0.43              |
| 9:LC:109:ARG:O     | 9:LC:109:ARG:HG2   | 2.18                     | 0.43              |
| 19:LH:12:ILE:HD12  | 19:LH:53:LYS:C     | 2.43                     | 0.43              |
| 46:S2:151:C:O2'    | 59:SG:132:ARG:NH1  | 2.52                     | 0.43              |
| 1:L5:955:C:HO2'    | 1:L5:1028:G:H1     | 1.61                     | 0.43              |
| 1:L5:2618:A:H2'    | 1:L5:2619:U:H6     | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L5:4278:C:O2'    | 1:L5:4279:A:H5'    | 2.18                     | 0.43              |
| 3:L8:67:U:H2'      | 3:L8:68:G:H8       | 1.83                     | 0.43              |
| 6:Lb:93:ARG:HG2    | 6:Lb:93:ARG:NH1    | 2.29                     | 0.43              |
| 6:Lb:110:MET:O     | 6:Lb:114:GLN:HG2   | 2.18                     | 0.43              |
| 12:Le:32:LYS:HE2   | 12:Le:32:LYS:HB2   | 1.56                     | 0.43              |
| 46:S2:1103:G:H2'   | 46:S2:1104:C:C6    | 2.54                     | 0.43              |
| 46:S2:1227:G:N1    | 46:S2:1640:G:OP2   | 2.50                     | 0.43              |
| 50:SB:179:ASN:OD1  | 50:SB:179:ASN:N    | 2.51                     | 0.43              |
| 51:Sc:49:PRO:HB2   | 57:SF:61:PHE:CE1   | 2.53                     | 0.43              |
| 59:SG:52:ILE:HD12  | 59:SG:52:ILE:O     | 2.17                     | 0.43              |
| 64:SL:120:VAL:HG22 | 64:SL:145:VAL:HG11 | 1.99                     | 0.43              |
| 70:SS:65:GLU:O     | 70:SS:69:THR:HG22  | 2.19                     | 0.43              |
| 1:L5:950:G:H22     | 1:L5:1035:U:H3     | 1.65                     | 0.43              |
| 1:L5:954:G:H2'     | 1:L5:955:C:O4'     | 2.18                     | 0.43              |
| 1:L5:2512:G:H2'    | 1:L5:2513:G:C8     | 2.53                     | 0.43              |
| 1:L5:3574:A:H2'    | 1:L5:3575:G:H8     | 1.82                     | 0.43              |
| 1:L5:3992:A:H2'    | 1:L5:3993:U:H6     | 1.83                     | 0.43              |
| 9:LC:218:ILE:HG12  | 9:LC:229:LEU:HG    | 2.01                     | 0.43              |
| 19:LH:28:LYS:HB2   | 19:LH:28:LYS:NZ    | 2.33                     | 0.43              |
| 20:Li:81:ILE:HD12  | 20:Li:81:ILE:HA    | 1.86                     | 0.43              |
| 30:LN:140:LYS:HG3  | 30:LN:144:ARG:HD3  | 2.01                     | 0.43              |
| 56:SE:126:VAL:HG13 | 56:SE:158:ASP:H    | 1.82                     | 0.43              |
| 56:SE:212:ASP:OD1  | 56:SE:216:ASN:HB2  | 2.18                     | 0.43              |
| 56:SE:246:LEU:O    | 56:SE:247:THR:HB   | 2.18                     | 0.43              |
| 57:SF:201:LYS:HD3  | 57:SF:201:LYS:HA   | 1.61                     | 0.43              |
| 59:SG:196:LYS:HA   | 59:SG:199:THR:HG22 | 2.01                     | 0.43              |
| 75:Sx:32:A:O2'     | 75:Sx:33:U:OP2     | 2.33                     | 0.43              |
| 76:SX:60:LYS:HG3   | 76:SX:61:GLN:HG2   | 2.01                     | 0.43              |
| 1:L5:150:U:OP2     | 17:LG:200:THR:OG1  | 2.37                     | 0.43              |
| 1:L5:267:G:H2'     | 1:L5:268:G:C8      | 2.54                     | 0.43              |
| 1:L5:2337:C:OP2    | 16:Lg:76:ARG:NH1   | 2.42                     | 0.43              |
| 5:LA:14:SER:OG     | 5:LA:15:VAL:N      | 2.52                     | 0.43              |
| 30:LN:145:ASN:HB3  | 30:LN:148:THR:HG22 | 2.00                     | 0.43              |
| 40:LU:44:GLN:HG2   | 40:LU:63:ILE:HD12  | 2.01                     | 0.43              |
| 46:S2:219:A:H2'    | 46:S2:220:U:C6     | 2.53                     | 0.43              |
| 46:S2:542:U:H2'    | 46:S2:543:U:H5''   | 2.00                     | 0.43              |
| 48:SA:147:LEU:HD22 | 48:SA:163:CYS:SG   | 2.58                     | 0.43              |
| 56:SE:35:PRO:HB2   | 56:SE:143:ASP:OD1  | 2.19                     | 0.43              |
| 69:SR:33:ARG:HD2   | 69:SR:33:ARG:HA    | 1.71                     | 0.43              |
| 1:L5:1562:G:H1     | 1:L5:1576:U:H3     | 1.67                     | 0.43              |
| 1:L5:2540:C:O2'    | 1:L5:2541:A:OP2    | 2.31                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:LC:283:LYS:HD3   | 35:LQ:103:LEU:HD22 | 2.00                     | 0.43              |
| 11:LD:152:ARG:HD2  | 11:LD:154:THR:HG23 | 2.01                     | 0.43              |
| 17:LG:89:ARG:HH11  | 17:LG:89:ARG:HG3   | 1.82                     | 0.43              |
| 17:LG:132:ARG:HA   | 17:LG:132:ARG:HD2  | 1.41                     | 0.43              |
| 17:LG:162:ASP:OD1  | 17:LG:187:LYS:NZ   | 2.51                     | 0.43              |
| 19:LH:12:ILE:HG12  | 19:LH:17:GLU:OE2   | 2.19                     | 0.43              |
| 39:LT:94:GLU:OE1   | 39:LT:94:GLU:N     | 2.50                     | 0.43              |
| 46:S2:120:U:H5'    | 46:S2:121:U:H5     | 1.83                     | 0.43              |
| 1:L5:1536:G:N3     | 1:L5:3867:A:H2'    | 2.33                     | 0.43              |
| 1:L5:4148:G:C2     | 1:L5:4149:A:N7     | 2.87                     | 0.43              |
| 2:L7:12:U:OP2      | 2:L7:67:C:O2'      | 2.36                     | 0.43              |
| 2:L7:52:C:HO2'     | 2:L7:53:U:P        | 2.41                     | 0.43              |
| 3:L8:66:A:H2'      | 3:L8:67:U:C6       | 2.53                     | 0.43              |
| 8:Lc:13:SER:O      | 8:Lc:17:ARG:HG3    | 2.19                     | 0.43              |
| 14:Lf:110:ILE:HD13 | 14:Lf:110:ILE:HA   | 1.90                     | 0.43              |
| 46:S2:47:G:H1      | 46:S2:479:G:N2     | 2.16                     | 0.43              |
| 46:S2:154:U:OP1    | 59:SG:15:LEU:HD21  | 2.18                     | 0.43              |
| 52:SC:188:CYS:O    | 52:SC:191:VAL:HG12 | 2.19                     | 0.43              |
| 76:SX:41:PHE:HZ    | 76:SX:102:VAL:HG12 | 1.84                     | 0.43              |
| 1:L5:2345:A:H2'    | 1:L5:2346:U:C6     | 2.53                     | 0.43              |
| 1:L5:4357:C:H2'    | 1:L5:4358:A:C8     | 2.54                     | 0.43              |
| 15:LF:221:LYS:H    | 15:LF:221:LYS:HG2  | 1.67                     | 0.43              |
| 17:LG:182:CYS:HB3  | 17:LG:222:ILE:HD13 | 2.00                     | 0.43              |
| 21:LI:190:LEU:HD22 | 21:LI:197:VAL:HG13 | 2.00                     | 0.43              |
| 22:Lj:36:LYS:HE2   | 22:Lj:36:LYS:HB2   | 1.84                     | 0.43              |
| 23:LJ:167:GLN:HA   | 23:LJ:171:ASP:O    | 2.18                     | 0.43              |
| 30:LN:83:LYS:O     | 30:LN:85:VAL:N     | 2.52                     | 0.43              |
| 38:LS:21:LYS:HE3   | 38:LS:21:LYS:HB3   | 1.87                     | 0.43              |
| 39:LT:43:LYS:O     | 39:LT:95:HIS:HB3   | 2.19                     | 0.43              |
| 46:S2:798:C:H3'    | 46:S2:800:U:H5'    | 2.00                     | 0.43              |
| 46:S2:1423:G:C8    | 46:S2:1425:G:H1'   | 2.54                     | 0.43              |
| 46:S2:1650:U:OP1   | 68:SQ:128:GLU:HB3  | 2.19                     | 0.43              |
| 58:Sg:14:HIS:HE1   | 58:Sg:18:VAL:HG22  | 1.84                     | 0.43              |
| 72:SU:56:MET:HE2   | 72:SU:56:MET:HA    | 2.01                     | 0.43              |
| 1:L5:949:C:H2'     | 1:L5:950:G:C8      | 2.54                     | 0.43              |
| 1:L5:1766:C:H2'    | 1:L5:1767:A:H8     | 1.84                     | 0.43              |
| 1:L5:3377:G:H22    | 1:L5:3390:A:H2     | 1.66                     | 0.43              |
| 3:L8:65:A:C4       | 3:L8:66:A:C8       | 3.07                     | 0.43              |
| 35:LQ:39:THR:HG22  | 35:LQ:41:SER:H     | 1.84                     | 0.43              |
| 46:S2:17:C:H2'     | 46:S2:18:C:C6      | 2.54                     | 0.43              |
| 46:S2:158:A:H5'    | 46:S2:465:A:N6     | 2.34                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:S2:311:C:H1'    | 46:S2:341:C:H4'   | 2.01                     | 0.43              |
| 60:SH:101:LEU:HD12 | 60:SH:101:LEU:HA  | 1.88                     | 0.43              |
| 69:SR:32:LYS:HD2   | 69:SR:47:ARG:HH21 | 1.83                     | 0.43              |
| 77:SY:20:ARG:HD3   | 77:SY:74:MET:HE3  | 2.01                     | 0.43              |
| 1:L5:1766:C:H2'    | 1:L5:1767:A:C8    | 2.54                     | 0.42              |
| 1:L5:2386:U:H2'    | 1:L5:2387:U:C6    | 2.54                     | 0.42              |
| 1:L5:3891:G:H2'    | 1:L5:3892:A:C8    | 2.54                     | 0.42              |
| 1:L5:4664:A:H2'    | 1:L5:4664:A:N3    | 2.33                     | 0.42              |
| 1:L5:4686:A:O2'    | 1:L5:4687:U:OP1   | 2.34                     | 0.42              |
| 41:LV:69:LYS:HB2   | 41:LV:69:LYS:HE2  | 1.92                     | 0.42              |
| 42:LW:12:LYS:HE3   | 42:LW:12:LYS:HB3  | 1.82                     | 0.42              |
| 46:S2:563:U:C2     | 46:S2:564:G:H8    | 2.37                     | 0.42              |
| 46:S2:1840:U:H2'   | 46:S2:1841:U:C6   | 2.54                     | 0.42              |
| 48:SA:50:ASN:OD1   | 48:SA:52:LYS:HG3  | 2.19                     | 0.42              |
| 79:S6:27:C:H2'     | 79:S6:28:U:C6     | 2.54                     | 0.42              |
| 1:L5:952:C:H2'     | 1:L5:953:C:C6     | 2.54                     | 0.42              |
| 1:L5:2214:G:O2'    | 1:L5:3329:G:H8    | 2.03                     | 0.42              |
| 1:L5:4527:U:C4     | 28:LM:113:MET:HG3 | 2.54                     | 0.42              |
| 7:LB:29:VAL:HG12   | 7:LB:31:SER:H     | 1.84                     | 0.42              |
| 7:LB:168:MET:HE3   | 7:LB:168:MET:HB3  | 1.80                     | 0.42              |
| 7:LB:305:THR:C     | 7:LB:307:TYR:H    | 2.27                     | 0.42              |
| 13:LE:51:CYS:SG    | 13:LE:52:SER:N    | 2.91                     | 0.42              |
| 16:Lg:107:LEU:HD23 | 16:Lg:107:LEU:HA  | 1.82                     | 0.42              |
| 39:LT:97:LYS:HB3   | 39:LT:97:LYS:HE2  | 1.56                     | 0.42              |
| 40:LU:65:ARG:HH11  | 40:LU:67:LYS:HA   | 1.84                     | 0.42              |
| 46:S2:69:C:H2'     | 46:S2:70:G:O4'    | 2.19                     | 0.42              |
| 46:S2:220:U:C4     | 46:S2:221:U:H5    | 2.37                     | 0.42              |
| 46:S2:509:A:H3'    | 62:SJ:3:VAL:HG12  | 2.01                     | 0.42              |
| 46:S2:798:C:H5''   | 46:S2:801:U:OP1   | 2.20                     | 0.42              |
| 46:S2:1388:G:H2'   | 46:S2:1389:A:O4'  | 2.18                     | 0.42              |
| 46:S2:1790:G:H5'   | 46:S2:1791:A:OP1  | 2.19                     | 0.42              |
| 50:SB:120:MET:HG3  | 50:SB:142:PHE:CE2 | 2.53                     | 0.42              |
| 55:Se:116:PHE:HE1  | 62:SJ:29:LEU:HD23 | 1.84                     | 0.42              |
| 57:SF:192:LYS:HB2  | 57:SF:192:LYS:HE2 | 1.91                     | 0.42              |
| 70:SS:117:ILE:HD13 | 70:SS:117:ILE:HA  | 1.85                     | 0.42              |
| 1:L5:3441:A:O2'    | 1:L5:3443:U:OP2   | 2.28                     | 0.42              |
| 1:L5:4387:A:H1'    | 1:L5:4388:G:C8    | 2.54                     | 0.42              |
| 3:L8:94:G:C5       | 22:Lj:84:PRO:HG3  | 2.53                     | 0.42              |
| 13:LE:284:SER:HB2  | 14:Lf:3:GLY:HA3   | 2.02                     | 0.42              |
| 20:Li:51:ALA:HB3   | 20:Li:54:GLU:OE1  | 2.19                     | 0.42              |
| 34:LP:140:MET:HE3  | 34:LP:140:MET:HB3 | 1.89                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:1202:U:H2'   | 46:S2:1203:U:C6    | 2.54                     | 0.42              |
| 48:SA:116:PHE:C    | 48:SA:117:ARG:HD3  | 2.44                     | 0.42              |
| 48:SA:191:ARG:NH2  | 73:SV:44:GLY:O     | 2.52                     | 0.42              |
| 52:SC:173:LYS:HB3  | 52:SC:173:LYS:HE3  | 1.65                     | 0.42              |
| 78:SZ:68:ILE:O     | 78:SZ:68:ILE:HG13  | 2.20                     | 0.42              |
| 1:L5:268:G:H2'     | 1:L5:269:U:C6      | 2.54                     | 0.42              |
| 1:L5:1122:A:H2'    | 1:L5:1123:C:H6     | 1.85                     | 0.42              |
| 8:Lc:82:GLY:HA2    | 8:Lc:91:VAL:HG12   | 2.01                     | 0.42              |
| 9:LC:62:THR:OG1    | 9:LC:63:SER:N      | 2.52                     | 0.42              |
| 18:Lh:107:GLN:O    | 18:Lh:111:GLU:HG3  | 2.20                     | 0.42              |
| 21:LI:86:HIS:HB3   | 21:LI:139:ARG:HG2  | 1.99                     | 0.42              |
| 23:LJ:96:LYS:HB3   | 23:LJ:176:PRO:HG2  | 2.00                     | 0.42              |
| 46:S2:87:U:O4      | 46:S2:501:A:H2     | 2.01                     | 0.42              |
| 46:S2:290:G:OP1    | 56:SE:155:LYS:HE2  | 2.19                     | 0.42              |
| 46:S2:535:G:H2'    | 46:S2:536:G:H8     | 1.83                     | 0.42              |
| 49:Sb:36:LYS:HB2   | 49:Sb:43:ILE:HG22  | 2.01                     | 0.42              |
| 59:SG:116:LYS:NZ   | 59:SG:120:ASP:OD1  | 2.45                     | 0.42              |
| 60:SH:107:LYS:HA   | 60:SH:107:LYS:HD3  | 1.66                     | 0.42              |
| 79:S6:35:A:H2'     | 79:S6:36:U:C6      | 2.54                     | 0.42              |
| 1:L5:266:G:H2'     | 1:L5:267:G:H8      | 1.84                     | 0.42              |
| 1:L5:829:G:O2'     | 1:L5:830:C:H5'     | 2.20                     | 0.42              |
| 1:L5:950:G:C2      | 1:L5:1037:G:C2     | 3.07                     | 0.42              |
| 7:LB:181:MET:HG2   | 7:LB:182:GLU:N     | 2.35                     | 0.42              |
| 7:LB:261:ARG:HB2   | 32:LO:64:THR:HG21  | 2.01                     | 0.42              |
| 9:LC:101:MET:HE2   | 9:LC:104:PRO:HA    | 2.01                     | 0.42              |
| 13:LE:188:VAL:HG21 | 13:LE:266:LEU:HD11 | 2.00                     | 0.42              |
| 46:S2:224:U:O2'    | 46:S2:225:C:H5'    | 2.20                     | 0.42              |
| 46:S2:375:G:C1'    | 64:SL:83:GLN:HE21  | 2.33                     | 0.42              |
| 46:S2:482:C:H2'    | 46:S2:483:G:H21    | 1.84                     | 0.42              |
| 46:S2:1126:C:OP1   | 69:SR:129:LYS:HD2  | 2.20                     | 0.42              |
| 46:S2:1311:U:H2'   | 46:S2:1312:C:C5    | 2.54                     | 0.42              |
| 46:S2:1745:G:HO2'  | 46:S2:1746:A:H8    | 1.60                     | 0.42              |
| 60:SH:160:LYS:HD3  | 60:SH:190:PRO:O    | 2.20                     | 0.42              |
| 60:SH:186:ASN:C    | 60:SH:186:ASN:OD1  | 2.62                     | 0.42              |
| 77:SY:41:ARG:NH1   | 77:SY:57:VAL:H     | 2.16                     | 0.42              |
| 78:SZ:65:TYR:CD1   | 78:SZ:68:ILE:HG22  | 2.55                     | 0.42              |
| 79:S7:20:A:O2'     | 79:S7:21:A:O5'     | 2.38                     | 0.42              |
| 3:L8:86:U:H1'      | 3:L8:87:G:H5'      | 2.02                     | 0.42              |
| 11:LD:117:LYS:HA   | 11:LD:117:LYS:HD3  | 1.75                     | 0.42              |
| 26:LL:108:GLU:H    | 26:LL:108:GLU:CD   | 2.26                     | 0.42              |
| 39:LT:120:LYS:HE2  | 39:LT:120:LYS:HB2  | 1.57                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:77:A:OP2     | 59:SG:154:ARG:NE   | 2.43                     | 0.42              |
| 46:S2:981:A:H2'    | 46:S2:982:A:C8     | 2.55                     | 0.42              |
| 48:SA:10:MET:O     | 48:SA:11:LYS:HB2   | 2.20                     | 0.42              |
| 56:SE:174:LYS:HD3  | 56:SE:174:LYS:HA   | 1.85                     | 0.42              |
| 58:Sg:92:LEU:HD23  | 58:Sg:93:THR:N     | 2.35                     | 0.42              |
| 72:SU:66:ARG:HG3   | 72:SU:68:THR:HG22  | 2.02                     | 0.42              |
| 1:L5:2652:G:H2'    | 1:L5:2653:C:C6     | 2.54                     | 0.42              |
| 1:L5:2657:G:N2     | 1:L5:2657:G:OP1    | 2.32                     | 0.42              |
| 1:L5:3587:U:H2'    | 1:L5:3588:C:C6     | 2.55                     | 0.42              |
| 7:LB:194:LEU:HD12  | 7:LB:194:LEU:HA    | 1.83                     | 0.42              |
| 9:LC:293:LEU:HD23  | 9:LC:293:LEU:HA    | 1.91                     | 0.42              |
| 12:Le:89:LEU:HD13  | 12:Le:118:LEU:HD22 | 2.02                     | 0.42              |
| 17:LG:89:ARG:HG3   | 17:LG:89:ARG:NH1   | 2.34                     | 0.42              |
| 37:LR:148:ASP:OD1  | 37:LR:148:ASP:N    | 2.50                     | 0.42              |
| 46:S2:837:G:H2'    | 46:S2:838:A:H4'    | 2.01                     | 0.42              |
| 53:Sd:52:PHE:HB3   | 72:SU:80:PHE:HB3   | 2.02                     | 0.42              |
| 54:SD:97:CYS:O     | 54:SD:101:GLN:HG2  | 2.20                     | 0.42              |
| 59:SG:23:LYS:HB2   | 59:SG:41:LEU:HD23  | 2.01                     | 0.42              |
| 68:SQ:98:LYS:HD3   | 68:SQ:99:TYR:CZ    | 2.55                     | 0.42              |
| 1:L5:2:G:H2'       | 1:L5:3:C:H6        | 1.84                     | 0.42              |
| 1:L5:99:A:H2'      | 1:L5:100:C:O2      | 2.20                     | 0.42              |
| 1:L5:4549:G:O6     | 1:L5:4565:G:H1'    | 2.20                     | 0.42              |
| 12:Le:124:ASN:OD1  | 12:Le:124:ASN:N    | 2.52                     | 0.42              |
| 20:Li:63:VAL:HG12  | 20:Li:65:LYS:HG3   | 2.01                     | 0.42              |
| 32:LO:175:LEU:HD12 | 32:LO:175:LEU:HA   | 1.85                     | 0.42              |
| 46:S2:345:U:H2'    | 46:S2:346:U:C6     | 2.55                     | 0.42              |
| 46:S2:516:G:H4'    | 46:S2:518:C:OP1    | 2.20                     | 0.42              |
| 46:S2:1017:U:O2    | 46:S2:1017:U:H2'   | 2.20                     | 0.42              |
| 46:S2:1113:U:O2'   | 46:S2:1114:A:H5'   | 2.19                     | 0.42              |
| 61:SI:142:SER:O    | 61:SI:145:ILE:HG12 | 2.20                     | 0.42              |
| 1:L5:1003:G:C2     | 1:L5:1004:G:H1'    | 2.55                     | 0.42              |
| 1:L5:1649:G:H2'    | 1:L5:1650:C:C6     | 2.54                     | 0.42              |
| 5:LA:10:LYS:HE3    | 5:LA:10:LYS:HB2    | 1.85                     | 0.42              |
| 9:LC:66:SER:HA     | 9:LC:77:PRO:HA     | 2.01                     | 0.42              |
| 26:LL:134:PRO:C    | 26:LL:135:LYS:HG2  | 2.44                     | 0.42              |
| 46:S2:185:G:H2'    | 46:S2:186:C:O4'    | 2.19                     | 0.42              |
| 46:S2:812:A:H2'    | 46:S2:813:A:C8     | 2.54                     | 0.42              |
| 46:S2:830:C:H4'    | 46:S2:831:A:OP1    | 2.20                     | 0.42              |
| 46:S2:1420:C:H2'   | 46:S2:1421:G:C6    | 2.54                     | 0.42              |
| 50:SB:83:LYS:HB2   | 50:SB:83:LYS:HE3   | 1.64                     | 0.42              |
| 62:SJ:94:LEU:HD23  | 62:SJ:94:LEU:HA    | 1.90                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:SK:79:LEU:HD12 | 63:SK:79:LEU:HA    | 1.86                     | 0.42              |
| 1:L5:25:A:H2'     | 1:L5:26:C:H6       | 1.85                     | 0.42              |
| 1:L5:1499:G:H2'   | 1:L5:1500:C:H6     | 1.85                     | 0.42              |
| 1:L5:2618:A:H2'   | 1:L5:2619:U:C6     | 2.54                     | 0.42              |
| 1:L5:3321:G:H2'   | 1:L5:3322:G:H8     | 1.84                     | 0.42              |
| 1:L5:3722:U:H2'   | 1:L5:3723:C:C6     | 2.54                     | 0.42              |
| 1:L5:4677:C:HO2'  | 1:L5:4678:U:H6     | 1.68                     | 0.42              |
| 7:LB:34:LYS:HE3   | 7:LB:34:LYS:HB3    | 1.85                     | 0.42              |
| 18:Lh:6:ALA:O     | 18:Lh:10:ARG:HG3   | 2.20                     | 0.42              |
| 20:Li:64:SER:O    | 20:Li:64:SER:OG    | 2.32                     | 0.42              |
| 46:S2:225:C:O2'   | 46:S2:226:A:H5'    | 2.19                     | 0.42              |
| 46:S2:1540:U:H1'  | 71:ST:48:TYR:CZ    | 2.54                     | 0.42              |
| 46:S2:1728:G:H2'  | 46:S2:1729:U:C6    | 2.55                     | 0.42              |
| 48:SA:69:GLU:OE2  | 52:SC:270:THR:HB   | 2.19                     | 0.42              |
| 50:SB:94:LYS:HD3  | 50:SB:94:LYS:HA    | 1.79                     | 0.42              |
| 54:SD:151:LYS:HB3 | 54:SD:151:LYS:HE2  | 1.86                     | 0.42              |
| 58:Sg:131:LEU:O   | 58:Sg:139:LYS:N    | 2.46                     | 0.42              |
| 61:SI:107:THR:O   | 61:SI:111:GLN:HG3  | 2.19                     | 0.42              |
| 69:SR:91:LEU:HD12 | 69:SR:91:LEU:HA    | 1.88                     | 0.42              |
| 71:ST:65:TYR:HB2  | 71:ST:123:LEU:HD22 | 2.02                     | 0.42              |
| 77:SY:46:LYS:HE2  | 77:SY:46:LYS:HB2   | 1.76                     | 0.42              |
| 79:S6:15:A:H2'    | 79:S6:16:G:O4'     | 2.19                     | 0.42              |
| 1:L5:384:A:N3     | 1:L5:386:G:H5''    | 2.34                     | 0.41              |
| 1:L5:667:G:HO2'   | 1:L5:668:G:H8      | 1.68                     | 0.41              |
| 1:L5:857:A:H8     | 1:L5:857:A:OP2     | 2.03                     | 0.41              |
| 1:L5:4333:G:H2'   | 1:L5:4334:A:C8     | 2.55                     | 0.41              |
| 5:LA:31:ALA:HB2   | 5:LA:123:ARG:NH2   | 2.35                     | 0.41              |
| 15:LF:62:LYS:HB3  | 15:LF:62:LYS:HE2   | 1.76                     | 0.41              |
| 15:LF:69:ARG:HA   | 15:LF:69:ARG:HD2   | 1.85                     | 0.41              |
| 31:Lo:93:LEU:HD23 | 31:Lo:93:LEU:HA    | 1.92                     | 0.41              |
| 35:LQ:49:LYS:HE2  | 35:LQ:49:LYS:HB3   | 1.58                     | 0.41              |
| 46:S2:381:G:OP1   | 61:SI:31:ARG:HD2   | 2.20                     | 0.41              |
| 46:S2:1422:A:H2'  | 46:S2:1423:G:C8    | 2.54                     | 0.41              |
| 46:S2:1809:U:N3   | 46:S2:1810:A:N7    | 2.67                     | 0.41              |
| 54:SD:25:LEU:HB3  | 54:SD:34:TYR:CE1   | 2.55                     | 0.41              |
| 54:SD:92:ALA:O    | 54:SD:93:THR:OG1   | 2.34                     | 0.41              |
| 67:SP:59:ARG:HG3  | 67:SP:76:VAL:HG11  | 2.00                     | 0.41              |
| 1:L5:1001:G:C6    | 1:L5:1026:C:C4     | 3.08                     | 0.41              |
| 1:L5:1018:G:O2'   | 1:L5:1019:U:H6     | 2.03                     | 0.41              |
| 1:L5:1761:A:H2'   | 1:L5:1762:U:O4'    | 2.20                     | 0.41              |
| 1:L5:3443:U:OP1   | 1:L5:4203:G:O2'    | 2.36                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:L8:19:C:H2'      | 3:L8:20:A:C8      | 2.54                     | 0.41              |
| 15:LF:206:ILE:HG23 | 15:LF:211:ASP:HB2 | 2.02                     | 0.41              |
| 35:LQ:97:LYS:HE2   | 35:LQ:97:LYS:HB3  | 1.87                     | 0.41              |
| 46:S2:508:G:C8     | 56:SE:27:PHE:CE2  | 3.08                     | 0.41              |
| 58:Sg:34:ALA:HB1   | 58:Sg:66:VAL:HG23 | 2.02                     | 0.41              |
| 59:SG:79:LYS:HG2   | 59:SG:86:PRO:HG3  | 2.01                     | 0.41              |
| 63:SK:7:ASN:O      | 63:SK:11:ILE:HG12 | 2.21                     | 0.41              |
| 71:ST:65:TYR:CD1   | 71:ST:65:TYR:C    | 2.98                     | 0.41              |
| 72:SU:23:THR:HG22  | 72:SU:113:GLU:HB2 | 2.01                     | 0.41              |
| 76:SX:61:GLN:HB3   | 76:SX:62:PRO:CD   | 2.50                     | 0.41              |
| 1:L5:477:G:OP1     | 36:Lr:66:ARG:NH2  | 2.53                     | 0.41              |
| 1:L5:2046:C:N4     | 36:Lr:19:LYS:HB3  | 2.34                     | 0.41              |
| 5:LA:115:CYS:O     | 5:LA:164:ALA:HA   | 2.20                     | 0.41              |
| 11:LD:278:ASP:OD2  | 11:LD:282:GLN:NE2 | 2.52                     | 0.41              |
| 15:LF:96:MET:HE2   | 15:LF:96:MET:HB3  | 1.89                     | 0.41              |
| 26:LL:94:ILE:HD13  | 26:LL:94:ILE:HA   | 1.80                     | 0.41              |
| 28:LM:11:ARG:NH1   | 28:LM:58:THR:O    | 2.51                     | 0.41              |
| 46:S2:508:G:N7     | 56:SE:27:PHE:CE2  | 2.88                     | 0.41              |
| 46:S2:615:C:H2'    | 46:S2:627:G:C8    | 2.55                     | 0.41              |
| 46:S2:687:U:OP1    | 74:SW:32:LYS:HG3  | 2.21                     | 0.41              |
| 56:SE:52:LEU:HD23  | 56:SE:52:LEU:HA   | 1.84                     | 0.41              |
| 58:Sg:101:PHE:CD1  | 58:Sg:136:GLY:HA2 | 2.56                     | 0.41              |
| 79:S7:34:C:H2'     | 79:S7:35:A:C8     | 2.55                     | 0.41              |
| 1:L5:1226:G:O2'    | 1:L5:1227:G:O4'   | 2.30                     | 0.41              |
| 1:L5:3733:G:H2'    | 1:L5:3734:U:C6    | 2.56                     | 0.41              |
| 1:L5:3891:G:H2'    | 1:L5:3892:A:H8    | 1.85                     | 0.41              |
| 1:L5:4194:G:N2     | 1:L5:4197:A:OP2   | 2.37                     | 0.41              |
| 3:L8:86:U:O2'      | 3:L8:87:G:O5'     | 2.38                     | 0.41              |
| 13:LE:207:THR:HG21 | 28:LM:107:PHE:HB2 | 2.01                     | 0.41              |
| 46:S2:564:G:H5''   | 46:S2:587:G:N2    | 2.35                     | 0.41              |
| 46:S2:864:U:C2     | 46:S2:865:A:C8    | 3.09                     | 0.41              |
| 46:S2:1504:C:H2'   | 46:S2:1505:U:H6   | 1.85                     | 0.41              |
| 46:S2:1518:G:OP1   | 67:SP:122:THR:OG1 | 2.32                     | 0.41              |
| 77:SY:55:ILE:HD12  | 77:SY:55:ILE:O    | 2.20                     | 0.41              |
| 77:SY:61:ARG:HG2   | 77:SY:61:ARG:NH1  | 2.34                     | 0.41              |
| 79:S7:43:G:H2'     | 79:S7:44:A:C8     | 2.55                     | 0.41              |
| 1:L5:108:A:H4'     | 1:L5:109:G:OP1    | 2.20                     | 0.41              |
| 1:L5:2301:G:N2     | 3:L8:126:C:O4'    | 2.54                     | 0.41              |
| 1:L5:3298:U:H5     | 1:L5:3303:A:N7    | 2.18                     | 0.41              |
| 1:L5:3568:C:H2'    | 1:L5:3569:U:C6    | 2.54                     | 0.41              |
| 36:Lr:7:TRP:O      | 36:Lr:11:ARG:HB2  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:Lr:52:GLU:OE1   | 36:Lr:79:ARG:NH2   | 2.53                     | 0.41              |
| 46:S2:922:G:C5     | 74:SW:28:ARG:HD2   | 2.55                     | 0.41              |
| 52:SC:88:ILE:HG22  | 52:SC:160:LEU:HD13 | 2.01                     | 0.41              |
| 54:SD:178:ARG:H    | 54:SD:178:ARG:HG3  | 1.67                     | 0.41              |
| 62:SJ:110:LEU:HD22 | 62:SJ:147:PHE:HB3  | 2.02                     | 0.41              |
| 1:L5:3942:U:H2'    | 1:L5:3943:U:C6     | 2.55                     | 0.41              |
| 9:LC:235:LEU:HD23  | 9:LC:235:LEU:HA    | 1.91                     | 0.41              |
| 9:LC:290:SER:O     | 9:LC:294:LYS:HG2   | 2.19                     | 0.41              |
| 21:LI:45:GLU:OE1   | 21:LI:45:GLU:N     | 2.53                     | 0.41              |
| 34:LP:37:LYS:HG3   | 34:LP:117:ILE:HG22 | 2.03                     | 0.41              |
| 37:LR:19:LYS:HB2   | 37:LR:19:LYS:HE2   | 1.88                     | 0.41              |
| 39:LT:107:LYS:O    | 39:LT:111:GLU:HG2  | 2.20                     | 0.41              |
| 46:S2:904:A:N7     | 46:S2:905:A:N6     | 2.69                     | 0.41              |
| 46:S2:1392:C:H4'   | 53:Sd:55:LEU:HD13  | 2.03                     | 0.41              |
| 46:S2:1610:C:OP2   | 70:SS:132:ARG:HD2  | 2.21                     | 0.41              |
| 53:Sd:54:LYS:HD3   | 72:SU:78:ASP:OD1   | 2.20                     | 0.41              |
| 59:SG:115:LYS:HG3  | 59:SG:116:LYS:O    | 2.21                     | 0.41              |
| 70:SS:5:ILE:HA     | 78:SZ:49:LEU:HD23  | 2.02                     | 0.41              |
| 1:L5:258:C:O2'     | 1:L5:259:C:O4'     | 2.31                     | 0.41              |
| 1:L5:1234:A:N3     | 1:L5:1234:A:H2'    | 2.36                     | 0.41              |
| 1:L5:3512:C:H2'    | 1:L5:3513:A:H8     | 1.85                     | 0.41              |
| 1:L5:3528:A:H2'    | 1:L5:3529:A:H8     | 1.84                     | 0.41              |
| 1:L5:3536:G:O2'    | 1:L5:3538:G:OP2    | 2.31                     | 0.41              |
| 1:L5:4191:G:H2'    | 1:L5:4192:U:C6     | 2.55                     | 0.41              |
| 1:L5:4216:U:H2'    | 1:L5:4217:A:H8     | 1.85                     | 0.41              |
| 3:L8:62:A:OP1      | 18:Lh:51:ARG:NH2   | 2.52                     | 0.41              |
| 8:Lc:37:MET:HG3    | 8:Lc:97:ILE:HD11   | 2.02                     | 0.41              |
| 9:LC:25:PRO:HG2    | 9:LC:28:PHE:CE2    | 2.56                     | 0.41              |
| 37:LR:173:ARG:HH21 | 46:S2:910:G:H5'    | 1.86                     | 0.41              |
| 41:LV:131:ARG:NH1  | 41:LV:131:ARG:HG2  | 2.35                     | 0.41              |
| 46:S2:55:U:H4'     | 46:S2:56:G:OP1     | 2.18                     | 0.41              |
| 59:SG:30:LYS:O     | 59:SG:102:VAL:HG12 | 2.21                     | 0.41              |
| 60:SH:174:SER:OG   | 60:SH:185:VAL:O    | 2.39                     | 0.41              |
| 69:SR:103:LYS:C    | 69:SR:103:LYS:HD3  | 2.46                     | 0.41              |
| 77:SY:37:LYS:HB3   | 77:SY:37:LYS:HE3   | 1.85                     | 0.41              |
| 1:L5:955:C:H1'     | 1:L5:1029:G:O6     | 2.20                     | 0.41              |
| 1:L5:3309:A:H2'    | 1:L5:3310:A:N7     | 2.36                     | 0.41              |
| 1:L5:3827:U:H2'    | 1:L5:3828:G:H8     | 1.85                     | 0.41              |
| 8:Lc:40:GLN:H      | 8:Lc:40:GLN:HG3    | 1.70                     | 0.41              |
| 15:LF:108:GLU:HB2  | 39:LT:135:PRO:HB3  | 2.03                     | 0.41              |
| 17:LG:257:LYS:HB3  | 17:LG:257:LYS:HE2  | 1.90                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:LM:51:PRO:HG2   | 28:LM:54:CYS:SG    | 2.61                     | 0.41              |
| 38:LS:25:PRO:HA    | 38:LS:26:PRO:HD3   | 1.93                     | 0.41              |
| 46:S2:847:G:C4     | 56:SE:19:MET:SD    | 3.14                     | 0.41              |
| 46:S2:1292:A:OP1   | 53:Sd:3:HIS:HB2    | 2.20                     | 0.41              |
| 46:S2:1667:C:H2'   | 46:S2:1668:U:C6    | 2.56                     | 0.41              |
| 54:SD:198:ILE:HD12 | 54:SD:198:ILE:HA   | 1.86                     | 0.41              |
| 62:SJ:84:ILE:HD13  | 62:SJ:84:ILE:HA    | 1.84                     | 0.41              |
| 70:SS:89:ASP:HB3   | 70:SS:93:GLY:H     | 1.85                     | 0.41              |
| 71:ST:27:LYS:HE2   | 71:ST:27:LYS:HB2   | 1.90                     | 0.41              |
| 1:L5:490:C:H2'     | 1:L5:491:C:H6      | 1.86                     | 0.41              |
| 1:L5:761:C:H5      | 1:L5:810:G:N1      | 2.11                     | 0.41              |
| 1:L5:950:G:H2'     | 1:L5:951:A:C8      | 2.56                     | 0.41              |
| 1:L5:1110:U:H4'    | 1:L5:1111:G:O4'    | 2.20                     | 0.41              |
| 1:L5:1225:G:N7     | 1:L5:1303:G:N2     | 2.69                     | 0.41              |
| 1:L5:1271:G:H4'    | 1:L5:1272:C:OP1    | 2.21                     | 0.41              |
| 1:L5:1338:A:H2     | 1:L5:3572:U:HO2'   | 1.67                     | 0.41              |
| 1:L5:1523:C:H5''   | 1:L5:1524:G:C8     | 2.56                     | 0.41              |
| 1:L5:2512:G:O2'    | 1:L5:2513:G:O5'    | 2.30                     | 0.41              |
| 1:L5:3420:A:O2'    | 1:L5:3421:U:H6     | 2.04                     | 0.41              |
| 1:L5:4068:A:OP1    | 21:LI:154:ARG:NH1  | 2.54                     | 0.41              |
| 3:L8:5:U:H2'       | 3:L8:6:C:C6        | 2.56                     | 0.41              |
| 3:L8:141:C:H2'     | 3:L8:142:U:H6      | 1.86                     | 0.41              |
| 32:LO:61:ARG:HA    | 32:LO:70:PRO:HD2   | 2.03                     | 0.41              |
| 35:LQ:43:PHE:CD2   | 35:LQ:133:GLY:HA3  | 2.56                     | 0.41              |
| 46:S2:219:A:H2'    | 46:S2:220:U:O4'    | 2.21                     | 0.41              |
| 46:S2:476:C:O2'    | 46:S2:477:A:H8     | 2.04                     | 0.41              |
| 46:S2:798:C:H2'    | 46:S2:801:U:P      | 2.61                     | 0.41              |
| 46:S2:825:C:H1'    | 62:SJ:144:ILE:HG21 | 2.01                     | 0.41              |
| 46:S2:965:A:H2'    | 46:S2:966:U:C6     | 2.51                     | 0.41              |
| 46:S2:986:G:H4'    | 66:SO:138:ASP:OD2  | 2.20                     | 0.41              |
| 46:S2:1556:U:C4    | 53:Sd:19:ARG:HA    | 2.56                     | 0.41              |
| 46:S2:1586:U:C4    | 71:ST:67:ARG:HD2   | 2.55                     | 0.41              |
| 46:S2:1750:G:H2'   | 46:S2:1751:C:C6    | 2.56                     | 0.41              |
| 48:SA:81:ASN:OD1   | 48:SA:82:THR:N     | 2.54                     | 0.41              |
| 49:Sb:8:LEU:HD12   | 49:Sb:8:LEU:HA     | 1.92                     | 0.41              |
| 50:SB:68:GLU:OE1   | 50:SB:83:LYS:HB3   | 2.21                     | 0.41              |
| 52:SC:84:PHE:HA    | 73:SV:15:ARG:NH1   | 2.36                     | 0.41              |
| 52:SC:246:LYS:HE2  | 52:SC:246:LYS:HB3  | 1.86                     | 0.41              |
| 56:SE:57:THR:HG22  | 56:SE:59:ASP:H     | 1.85                     | 0.41              |
| 56:SE:103:TYR:CD1  | 56:SE:189:LEU:HD21 | 2.56                     | 0.41              |
| 57:SF:16:ASP:C     | 57:SF:17:ILE:HD12  | 2.46                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:Sg:174:VAL:CG2  | 58:Sg:188:HIS:HB2  | 2.50                     | 0.41              |
| 58:Sg:245:ARG:HH22 | 58:Sg:247:TRP:HB2  | 1.86                     | 0.41              |
| 59:SG:32:MET:HA    | 59:SG:52:ILE:HD13  | 2.03                     | 0.41              |
| 60:SH:36:LEU:HA    | 60:SH:36:LEU:HD23  | 1.83                     | 0.41              |
| 61:SI:201:LYS:HD3  | 61:SI:201:LYS:HA   | 1.88                     | 0.41              |
| 63:SK:57:TYR:O     | 63:SK:72:THR:OG1   | 2.27                     | 0.41              |
| 68:SQ:49:TYR:O     | 68:SQ:53:GLU:HG2   | 2.21                     | 0.41              |
| 72:SU:22:ILE:HG23  | 72:SU:114:VAL:HG22 | 2.02                     | 0.41              |
| 79:S7:2:A:H2'      | 79:S7:3:G:H8       | 1.86                     | 0.41              |
| 1:L5:750:G:H2'     | 1:L5:751:G:O4'     | 2.22                     | 0.41              |
| 1:L5:1581:C:H5''   | 11:LD:5:LYS:HG2    | 2.03                     | 0.41              |
| 11:LD:289:ARG:O    | 11:LD:292:GLU:HG3  | 2.20                     | 0.41              |
| 17:LG:259:LYS:HE3  | 17:LG:259:LYS:HB3  | 1.86                     | 0.41              |
| 26:LL:194:ILE:HD12 | 26:LL:194:ILE:HA   | 1.78                     | 0.41              |
| 40:LU:41:GLN:O     | 40:LU:45:GLU:HG2   | 2.21                     | 0.41              |
| 46:S2:95:G:H1      | 46:S2:435:G:N2     | 2.10                     | 0.41              |
| 46:S2:493:C:H5''   | 46:S2:510:G:N1     | 2.35                     | 0.41              |
| 46:S2:544:C:H3'    | 46:S2:545:G:H8     | 1.85                     | 0.41              |
| 46:S2:836:C:H4'    | 46:S2:837:G:N7     | 2.36                     | 0.41              |
| 46:S2:864:U:N3     | 46:S2:865:A:N7     | 2.69                     | 0.41              |
| 46:S2:1426:G:H2'   | 46:S2:1427:U:C6    | 2.56                     | 0.41              |
| 46:S2:1644:U:H2'   | 46:S2:1645:C:C6    | 2.56                     | 0.41              |
| 46:S2:1679:A:O2'   | 46:S2:1680:A:H5'   | 2.20                     | 0.41              |
| 46:S2:1789:A:H2'   | 46:S2:1790:G:O4'   | 2.21                     | 0.41              |
| 56:SE:29:PRO:HG2   | 56:SE:46:ILE:HD11  | 2.01                     | 0.41              |
| 60:SH:160:LYS:O    | 60:SH:160:LYS:HG3  | 2.20                     | 0.41              |
| 66:SO:133:THR:HA   | 66:SO:134:PRO:HD3  | 1.96                     | 0.41              |
| 69:SR:89:SER:HB2   | 69:SR:92:ASP:HB2   | 2.03                     | 0.41              |
| 79:S7:19:G:H5'     | 79:S7:60:A:H61     | 1.86                     | 0.41              |
| 1:L5:415:U:HO2'    | 1:L5:416:G:P       | 2.43                     | 0.40              |
| 1:L5:677:C:O2'     | 1:L5:678:G:O5'     | 2.36                     | 0.40              |
| 1:L5:1765:A:C5     | 1:L5:1766:C:C6     | 3.09                     | 0.40              |
| 1:L5:3976:A:C2     | 11:LD:146:LEU:HD23 | 2.56                     | 0.40              |
| 1:L5:4404:G:H2'    | 1:L5:4405:G:C8     | 2.56                     | 0.40              |
| 4:La:94:LYS:H      | 4:La:94:LYS:HG2    | 1.56                     | 0.40              |
| 7:LB:84:MET:O      | 7:LB:204:GLN:HA    | 2.21                     | 0.40              |
| 13:LE:206:SER:OG   | 13:LE:296:PHE:OXT  | 2.38                     | 0.40              |
| 17:LG:193:LEU:HD23 | 17:LG:193:LEU:HA   | 1.90                     | 0.40              |
| 19:LH:18:ILE:HD12  | 19:LH:18:ILE:N     | 2.36                     | 0.40              |
| 39:LT:146:LYS:HB3  | 39:LT:146:LYS:HE3  | 1.82                     | 0.40              |
| 46:S2:547:G:H1'    | 46:S2:548:G:N7     | 2.36                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:S2:854:C:C2     | 46:S2:855:A:C8     | 3.09                     | 0.40              |
| 46:S2:1020:C:H2'   | 46:S2:1021:A:O4'   | 2.21                     | 0.40              |
| 46:S2:1281:G:H2'   | 46:S2:1282:G:H8    | 1.85                     | 0.40              |
| 56:SE:98:ASN:O     | 56:SE:114:ILE:HG12 | 2.21                     | 0.40              |
| 58:Sg:27:PHE:HE2   | 58:Sg:75:GLY:HA3   | 1.86                     | 0.40              |
| 69:SR:31:ASN:OD1   | 69:SR:31:ASN:N     | 2.54                     | 0.40              |
| 70:SS:87:GLN:HB3   | 70:SS:95:TYR:CE2   | 2.56                     | 0.40              |
| 77:SY:105:LYS:HA   | 77:SY:105:LYS:HD2  | 1.69                     | 0.40              |
| 1:L5:423:U:H2'     | 1:L5:424:U:H6      | 1.86                     | 0.40              |
| 1:L5:686:C:H2'     | 1:L5:687:C:H6      | 1.87                     | 0.40              |
| 1:L5:1374:A:H2'    | 1:L5:1375:G:H8     | 1.81                     | 0.40              |
| 1:L5:1377:A:H2'    | 1:L5:1378:A:N3     | 2.37                     | 0.40              |
| 1:L5:2655:G:C2     | 1:L5:3256:A:C2     | 3.10                     | 0.40              |
| 1:L5:3264:U:H2'    | 1:L5:3265:A:C8     | 2.56                     | 0.40              |
| 1:L5:3364:U:H2'    | 1:L5:3365:C:H6     | 1.85                     | 0.40              |
| 6:Lb:51:LYS:O      | 6:Lb:54:LEU:HD23   | 2.21                     | 0.40              |
| 46:S2:918:U:H2'    | 46:S2:919:U:C6     | 2.56                     | 0.40              |
| 46:S2:922:G:C6     | 74:SW:28:ARG:HD2   | 2.57                     | 0.40              |
| 46:S2:929:G:H1     | 46:S2:1014:U:H3    | 1.68                     | 0.40              |
| 47:Sa:13:LYS:HA    | 47:Sa:13:LYS:HD3   | 1.90                     | 0.40              |
| 61:SI:3:ILE:O      | 61:SI:30:GLY:N     | 2.51                     | 0.40              |
| 61:SI:42:ARG:HH12  | 61:SI:59:ARG:HH21  | 1.69                     | 0.40              |
| 65:SN:78:LYS:HA    | 65:SN:78:LYS:HD3   | 1.83                     | 0.40              |
| 71:ST:85:ASN:OD1   | 71:ST:88:ARG:HB2   | 2.20                     | 0.40              |
| 79:S6:13:G:N1      | 79:S6:24:G:C2      | 2.89                     | 0.40              |
| 79:S6:43:G:H2'     | 79:S6:44:A:H8      | 1.85                     | 0.40              |
| 1:L5:1004:G:H22    | 1:L5:1022:G:H1     | 1.68                     | 0.40              |
| 1:L5:2060:C:H5''   | 12:Le:104:SER:HB3  | 2.03                     | 0.40              |
| 1:L5:3420:A:H61    | 46:S2:1710:G:HO2'  | 1.67                     | 0.40              |
| 1:L5:4397:G:H2'    | 1:L5:4398:A:C8     | 2.56                     | 0.40              |
| 1:L5:4618:C:C2     | 1:L5:4619:A:C8     | 3.08                     | 0.40              |
| 9:LC:132:ALA:C     | 9:LC:150:LEU:HD23  | 2.47                     | 0.40              |
| 11:LD:187:SER:HB2  | 11:LD:189:GLU:OE2  | 2.22                     | 0.40              |
| 18:Lh:123:ALA:HB3  | 26:LL:150:LEU:HD11 | 2.02                     | 0.40              |
| 19:LH:96:TYR:CE2   | 19:LH:100:PRO:HA   | 2.56                     | 0.40              |
| 26:LL:169:ILE:HG22 | 26:LL:174:LYS:HG2  | 2.02                     | 0.40              |
| 46:S2:82:G:H8      | 46:S2:82:G:OP2     | 2.04                     | 0.40              |
| 46:S2:219:A:C6     | 46:S2:220:U:N3     | 2.89                     | 0.40              |
| 46:S2:221:U:O2'    | 61:SI:186:ASP:OD2  | 2.36                     | 0.40              |
| 46:S2:339:G:H2'    | 46:S2:340:A:O4'    | 2.21                     | 0.40              |
| 46:S2:430:C:OP1    | 56:SE:10:LYS:HE2   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:S2:1519:C:H5'' | 46:S2:1520:U:H2'   | 2.04                     | 0.40              |
| 46:S2:1680:A:P    | 57:SF:60:ARG:HE    | 2.45                     | 0.40              |
| 46:S2:1734:U:H2'  | 46:S2:1735:G:O4'   | 2.21                     | 0.40              |
| 47:Sa:94:ASP:OD1  | 47:Sa:94:ASP:N     | 2.39                     | 0.40              |
| 49:Sb:34:ASP:HA   | 49:Sb:44:THR:O     | 2.21                     | 0.40              |
| 52:SC:125:LYS:HG3 | 52:SC:143:CYS:HB2  | 2.03                     | 0.40              |
| 71:ST:39:LEU:O    | 71:ST:96:SER:HB2   | 2.21                     | 0.40              |
| 1:L5:822:U:H2'    | 1:L5:823:C:C6      | 2.57                     | 0.40              |
| 1:L5:2513:G:O2'   | 1:L5:2514:G:O4'    | 2.24                     | 0.40              |
| 1:L5:2602:G:O2'   | 1:L5:3495:U:O4     | 2.37                     | 0.40              |
| 1:L5:3269:C:H1'   | 1:L5:4664:A:H8     | 1.84                     | 0.40              |
| 5:LA:54:ARG:HG2   | 5:LA:56:ALA:H      | 1.86                     | 0.40              |
| 9:LC:50:GLN:HA    | 9:LC:51:PRO:HD3    | 1.96                     | 0.40              |
| 15:LF:138:GLN:O   | 15:LF:141:ASN:HB2  | 2.22                     | 0.40              |
| 38:LS:113:MET:HE3 | 38:LS:113:MET:HB3  | 1.98                     | 0.40              |
| 46:S2:128:U:H4'   | 46:S2:217:G:H5'    | 2.04                     | 0.40              |
| 46:S2:155:G:C2'   | 46:S2:156:G:H5'    | 2.52                     | 0.40              |
| 46:S2:849:U:H2'   | 46:S2:850:A:C8     | 2.56                     | 0.40              |
| 46:S2:946:U:H2'   | 46:S2:947:U:H6     | 1.87                     | 0.40              |
| 46:S2:1502:C:H2'  | 46:S2:1503:C:C6    | 2.56                     | 0.40              |
| 46:S2:1736:A:H5'  | 46:S2:1737:G:OP2   | 2.22                     | 0.40              |
| 46:S2:1857:C:H2'  | 46:S2:1858:G:C8    | 2.57                     | 0.40              |
| 56:SE:175:PHE:CE1 | 56:SE:195:ILE:HD13 | 2.56                     | 0.40              |
| 67:SP:33:LEU:HD23 | 67:SP:33:LEU:HA    | 1.85                     | 0.40              |
| 76:SX:68:LYS:H    | 76:SX:68:LYS:HG2   | 1.74                     | 0.40              |
| 78:SZ:49:LEU:N    | 78:SZ:83:LEU:HD22  | 2.37                     | 0.40              |
| 1:L5:3318:G:H4'   | 1:L5:3319:A:H5'    | 2.04                     | 0.40              |
| 1:L5:4059:U:C2    | 1:L5:4060:G:C8     | 3.09                     | 0.40              |
| 7:LB:4:ARG:HD3    | 7:LB:5:LYS:N       | 2.37                     | 0.40              |
| 7:LB:258:HIS:C    | 7:LB:260:ALA:N     | 2.78                     | 0.40              |
| 9:LC:150:LEU:HD12 | 9:LC:150:LEU:HA    | 1.83                     | 0.40              |
| 11:LD:259:ARG:HD2 | 11:LD:259:ARG:HA   | 1.87                     | 0.40              |
| 17:LG:48:LYS:HD3  | 17:LG:48:LYS:HA    | 1.82                     | 0.40              |
| 25:Ll:34:LYS:HB3  | 25:Ll:34:LYS:HE2   | 1.78                     | 0.40              |
| 46:S2:66:G:OP1    | 46:S2:82:G:N2      | 2.52                     | 0.40              |
| 46:S2:454:C:H2'   | 46:S2:455:U:C6     | 2.55                     | 0.40              |
| 46:S2:593:C:C2    | 46:S2:594:C:H5''   | 2.57                     | 0.40              |
| 46:S2:1553:G:H2'  | 46:S2:1557:A:OP1   | 2.21                     | 0.40              |
| 46:S2:1706:C:H2'  | 46:S2:1707:G:C8    | 2.56                     | 0.40              |
| 48:SA:174:MET:HB2 | 48:SA:174:MET:HE3  | 1.66                     | 0.40              |
| 52:SC:132:ASP:OD1 | 52:SC:133:TYR:N    | 2.55                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:SE:18:TRP:C     | 56:SE:18:TRP:CD1   | 3.00                     | 0.40              |
| 56:SE:51:ARG:HG3   | 56:SE:51:ARG:HH11  | 1.87                     | 0.40              |
| 57:SF:42:LYS:HG3   | 57:SF:43:GLU:H     | 1.87                     | 0.40              |
| 58:Sg:105:THR:HG23 | 58:Sg:106:LYS:HG2  | 2.02                     | 0.40              |
| 59:SG:103:ASP:O    | 59:SG:106:LEU:HD23 | 2.22                     | 0.40              |
| 59:SG:121:ILE:HD13 | 59:SG:121:ILE:HA   | 1.88                     | 0.40              |
| 62:SJ:111:GLN:OE1  | 62:SJ:127:ARG:HD2  | 2.21                     | 0.40              |
| 63:SK:2:LEU:HD12   | 63:SK:2:LEU:HA     | 1.89                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | La    | 145/148 (98%) | 136 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 5   | LA    | 246/257 (96%) | 228 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 6   | Lb    | 95/160 (59%)  | 93 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 7   | LB    | 395/403 (98%) | 372 (94%) | 23 (6%)  | 0        | 100         | 100 |
| 8   | Lc    | 92/115 (80%)  | 90 (98%)  | 1 (1%)   | 1 (1%)   | 11          | 16  |
| 9   | LC    | 355/419 (85%) | 335 (94%) | 20 (6%)  | 0        | 100         | 100 |
| 10  | Ld    | 106/125 (85%) | 103 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 11  | LD    | 291/297 (98%) | 263 (90%) | 28 (10%) | 0        | 100         | 100 |
| 12  | Le    | 126/135 (93%) | 119 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 13  | LE    | 210/296 (71%) | 200 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 14  | Lf    | 107/110 (97%) | 104 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 15  | LF    | 212/270 (78%) | 201 (95%) | 11 (5%)  | 0        | 100         | 100 |
| 16  | Lg    | 108/117 (92%) | 107 (99%) | 1 (1%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 17  | LG    | 225/266 (85%) | 215 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 18  | Lh    | 120/123 (98%) | 118 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 19  | LH    | 188/190 (99%) | 175 (93%) | 10 (5%)  | 3 (2%)   | 7           | 10  |
| 20  | Li    | 100/105 (95%) | 93 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 21  | LI    | 197/214 (92%) | 194 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 22  | Lj    | 84/97 (87%)   | 81 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 23  | LJ    | 165/178 (93%) | 158 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 24  | Lk    | 67/70 (96%)   | 64 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 25  | Ll    | 48/51 (94%)   | 46 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 26  | LL    | 204/211 (97%) | 191 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 27  | Lm    | 49/128 (38%)  | 49 (100%) | 0        | 0        | 100         | 100 |
| 28  | LM    | 134/217 (62%) | 129 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 29  | Ln    | 23/25 (92%)   | 23 (100%) | 0        | 0        | 100         | 100 |
| 30  | LN    | 201/204 (98%) | 193 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 31  | Lo    | 101/106 (95%) | 95 (94%)  | 5 (5%)   | 1 (1%)   | 12          | 18  |
| 32  | LO    | 199/203 (98%) | 188 (94%) | 10 (5%)  | 1 (0%)   | 24          | 36  |
| 33  | Lp    | 89/92 (97%)   | 84 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 34  | LP    | 152/184 (83%) | 148 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 35  | LQ    | 185/188 (98%) | 178 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 36  | Lr    | 122/137 (89%) | 113 (93%) | 8 (7%)   | 1 (1%)   | 16          | 24  |
| 37  | LR    | 172/196 (88%) | 169 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 38  | LS    | 173/176 (98%) | 165 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 39  | LT    | 158/160 (99%) | 154 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 40  | LU    | 98/128 (77%)  | 87 (89%)  | 11 (11%) | 0        | 100         | 100 |
| 41  | LV    | 128/140 (91%) | 125 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 42  | LW    | 60/157 (38%)  | 59 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 43  | LX    | 116/156 (74%) | 113 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 44  | LY    | 130/145 (90%) | 129 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 45  | LZ    | 133/136 (98%) | 128 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 47  | Sa    | 97/115 (84%)  | 91 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 48  | SA    | 205/295 (70%) | 189 (92%) | 16 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 49  | Sb    | 81/84 (96%)       | 73 (90%)    | 8 (10%)  | 0        | 100         | 100 |
| 50  | SB    | 211/264 (80%)     | 197 (93%)   | 14 (7%)  | 0        | 100         | 100 |
| 51  | Sc    | 52/69 (75%)       | 46 (88%)    | 5 (10%)  | 1 (2%)   | 6           | 8   |
| 52  | SC    | 213/293 (73%)     | 206 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 53  | Sd    | 52/56 (93%)       | 50 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 54  | SD    | 207/243 (85%)     | 193 (93%)   | 13 (6%)  | 1 (0%)   | 24          | 36  |
| 55  | Se    | 44/133 (33%)      | 39 (89%)    | 5 (11%)  | 0        | 100         | 100 |
| 56  | SE    | 256/263 (97%)     | 242 (94%)   | 13 (5%)  | 1 (0%)   | 30          | 42  |
| 57  | SF    | 175/204 (86%)     | 165 (94%)   | 10 (6%)  | 0        | 100         | 100 |
| 58  | Sg    | 270/317 (85%)     | 244 (90%)   | 26 (10%) | 0        | 100         | 100 |
| 59  | SG    | 200/249 (80%)     | 191 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 60  | SH    | 176/194 (91%)     | 162 (92%)   | 14 (8%)  | 0        | 100         | 100 |
| 61  | SI    | 179/208 (86%)     | 173 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 62  | SJ    | 130/194 (67%)     | 123 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 63  | SK    | 86/165 (52%)      | 75 (87%)    | 11 (13%) | 0        | 100         | 100 |
| 64  | SL    | 131/158 (83%)     | 126 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 65  | SN    | 148/151 (98%)     | 147 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 66  | SO    | 132/151 (87%)     | 123 (93%)   | 9 (7%)   | 0        | 100         | 100 |
| 67  | SP    | 116/145 (80%)     | 111 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 68  | SQ    | 137/146 (94%)     | 125 (91%)   | 12 (9%)  | 0        | 100         | 100 |
| 69  | SR    | 129/135 (96%)     | 116 (90%)   | 13 (10%) | 0        | 100         | 100 |
| 70  | SS    | 138/152 (91%)     | 128 (93%)   | 10 (7%)  | 0        | 100         | 100 |
| 71  | ST    | 138/145 (95%)     | 130 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 72  | SU    | 93/119 (78%)      | 86 (92%)    | 7 (8%)   | 0        | 100         | 100 |
| 73  | SV    | 79/83 (95%)       | 74 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 74  | SW    | 127/130 (98%)     | 120 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 76  | SX    | 137/143 (96%)     | 126 (92%)   | 10 (7%)  | 1 (1%)   | 18          | 27  |
| 77  | SY    | 108/133 (81%)     | 102 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 78  | SZ    | 70/125 (56%)      | 62 (89%)    | 8 (11%)  | 0        | 100         | 100 |
| All | All   | 10626/12497 (85%) | 10050 (95%) | 565 (5%) | 11 (0%)  | 49          | 64  |

All (11) Ramachandran outliers are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | Lc    | 99  | PRO  |
| 19  | LH    | 13  | PRO  |
| 32  | LO    | 187 | LYS  |
| 36  | Lr    | 123 | PRO  |
| 51  | Sc    | 51  | ARG  |
| 76  | SX    | 61  | GLN  |
| 31  | Lo    | 59  | LYS  |
| 54  | SD    | 93  | THR  |
| 19  | LH    | 189 | GLN  |
| 19  | LH    | 53  | LYS  |
| 56  | SE    | 247 | THR  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | La    | 120/121 (99%)  | 117 (98%) | 3 (2%)   | 42          | 63 |
| 5   | LA    | 190/199 (96%)  | 187 (98%) | 3 (2%)   | 55          | 73 |
| 6   | Lb    | 83/124 (67%)   | 82 (99%)  | 1 (1%)   | 63          | 78 |
| 7   | LB    | 344/348 (99%)  | 334 (97%) | 10 (3%)  | 37          | 57 |
| 8   | Lc    | 79/97 (81%)    | 78 (99%)  | 1 (1%)   | 61          | 76 |
| 9   | LC    | 301/348 (86%)  | 297 (99%) | 4 (1%)   | 61          | 76 |
| 10  | Ld    | 99/110 (90%)   | 96 (97%)  | 3 (3%)   | 36          | 56 |
| 11  | LD    | 246/249 (99%)  | 236 (96%) | 10 (4%)  | 27          | 44 |
| 12  | Le    | 114/121 (94%)  | 110 (96%) | 4 (4%)   | 32          | 51 |
| 13  | LE    | 194/256 (76%)  | 187 (96%) | 7 (4%)   | 31          | 50 |
| 14  | Lf    | 88/89 (99%)    | 87 (99%)  | 1 (1%)   | 65          | 79 |
| 15  | LF    | 185/234 (79%)  | 182 (98%) | 3 (2%)   | 55          | 73 |
| 16  | Lg    | 94/100 (94%)   | 93 (99%)  | 1 (1%)   | 65          | 79 |
| 17  | LG    | 197/223 (88%)  | 189 (96%) | 8 (4%)   | 27          | 44 |
| 18  | Lh    | 109/110 (99%)  | 108 (99%) | 1 (1%)   | 70          | 82 |
| 19  | LH    | 169/169 (100%) | 162 (96%) | 7 (4%)   | 27          | 44 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 20  | Li    | 86/89 (97%)    | 85 (99%)   | 1 (1%)   | 63          | 78  |
| 21  | LI    | 170/180 (94%)  | 165 (97%)  | 5 (3%)   | 37          | 57  |
| 22  | Lj    | 73/80 (91%)    | 73 (100%)  | 0        | 100         | 100 |
| 23  | LJ    | 141/149 (95%)  | 133 (94%)  | 8 (6%)   | 18          | 31  |
| 24  | Lk    | 64/65 (98%)    | 62 (97%)   | 2 (3%)   | 35          | 55  |
| 25  | Ll    | 46/47 (98%)    | 45 (98%)   | 1 (2%)   | 45          | 66  |
| 26  | LL    | 173/178 (97%)  | 164 (95%)  | 9 (5%)   | 21          | 34  |
| 27  | Lm    | 47/116 (40%)   | 45 (96%)   | 2 (4%)   | 26          | 42  |
| 28  | LM    | 116/157 (74%)  | 114 (98%)  | 2 (2%)   | 53          | 72  |
| 29  | Ln    | 24/24 (100%)   | 24 (100%)  | 0        | 100         | 100 |
| 30  | LN    | 171/172 (99%)  | 170 (99%)  | 1 (1%)   | 78          | 87  |
| 31  | Lo    | 91/94 (97%)    | 91 (100%)  | 0        | 100         | 100 |
| 32  | LO    | 172/173 (99%)  | 168 (98%)  | 4 (2%)   | 44          | 65  |
| 33  | Lp    | 74/75 (99%)    | 71 (96%)   | 3 (4%)   | 27          | 44  |
| 34  | LP    | 135/163 (83%)  | 132 (98%)  | 3 (2%)   | 45          | 66  |
| 35  | LQ    | 164/165 (99%)  | 163 (99%)  | 1 (1%)   | 78          | 87  |
| 36  | Lr    | 108/121 (89%)  | 105 (97%)  | 3 (3%)   | 38          | 58  |
| 37  | LR    | 154/175 (88%)  | 149 (97%)  | 5 (3%)   | 34          | 54  |
| 38  | LS    | 155/156 (99%)  | 149 (96%)  | 6 (4%)   | 28          | 47  |
| 39  | LT    | 140/140 (100%) | 137 (98%)  | 3 (2%)   | 47          | 67  |
| 40  | LU    | 90/114 (79%)   | 88 (98%)   | 2 (2%)   | 45          | 66  |
| 41  | LV    | 100/107 (94%)  | 97 (97%)   | 3 (3%)   | 36          | 56  |
| 42  | LW    | 54/126 (43%)   | 54 (100%)  | 0        | 100         | 100 |
| 43  | LX    | 106/133 (80%)  | 103 (97%)  | 3 (3%)   | 38          | 58  |
| 44  | LY    | 123/135 (91%)  | 122 (99%)  | 1 (1%)   | 73          | 84  |
| 45  | LZ    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 47  | Sa    | 86/98 (88%)    | 81 (94%)   | 5 (6%)   | 18          | 30  |
| 48  | SA    | 173/242 (72%)  | 170 (98%)  | 3 (2%)   | 53          | 72  |
| 49  | Sb    | 75/76 (99%)    | 67 (89%)   | 8 (11%)  | 6           | 9   |
| 50  | SB    | 194/229 (85%)  | 191 (98%)  | 3 (2%)   | 57          | 74  |
| 51  | Sc    | 48/62 (77%)    | 46 (96%)   | 2 (4%)   | 26          | 44  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 52  | SC    | 181/224 (81%)    | 176 (97%)  | 5 (3%)   | 38          | 58  |
| 53  | Sd    | 48/49 (98%)      | 45 (94%)   | 3 (6%)   | 16          | 27  |
| 54  | SD    | 173/202 (86%)    | 166 (96%)  | 7 (4%)   | 28          | 45  |
| 55  | Se    | 39/106 (37%)     | 38 (97%)   | 1 (3%)   | 40          | 61  |
| 56  | SE    | 221/225 (98%)    | 207 (94%)  | 14 (6%)  | 16          | 27  |
| 57  | SF    | 152/170 (89%)    | 149 (98%)  | 3 (2%)   | 48          | 68  |
| 58  | Sg    | 237/275 (86%)    | 231 (98%)  | 6 (2%)   | 42          | 63  |
| 59  | SG    | 178/218 (82%)    | 172 (97%)  | 6 (3%)   | 32          | 52  |
| 60  | SH    | 161/174 (92%)    | 150 (93%)  | 11 (7%)  | 14          | 23  |
| 61  | SI    | 159/180 (88%)    | 154 (97%)  | 5 (3%)   | 35          | 55  |
| 62  | SJ    | 126/168 (75%)    | 123 (98%)  | 3 (2%)   | 43          | 64  |
| 63  | SK    | 81/136 (60%)     | 80 (99%)   | 1 (1%)   | 63          | 78  |
| 64  | SL    | 123/142 (87%)    | 120 (98%)  | 3 (2%)   | 43          | 64  |
| 65  | SN    | 130/131 (99%)    | 127 (98%)  | 3 (2%)   | 44          | 65  |
| 66  | SO    | 104/119 (87%)    | 101 (97%)  | 3 (3%)   | 37          | 57  |
| 67  | SP    | 107/130 (82%)    | 101 (94%)  | 6 (6%)   | 19          | 31  |
| 68  | SQ    | 115/121 (95%)    | 108 (94%)  | 7 (6%)   | 17          | 29  |
| 69  | SR    | 119/121 (98%)    | 116 (98%)  | 3 (2%)   | 42          | 63  |
| 70  | SS    | 122/132 (92%)    | 113 (93%)  | 9 (7%)   | 13          | 20  |
| 71  | ST    | 110/115 (96%)    | 104 (94%)  | 6 (6%)   | 19          | 32  |
| 72  | SU    | 88/107 (82%)     | 86 (98%)   | 2 (2%)   | 44          | 65  |
| 73  | SV    | 65/67 (97%)      | 62 (95%)   | 3 (5%)   | 24          | 39  |
| 74  | SW    | 112/113 (99%)    | 106 (95%)  | 6 (5%)   | 20          | 33  |
| 76  | SX    | 111/115 (96%)    | 104 (94%)  | 7 (6%)   | 16          | 27  |
| 77  | SY    | 93/115 (81%)     | 93 (100%)  | 0        | 100         | 100 |
| 78  | SZ    | 64/103 (62%)     | 63 (98%)   | 1 (2%)   | 55          | 73  |
| All | All   | 9301/10615 (88%) | 9021 (97%) | 280 (3%) | 37          | 56  |

All (280) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | La    | 92  | LYS  |
| 4   | La    | 103 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | La    | 140 | VAL  |
| 5   | LA    | 15  | VAL  |
| 5   | LA    | 136 | VAL  |
| 5   | LA    | 237 | LEU  |
| 6   | Lb    | 115 | ARG  |
| 7   | LB    | 17  | LEU  |
| 7   | LB    | 31  | SER  |
| 7   | LB    | 43  | LEU  |
| 7   | LB    | 60  | VAL  |
| 7   | LB    | 162 | ILE  |
| 7   | LB    | 258 | HIS  |
| 7   | LB    | 328 | ASN  |
| 7   | LB    | 329 | ASP  |
| 7   | LB    | 331 | ILE  |
| 7   | LB    | 362 | LYS  |
| 8   | Lc    | 58  | SER  |
| 9   | LC    | 62  | THR  |
| 9   | LC    | 105 | THR  |
| 9   | LC    | 107 | THR  |
| 9   | LC    | 228 | THR  |
| 10  | Ld    | 36  | VAL  |
| 10  | Ld    | 57  | MET  |
| 10  | Ld    | 89  | SER  |
| 11  | LD    | 7   | VAL  |
| 11  | LD    | 44  | TYR  |
| 11  | LD    | 118 | ILE  |
| 11  | LD    | 171 | LEU  |
| 11  | LD    | 194 | VAL  |
| 11  | LD    | 217 | ASP  |
| 11  | LD    | 224 | SER  |
| 11  | LD    | 226 | TYR  |
| 11  | LD    | 267 | ASN  |
| 11  | LD    | 286 | SER  |
| 12  | Le    | 4   | LEU  |
| 12  | Le    | 31  | ILE  |
| 12  | Le    | 86  | GLU  |
| 12  | Le    | 117 | GLN  |
| 13  | LE    | 101 | THR  |
| 13  | LE    | 183 | VAL  |
| 13  | LE    | 202 | VAL  |
| 13  | LE    | 206 | SER  |
| 13  | LE    | 207 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | LE    | 209 | VAL  |
| 13  | LE    | 295 | VAL  |
| 14  | Lf    | 59  | THR  |
| 15  | LF    | 218 | THR  |
| 15  | LF    | 247 | THR  |
| 15  | LF    | 250 | VAL  |
| 16  | Lg    | 17  | SER  |
| 17  | LG    | 33  | GLU  |
| 17  | LG    | 97  | LYS  |
| 17  | LG    | 106 | THR  |
| 17  | LG    | 108 | GLN  |
| 17  | LG    | 112 | GLN  |
| 17  | LG    | 132 | ARG  |
| 17  | LG    | 166 | LEU  |
| 17  | LG    | 168 | VAL  |
| 18  | Lh    | 14  | LYS  |
| 19  | LH    | 58  | ASP  |
| 19  | LH    | 65  | LYS  |
| 19  | LH    | 95  | VAL  |
| 19  | LH    | 137 | SER  |
| 19  | LH    | 155 | SER  |
| 19  | LH    | 183 | GLU  |
| 19  | LH    | 188 | GLN  |
| 20  | Li    | 64  | SER  |
| 21  | LI    | 43  | VAL  |
| 21  | LI    | 59  | GLN  |
| 21  | LI    | 179 | ASP  |
| 21  | LI    | 195 | CYS  |
| 21  | LI    | 197 | VAL  |
| 23  | LJ    | 56  | THR  |
| 23  | LJ    | 72  | CYS  |
| 23  | LJ    | 78  | LYS  |
| 23  | LJ    | 81  | GLU  |
| 23  | LJ    | 90  | ARG  |
| 23  | LJ    | 132 | VAL  |
| 23  | LJ    | 146 | ARG  |
| 23  | LJ    | 173 | ILE  |
| 24  | Lk    | 5   | ILE  |
| 24  | Lk    | 59  | SER  |
| 25  | LI    | 47  | THR  |
| 26  | LL    | 17  | ASP  |
| 26  | LL    | 59  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | LL    | 63  | THR  |
| 26  | LL    | 64  | VAL  |
| 26  | LL    | 67  | HIS  |
| 26  | LL    | 107 | THR  |
| 26  | LL    | 115 | GLN  |
| 26  | LL    | 204 | GLU  |
| 26  | LL    | 206 | ASP  |
| 27  | Lm    | 103 | LEU  |
| 27  | Lm    | 126 | LYS  |
| 28  | LM    | 31  | ILE  |
| 28  | LM    | 136 | LEU  |
| 30  | LN    | 34  | SER  |
| 32  | LO    | 32  | LYS  |
| 32  | LO    | 120 | VAL  |
| 32  | LO    | 175 | LEU  |
| 32  | LO    | 187 | LYS  |
| 33  | Lp    | 21  | SER  |
| 33  | Lp    | 26  | VAL  |
| 33  | Lp    | 52  | VAL  |
| 34  | LP    | 24  | VAL  |
| 34  | LP    | 57  | CYS  |
| 34  | LP    | 93  | HIS  |
| 35  | LQ    | 119 | LYS  |
| 36  | Lr    | 91  | SER  |
| 36  | Lr    | 122 | LYS  |
| 36  | Lr    | 123 | PRO  |
| 37  | LR    | 91  | GLU  |
| 37  | LR    | 93  | VAL  |
| 37  | LR    | 112 | SER  |
| 37  | LR    | 149 | LYS  |
| 37  | LR    | 152 | LYS  |
| 38  | LS    | 23  | HIS  |
| 38  | LS    | 48  | VAL  |
| 38  | LS    | 82  | LEU  |
| 38  | LS    | 90  | THR  |
| 38  | LS    | 148 | SER  |
| 38  | LS    | 161 | ARG  |
| 39  | LT    | 2   | THR  |
| 39  | LT    | 29  | THR  |
| 39  | LT    | 76  | VAL  |
| 40  | LU    | 109 | SER  |
| 40  | LU    | 115 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | LV    | 18  | LEU  |
| 41  | LV    | 92  | ASP  |
| 41  | LV    | 115 | SER  |
| 43  | LX    | 85  | SER  |
| 43  | LX    | 119 | ILE  |
| 43  | LX    | 148 | ASP  |
| 44  | LY    | 43  | ASN  |
| 47  | Sa    | 24  | THR  |
| 47  | Sa    | 30  | VAL  |
| 47  | Sa    | 54  | SER  |
| 47  | Sa    | 66  | LYS  |
| 47  | Sa    | 81  | SER  |
| 48  | SA    | 6   | ASP  |
| 48  | SA    | 7   | VAL  |
| 48  | SA    | 54  | THR  |
| 49  | Sb    | 8   | LEU  |
| 49  | Sb    | 13  | GLU  |
| 49  | Sb    | 43  | ILE  |
| 49  | Sb    | 44  | THR  |
| 49  | Sb    | 46  | VAL  |
| 49  | Sb    | 57  | VAL  |
| 49  | Sb    | 65  | GLN  |
| 49  | Sb    | 78  | SER  |
| 50  | SB    | 38  | MET  |
| 50  | SB    | 55  | THR  |
| 50  | SB    | 91  | VAL  |
| 51  | Sc    | 15  | THR  |
| 51  | Sc    | 17  | VAL  |
| 52  | SC    | 137 | VAL  |
| 52  | SC    | 147 | VAL  |
| 52  | SC    | 149 | THR  |
| 52  | SC    | 184 | VAL  |
| 52  | SC    | 211 | LYS  |
| 53  | Sd    | 31  | ILE  |
| 53  | Sd    | 36  | LEU  |
| 53  | Sd    | 53  | ILE  |
| 54  | SD    | 17  | PHE  |
| 54  | SD    | 20  | GLU  |
| 54  | SD    | 32  | ASP  |
| 54  | SD    | 48  | ILE  |
| 54  | SD    | 110 | LEU  |
| 54  | SD    | 206 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | SD    | 208 | VAL  |
| 55  | Se    | 132 | ASN  |
| 56  | SE    | 12  | VAL  |
| 56  | SE    | 18  | TRP  |
| 56  | SE    | 19  | MET  |
| 56  | SE    | 56  | LEU  |
| 56  | SE    | 126 | VAL  |
| 56  | SE    | 131 | VAL  |
| 56  | SE    | 140 | VAL  |
| 56  | SE    | 166 | THR  |
| 56  | SE    | 196 | THR  |
| 56  | SE    | 210 | VAL  |
| 56  | SE    | 217 | SER  |
| 56  | SE    | 220 | THR  |
| 56  | SE    | 222 | LEU  |
| 56  | SE    | 248 | ILE  |
| 57  | SF    | 34  | SER  |
| 57  | SF    | 82  | ASN  |
| 57  | SF    | 147 | VAL  |
| 58  | Sg    | 69  | VAL  |
| 58  | Sg    | 135 | LEU  |
| 58  | Sg    | 146 | SER  |
| 58  | Sg    | 178 | ASN  |
| 58  | Sg    | 297 | THR  |
| 58  | Sg    | 309 | VAL  |
| 59  | SG    | 26  | THR  |
| 59  | SG    | 114 | VAL  |
| 59  | SG    | 129 | VAL  |
| 59  | SG    | 141 | ILE  |
| 59  | SG    | 172 | LYS  |
| 59  | SG    | 178 | ARG  |
| 60  | SH    | 30  | LEU  |
| 60  | SH    | 40  | LEU  |
| 60  | SH    | 52  | GLU  |
| 60  | SH    | 61  | ILE  |
| 60  | SH    | 64  | VAL  |
| 60  | SH    | 114 | GLN  |
| 60  | SH    | 151 | SER  |
| 60  | SH    | 166 | VAL  |
| 60  | SH    | 172 | THR  |
| 60  | SH    | 174 | SER  |
| 60  | SH    | 184 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | SI    | 38  | ILE  |
| 61  | SI    | 91  | VAL  |
| 61  | SI    | 97  | VAL  |
| 61  | SI    | 121 | LEU  |
| 61  | SI    | 157 | LYS  |
| 62  | SJ    | 114 | VAL  |
| 62  | SJ    | 123 | ILE  |
| 62  | SJ    | 149 | VAL  |
| 63  | SK    | 7   | ASN  |
| 64  | SL    | 87  | VAL  |
| 64  | SL    | 130 | GLU  |
| 64  | SL    | 146 | THR  |
| 65  | SN    | 63  | VAL  |
| 65  | SN    | 67  | THR  |
| 65  | SN    | 87  | ASP  |
| 66  | SO    | 65  | ASP  |
| 66  | SO    | 98  | ARG  |
| 66  | SO    | 129 | ILE  |
| 67  | SP    | 26  | LEU  |
| 67  | SP    | 57  | LEU  |
| 67  | SP    | 58  | LYS  |
| 67  | SP    | 59  | ARG  |
| 67  | SP    | 61  | ARG  |
| 67  | SP    | 79  | HIS  |
| 68  | SQ    | 18  | THR  |
| 68  | SQ    | 34  | VAL  |
| 68  | SQ    | 48  | GLN  |
| 68  | SQ    | 70  | VAL  |
| 68  | SQ    | 89  | SER  |
| 68  | SQ    | 105 | LYS  |
| 68  | SQ    | 113 | ILE  |
| 69  | SR    | 6   | THR  |
| 69  | SR    | 27  | ASP  |
| 69  | SR    | 62  | GLN  |
| 70  | SS    | 12  | ILE  |
| 70  | SS    | 15  | VAL  |
| 70  | SS    | 33  | ILE  |
| 70  | SS    | 52  | LEU  |
| 70  | SS    | 67  | VAL  |
| 70  | SS    | 99  | LEU  |
| 70  | SS    | 109 | GLU  |
| 70  | SS    | 111 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70  | SS    | 116 | LYS  |
| 71  | ST    | 6   | VAL  |
| 71  | ST    | 28  | LEU  |
| 71  | ST    | 39  | LEU  |
| 71  | ST    | 90  | SER  |
| 71  | ST    | 93  | SER  |
| 71  | ST    | 113 | VAL  |
| 72  | SU    | 40  | ILE  |
| 72  | SU    | 65  | THR  |
| 73  | SV    | 10  | ASP  |
| 73  | SV    | 70  | LEU  |
| 73  | SV    | 74  | LYS  |
| 74  | SW    | 6   | VAL  |
| 74  | SW    | 66  | THR  |
| 74  | SW    | 80  | ASP  |
| 74  | SW    | 81  | VAL  |
| 74  | SW    | 103 | VAL  |
| 74  | SW    | 118 | ARG  |
| 76  | SX    | 4   | CYS  |
| 76  | SX    | 24  | ASP  |
| 76  | SX    | 26  | GLN  |
| 76  | SX    | 51  | VAL  |
| 76  | SX    | 71  | ARG  |
| 76  | SX    | 112 | VAL  |
| 76  | SX    | 128 | VAL  |
| 78  | SZ    | 73  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | La    | 28  | HIS  |
| 4   | La    | 39  | HIS  |
| 4   | La    | 66  | ASN  |
| 4   | La    | 67  | GLN  |
| 5   | LA    | 50  | HIS  |
| 6   | Lb    | 19  | ASN  |
| 7   | LB    | 184 | GLN  |
| 7   | LB    | 376 | HIS  |
| 9   | LC    | 60  | HIS  |
| 9   | LC    | 61  | GLN  |
| 9   | LC    | 89  | GLN  |
| 9   | LC    | 212 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | LC    | 329 | ASN  |
| 10  | Ld    | 93  | ASN  |
| 11  | LD    | 157 | ASN  |
| 11  | LD    | 267 | ASN  |
| 15  | LF    | 102 | ASN  |
| 15  | LF    | 121 | ASN  |
| 15  | LF    | 148 | ASN  |
| 17  | LG    | 81  | ASN  |
| 17  | LG    | 100 | HIS  |
| 17  | LG    | 141 | ASN  |
| 18  | Lh    | 108 | GLN  |
| 19  | LH    | 163 | GLN  |
| 21  | LI    | 144 | ASN  |
| 22  | Lj    | 13  | ASN  |
| 23  | LJ    | 65  | ASN  |
| 23  | LJ    | 98  | ASN  |
| 23  | LJ    | 104 | ASN  |
| 27  | Lm    | 109 | ASN  |
| 30  | LN    | 91  | GLN  |
| 30  | LN    | 156 | HIS  |
| 32  | LO    | 26  | GLN  |
| 32  | LO    | 42  | ASN  |
| 32  | LO    | 63  | ASN  |
| 34  | LP    | 97  | ASN  |
| 34  | LP    | 116 | HIS  |
| 34  | LP    | 133 | HIS  |
| 35  | LQ    | 162 | HIS  |
| 36  | Lr    | 4   | HIS  |
| 36  | Lr    | 21  | ASN  |
| 37  | LR    | 141 | HIS  |
| 38  | LS    | 77  | ASN  |
| 38  | LS    | 91  | HIS  |
| 38  | LS    | 108 | GLN  |
| 39  | LT    | 66  | ASN  |
| 40  | LU    | 27  | HIS  |
| 41  | LV    | 108 | ASN  |
| 43  | LX    | 57  | GLN  |
| 43  | LX    | 69  | ASN  |
| 43  | LX    | 111 | GLN  |
| 44  | LY    | 43  | ASN  |
| 44  | LY    | 100 | HIS  |
| 47  | Sa    | 8   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | SC    | 113 | GLN  |
| 52  | SC    | 267 | GLN  |
| 53  | Sd    | 26  | ASN  |
| 53  | Sd    | 37  | ASN  |
| 54  | SD    | 22  | ASN  |
| 55  | Se    | 132 | ASN  |
| 56  | SE    | 214 | ASN  |
| 57  | SF    | 149 | GLN  |
| 57  | SF    | 203 | ASN  |
| 60  | SH    | 33  | ASN  |
| 60  | SH    | 39  | GLN  |
| 60  | SH    | 165 | ASN  |
| 61  | SI    | 35  | ASN  |
| 63  | SK    | 61  | GLN  |
| 64  | SL    | 18  | GLN  |
| 64  | SL    | 19  | ASN  |
| 64  | SL    | 83  | GLN  |
| 64  | SL    | 100 | ASN  |
| 64  | SL    | 112 | HIS  |
| 65  | SN    | 62  | GLN  |
| 66  | SO    | 32  | HIS  |
| 67  | SP    | 32  | GLN  |
| 68  | SQ    | 80  | GLN  |
| 68  | SQ    | 142 | GLN  |
| 69  | SR    | 74  | GLN  |
| 69  | SR    | 121 | GLN  |
| 70  | SS    | 17  | ASN  |
| 70  | SS    | 72  | GLN  |
| 71  | ST    | 42  | HIS  |
| 71  | ST    | 91  | HIS  |
| 74  | SW    | 24  | GLN  |
| 74  | SW    | 64  | ASN  |
| 74  | SW    | 82  | GLN  |
| 76  | SX    | 61  | GLN  |
| 76  | SX    | 77  | ASN  |
| 78  | SZ    | 106 | GLN  |

### 5.3.3 RNA

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | L5    | 3377/4731 (71%) | 685 (20%)         | 33 (0%)         |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2   | L7    | 119/120 (99%)   | 10 (8%)           | 3 (2%)          |
| 3   | L8    | 149/158 (94%)   | 28 (18%)          | 1 (0%)          |
| 46  | S2    | 1618/1870 (86%) | 508 (31%)         | 35 (2%)         |
| 75  | Sx    | 9/10 (90%)      | 1 (11%)           | 0               |
| 79  | S6    | 74/75 (98%)     | 23 (31%)          | 3 (4%)          |
| 79  | S7    | 74/75 (98%)     | 27 (36%)          | 1 (1%)          |
| All | All   | 5420/7039 (76%) | 1282 (23%)        | 76 (1%)         |

All (1282) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L5    | 2   | G    |
| 1   | L5    | 3   | C    |
| 1   | L5    | 21  | G    |
| 1   | L5    | 25  | A    |
| 1   | L5    | 39  | A    |
| 1   | L5    | 42  | A    |
| 1   | L5    | 48  | G    |
| 1   | L5    | 56  | A    |
| 1   | L5    | 59  | A    |
| 1   | L5    | 64  | A    |
| 1   | L5    | 65  | A    |
| 1   | L5    | 66  | A    |
| 1   | L5    | 71  | C    |
| 1   | L5    | 72  | C    |
| 1   | L5    | 76  | A    |
| 1   | L5    | 85  | G    |
| 1   | L5    | 91  | G    |
| 1   | L5    | 99  | A    |
| 1   | L5    | 104 | G    |
| 1   | L5    | 108 | A    |
| 1   | L5    | 109 | G    |
| 1   | L5    | 119 | G    |
| 1   | L5    | 120 | A    |
| 1   | L5    | 132 | G    |
| 1   | L5    | 133 | C    |
| 1   | L5    | 134 | G    |
| 1   | L5    | 135 | U    |
| 1   | L5    | 136 | C    |
| 1   | L5    | 137 | G    |
| 1   | L5    | 138 | C    |
| 1   | L5    | 139 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L5    | 140 | G    |
| 1   | L5    | 141 | C    |
| 1   | L5    | 143 | U    |
| 1   | L5    | 144 | G    |
| 1   | L5    | 159 | C    |
| 1   | L5    | 160 | G    |
| 1   | L5    | 170 | C    |
| 1   | L5    | 172 | C    |
| 1   | L5    | 173 | C    |
| 1   | L5    | 195 | C    |
| 1   | L5    | 197 | A    |
| 1   | L5    | 200 | U    |
| 1   | L5    | 209 | U    |
| 1   | L5    | 210 | C    |
| 1   | L5    | 217 | C    |
| 1   | L5    | 218 | A    |
| 1   | L5    | 219 | G    |
| 1   | L5    | 228 | C    |
| 1   | L5    | 233 | U    |
| 1   | L5    | 234 | G    |
| 1   | L5    | 235 | A    |
| 1   | L5    | 241 | G    |
| 1   | L5    | 252 | G    |
| 1   | L5    | 256 | C    |
| 1   | L5    | 258 | C    |
| 1   | L5    | 259 | C    |
| 1   | L5    | 260 | G    |
| 1   | L5    | 264 | U    |
| 1   | L5    | 265 | C    |
| 1   | L5    | 267 | G    |
| 1   | L5    | 269 | U    |
| 1   | L5    | 279 | G    |
| 1   | L5    | 296 | U    |
| 1   | L5    | 305 | A    |
| 1   | L5    | 315 | U    |
| 1   | L5    | 333 | A    |
| 1   | L5    | 339 | C    |
| 1   | L5    | 349 | C    |
| 1   | L5    | 360 | C    |
| 1   | L5    | 361 | A    |
| 1   | L5    | 372 | G    |
| 1   | L5    | 386 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L5    | 387 | A    |
| 1   | L5    | 388 | A    |
| 1   | L5    | 398 | G    |
| 1   | L5    | 408 | G    |
| 1   | L5    | 409 | A    |
| 1   | L5    | 411 | G    |
| 1   | L5    | 416 | G    |
| 1   | L5    | 430 | G    |
| 1   | L5    | 431 | U    |
| 1   | L5    | 443 | G    |
| 1   | L5    | 448 | C    |
| 1   | L5    | 449 | G    |
| 1   | L5    | 452 | G    |
| 1   | L5    | 453 | U    |
| 1   | L5    | 454 | C    |
| 1   | L5    | 455 | C    |
| 1   | L5    | 456 | G    |
| 1   | L5    | 457 | C    |
| 1   | L5    | 458 | C    |
| 1   | L5    | 459 | C    |
| 1   | L5    | 466 | U    |
| 1   | L5    | 467 | U    |
| 1   | L5    | 487 | C    |
| 1   | L5    | 491 | C    |
| 1   | L5    | 494 | G    |
| 1   | L5    | 497 | C    |
| 1   | L5    | 512 | A    |
| 1   | L5    | 513 | U    |
| 1   | L5    | 654 | G    |
| 1   | L5    | 660 | G    |
| 1   | L5    | 661 | U    |
| 1   | L5    | 667 | G    |
| 1   | L5    | 668 | G    |
| 1   | L5    | 669 | C    |
| 1   | L5    | 671 | G    |
| 1   | L5    | 673 | C    |
| 1   | L5    | 674 | G    |
| 1   | L5    | 675 | A    |
| 1   | L5    | 676 | C    |
| 1   | L5    | 677 | C    |
| 1   | L5    | 678 | G    |
| 1   | L5    | 680 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L5    | 682 | G    |
| 1   | L5    | 691 | C    |
| 1   | L5    | 693 | C    |
| 1   | L5    | 695 | C    |
| 1   | L5    | 696 | U    |
| 1   | L5    | 697 | U    |
| 1   | L5    | 701 | C    |
| 1   | L5    | 704 | U    |
| 1   | L5    | 705 | G    |
| 1   | L5    | 712 | C    |
| 1   | L5    | 714 | C    |
| 1   | L5    | 739 | G    |
| 1   | L5    | 746 | C    |
| 1   | L5    | 747 | G    |
| 1   | L5    | 748 | G    |
| 1   | L5    | 749 | U    |
| 1   | L5    | 750 | G    |
| 1   | L5    | 754 | A    |
| 1   | L5    | 757 | G    |
| 1   | L5    | 761 | C    |
| 1   | L5    | 766 | G    |
| 1   | L5    | 806 | C    |
| 1   | L5    | 807 | C    |
| 1   | L5    | 810 | G    |
| 1   | L5    | 813 | U    |
| 1   | L5    | 815 | A    |
| 1   | L5    | 817 | A    |
| 1   | L5    | 824 | C    |
| 1   | L5    | 825 | G    |
| 1   | L5    | 830 | C    |
| 1   | L5    | 831 | G    |
| 1   | L5    | 833 | U    |
| 1   | L5    | 834 | U    |
| 1   | L5    | 835 | U    |
| 1   | L5    | 842 | A    |
| 1   | L5    | 843 | U    |
| 1   | L5    | 857 | A    |
| 1   | L5    | 858 | A    |
| 1   | L5    | 860 | C    |
| 1   | L5    | 882 | U    |
| 1   | L5    | 886 | U    |
| 1   | L5    | 924 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 926  | G    |
| 1   | L5    | 927  | C    |
| 1   | L5    | 928  | C    |
| 1   | L5    | 938  | C    |
| 1   | L5    | 940  | C    |
| 1   | L5    | 953  | C    |
| 1   | L5    | 954  | G    |
| 1   | L5    | 1003 | G    |
| 1   | L5    | 1005 | C    |
| 1   | L5    | 1006 | G    |
| 1   | L5    | 1007 | G    |
| 1   | L5    | 1009 | C    |
| 1   | L5    | 1010 | U    |
| 1   | L5    | 1011 | G    |
| 1   | L5    | 1012 | U    |
| 1   | L5    | 1013 | C    |
| 1   | L5    | 1014 | C    |
| 1   | L5    | 1015 | C    |
| 1   | L5    | 1016 | C    |
| 1   | L5    | 1017 | A    |
| 1   | L5    | 1018 | G    |
| 1   | L5    | 1019 | U    |
| 1   | L5    | 1020 | G    |
| 1   | L5    | 1021 | C    |
| 1   | L5    | 1022 | G    |
| 1   | L5    | 1026 | C    |
| 1   | L5    | 1027 | G    |
| 1   | L5    | 1028 | G    |
| 1   | L5    | 1029 | G    |
| 1   | L5    | 1031 | G    |
| 1   | L5    | 1032 | U    |
| 1   | L5    | 1033 | G    |
| 1   | L5    | 1034 | G    |
| 1   | L5    | 1036 | C    |
| 1   | L5    | 1037 | G    |
| 1   | L5    | 1038 | C    |
| 1   | L5    | 1039 | G    |
| 1   | L5    | 1044 | C    |
| 1   | L5    | 1045 | G    |
| 1   | L5    | 1048 | U    |
| 1   | L5    | 1049 | C    |
| 1   | L5    | 1050 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 1051 | G    |
| 1   | L5    | 1053 | G    |
| 1   | L5    | 1055 | G    |
| 1   | L5    | 1095 | C    |
| 1   | L5    | 1099 | G    |
| 1   | L5    | 1100 | U    |
| 1   | L5    | 1102 | G    |
| 1   | L5    | 1108 | G    |
| 1   | L5    | 1116 | C    |
| 1   | L5    | 1141 | A    |
| 1   | L5    | 1152 | A    |
| 1   | L5    | 1154 | U    |
| 1   | L5    | 1160 | G    |
| 1   | L5    | 1169 | A    |
| 1   | L5    | 1173 | A    |
| 1   | L5    | 1174 | G    |
| 1   | L5    | 1180 | C    |
| 1   | L5    | 1193 | C    |
| 1   | L5    | 1194 | C    |
| 1   | L5    | 1202 | A    |
| 1   | L5    | 1209 | G    |
| 1   | L5    | 1212 | A    |
| 1   | L5    | 1221 | G    |
| 1   | L5    | 1222 | C    |
| 1   | L5    | 1223 | C    |
| 1   | L5    | 1224 | C    |
| 1   | L5    | 1225 | G    |
| 1   | L5    | 1226 | G    |
| 1   | L5    | 1227 | G    |
| 1   | L5    | 1228 | G    |
| 1   | L5    | 1229 | G    |
| 1   | L5    | 1230 | C    |
| 1   | L5    | 1232 | C    |
| 1   | L5    | 1234 | A    |
| 1   | L5    | 1254 | U    |
| 1   | L5    | 1256 | C    |
| 1   | L5    | 1257 | A    |
| 1   | L5    | 1261 | C    |
| 1   | L5    | 1266 | A    |
| 1   | L5    | 1272 | C    |
| 1   | L5    | 1289 | G    |
| 1   | L5    | 1290 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 1295 | C    |
| 1   | L5    | 1296 | G    |
| 1   | L5    | 1297 | C    |
| 1   | L5    | 1298 | G    |
| 1   | L5    | 1299 | C    |
| 1   | L5    | 1311 | A    |
| 1   | L5    | 1312 | G    |
| 1   | L5    | 1316 | G    |
| 1   | L5    | 1317 | A    |
| 1   | L5    | 1328 | U    |
| 1   | L5    | 1329 | A    |
| 1   | L5    | 1344 | G    |
| 1   | L5    | 1348 | A    |
| 1   | L5    | 1361 | A    |
| 1   | L5    | 1379 | A    |
| 1   | L5    | 1380 | C    |
| 1   | L5    | 1389 | A    |
| 1   | L5    | 1392 | U    |
| 1   | L5    | 1405 | U    |
| 1   | L5    | 1410 | U    |
| 1   | L5    | 1415 | A    |
| 1   | L5    | 1428 | C    |
| 1   | L5    | 1438 | G    |
| 1   | L5    | 1439 | G    |
| 1   | L5    | 1445 | A    |
| 1   | L5    | 1447 | G    |
| 1   | L5    | 1448 | A    |
| 1   | L5    | 1454 | C    |
| 1   | L5    | 1456 | A    |
| 1   | L5    | 1465 | G    |
| 1   | L5    | 1468 | G    |
| 1   | L5    | 1475 | C    |
| 1   | L5    | 1490 | C    |
| 1   | L5    | 1491 | U    |
| 1   | L5    | 1508 | C    |
| 1   | L5    | 1511 | G    |
| 1   | L5    | 1524 | G    |
| 1   | L5    | 1537 | G    |
| 1   | L5    | 1553 | G    |
| 1   | L5    | 1556 | G    |
| 1   | L5    | 1557 | U    |
| 1   | L5    | 1560 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 1561 | G    |
| 1   | L5    | 1563 | G    |
| 1   | L5    | 1564 | G    |
| 1   | L5    | 1575 | C    |
| 1   | L5    | 1578 | A    |
| 1   | L5    | 1586 | C    |
| 1   | L5    | 1590 | A    |
| 1   | L5    | 1607 | A    |
| 1   | L5    | 1615 | C    |
| 1   | L5    | 1625 | U    |
| 1   | L5    | 1627 | G    |
| 1   | L5    | 1639 | G    |
| 1   | L5    | 1640 | A    |
| 1   | L5    | 1645 | G    |
| 1   | L5    | 1658 | G    |
| 1   | L5    | 1672 | G    |
| 1   | L5    | 1673 | C    |
| 1   | L5    | 1685 | U    |
| 1   | L5    | 1700 | A    |
| 1   | L5    | 1713 | G    |
| 1   | L5    | 1721 | U    |
| 1   | L5    | 1722 | G    |
| 1   | L5    | 1723 | C    |
| 1   | L5    | 1724 | C    |
| 1   | L5    | 1725 | G    |
| 1   | L5    | 1728 | G    |
| 1   | L5    | 1734 | C    |
| 1   | L5    | 1735 | A    |
| 1   | L5    | 1743 | G    |
| 1   | L5    | 1751 | G    |
| 1   | L5    | 1762 | U    |
| 1   | L5    | 1763 | A    |
| 1   | L5    | 1764 | G    |
| 1   | L5    | 1765 | A    |
| 1   | L5    | 1766 | C    |
| 1   | L5    | 1767 | A    |
| 1   | L5    | 1831 | C    |
| 1   | L5    | 1832 | A    |
| 1   | L5    | 1847 | U    |
| 1   | L5    | 1851 | U    |
| 1   | L5    | 1858 | G    |
| 1   | L5    | 1859 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 1872 | A    |
| 1   | L5    | 1887 | C    |
| 1   | L5    | 1892 | G    |
| 1   | L5    | 1903 | A    |
| 1   | L5    | 1904 | C    |
| 1   | L5    | 1905 | G    |
| 1   | L5    | 1907 | G    |
| 1   | L5    | 1908 | A    |
| 1   | L5    | 1909 | C    |
| 1   | L5    | 1910 | G    |
| 1   | L5    | 2016 | G    |
| 1   | L5    | 2046 | C    |
| 1   | L5    | 2057 | A    |
| 1   | L5    | 2058 | G    |
| 1   | L5    | 2070 | A    |
| 1   | L5    | 2073 | G    |
| 1   | L5    | 2089 | A    |
| 1   | L5    | 2090 | G    |
| 1   | L5    | 2105 | G    |
| 1   | L5    | 2108 | C    |
| 1   | L5    | 2121 | G    |
| 1   | L5    | 2141 | U    |
| 1   | L5    | 2152 | A    |
| 1   | L5    | 2153 | A    |
| 1   | L5    | 2154 | G    |
| 1   | L5    | 2178 | G    |
| 1   | L5    | 2179 | C    |
| 1   | L5    | 2180 | A    |
| 1   | L5    | 2182 | U    |
| 1   | L5    | 2207 | G    |
| 1   | L5    | 2210 | A    |
| 1   | L5    | 2222 | C    |
| 1   | L5    | 2227 | C    |
| 1   | L5    | 2228 | G    |
| 1   | L5    | 2230 | A    |
| 1   | L5    | 2231 | G    |
| 1   | L5    | 2232 | G    |
| 1   | L5    | 2235 | C    |
| 1   | L5    | 2236 | G    |
| 1   | L5    | 2237 | G    |
| 1   | L5    | 2241 | A    |
| 1   | L5    | 2242 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 2243 | G    |
| 1   | L5    | 2254 | C    |
| 1   | L5    | 2255 | C    |
| 1   | L5    | 2260 | G    |
| 1   | L5    | 2261 | C    |
| 1   | L5    | 2263 | G    |
| 1   | L5    | 2269 | A    |
| 1   | L5    | 2270 | A    |
| 1   | L5    | 2274 | A    |
| 1   | L5    | 2285 | G    |
| 1   | L5    | 2300 | A    |
| 1   | L5    | 2301 | G    |
| 1   | L5    | 2302 | U    |
| 1   | L5    | 2303 | G    |
| 1   | L5    | 2304 | G    |
| 1   | L5    | 2311 | U    |
| 1   | L5    | 2312 | G    |
| 1   | L5    | 2315 | C    |
| 1   | L5    | 2324 | G    |
| 1   | L5    | 2337 | C    |
| 1   | L5    | 2340 | G    |
| 1   | L5    | 2341 | A    |
| 1   | L5    | 2343 | C    |
| 1   | L5    | 2346 | U    |
| 1   | L5    | 2355 | A    |
| 1   | L5    | 2356 | G    |
| 1   | L5    | 2381 | C    |
| 1   | L5    | 2392 | G    |
| 1   | L5    | 2401 | A    |
| 1   | L5    | 2406 | G    |
| 1   | L5    | 2407 | C    |
| 1   | L5    | 2414 | A    |
| 1   | L5    | 2416 | G    |
| 1   | L5    | 2423 | C    |
| 1   | L5    | 2435 | G    |
| 1   | L5    | 2441 | U    |
| 1   | L5    | 2448 | G    |
| 1   | L5    | 2449 | A    |
| 1   | L5    | 2450 | A    |
| 1   | L5    | 2457 | G    |
| 1   | L5    | 2460 | G    |
| 1   | L5    | 2461 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 2462 | U    |
| 1   | L5    | 2463 | C    |
| 1   | L5    | 2464 | C    |
| 1   | L5    | 2465 | G    |
| 1   | L5    | 2466 | G    |
| 1   | L5    | 2480 | G    |
| 1   | L5    | 2493 | C    |
| 1   | L5    | 2497 | A    |
| 1   | L5    | 2498 | A    |
| 1   | L5    | 2508 | G    |
| 1   | L5    | 2513 | G    |
| 1   | L5    | 2515 | U    |
| 1   | L5    | 2516 | G    |
| 1   | L5    | 2517 | U    |
| 1   | L5    | 2518 | A    |
| 1   | L5    | 2519 | A    |
| 1   | L5    | 2520 | A    |
| 1   | L5    | 2524 | C    |
| 1   | L5    | 2532 | G    |
| 1   | L5    | 2541 | A    |
| 1   | L5    | 2542 | U    |
| 1   | L5    | 2544 | U    |
| 1   | L5    | 2552 | A    |
| 1   | L5    | 2561 | A    |
| 1   | L5    | 2569 | A    |
| 1   | L5    | 2576 | G    |
| 1   | L5    | 2580 | U    |
| 1   | L5    | 2581 | G    |
| 1   | L5    | 2583 | U    |
| 1   | L5    | 2592 | G    |
| 1   | L5    | 2609 | G    |
| 1   | L5    | 2646 | C    |
| 1   | L5    | 2650 | G    |
| 1   | L5    | 2651 | G    |
| 1   | L5    | 2653 | C    |
| 1   | L5    | 2657 | G    |
| 1   | L5    | 3263 | U    |
| 1   | L5    | 3273 | U    |
| 1   | L5    | 3275 | C    |
| 1   | L5    | 3283 | G    |
| 1   | L5    | 3292 | A    |
| 1   | L5    | 3301 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 3319 | A    |
| 1   | L5    | 3330 | C    |
| 1   | L5    | 3331 | G    |
| 1   | L5    | 3349 | A    |
| 1   | L5    | 3353 | C    |
| 1   | L5    | 3368 | A    |
| 1   | L5    | 3375 | A    |
| 1   | L5    | 3398 | C    |
| 1   | L5    | 3399 | G    |
| 1   | L5    | 3400 | G    |
| 1   | L5    | 3405 | A    |
| 1   | L5    | 3407 | G    |
| 1   | L5    | 3410 | G    |
| 1   | L5    | 3411 | G    |
| 1   | L5    | 3416 | A    |
| 1   | L5    | 3417 | A    |
| 1   | L5    | 3418 | C    |
| 1   | L5    | 3420 | A    |
| 1   | L5    | 3421 | U    |
| 1   | L5    | 3423 | A    |
| 1   | L5    | 3428 | C    |
| 1   | L5    | 3430 | U    |
| 1   | L5    | 3431 | A    |
| 1   | L5    | 3433 | G    |
| 1   | L5    | 3434 | G    |
| 1   | L5    | 3441 | A    |
| 1   | L5    | 3443 | U    |
| 1   | L5    | 3449 | G    |
| 1   | L5    | 3468 | G    |
| 1   | L5    | 3471 | U    |
| 1   | L5    | 3474 | A    |
| 1   | L5    | 3475 | U    |
| 1   | L5    | 3476 | G    |
| 1   | L5    | 3495 | U    |
| 1   | L5    | 3497 | U    |
| 1   | L5    | 3508 | U    |
| 1   | L5    | 3524 | A    |
| 1   | L5    | 3534 | A    |
| 1   | L5    | 3535 | C    |
| 1   | L5    | 3536 | G    |
| 1   | L5    | 3544 | C    |
| 1   | L5    | 3549 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 3553 | C    |
| 1   | L5    | 3554 | G    |
| 1   | L5    | 3558 | A    |
| 1   | L5    | 3562 | A    |
| 1   | L5    | 3563 | A    |
| 1   | L5    | 3564 | G    |
| 1   | L5    | 3565 | A    |
| 1   | L5    | 3572 | U    |
| 1   | L5    | 3596 | G    |
| 1   | L5    | 3597 | U    |
| 1   | L5    | 3599 | A    |
| 1   | L5    | 3601 | G    |
| 1   | L5    | 3603 | G    |
| 1   | L5    | 3605 | C    |
| 1   | L5    | 3606 | A    |
| 1   | L5    | 3608 | G    |
| 1   | L5    | 3712 | C    |
| 1   | L5    | 3713 | A    |
| 1   | L5    | 3714 | U    |
| 1   | L5    | 3715 | C    |
| 1   | L5    | 3716 | G    |
| 1   | L5    | 3717 | U    |
| 1   | L5    | 3718 | U    |
| 1   | L5    | 3727 | G    |
| 1   | L5    | 3744 | G    |
| 1   | L5    | 3745 | G    |
| 1   | L5    | 3747 | C    |
| 1   | L5    | 3768 | U    |
| 1   | L5    | 3770 | C    |
| 1   | L5    | 3773 | G    |
| 1   | L5    | 3778 | A    |
| 1   | L5    | 3786 | G    |
| 1   | L5    | 3787 | U    |
| 1   | L5    | 3788 | C    |
| 1   | L5    | 3789 | C    |
| 1   | L5    | 3816 | U    |
| 1   | L5    | 3821 | G    |
| 1   | L5    | 3823 | A    |
| 1   | L5    | 3836 | G    |
| 1   | L5    | 3837 | G    |
| 1   | L5    | 3842 | U    |
| 1   | L5    | 3844 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 3849 | G    |
| 1   | L5    | 3856 | A    |
| 1   | L5    | 3878 | G    |
| 1   | L5    | 3882 | U    |
| 1   | L5    | 3886 | A    |
| 1   | L5    | 3904 | A    |
| 1   | L5    | 3905 | C    |
| 1   | L5    | 3907 | G    |
| 1   | L5    | 3909 | A    |
| 1   | L5    | 3910 | A    |
| 1   | L5    | 3911 | C    |
| 1   | L5    | 3921 | A    |
| 1   | L5    | 3924 | A    |
| 1   | L5    | 3926 | A    |
| 1   | L5    | 3933 | A    |
| 1   | L5    | 3934 | A    |
| 1   | L5    | 3944 | G    |
| 1   | L5    | 3950 | G    |
| 1   | L5    | 3958 | G    |
| 1   | L5    | 3959 | U    |
| 1   | L5    | 3967 | C    |
| 1   | L5    | 3977 | A    |
| 1   | L5    | 3982 | G    |
| 1   | L5    | 3983 | G    |
| 1   | L5    | 3985 | C    |
| 1   | L5    | 3992 | A    |
| 1   | L5    | 4001 | A    |
| 1   | L5    | 4021 | G    |
| 1   | L5    | 4026 | G    |
| 1   | L5    | 4029 | A    |
| 1   | L5    | 4030 | G    |
| 1   | L5    | 4031 | A    |
| 1   | L5    | 4033 | A    |
| 1   | L5    | 4040 | C    |
| 1   | L5    | 4044 | G    |
| 1   | L5    | 4047 | A    |
| 1   | L5    | 4068 | A    |
| 1   | L5    | 4073 | U    |
| 1   | L5    | 4074 | C    |
| 1   | L5    | 4075 | A    |
| 1   | L5    | 4090 | U    |
| 1   | L5    | 4101 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 4103 | U    |
| 1   | L5    | 4106 | C    |
| 1   | L5    | 4117 | A    |
| 1   | L5    | 4128 | G    |
| 1   | L5    | 4146 | U    |
| 1   | L5    | 4165 | U    |
| 1   | L5    | 4166 | A    |
| 1   | L5    | 4171 | A    |
| 1   | L5    | 4172 | C    |
| 1   | L5    | 4177 | G    |
| 1   | L5    | 4181 | G    |
| 1   | L5    | 4201 | A    |
| 1   | L5    | 4208 | U    |
| 1   | L5    | 4210 | U    |
| 1   | L5    | 4213 | C    |
| 1   | L5    | 4220 | G    |
| 1   | L5    | 4228 | G    |
| 1   | L5    | 4237 | A    |
| 1   | L5    | 4243 | A    |
| 1   | L5    | 4253 | G    |
| 1   | L5    | 4259 | G    |
| 1   | L5    | 4263 | A    |
| 1   | L5    | 4287 | U    |
| 1   | L5    | 4288 | A    |
| 1   | L5    | 4289 | U    |
| 1   | L5    | 4290 | G    |
| 1   | L5    | 4309 | A    |
| 1   | L5    | 4310 | U    |
| 1   | L5    | 4323 | C    |
| 1   | L5    | 4325 | A    |
| 1   | L5    | 4330 | U    |
| 1   | L5    | 4353 | A    |
| 1   | L5    | 4360 | A    |
| 1   | L5    | 4361 | A    |
| 1   | L5    | 4362 | U    |
| 1   | L5    | 4373 | C    |
| 1   | L5    | 4381 | U    |
| 1   | L5    | 4383 | C    |
| 1   | L5    | 4384 | G    |
| 1   | L5    | 4385 | G    |
| 1   | L5    | 4386 | C    |
| 1   | L5    | 4387 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 4393 | G    |
| 1   | L5    | 4394 | A    |
| 1   | L5    | 4395 | A    |
| 1   | L5    | 4396 | G    |
| 1   | L5    | 4399 | G    |
| 1   | L5    | 4408 | G    |
| 1   | L5    | 4411 | C    |
| 1   | L5    | 4413 | C    |
| 1   | L5    | 4415 | G    |
| 1   | L5    | 4419 | G    |
| 1   | L5    | 4428 | C    |
| 1   | L5    | 4507 | G    |
| 1   | L5    | 4516 | G    |
| 1   | L5    | 4517 | C    |
| 1   | L5    | 4528 | U    |
| 1   | L5    | 4529 | C    |
| 1   | L5    | 4531 | U    |
| 1   | L5    | 4532 | C    |
| 1   | L5    | 4549 | G    |
| 1   | L5    | 4550 | G    |
| 1   | L5    | 4552 | C    |
| 1   | L5    | 4553 | G    |
| 1   | L5    | 4554 | G    |
| 1   | L5    | 4558 | G    |
| 1   | L5    | 4559 | G    |
| 1   | L5    | 4565 | G    |
| 1   | L5    | 4567 | C    |
| 1   | L5    | 4568 | C    |
| 1   | L5    | 4569 | U    |
| 1   | L5    | 4579 | C    |
| 1   | L5    | 4580 | A    |
| 1   | L5    | 4583 | U    |
| 1   | L5    | 4584 | U    |
| 1   | L5    | 4588 | C    |
| 1   | L5    | 4589 | G    |
| 1   | L5    | 4591 | A    |
| 1   | L5    | 4592 | C    |
| 1   | L5    | 4593 | G    |
| 1   | L5    | 4599 | G    |
| 1   | L5    | 4604 | A    |
| 1   | L5    | 4605 | C    |
| 1   | L5    | 4613 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 4621 | U    |
| 1   | L5    | 4624 | U    |
| 1   | L5    | 4636 | U    |
| 1   | L5    | 4638 | C    |
| 1   | L5    | 4639 | U    |
| 1   | L5    | 4654 | U    |
| 1   | L5    | 4662 | A    |
| 1   | L5    | 4664 | A    |
| 1   | L5    | 4665 | G    |
| 1   | L5    | 4668 | G    |
| 1   | L5    | 4669 | C    |
| 1   | L5    | 4676 | G    |
| 1   | L5    | 4677 | C    |
| 1   | L5    | 4678 | U    |
| 1   | L5    | 4682 | A    |
| 1   | L5    | 4687 | U    |
| 1   | L5    | 4689 | G    |
| 1   | L5    | 4698 | C    |
| 1   | L5    | 4702 | C    |
| 1   | L5    | 4703 | G    |
| 1   | L5    | 4706 | A    |
| 1   | L5    | 4709 | A    |
| 1   | L5    | 4710 | G    |
| 1   | L5    | 4717 | U    |
| 2   | L7    | 4    | U    |
| 2   | L7    | 22   | A    |
| 2   | L7    | 24   | C    |
| 2   | L7    | 53   | U    |
| 2   | L7    | 61   | G    |
| 2   | L7    | 64   | G    |
| 2   | L7    | 100  | A    |
| 2   | L7    | 103  | A    |
| 2   | L7    | 110  | G    |
| 2   | L7    | 120  | U    |
| 3   | L8    | 6    | C    |
| 3   | L8    | 23   | C    |
| 3   | L8    | 34   | U    |
| 3   | L8    | 35   | C    |
| 3   | L8    | 52   | A    |
| 3   | L8    | 59   | A    |
| 3   | L8    | 60   | G    |
| 3   | L8    | 62   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L8    | 63  | U    |
| 3   | L8    | 71  | A    |
| 3   | L8    | 72  | A    |
| 3   | L8    | 75  | G    |
| 3   | L8    | 80  | A    |
| 3   | L8    | 87  | G    |
| 3   | L8    | 94  | G    |
| 3   | L8    | 96  | C    |
| 3   | L8    | 103 | A    |
| 3   | L8    | 105 | C    |
| 3   | L8    | 109 | C    |
| 3   | L8    | 110 | U    |
| 3   | L8    | 111 | U    |
| 3   | L8    | 114 | G    |
| 3   | L8    | 121 | G    |
| 3   | L8    | 123 | U    |
| 3   | L8    | 125 | C    |
| 3   | L8    | 126 | C    |
| 3   | L8    | 150 | C    |
| 3   | L8    | 151 | G    |
| 46  | S2    | 2   | A    |
| 46  | S2    | 17  | C    |
| 46  | S2    | 23  | G    |
| 46  | S2    | 26  | U    |
| 46  | S2    | 33  | G    |
| 46  | S2    | 35  | C    |
| 46  | S2    | 40  | A    |
| 46  | S2    | 41  | G    |
| 46  | S2    | 43  | U    |
| 46  | S2    | 46  | A    |
| 46  | S2    | 49  | C    |
| 46  | S2    | 50  | A    |
| 46  | S2    | 52  | G    |
| 46  | S2    | 53  | C    |
| 46  | S2    | 56  | G    |
| 46  | S2    | 57  | U    |
| 46  | S2    | 59  | U    |
| 46  | S2    | 60  | A    |
| 46  | S2    | 61  | A    |
| 46  | S2    | 62  | G    |
| 46  | S2    | 65  | C    |
| 46  | S2    | 67  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 68  | A    |
| 46  | S2    | 72  | C    |
| 46  | S2    | 73  | C    |
| 46  | S2    | 74  | G    |
| 46  | S2    | 75  | G    |
| 46  | S2    | 76  | U    |
| 46  | S2    | 78  | C    |
| 46  | S2    | 79  | A    |
| 46  | S2    | 80  | G    |
| 46  | S2    | 83  | A    |
| 46  | S2    | 86  | C    |
| 46  | S2    | 87  | U    |
| 46  | S2    | 88  | G    |
| 46  | S2    | 90  | G    |
| 46  | S2    | 91  | A    |
| 46  | S2    | 92  | A    |
| 46  | S2    | 93  | U    |
| 46  | S2    | 94  | G    |
| 46  | S2    | 95  | G    |
| 46  | S2    | 96  | C    |
| 46  | S2    | 97  | U    |
| 46  | S2    | 98  | C    |
| 46  | S2    | 99  | A    |
| 46  | S2    | 100 | U    |
| 46  | S2    | 102 | A    |
| 46  | S2    | 103 | A    |
| 46  | S2    | 113 | G    |
| 46  | S2    | 114 | G    |
| 46  | S2    | 115 | U    |
| 46  | S2    | 116 | U    |
| 46  | S2    | 117 | C    |
| 46  | S2    | 118 | C    |
| 46  | S2    | 119 | U    |
| 46  | S2    | 120 | U    |
| 46  | S2    | 121 | U    |
| 46  | S2    | 126 | G    |
| 46  | S2    | 127 | C    |
| 46  | S2    | 129 | C    |
| 46  | S2    | 142 | C    |
| 46  | S2    | 143 | U    |
| 46  | S2    | 149 | A    |
| 46  | S2    | 151 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 152 | U    |
| 46  | S2    | 153 | G    |
| 46  | S2    | 156 | G    |
| 46  | S2    | 158 | A    |
| 46  | S2    | 161 | U    |
| 46  | S2    | 162 | C    |
| 46  | S2    | 163 | U    |
| 46  | S2    | 165 | G    |
| 46  | S2    | 168 | C    |
| 46  | S2    | 169 | U    |
| 46  | S2    | 171 | A    |
| 46  | S2    | 173 | A    |
| 46  | S2    | 177 | G    |
| 46  | S2    | 179 | C    |
| 46  | S2    | 181 | A    |
| 46  | S2    | 182 | C    |
| 46  | S2    | 222 | U    |
| 46  | S2    | 226 | A    |
| 46  | S2    | 289 | G    |
| 46  | S2    | 292 | G    |
| 46  | S2    | 294 | C    |
| 46  | S2    | 299 | G    |
| 46  | S2    | 303 | A    |
| 46  | S2    | 311 | C    |
| 46  | S2    | 313 | G    |
| 46  | S2    | 314 | A    |
| 46  | S2    | 315 | U    |
| 46  | S2    | 316 | C    |
| 46  | S2    | 317 | G    |
| 46  | S2    | 319 | A    |
| 46  | S2    | 320 | C    |
| 46  | S2    | 323 | C    |
| 46  | S2    | 338 | C    |
| 46  | S2    | 341 | C    |
| 46  | S2    | 342 | C    |
| 46  | S2    | 343 | C    |
| 46  | S2    | 344 | A    |
| 46  | S2    | 348 | G    |
| 46  | S2    | 357 | C    |
| 46  | S2    | 363 | C    |
| 46  | S2    | 365 | A    |
| 46  | S2    | 370 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 371 | G    |
| 46  | S2    | 384 | G    |
| 46  | S2    | 386 | G    |
| 46  | S2    | 387 | C    |
| 46  | S2    | 408 | G    |
| 46  | S2    | 409 | A    |
| 46  | S2    | 410 | C    |
| 46  | S2    | 419 | A    |
| 46  | S2    | 445 | G    |
| 46  | S2    | 447 | G    |
| 46  | S2    | 449 | A    |
| 46  | S2    | 450 | A    |
| 46  | S2    | 451 | C    |
| 46  | S2    | 455 | U    |
| 46  | S2    | 464 | C    |
| 46  | S2    | 465 | A    |
| 46  | S2    | 466 | A    |
| 46  | S2    | 467 | G    |
| 46  | S2    | 469 | A    |
| 46  | S2    | 470 | A    |
| 46  | S2    | 472 | G    |
| 46  | S2    | 473 | C    |
| 46  | S2    | 474 | A    |
| 46  | S2    | 475 | G    |
| 46  | S2    | 476 | C    |
| 46  | S2    | 477 | A    |
| 46  | S2    | 478 | G    |
| 46  | S2    | 479 | G    |
| 46  | S2    | 483 | G    |
| 46  | S2    | 484 | C    |
| 46  | S2    | 485 | A    |
| 46  | S2    | 486 | A    |
| 46  | S2    | 487 | A    |
| 46  | S2    | 488 | U    |
| 46  | S2    | 489 | U    |
| 46  | S2    | 490 | A    |
| 46  | S2    | 491 | C    |
| 46  | S2    | 492 | C    |
| 46  | S2    | 493 | C    |
| 46  | S2    | 494 | A    |
| 46  | S2    | 495 | C    |
| 46  | S2    | 496 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 502 | C    |
| 46  | S2    | 503 | C    |
| 46  | S2    | 504 | C    |
| 46  | S2    | 505 | G    |
| 46  | S2    | 507 | G    |
| 46  | S2    | 508 | G    |
| 46  | S2    | 509 | A    |
| 46  | S2    | 510 | G    |
| 46  | S2    | 513 | A    |
| 46  | S2    | 515 | U    |
| 46  | S2    | 517 | A    |
| 46  | S2    | 518 | C    |
| 46  | S2    | 525 | U    |
| 46  | S2    | 526 | A    |
| 46  | S2    | 530 | A    |
| 46  | S2    | 531 | U    |
| 46  | S2    | 533 | C    |
| 46  | S2    | 534 | A    |
| 46  | S2    | 535 | G    |
| 46  | S2    | 537 | A    |
| 46  | S2    | 538 | C    |
| 46  | S2    | 539 | U    |
| 46  | S2    | 541 | U    |
| 46  | S2    | 543 | U    |
| 46  | S2    | 545 | G    |
| 46  | S2    | 546 | A    |
| 46  | S2    | 547 | G    |
| 46  | S2    | 548 | G    |
| 46  | S2    | 552 | U    |
| 46  | S2    | 557 | U    |
| 46  | S2    | 559 | G    |
| 46  | S2    | 560 | G    |
| 46  | S2    | 561 | A    |
| 46  | S2    | 562 | A    |
| 46  | S2    | 564 | G    |
| 46  | S2    | 565 | A    |
| 46  | S2    | 566 | G    |
| 46  | S2    | 567 | U    |
| 46  | S2    | 568 | C    |
| 46  | S2    | 569 | C    |
| 46  | S2    | 570 | A    |
| 46  | S2    | 572 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 577 | A    |
| 46  | S2    | 584 | A    |
| 46  | S2    | 585 | A    |
| 46  | S2    | 587 | G    |
| 46  | S2    | 588 | A    |
| 46  | S2    | 590 | G    |
| 46  | S2    | 591 | A    |
| 46  | S2    | 592 | U    |
| 46  | S2    | 593 | C    |
| 46  | S2    | 594 | C    |
| 46  | S2    | 595 | A    |
| 46  | S2    | 596 | U    |
| 46  | S2    | 600 | A    |
| 46  | S2    | 605 | A    |
| 46  | S2    | 607 | G    |
| 46  | S2    | 608 | U    |
| 46  | S2    | 609 | C    |
| 46  | S2    | 627 | G    |
| 46  | S2    | 629 | A    |
| 46  | S2    | 630 | A    |
| 46  | S2    | 632 | U    |
| 46  | S2    | 644 | A    |
| 46  | S2    | 645 | G    |
| 46  | S2    | 656 | A    |
| 46  | S2    | 661 | C    |
| 46  | S2    | 665 | A    |
| 46  | S2    | 669 | A    |
| 46  | S2    | 670 | A    |
| 46  | S2    | 672 | A    |
| 46  | S2    | 673 | A    |
| 46  | S2    | 674 | G    |
| 46  | S2    | 684 | G    |
| 46  | S2    | 689 | U    |
| 46  | S2    | 749 | C    |
| 46  | S2    | 750 | U    |
| 46  | S2    | 751 | C    |
| 46  | S2    | 795 | A    |
| 46  | S2    | 796 | A    |
| 46  | S2    | 798 | C    |
| 46  | S2    | 799 | G    |
| 46  | S2    | 800 | U    |
| 46  | S2    | 822 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | S2    | 823 | U    |
| 46  | S2    | 831 | A    |
| 46  | S2    | 832 | G    |
| 46  | S2    | 835 | C    |
| 46  | S2    | 837 | G    |
| 46  | S2    | 838 | A    |
| 46  | S2    | 839 | G    |
| 46  | S2    | 840 | C    |
| 46  | S2    | 841 | C    |
| 46  | S2    | 843 | C    |
| 46  | S2    | 844 | C    |
| 46  | S2    | 845 | U    |
| 46  | S2    | 846 | G    |
| 46  | S2    | 847 | G    |
| 46  | S2    | 848 | A    |
| 46  | S2    | 854 | C    |
| 46  | S2    | 863 | A    |
| 46  | S2    | 870 | A    |
| 46  | S2    | 871 | A    |
| 46  | S2    | 874 | G    |
| 46  | S2    | 875 | G    |
| 46  | S2    | 876 | A    |
| 46  | S2    | 882 | G    |
| 46  | S2    | 884 | U    |
| 46  | S2    | 885 | C    |
| 46  | S2    | 886 | U    |
| 46  | S2    | 890 | U    |
| 46  | S2    | 891 | U    |
| 46  | S2    | 892 | G    |
| 46  | S2    | 893 | U    |
| 46  | S2    | 894 | U    |
| 46  | S2    | 895 | G    |
| 46  | S2    | 896 | G    |
| 46  | S2    | 897 | U    |
| 46  | S2    | 898 | U    |
| 46  | S2    | 899 | U    |
| 46  | S2    | 900 | U    |
| 46  | S2    | 901 | C    |
| 46  | S2    | 902 | G    |
| 46  | S2    | 903 | G    |
| 46  | S2    | 904 | A    |
| 46  | S2    | 905 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 914  | A    |
| 46  | S2    | 917  | A    |
| 46  | S2    | 918  | U    |
| 46  | S2    | 921  | A    |
| 46  | S2    | 923  | A    |
| 46  | S2    | 931  | C    |
| 46  | S2    | 934  | G    |
| 46  | S2    | 957  | G    |
| 46  | S2    | 972  | G    |
| 46  | S2    | 991  | A    |
| 46  | S2    | 993  | A    |
| 46  | S2    | 1000 | G    |
| 46  | S2    | 1002 | A    |
| 46  | S2    | 1018 | U    |
| 46  | S2    | 1024 | A    |
| 46  | S2    | 1048 | C    |
| 46  | S2    | 1061 | A    |
| 46  | S2    | 1062 | U    |
| 46  | S2    | 1063 | A    |
| 46  | S2    | 1084 | A    |
| 46  | S2    | 1086 | C    |
| 46  | S2    | 1109 | G    |
| 46  | S2    | 1110 | C    |
| 46  | S2    | 1114 | A    |
| 46  | S2    | 1115 | U    |
| 46  | S2    | 1116 | U    |
| 46  | S2    | 1117 | C    |
| 46  | S2    | 1118 | C    |
| 46  | S2    | 1119 | C    |
| 46  | S2    | 1139 | C    |
| 46  | S2    | 1154 | C    |
| 46  | S2    | 1155 | U    |
| 46  | S2    | 1196 | A    |
| 46  | S2    | 1204 | G    |
| 46  | S2    | 1208 | G    |
| 46  | S2    | 1209 | A    |
| 46  | S2    | 1216 | C    |
| 46  | S2    | 1217 | C    |
| 46  | S2    | 1225 | G    |
| 46  | S2    | 1228 | G    |
| 46  | S2    | 1238 | C    |
| 46  | S2    | 1240 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1241 | A    |
| 46  | S2    | 1242 | A    |
| 46  | S2    | 1243 | U    |
| 46  | S2    | 1244 | U    |
| 46  | S2    | 1248 | C    |
| 46  | S2    | 1249 | U    |
| 46  | S2    | 1252 | A    |
| 46  | S2    | 1254 | A    |
| 46  | S2    | 1257 | G    |
| 46  | S2    | 1258 | G    |
| 46  | S2    | 1260 | A    |
| 46  | S2    | 1266 | A    |
| 46  | S2    | 1269 | C    |
| 46  | S2    | 1270 | G    |
| 46  | S2    | 1271 | G    |
| 46  | S2    | 1273 | C    |
| 46  | S2    | 1275 | G    |
| 46  | S2    | 1276 | G    |
| 46  | S2    | 1277 | A    |
| 46  | S2    | 1279 | A    |
| 46  | S2    | 1284 | C    |
| 46  | S2    | 1286 | G    |
| 46  | S2    | 1287 | G    |
| 46  | S2    | 1288 | A    |
| 46  | S2    | 1289 | U    |
| 46  | S2    | 1292 | A    |
| 46  | S2    | 1293 | C    |
| 46  | S2    | 1294 | A    |
| 46  | S2    | 1295 | G    |
| 46  | S2    | 1296 | A    |
| 46  | S2    | 1297 | U    |
| 46  | S2    | 1298 | U    |
| 46  | S2    | 1299 | G    |
| 46  | S2    | 1301 | U    |
| 46  | S2    | 1303 | G    |
| 46  | S2    | 1304 | C    |
| 46  | S2    | 1305 | U    |
| 46  | S2    | 1307 | U    |
| 46  | S2    | 1308 | U    |
| 46  | S2    | 1309 | U    |
| 46  | S2    | 1310 | C    |
| 46  | S2    | 1311 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1315 | U    |
| 46  | S2    | 1318 | C    |
| 46  | S2    | 1319 | G    |
| 46  | S2    | 1321 | G    |
| 46  | S2    | 1324 | U    |
| 46  | S2    | 1325 | G    |
| 46  | S2    | 1331 | G    |
| 46  | S2    | 1343 | U    |
| 46  | S2    | 1344 | U    |
| 46  | S2    | 1372 | U    |
| 46  | S2    | 1373 | U    |
| 46  | S2    | 1374 | C    |
| 46  | S2    | 1379 | A    |
| 46  | S2    | 1391 | U    |
| 46  | S2    | 1398 | U    |
| 46  | S2    | 1399 | G    |
| 46  | S2    | 1401 | U    |
| 46  | S2    | 1403 | A    |
| 46  | S2    | 1404 | C    |
| 46  | S2    | 1405 | U    |
| 46  | S2    | 1407 | G    |
| 46  | S2    | 1409 | U    |
| 46  | S2    | 1412 | G    |
| 46  | S2    | 1417 | C    |
| 46  | S2    | 1419 | C    |
| 46  | S2    | 1420 | C    |
| 46  | S2    | 1421 | G    |
| 46  | S2    | 1422 | A    |
| 46  | S2    | 1423 | G    |
| 46  | S2    | 1424 | C    |
| 46  | S2    | 1425 | G    |
| 46  | S2    | 1426 | G    |
| 46  | S2    | 1427 | U    |
| 46  | S2    | 1428 | C    |
| 46  | S2    | 1430 | G    |
| 46  | S2    | 1431 | C    |
| 46  | S2    | 1432 | G    |
| 46  | S2    | 1433 | U    |
| 46  | S2    | 1442 | U    |
| 46  | S2    | 1443 | U    |
| 46  | S2    | 1448 | G    |
| 46  | S2    | 1453 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1455 | A    |
| 46  | S2    | 1463 | U    |
| 46  | S2    | 1465 | C    |
| 46  | S2    | 1477 | A    |
| 46  | S2    | 1479 | U    |
| 46  | S2    | 1488 | A    |
| 46  | S2    | 1490 | A    |
| 46  | S2    | 1491 | G    |
| 46  | S2    | 1498 | G    |
| 46  | S2    | 1507 | A    |
| 46  | S2    | 1508 | G    |
| 46  | S2    | 1509 | A    |
| 46  | S2    | 1510 | U    |
| 46  | S2    | 1513 | C    |
| 46  | S2    | 1515 | G    |
| 46  | S2    | 1518 | G    |
| 46  | S2    | 1521 | G    |
| 46  | S2    | 1522 | C    |
| 46  | S2    | 1523 | A    |
| 46  | S2    | 1534 | A    |
| 46  | S2    | 1538 | A    |
| 46  | S2    | 1540 | U    |
| 46  | S2    | 1542 | G    |
| 46  | S2    | 1553 | G    |
| 46  | S2    | 1554 | C    |
| 46  | S2    | 1556 | U    |
| 46  | S2    | 1557 | A    |
| 46  | S2    | 1558 | C    |
| 46  | S2    | 1559 | C    |
| 46  | S2    | 1565 | C    |
| 46  | S2    | 1569 | C    |
| 46  | S2    | 1580 | A    |
| 46  | S2    | 1581 | A    |
| 46  | S2    | 1582 | C    |
| 46  | S2    | 1583 | C    |
| 46  | S2    | 1586 | U    |
| 46  | S2    | 1588 | G    |
| 46  | S2    | 1589 | A    |
| 46  | S2    | 1595 | A    |
| 46  | S2    | 1596 | U    |
| 46  | S2    | 1599 | G    |
| 46  | S2    | 1600 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1601 | G    |
| 46  | S2    | 1602 | A    |
| 46  | S2    | 1604 | G    |
| 46  | S2    | 1620 | A    |
| 46  | S2    | 1622 | U    |
| 46  | S2    | 1624 | A    |
| 46  | S2    | 1638 | A    |
| 46  | S2    | 1647 | C    |
| 46  | S2    | 1649 | G    |
| 46  | S2    | 1655 | G    |
| 46  | S2    | 1662 | A    |
| 46  | S2    | 1664 | A    |
| 46  | S2    | 1666 | G    |
| 46  | S2    | 1672 | G    |
| 46  | S2    | 1681 | G    |
| 46  | S2    | 1687 | G    |
| 46  | S2    | 1700 | A    |
| 46  | S2    | 1719 | G    |
| 46  | S2    | 1720 | A    |
| 46  | S2    | 1721 | U    |
| 46  | S2    | 1722 | U    |
| 46  | S2    | 1723 | G    |
| 46  | S2    | 1729 | U    |
| 46  | S2    | 1730 | U    |
| 46  | S2    | 1731 | U    |
| 46  | S2    | 1733 | G    |
| 46  | S2    | 1736 | A    |
| 46  | S2    | 1743 | C    |
| 46  | S2    | 1744 | G    |
| 46  | S2    | 1748 | C    |
| 46  | S2    | 1749 | G    |
| 46  | S2    | 1752 | C    |
| 46  | S2    | 1753 | C    |
| 46  | S2    | 1754 | C    |
| 46  | S2    | 1778 | G    |
| 46  | S2    | 1779 | C    |
| 46  | S2    | 1782 | A    |
| 46  | S2    | 1784 | C    |
| 46  | S2    | 1785 | G    |
| 46  | S2    | 1786 | C    |
| 46  | S2    | 1787 | U    |
| 46  | S2    | 1790 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 1791 | A    |
| 46  | S2    | 1807 | A    |
| 46  | S2    | 1809 | U    |
| 46  | S2    | 1810 | A    |
| 46  | S2    | 1811 | U    |
| 46  | S2    | 1818 | G    |
| 46  | S2    | 1819 | A    |
| 46  | S2    | 1825 | A    |
| 46  | S2    | 1826 | A    |
| 46  | S2    | 1827 | G    |
| 46  | S2    | 1828 | U    |
| 46  | S2    | 1830 | G    |
| 46  | S2    | 1832 | A    |
| 46  | S2    | 1836 | A    |
| 46  | S2    | 1839 | U    |
| 46  | S2    | 1850 | G    |
| 46  | S2    | 1852 | A    |
| 46  | S2    | 1853 | C    |
| 46  | S2    | 1862 | G    |
| 46  | S2    | 1863 | G    |
| 46  | S2    | 1864 | A    |
| 46  | S2    | 1865 | U    |
| 46  | S2    | 1866 | C    |
| 46  | S2    | 1870 | A    |
| 75  | Sx    | 33   | U    |
| 79  | S6    | 6    | G    |
| 79  | S6    | 10   | G    |
| 79  | S6    | 17   | C    |
| 79  | S6    | 18   | G    |
| 79  | S6    | 20   | A    |
| 79  | S6    | 21   | A    |
| 79  | S6    | 27   | C    |
| 79  | S6    | 32   | C    |
| 79  | S6    | 33   | C    |
| 79  | S6    | 34   | C    |
| 79  | S6    | 46   | G    |
| 79  | S6    | 48   | C    |
| 79  | S6    | 54   | A    |
| 79  | S6    | 55   | U    |
| 79  | S6    | 57   | G    |
| 79  | S6    | 58   | A    |
| 79  | S6    | 59   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S6    | 61  | C    |
| 79  | S6    | 62  | C    |
| 79  | S6    | 67  | U    |
| 79  | S6    | 69  | U    |
| 79  | S6    | 75  | C    |
| 79  | S6    | 76  | A    |
| 79  | S7    | 3   | G    |
| 79  | S7    | 11  | G    |
| 79  | S7    | 12  | C    |
| 79  | S7    | 14  | C    |
| 79  | S7    | 18  | G    |
| 79  | S7    | 19  | G    |
| 79  | S7    | 20  | A    |
| 79  | S7    | 21  | A    |
| 79  | S7    | 23  | C    |
| 79  | S7    | 24  | G    |
| 79  | S7    | 35  | A    |
| 79  | S7    | 40  | C    |
| 79  | S7    | 46  | G    |
| 79  | S7    | 47  | U    |
| 79  | S7    | 48  | C    |
| 79  | S7    | 50  | A    |
| 79  | S7    | 53  | G    |
| 79  | S7    | 54  | A    |
| 79  | S7    | 55  | U    |
| 79  | S7    | 58  | A    |
| 79  | S7    | 59  | A    |
| 79  | S7    | 62  | C    |
| 79  | S7    | 66  | C    |
| 79  | S7    | 67  | U    |
| 79  | S7    | 72  | U    |
| 79  | S7    | 75  | C    |
| 79  | S7    | 76  | A    |

All (76) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L5    | 1   | C    |
| 1   | L5    | 234 | G    |
| 1   | L5    | 266 | G    |
| 1   | L5    | 415 | U    |
| 1   | L5    | 453 | U    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L5    | 456  | G    |
| 1   | L5    | 458  | C    |
| 1   | L5    | 486  | C    |
| 1   | L5    | 676  | C    |
| 1   | L5    | 753  | G    |
| 1   | L5    | 760  | G    |
| 1   | L5    | 823  | C    |
| 1   | L5    | 830  | C    |
| 1   | L5    | 1054 | G    |
| 1   | L5    | 1192 | G    |
| 1   | L5    | 1227 | G    |
| 1   | L5    | 1271 | G    |
| 1   | L5    | 1447 | G    |
| 1   | L5    | 1563 | G    |
| 1   | L5    | 1585 | U    |
| 1   | L5    | 2345 | A    |
| 1   | L5    | 2519 | A    |
| 1   | L5    | 2540 | C    |
| 1   | L5    | 2649 | A    |
| 1   | L5    | 3416 | A    |
| 1   | L5    | 3422 | G    |
| 1   | L5    | 3427 | U    |
| 1   | L5    | 3605 | C    |
| 1   | L5    | 3714 | U    |
| 1   | L5    | 3904 | A    |
| 1   | L5    | 4352 | U    |
| 1   | L5    | 4612 | C    |
| 1   | L5    | 4686 | A    |
| 2   | L7    | 3    | C    |
| 2   | L7    | 52   | C    |
| 2   | L7    | 60   | G    |
| 3   | L8    | 5    | U    |
| 46  | S2    | 34   | U    |
| 46  | S2    | 55   | U    |
| 46  | S2    | 94   | G    |
| 46  | S2    | 96   | C    |
| 46  | S2    | 97   | U    |
| 46  | S2    | 118  | C    |
| 46  | S2    | 126  | G    |
| 46  | S2    | 293  | A    |
| 46  | S2    | 446  | A    |
| 46  | S2    | 454  | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | S2    | 483  | G    |
| 46  | S2    | 484  | C    |
| 46  | S2    | 485  | A    |
| 46  | S2    | 512  | U    |
| 46  | S2    | 536  | G    |
| 46  | S2    | 537  | A    |
| 46  | S2    | 565  | A    |
| 46  | S2    | 592  | U    |
| 46  | S2    | 593  | C    |
| 46  | S2    | 599  | G    |
| 46  | S2    | 629  | A    |
| 46  | S2    | 842  | G    |
| 46  | S2    | 862  | A    |
| 46  | S2    | 893  | U    |
| 46  | S2    | 1241 | A    |
| 46  | S2    | 1294 | A    |
| 46  | S2    | 1297 | U    |
| 46  | S2    | 1343 | U    |
| 46  | S2    | 1408 | U    |
| 46  | S2    | 1414 | G    |
| 46  | S2    | 1416 | C    |
| 46  | S2    | 1442 | U    |
| 46  | S2    | 1476 | G    |
| 46  | S2    | 1555 | C    |
| 46  | S2    | 1784 | C    |
| 79  | S6    | 53   | G    |
| 79  | S6    | 54   | A    |
| 79  | S6    | 74   | C    |
| 79  | S7    | 53   | G    |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 100 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

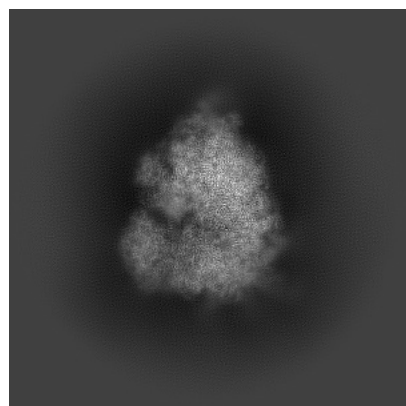
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62285. These allow visual inspection of the internal detail of the map and identification of artifacts.

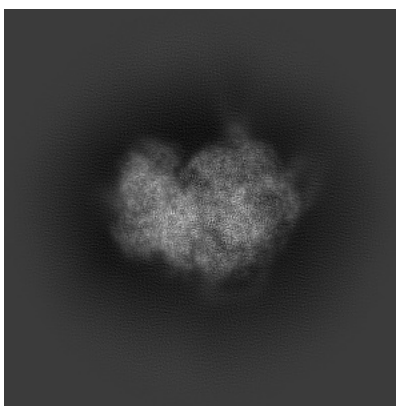
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

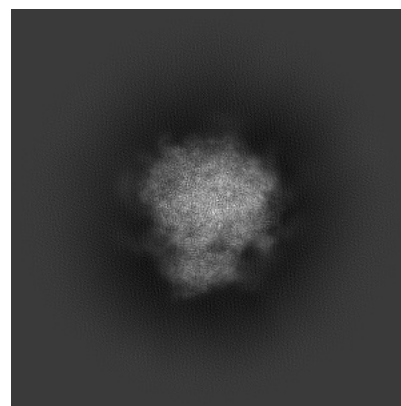
#### 6.1.1 Primary map



X

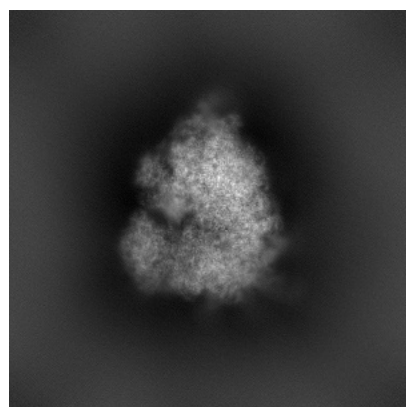


Y

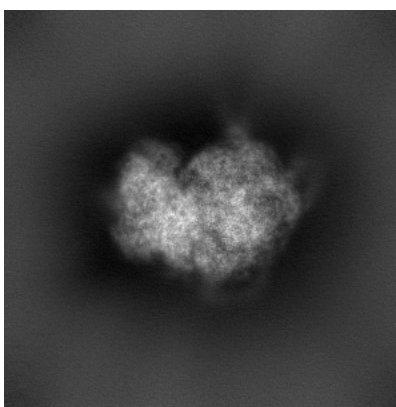


Z

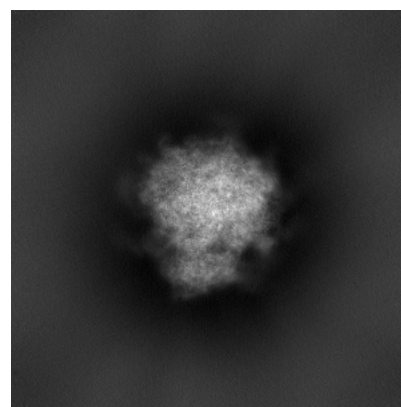
#### 6.1.2 Raw map



X



Y

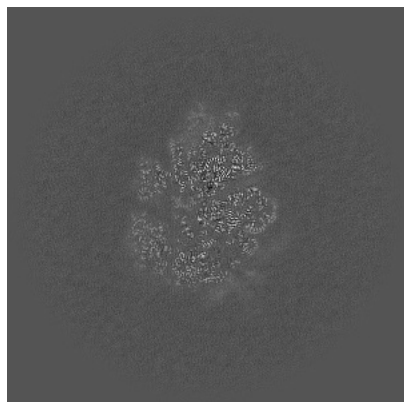


Z

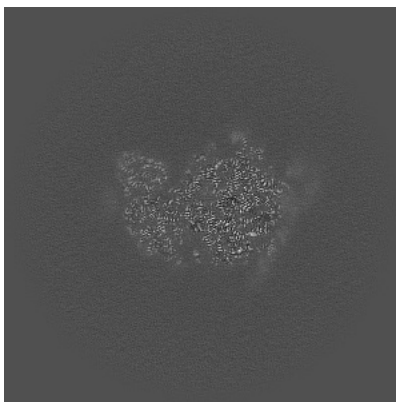
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

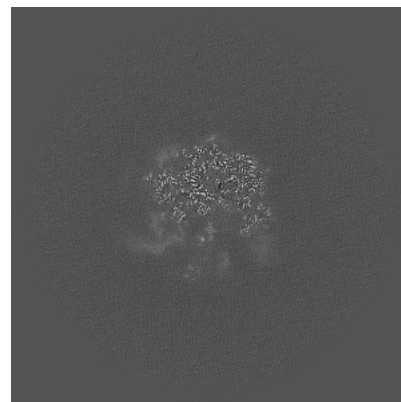
### 6.2.1 Primary map



X Index: 280

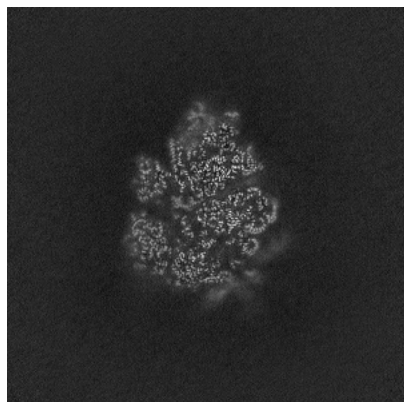


Y Index: 280

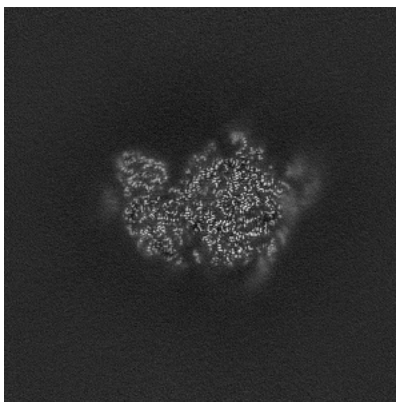


Z Index: 280

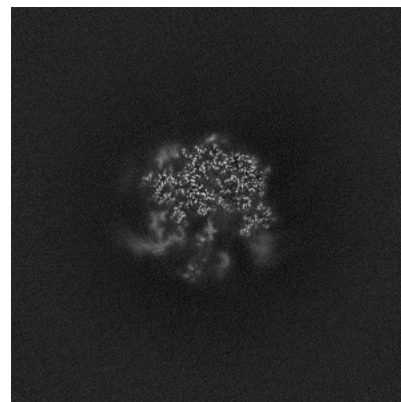
### 6.2.2 Raw map



X Index: 280



Y Index: 280

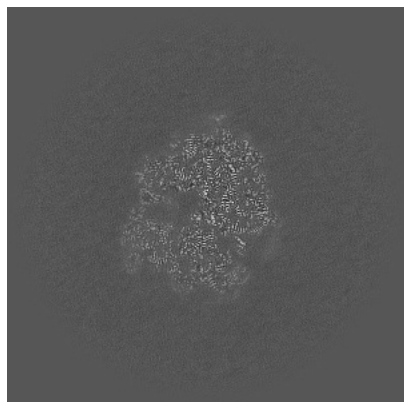


Z Index: 280

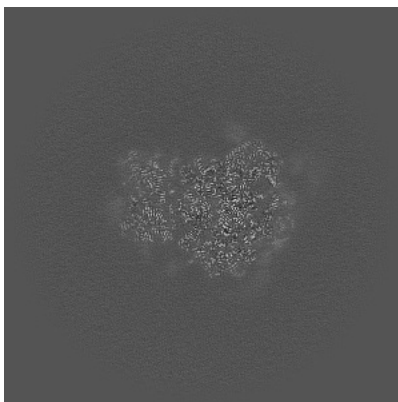
The images above show central slices of the map in three orthogonal directions.

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

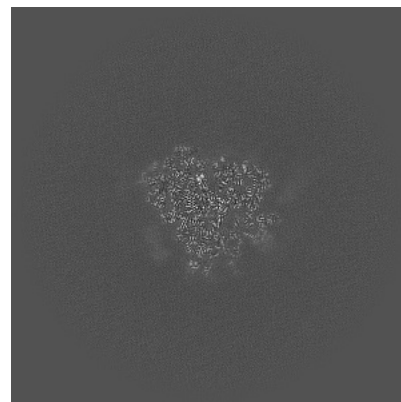
### 6.3.1 Primary map



X Index: 260

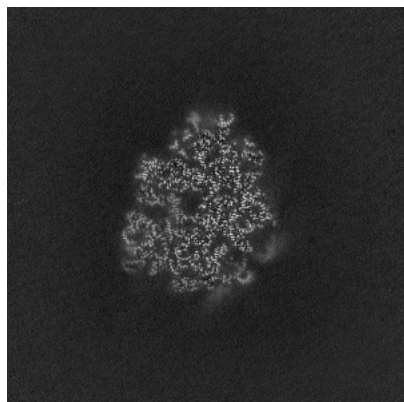


Y Index: 292

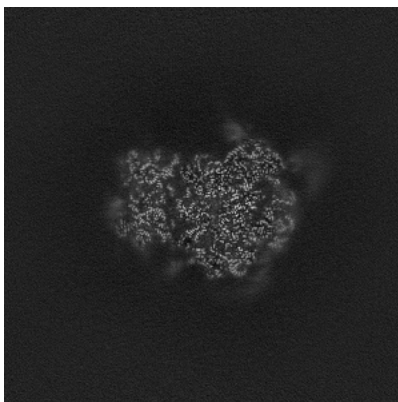


Z Index: 312

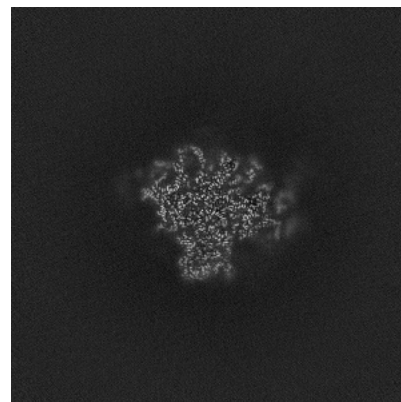
### 6.3.2 Raw map



X Index: 268



Y Index: 294



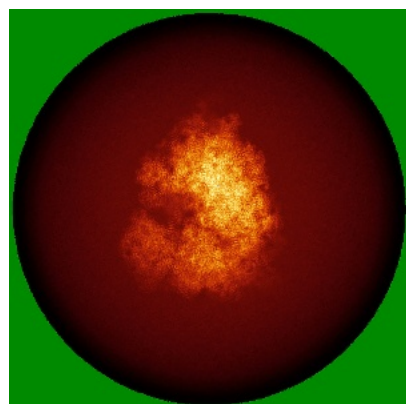
Z Index: 325

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

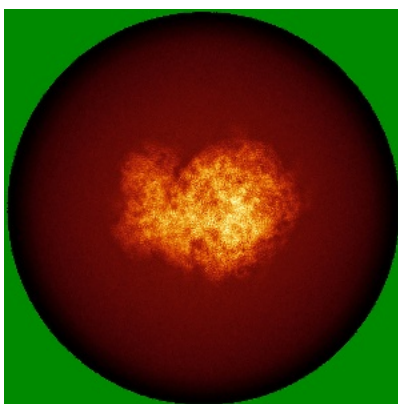


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

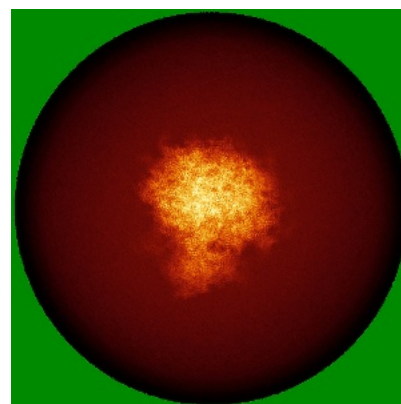
### 6.4.1 Primary map



X

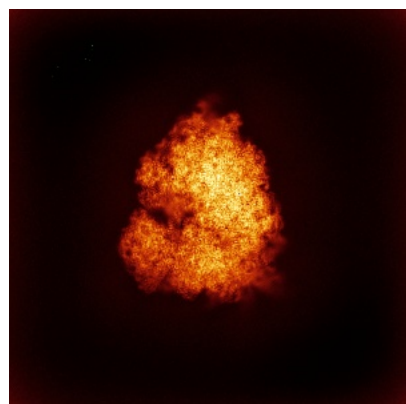


Y

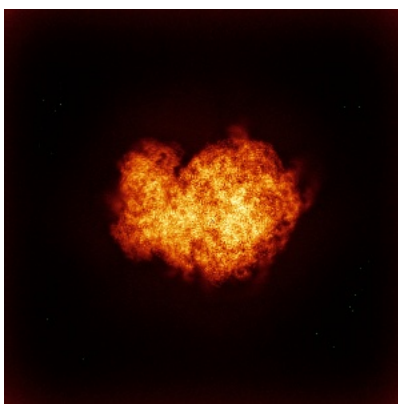


Z

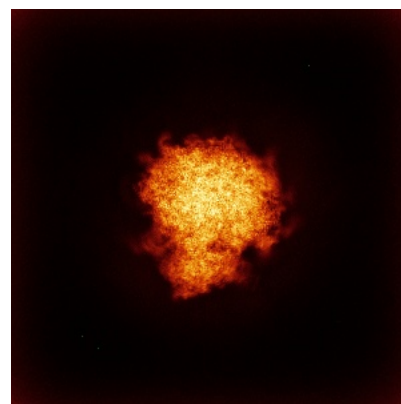
### 6.4.2 Raw map



X



Y

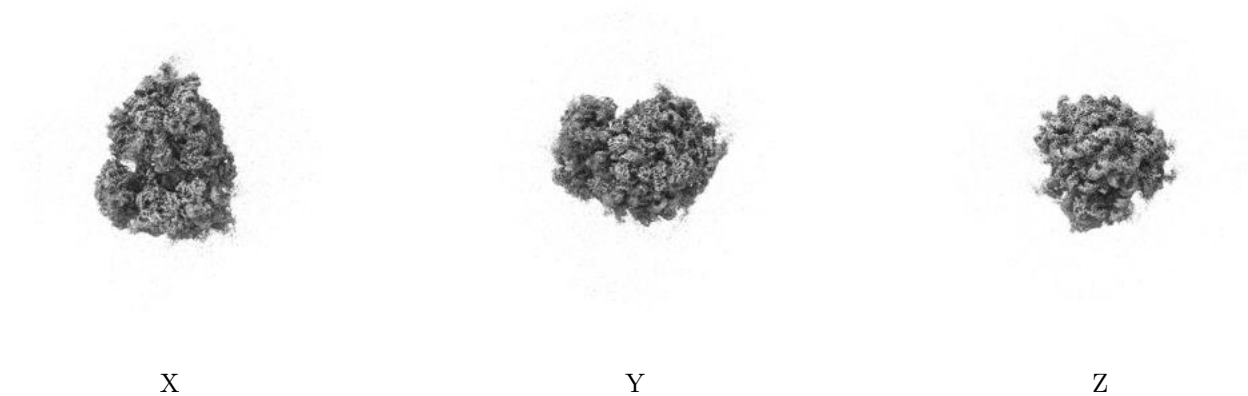


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

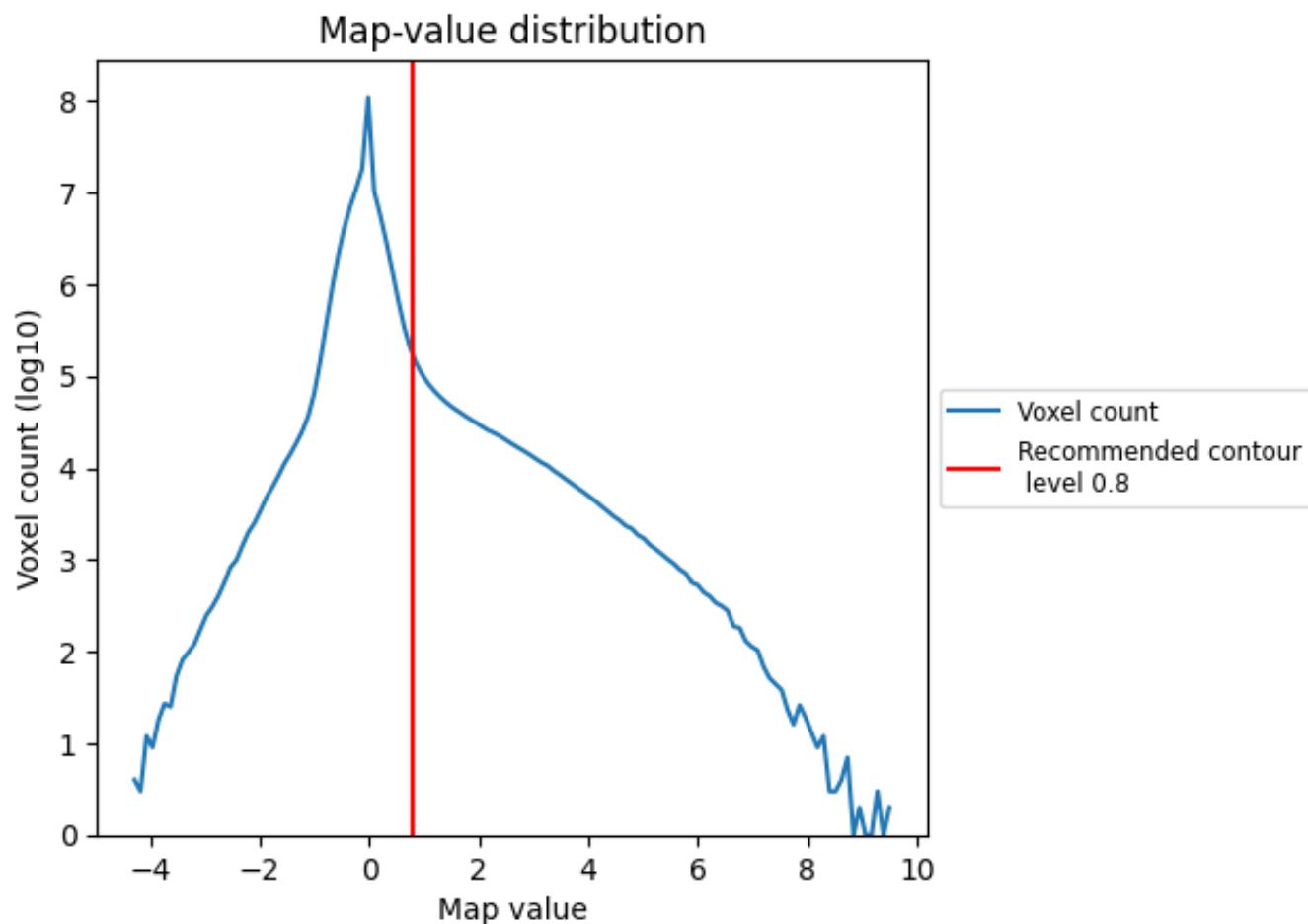
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

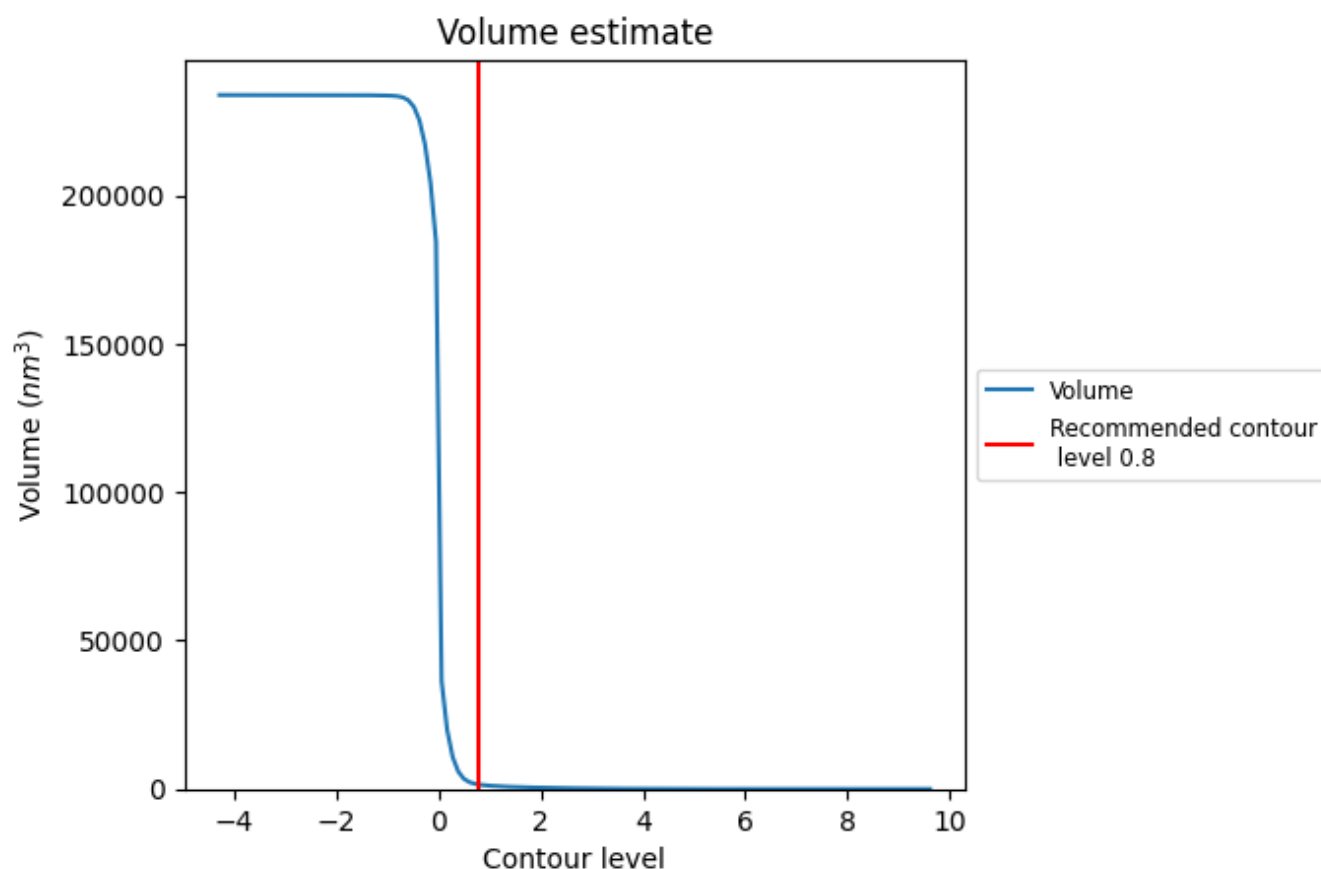
This section contains the results of statistical analysis of the map.

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



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

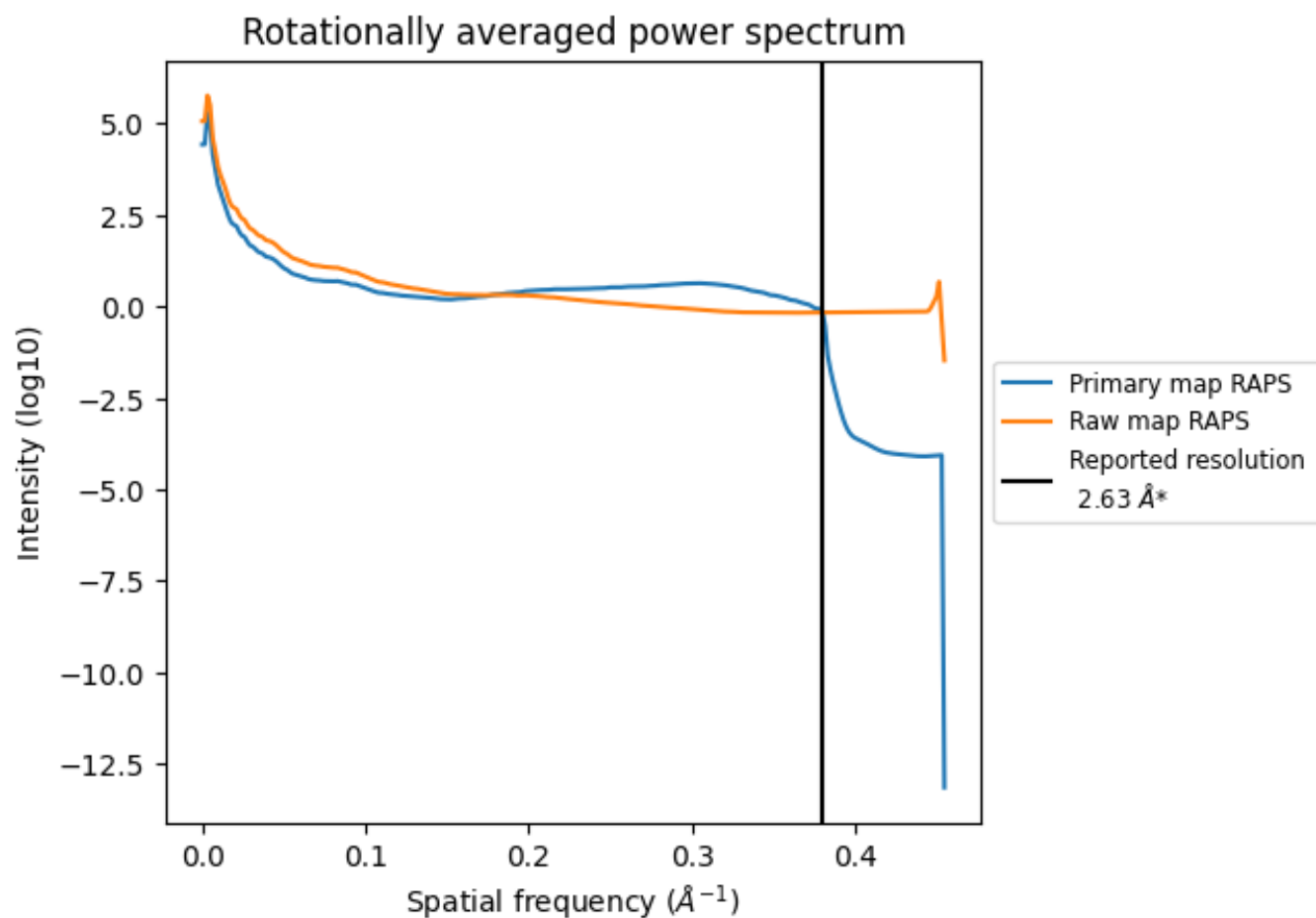
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1473 \text{ nm}^3$ ; this corresponds to an approximate mass of 1331 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 ⓘ

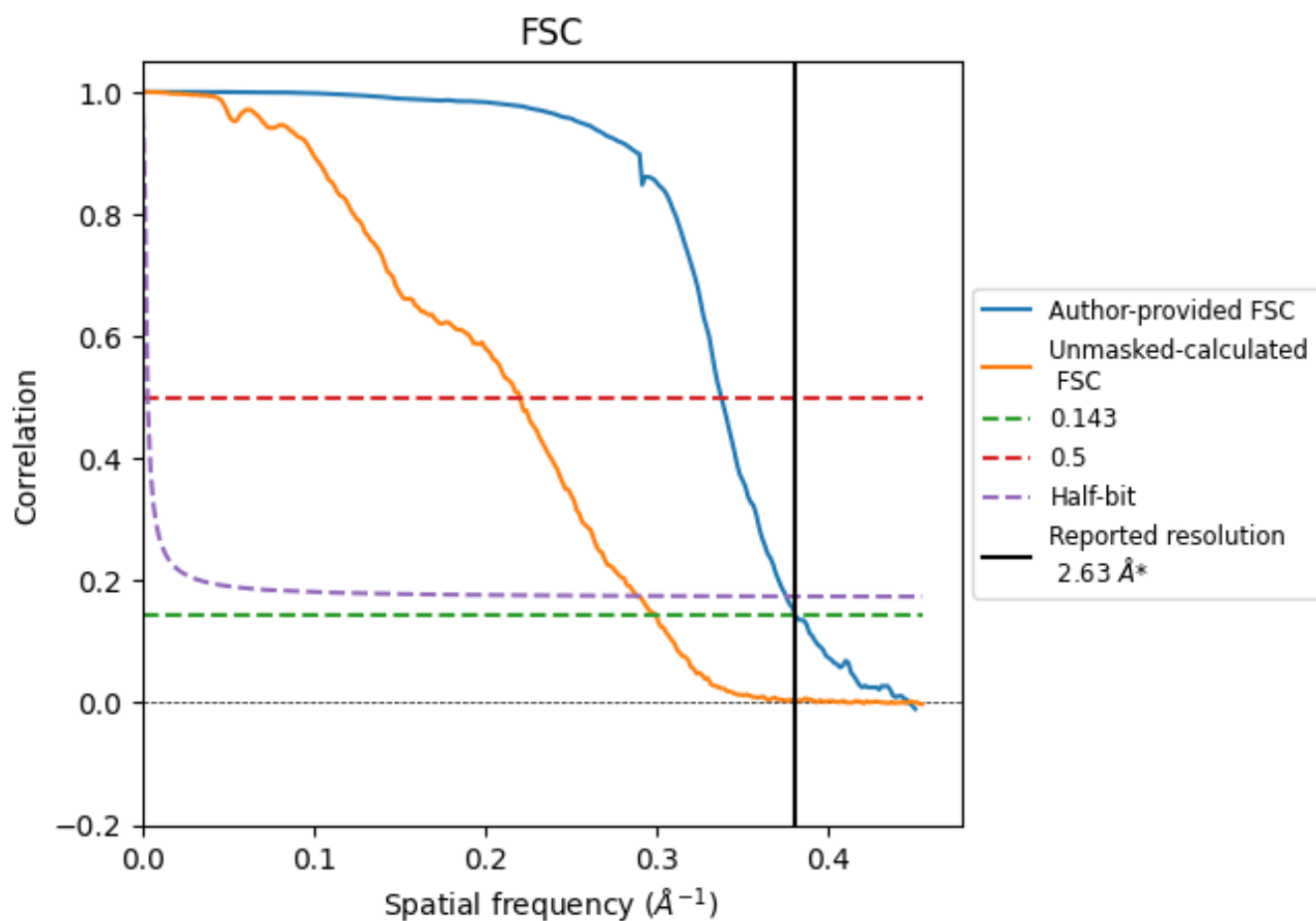


\*Reported resolution corresponds to spatial frequency of 0.380 Å<sup>-1</sup>

## 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 0.380 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

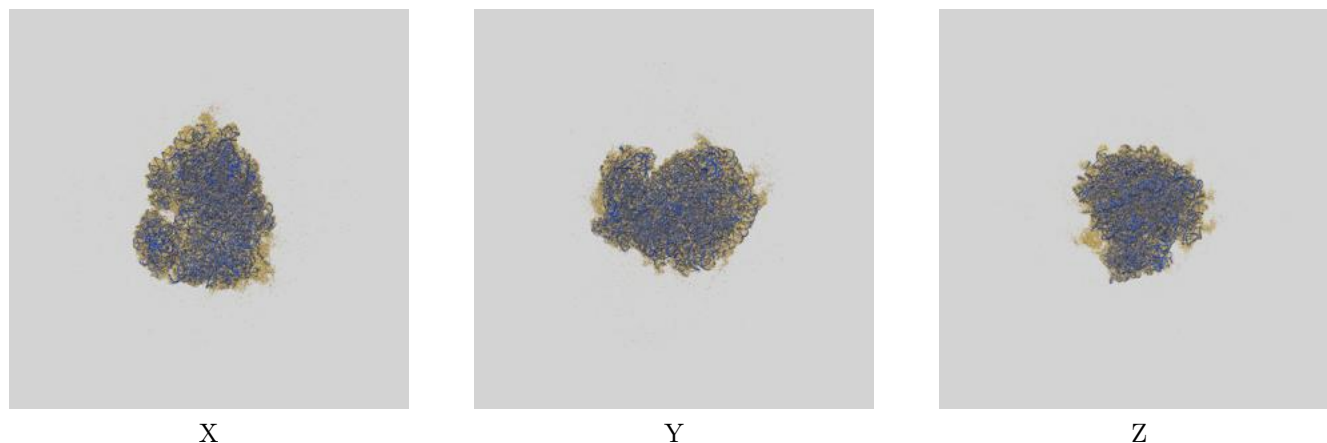
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.63                               | -    | -        |
| Author-provided FSC curve | 2.63                               | 2.96 | 2.67     |
| Unmasked-calculated*      | 3.34                               | 4.55 | 3.47     |

\*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 3.34 differs from the reported value 2.63 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-62285 and PDB model 9KDT. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

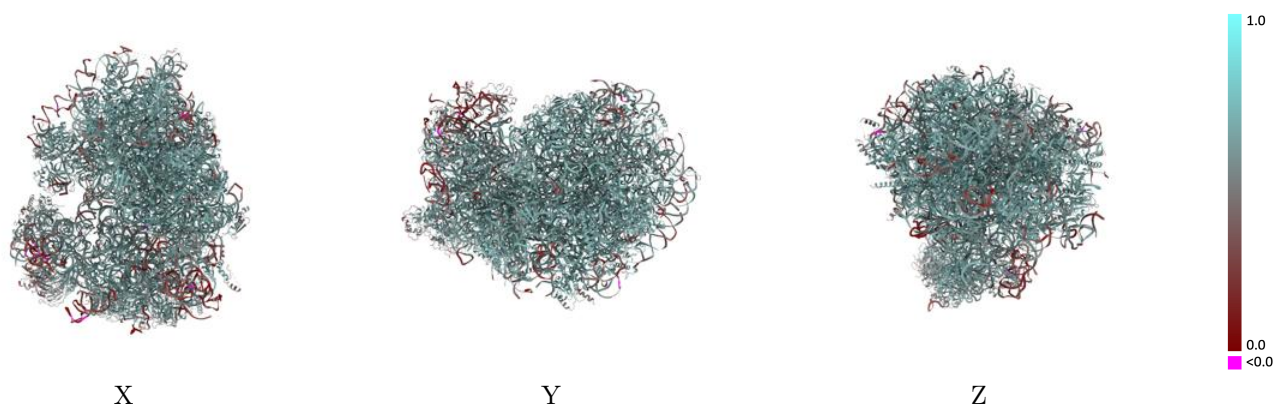
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

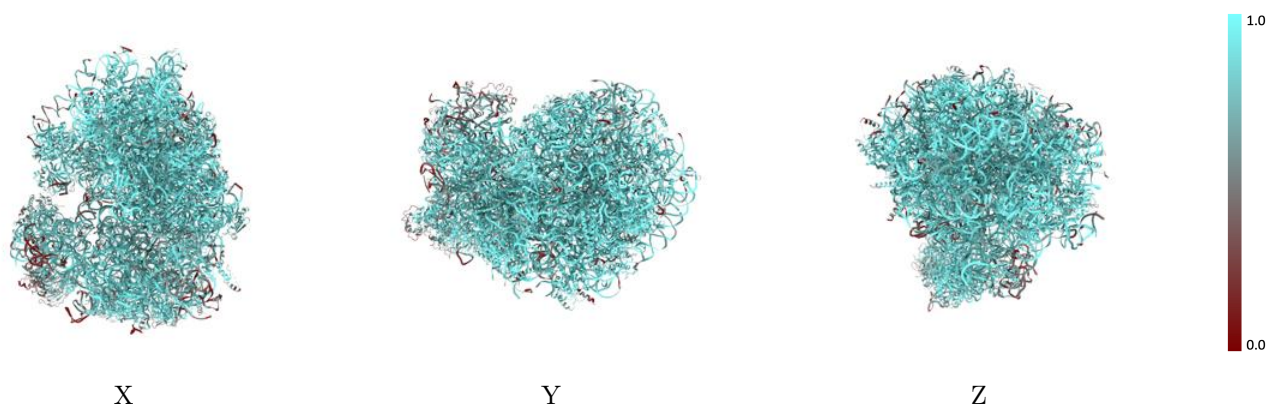


## 9.2 Q-score mapped to coordinate model [i](#)



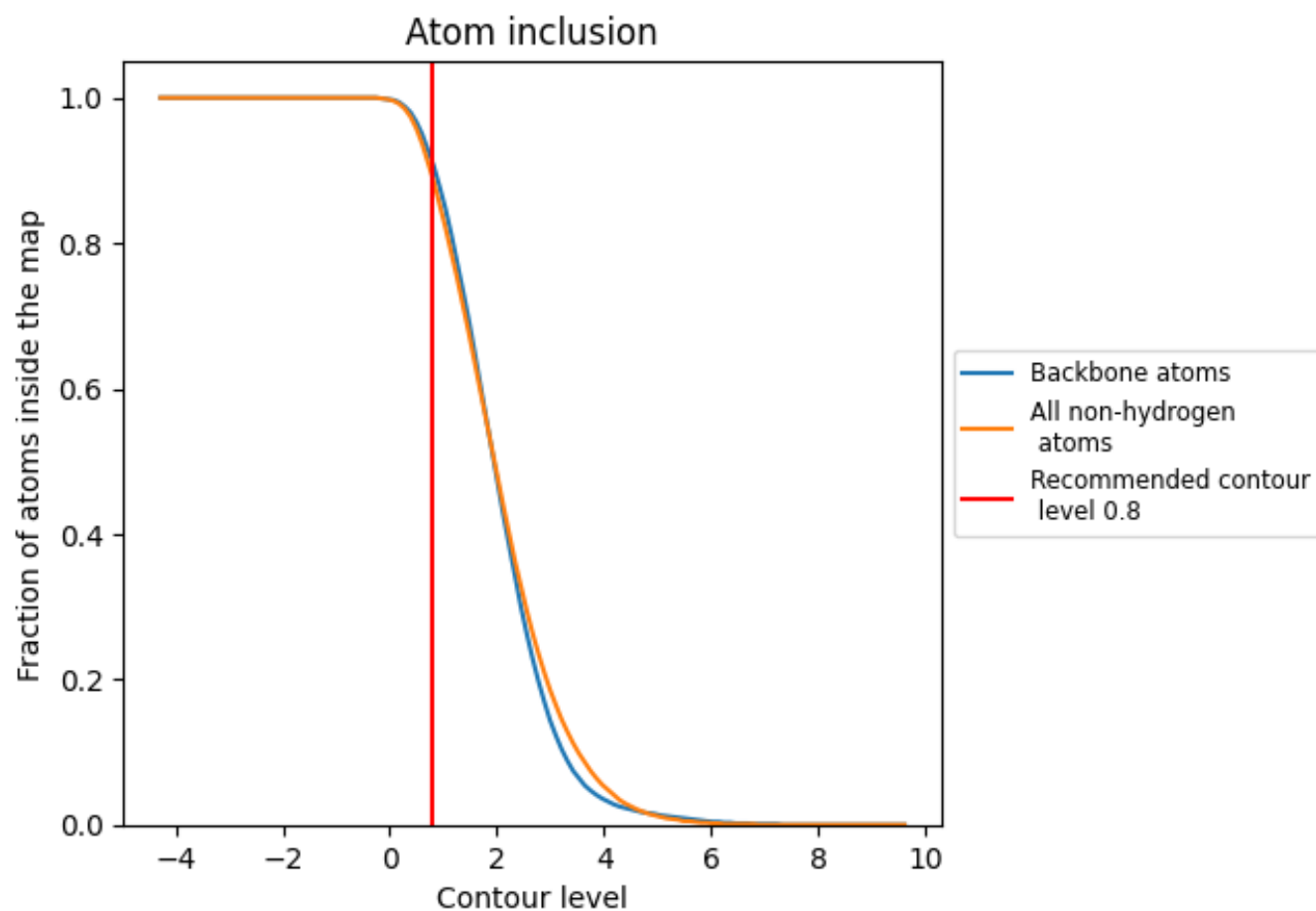
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.8) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8900   |  0.5870   |
| L5    |  0.9350   |  0.6010   |
| L7    |  0.9850   |  0.6320   |
| L8    |  0.9570   |  0.6200   |
| LA    |  0.9630   |  0.6540   |
| LB    |  0.9260   |  0.6360   |
| LC    |  0.9570   |  0.6470   |
| LD    |  0.8890   |  0.5990   |
| LE    |  0.9070   |  0.6080   |
| LF    |  0.9670   |  0.6540   |
| LG    |  0.8370   |  0.5950   |
| LH    |  0.8910   |  0.6110   |
| LI    |  0.8170   |  0.5950   |
| LJ    |  0.8650   |  0.5960   |
| LL    |  0.9110  |  0.6300  |
| LM    |  0.9360 |  0.6320 |
| LN    |  0.9870 |  0.6690 |
| LO    |  0.9570 |  0.6490 |
| LP    |  0.9490 |  0.6480 |
| LQ    |  0.9730 |  0.6660 |
| LR    |  0.9090 |  0.6310 |
| LS    |  0.9570 |  0.6490 |
| LT    |  0.9030 |  0.6310 |
| LU    |  0.8140 |  0.5640 |
| LV    |  0.9430 |  0.6480 |
| LW    |  0.9400 |  0.6400 |
| LX    |  0.9270 |  0.6430 |
| LY    |  0.9240 |  0.6310 |
| LZ    |  0.9280 |  0.6350 |
| La    |  0.9650 |  0.6620 |
| Lb    |  0.8730 |  0.5950 |
| Lc    |  0.9400 |  0.6350 |
| Ld    |  0.8870 |  0.6150 |
| Le    |  0.9710 |  0.6600 |
| Lf    |  0.9730 |  0.6600 |













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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Lg    |  0.9380   |  0.6440   |
| Lh    |  0.9160   |  0.6360   |
| Li    |  0.8920   |  0.6210   |
| Lj    |  0.9760   |  0.6600   |
| Lk    |  0.7970   |  0.5870   |
| Ll    |  0.9720   |  0.6510   |
| Lm    |  0.9380   |  0.6310   |
| Ln    |  0.9310   |  0.6480   |
| Lo    |  0.9290   |  0.6390   |
| Lp    |  0.9200   |  0.6420   |
| Lr    |  0.9720   |  0.6540   |
| S2    |  0.8490   |  0.5280   |
| S6    |  0.4630   |  0.2770   |
| S7    |  0.8640   |  0.5610   |
| SA    |  0.8780   |  0.6040   |
| SB    |  0.8540   |  0.6010   |
| SC    |  0.9060   |  0.6160   |
| SD    |  0.7170  |  0.5250  |
| SE    |  0.8800 |  0.5820 |
| SF    |  0.8500 |  0.5770 |
| SG    |  0.6310 |  0.4860 |
| SH    |  0.6690 |  0.5110 |
| SI    |  0.8960 |  0.6000 |
| SJ    |  0.9000 |  0.5850 |
| SK    |  0.5200 |  0.4220 |
| SL    |  0.9310 |  0.6370 |
| SN    |  0.9150 |  0.6250 |
| SO    |  0.8900 |  0.6140 |
| SP    |  0.6670 |  0.4970 |
| SQ    |  0.8420 |  0.5630 |
| SR    |  0.6850 |  0.5170 |
| SS    |  0.7910 |  0.5540 |
| ST    |  0.8240 |  0.5550 |
| SU    |  0.6130 |  0.4760 |
| SV    |  0.8340 |  0.5770 |
| SW    |  0.9440 |  0.6310 |
| SX    |  0.9050 |  0.6150 |
| SY    |  0.7000 |  0.4570 |
| SZ    |  0.7520 |  0.5140 |
| Sa    |  0.9030 |  0.6100 |
| Sb    |  0.7570 |  0.5450 |
| Sc    |  0.7870 |  0.5560 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Sd    |  0.7350 |  0.5090 |
| Se    |  0.7700 |  0.5480 |
| Sg    |  0.6290 |  0.4660 |
| Sx    |  0.5890 |  0.3720 |
| Z     |  0.3530 |  0.3540 |