



Full wwPDB EM Validation Report ⓘ

May 12, 2025 – 01:52 AM JST

PDB ID : 8ZHB / pdb_00008zhb
EMDB ID : EMD-60097
Title : 80S ribosome with A/A P/E tRNA and mRNA of WNV
Authors : Wu, M.; Yuan, S.
Deposited on : 2024-05-10
Resolution : 2.60 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

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>.

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

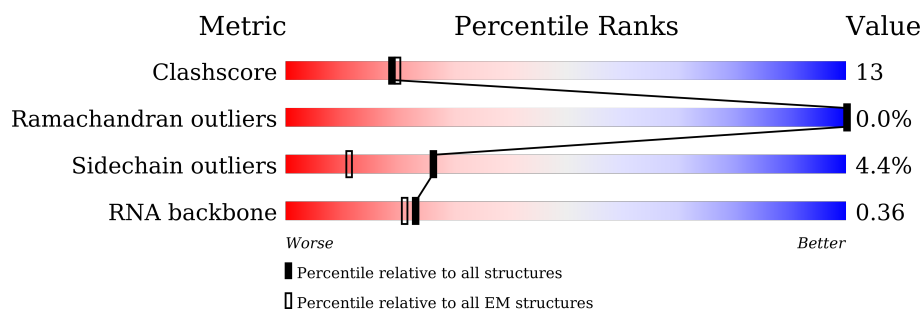
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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 (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 ≥ 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 | LA | 3393 | <div> <div>9%</div> <div>43%</div> <div>41%</div> <div>10%</div> <div>6%</div> </div> |
| 2 | LB | 121 | <div> <div>50%</div> <div>45%</div> <div>5%</div> </div> |
| 3 | LC | 158 | <div> <div>5%</div> <div>42%</div> <div>45%</div> <div>13%</div> </div> |
| 4 | LD | 251 | <div> <div>65%</div> <div>35%</div> </div> |
| 5 | LE | 386 | <div> <div>69%</div> <div>28%</div> <div>.</div> </div> |
| 6 | LF | 361 | <div> <div>69%</div> <div>29%</div> <div>.</div> </div> |
| 7 | LG | 294 | <div> <div>9%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | LH | 175 | |
| 9 | LI | 222 | |
| 10 | LJ | 233 | |
| 11 | LK | 191 | |
| 12 | LL | 218 | |
| 13 | LM | 169 | |
| 14 | LN | 193 | |
| 15 | LO | 136 | |
| 16 | LP | 203 | |
| 17 | LQ | 197 | |
| 18 | LR | 183 | |
| 19 | LS | 185 | |
| 20 | LT | 188 | |
| 21 | LU | 171 | |
| 22 | LV | 159 | |
| 23 | LW | 100 | |
| 24 | LX | 136 | |
| 25 | LY | 65 | |
| 26 | LZ | 121 | |
| 27 | La | 125 | |
| 28 | Lb | 135 | |
| 29 | Lc | 148 | |
| 30 | Ld | 58 | |
| 31 | Le | 96 | |
| 32 | Lf | 109 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 33 | Lg | 127 | |
| 34 | Lh | 106 | |
| 35 | Li | 112 | |
| 36 | Lj | 119 | |
| 37 | Lk | 99 | |
| 38 | Ll | 81 | |
| 39 | Lm | 77 | |
| 40 | Ln | 50 | |
| 41 | Lo | 52 | |
| 42 | Lp | 25 | |
| 43 | Lq | 103 | |
| 44 | Lr | 91 | |
| 45 | S2 | 1799 | |
| 46 | SA | 223 | |
| 47 | SB | 206 | |
| 48 | SC | 92 | |
| 49 | SD | 124 | |
| 50 | SE | 117 | |
| 51 | SF | 141 | |
| 52 | SG | 125 | |
| 53 | SH | 145 | |
| 54 | SI | 143 | |
| 55 | SJ | 101 | |
| 56 | SK | 82 | |
| 57 | SL | 63 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 58 | SM | 53 | |
| 59 | SN | 73 | |
| 60 | SO | 312 | |
| 61 | SP | 206 | |
| 62 | SQ | 232 | |
| 63 | SR | 217 | |
| 64 | SS | 260 | |
| 65 | ST | 228 | |
| 66 | SU | 185 | |
| 67 | SV | 199 | |
| 68 | SW | 185 | |
| 69 | SX | 146 | |
| 70 | SY | 150 | |
| 71 | SZ | 128 | |
| 72 | Sa | 87 | |
| 73 | Sb | 129 | |
| 74 | Sc | 144 | |
| 75 | Sd | 134 | |
| 76 | Se | 97 | |
| 77 | Sf | 81 | |
| 78 | Sg | 57 | |
| 79 | Ta | 77 | |
| 80 | Tb | 77 | |
| 81 | mR | 25 | |

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 202562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S rRNA (3393-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1 | LA | 3184 | Total | C | N | O | P | 0 | 0 |
| | | | 68091 | 30415 | 12259 | 22233 | 3184 | | |

- Molecule 2 is a RNA chain called 5S rRNA (121-MER).

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

- Molecule 3 is a RNA chain called 5.8S rRNA (158-MER).

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL2A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | LD | 251 | Total | C | N | O | S | 0 | 0 |
| | | | 1899 | 1182 | 385 | 331 | 1 | | |

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | LE | 386 | Total | C | N | O | S | 0 | 0 |
| | | | 3075 | 1950 | 584 | 533 | 8 | | |

- Molecule 6 is a protein called Large ribosomal subunit protein uL4A.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | LG | 294 | Total | C | N | O | S | 0 | 0 |
| | | | 2351 | 1484 | 410 | 455 | 2 | | |

- Molecule 8 is a protein called Large ribosomal subunit protein eL6B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | LH | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1307 | 843 | 234 | 230 | | | |

- Molecule 9 is a protein called Large ribosomal subunit protein uL30A.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL8A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | LJ | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1804 | 1151 | 323 | 327 | 3 | | |

- Molecule 11 is a protein called Large ribosomal subunit protein uL6A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | LK | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1508 | 957 | 274 | 273 | 4 | | |

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | LL | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1764 | 1117 | 334 | 306 | 7 | | |

- Molecule 13 is a protein called Large ribosomal subunit protein uL5B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | LM | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1346 | 843 | 252 | 247 | 4 | | |

- Molecule 14 is a protein called Large ribosomal subunit protein eL13A.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL14A.

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL15A.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL13A.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL22A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18 | LR | 183 | Total | C | N | O | 0 | 0 |
| | | | 1416 | 879 | 284 | 253 | | |

- Molecule 19 is a protein called Large ribosomal subunit protein eL18A.

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

- Molecule 20 is a protein called Large ribosomal subunit protein eL19A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20 | LT | 188 | Total | C | N | O | 0 | 0 |
| | | | 1515 | 932 | 323 | 260 | | |

- Molecule 21 is a protein called Large ribosomal subunit protein eL20A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | LU | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1437 | 925 | 266 | 243 | 3 | | |

- Molecule 22 is a protein called Large ribosomal subunit protein eL21A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | LV | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1272 | 802 | 245 | 221 | 4 | | |

- Molecule 23 is a protein called Large ribosomal subunit protein eL22A.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL14A.

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

- Molecule 25 is a protein called Large ribosomal subunit protein eL24A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 25 | LY | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 528 | 339 | 104 | 84 | 1 | | |

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | LZ | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 620 | 169 | 173 | 2 | | |

- Molecule 27 is a protein called Large ribosomal subunit protein uL24A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | La | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 984 | 620 | 191 | 173 | | | |

- Molecule 28 is a protein called Large ribosomal subunit protein eL27A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28 | Lb | 135 | Total | C | N | O | 0 | 0 |
| | | | 1080 | 701 | 199 | 180 | | |

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | Lc | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1169 | 747 | 231 | 188 | 3 | | |

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | Le | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 737 | 476 | 123 | 137 | 1 | | |

- Molecule 32 is a protein called Large ribosomal subunit protein eL31A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | Lf | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | |

- Molecule 33 is a protein called Large ribosomal subunit protein eL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | Lg | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1017 | 644 | 205 | 167 | 1 | | |

- Molecule 34 is a protein called Large ribosomal subunit protein eL33A.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL34A.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL29A.

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

- Molecule 37 is a protein called Large ribosomal subunit protein eL36A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | Lk | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 478 | 154 | 132 | 2 | | |

- Molecule 38 is a protein called Large ribosomal subunit protein eL37A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | Ll | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 645 | 393 | 141 | 106 | 5 | | |

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL40A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41 | Lo | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 410 | 254 | 86 | 65 | 5 | | |

- Molecule 42 is a protein called Large ribosomal subunit protein eL41A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42 | Lp | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 229 | 139 | 62 | 27 | 1 | | |

- Molecule 43 is a protein called Large ribosomal subunit protein eL42A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | Lq | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 824 | 517 | 167 | 135 | 5 | | |

- Molecule 44 is a protein called Large ribosomal subunit protein eL43A.

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

- Molecule 45 is a RNA chain called chain 2 18S rRNA (1799-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 45 | S2 | 1771 | Total | C | N | O | P | 0 | 0 |
| | | | 37739 | 16872 | 6683 | 12413 | 1771 | | |

- Molecule 46 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46 | SA | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1729 | 1098 | 312 | 313 | 6 | | |

- Molecule 47 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47 | SB | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1605 | 1005 | 299 | 298 | 3 | | |

- Molecule 48 is a protein called Small ribosomal subunit protein eS10A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | SC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 752 | 487 | 122 | 141 | 2 | | |

- Molecule 49 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | SD | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 875 | 551 | 153 | 169 | 2 | | |

- Molecule 50 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | SE | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 916 | 583 | 171 | 155 | 7 | | |

- Molecule 51 is a protein called Small ribosomal subunit protein uS9A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | SF | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1105 | 708 | 203 | 194 | | | |

- Molecule 52 is a protein called Small ribosomal subunit protein eS17A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | SG | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 948 | 596 | 179 | 171 | 2 | | |

- Molecule 53 is a protein called Small ribosomal subunit protein uS13A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | SH | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1188 | 741 | 237 | 208 | 2 | | |

- Molecule 54 is a protein called Small ribosomal subunit protein eS19A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54 | SI | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | |

- Molecule 55 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55 | SJ | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 797 | 506 | 144 | 146 | 1 | | |

- Molecule 56 is a protein called Small ribosomal subunit protein eS25A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 56 | SK | 82 | Total | C | N | O | 0 | 0 |
| | | | 651 | 416 | 123 | 112 | | |

- Molecule 57 is a protein called Small ribosomal subunit protein eS28A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 57 | SL | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 491 | 303 | 96 | 91 | 1 | | |

- Molecule 58 is a protein called Small ribosomal subunit protein uS14A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 58 | SM | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 442 | 274 | 92 | 72 | 4 | | |

- Molecule 59 is a protein called Small ribosomal subunit protein eS31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 59 | SN | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 556 | 352 | 105 | 95 | 4 | | |

- Molecule 60 is a protein called Small ribosomal subunit protein RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60 | SO | 312 | Total | C | N | O | S | 0 | 0 |
| | | | 2383 | 1514 | 409 | 452 | 8 | | |

- Molecule 61 is a protein called Small ribosomal subunit protein uS2A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 61 | SP | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1603 | 1030 | 284 | 287 | 2 | | |

- Molecule 62 is a protein called Small ribosomal subunit protein eS1A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 62 | SQ | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1798 | 1139 | 330 | 325 | 4 | | |

- Molecule 63 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 63 | SR | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1626 | 1042 | 287 | 295 | 2 | | |

- Molecule 64 is a protein called Small ribosomal subunit protein eS4A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 64 | SS | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 2056 | 1308 | 387 | 358 | 3 | | |

- Molecule 65 is a protein called Small ribosomal subunit protein eS6A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65 | ST | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1815 | 1138 | 351 | 323 | 3 | | |

- Molecule 66 is a protein called Small ribosomal subunit protein eS7A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 66 | SU | 184 | Total | C | N | O | | 0 | 0 |
| | | | 1473 | 946 | 263 | 264 | | | |

- Molecule 67 is a protein called Small ribosomal subunit protein eS8A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67 | SV | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1476 | 916 | 295 | 263 | 2 | | |

- Molecule 68 is a protein called Small ribosomal subunit protein uS4A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68 | SW | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1479 | 935 | 285 | 258 | 1 | | |

- Molecule 69 is a protein called Small ribosomal subunit protein uS17A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69 | SX | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1142 | 733 | 217 | 189 | 3 | | |

- Molecule 70 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70 | SY | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | |

- Molecule 71 is a protein called Small ribosomal subunit protein uS11B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71 | SZ | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 923 | 568 | 185 | 167 | 3 | | |

- Molecule 72 is a protein called Small ribosomal subunit protein eS21A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72 | Sa | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 673 | 415 | 125 | 131 | 2 | | |

- Molecule 73 is a protein called Small ribosomal subunit protein uS8A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73 | Sb | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | |

- Molecule 74 is a protein called Small ribosomal subunit protein uS12A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74 | Sc | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | |

- Molecule 75 is a protein called Small ribosomal subunit protein eS24A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 75 | Sd | 134 | Total | C | N | O | 0 | 0 |
| | | | 1032 | 651 | 195 | 186 | | |

- Molecule 76 is a protein called Small ribosomal subunit protein eS26B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76 | Se | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 765 | 473 | 160 | 127 | 5 | | |

- Molecule 77 is a protein called Small ribosomal subunit protein eS27A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77 | Sf | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | |

- Molecule 78 is a protein called Small ribosomal subunit protein eS30A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78 | Sg | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 451 | 284 | 93 | 73 | 1 | | |

- Molecule 79 is a RNA chain called tRNA (77-MER).

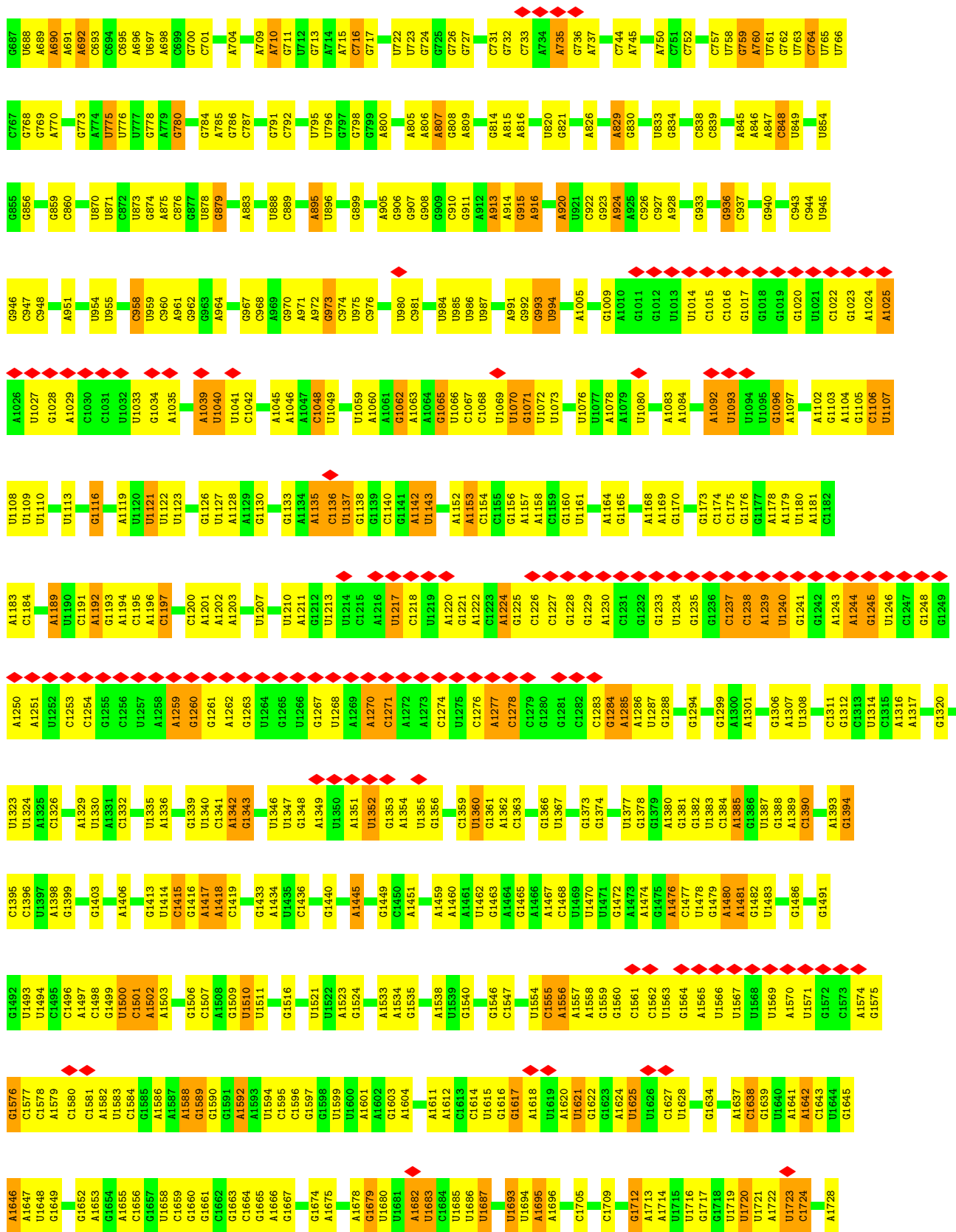
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 79 | Ta | 77 | Total | C | N | O | P | 0 | 0 |
| | | | 1650 | 734 | 303 | 536 | 77 | | |

- Molecule 80 is a RNA chain called tRNA (77-MER).

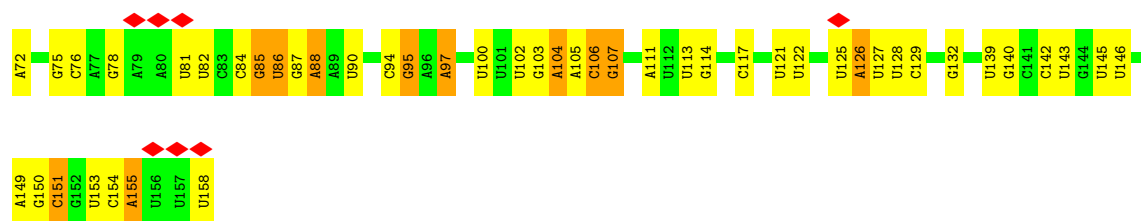
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 80 | Tb | 77 | Total | C | N | O | P | 0 | 0 |
| | | | 1645 | 732 | 298 | 538 | 77 | | |

- Molecule 81 is a RNA chain called RNA (5'-R(P*GP*AP*UP*UP*GP*AP*CP*CP*CP*UP*U)-3').

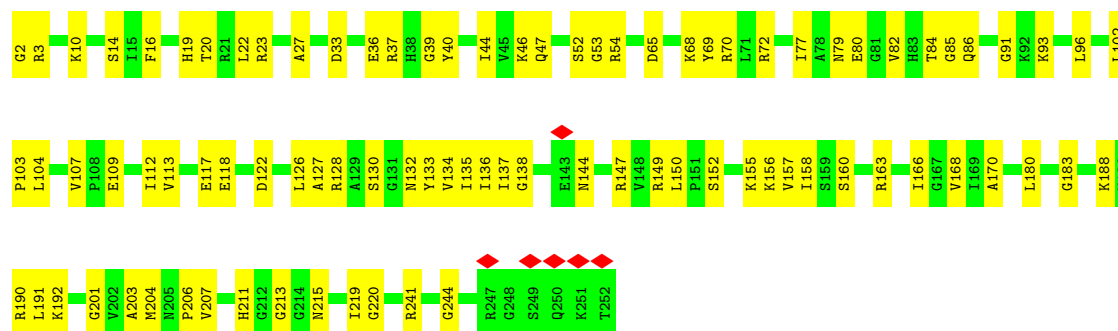
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 81 | mR | 11 | Total | C | N | O | P | 0 | 0 |
| | | | 230 | 103 | 37 | 79 | 11 | | |



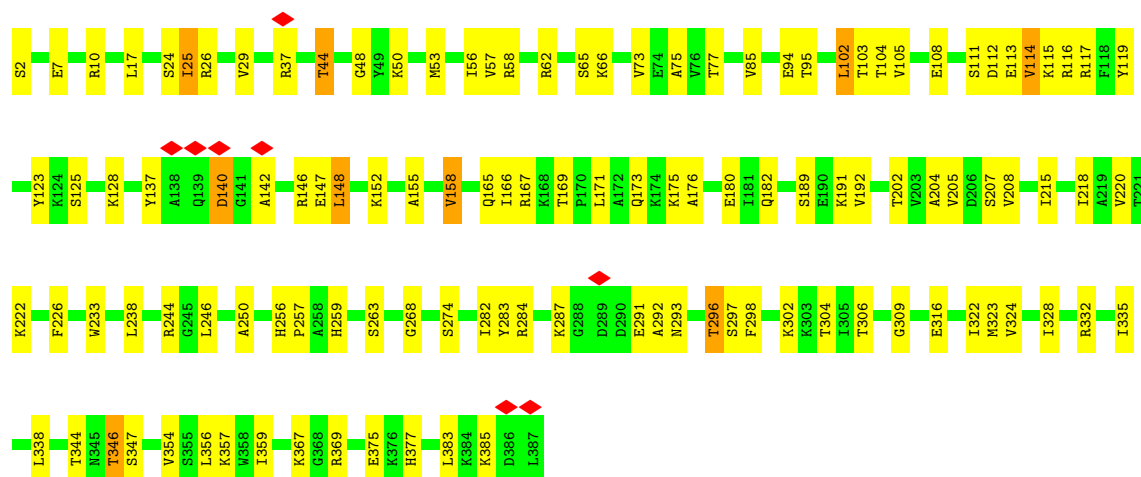




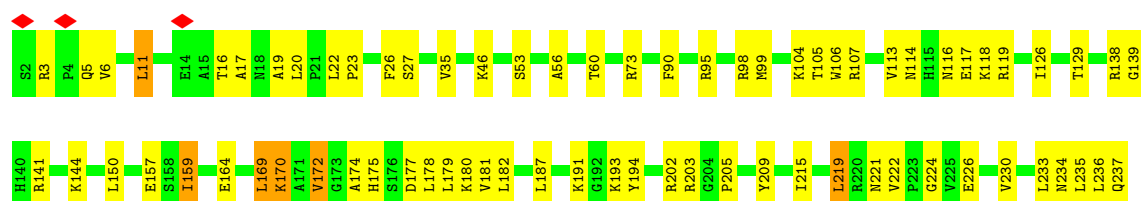
• Molecule 4: Large ribosomal subunit protein uL2A

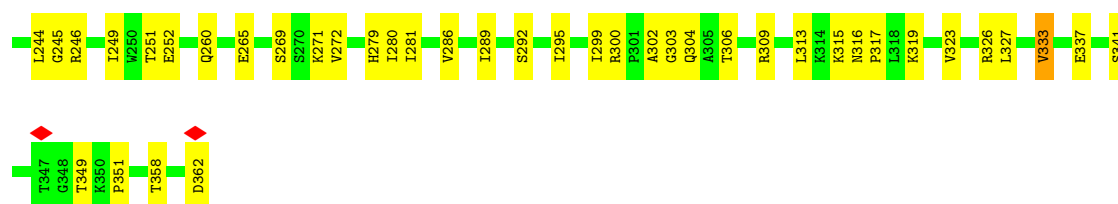


• Molecule 5: Large ribosomal subunit protein uL3

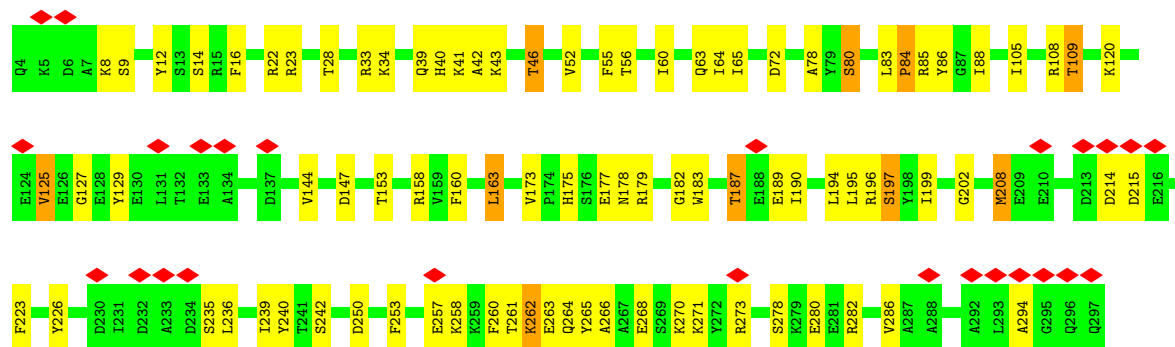


• Molecule 6: Large ribosomal subunit protein uL4A

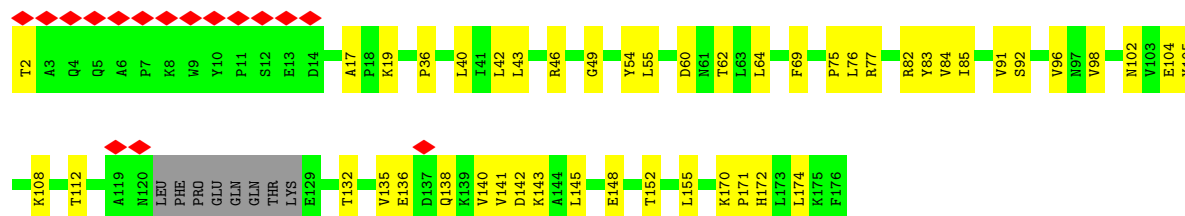




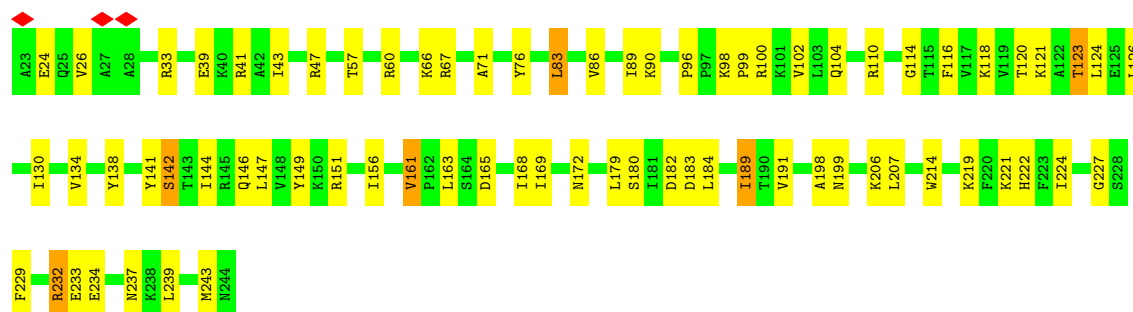
- Molecule 7: Large ribosomal subunit protein uL18



- Molecule 8: Large ribosomal subunit protein eL6B

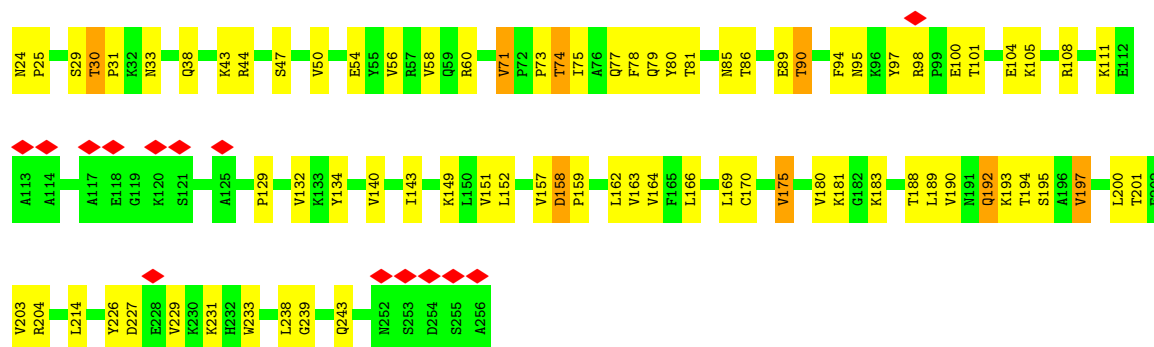


- Molecule 9: Large ribosomal subunit protein uL30A



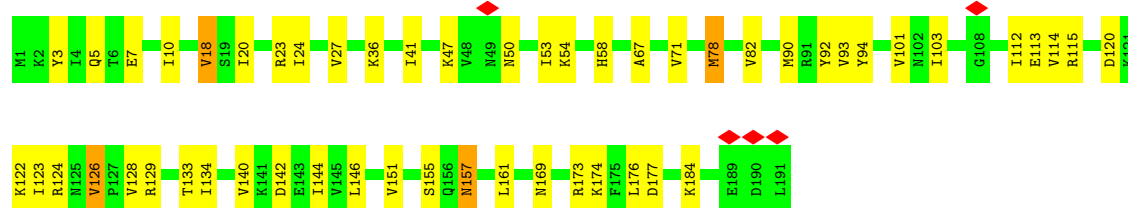
- Molecule 10: Large ribosomal subunit protein eL8A





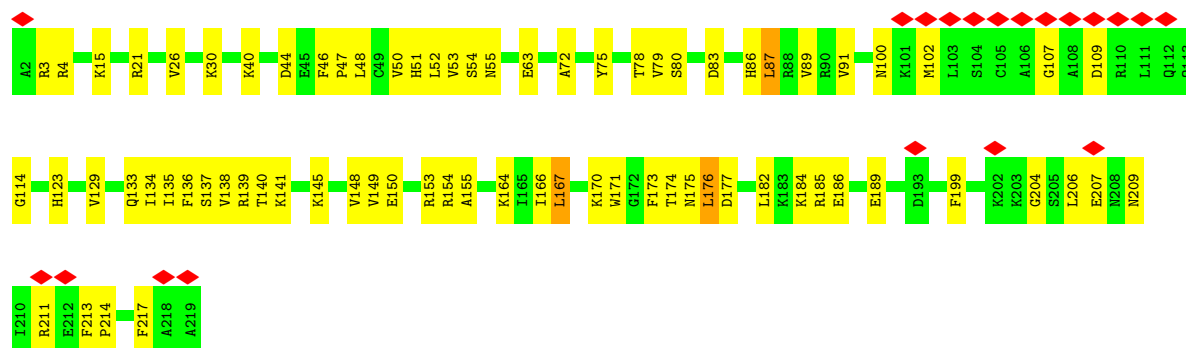
- Molecule 11: Large ribosomal subunit protein uL6A

Chain LK: 72% 26%



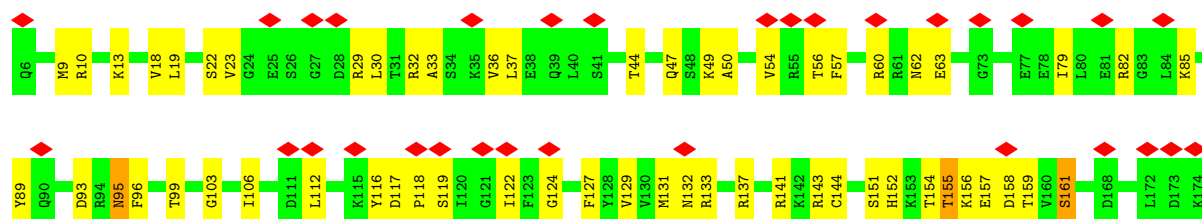
- Molecule 12: Large ribosomal subunit protein uL16

Chain LL: 9% 66% 33%

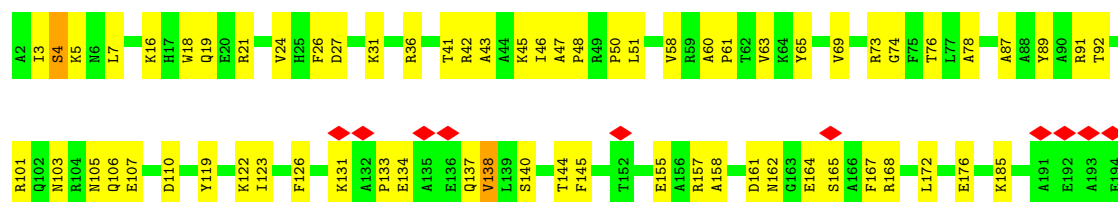


- Molecule 13: Large ribosomal subunit protein uL5B

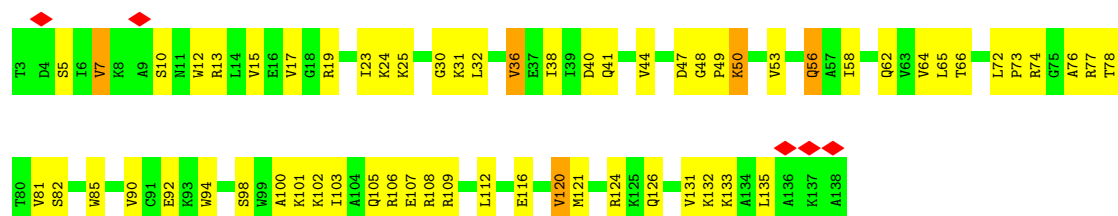
Chain LM: 18% 66% 33%



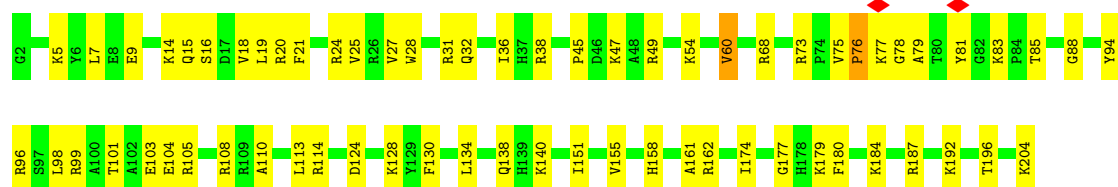
- Molecule 14: Large ribosomal subunit protein eL13A



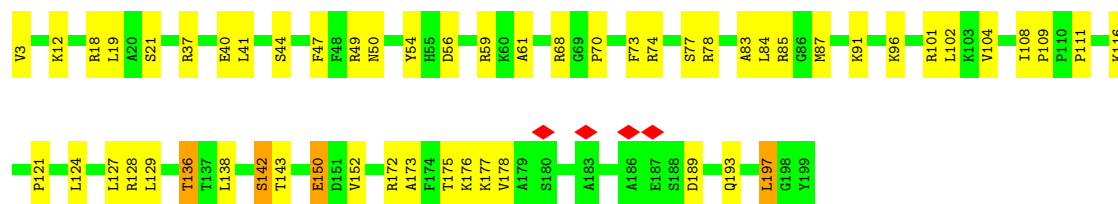
- Molecule 15: Large ribosomal subunit protein eL14A



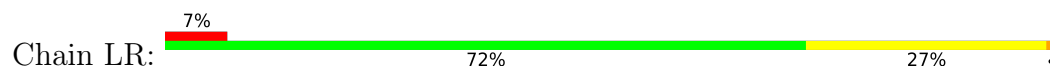
- Molecule 16: Large ribosomal subunit protein eL15A

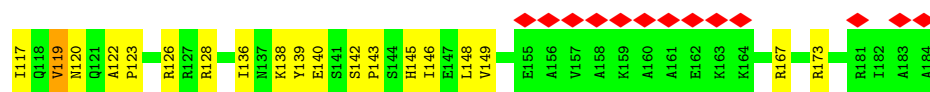


- Molecule 17: Large ribosomal subunit protein uL13A



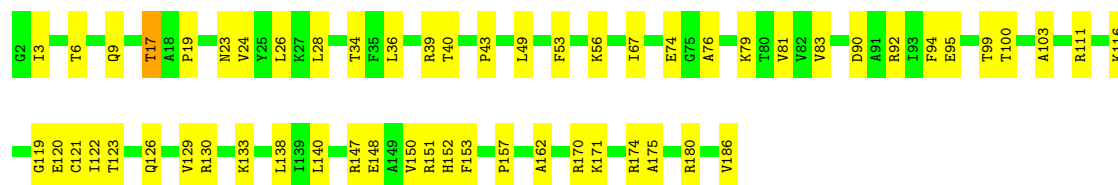
- Molecule 18: Large ribosomal subunit protein uL22A





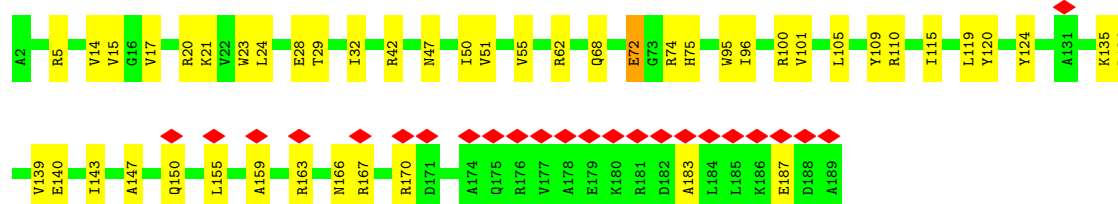
- Molecule 19: Large ribosomal subunit protein eL18A

Chain LS: 69% 30%



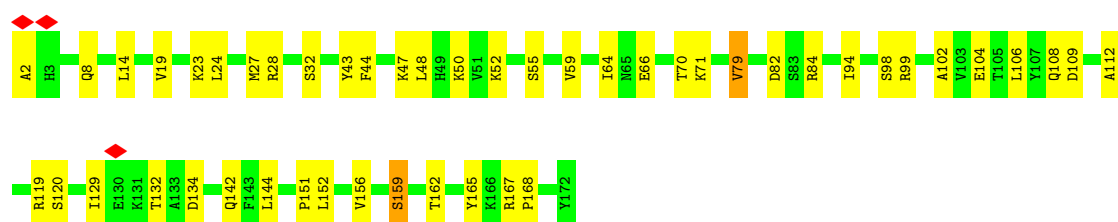
- Molecule 20: Large ribosomal subunit protein eL19A

Chain LT: 13% 75% 24%



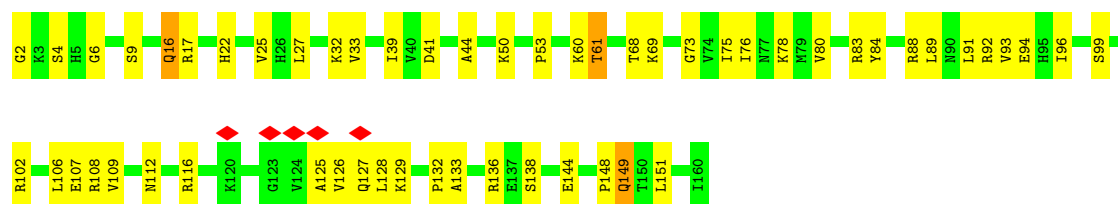
- Molecule 21: Large ribosomal subunit protein eL20A

Chain LU: 71% 27%



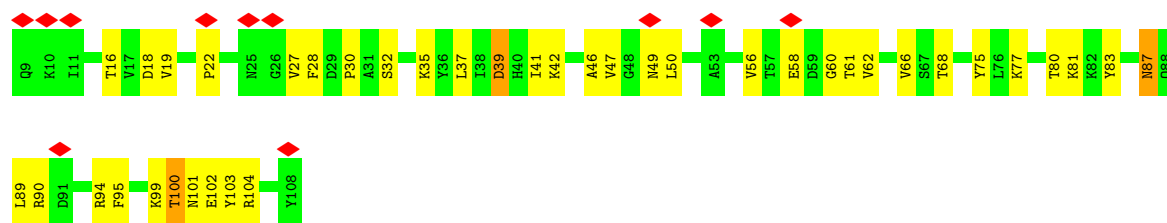
- Molecule 22: Large ribosomal subunit protein eL21A

Chain LV: 65% 33%

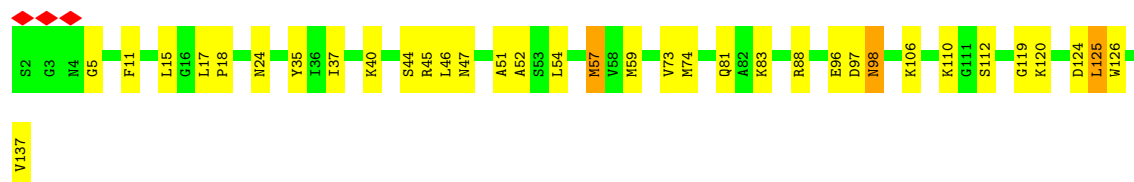
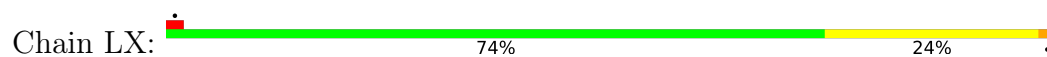


- Molecule 23: Large ribosomal subunit protein eL22A

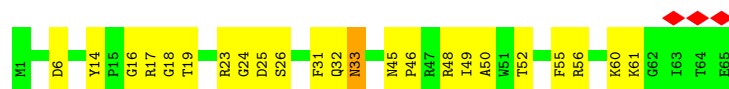
Chain LW: 11% 60% 37%



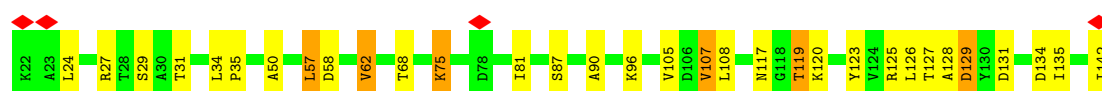
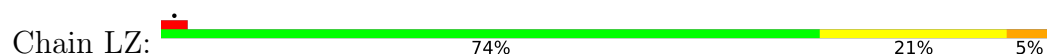
- Molecule 24: Large ribosomal subunit protein uL14A



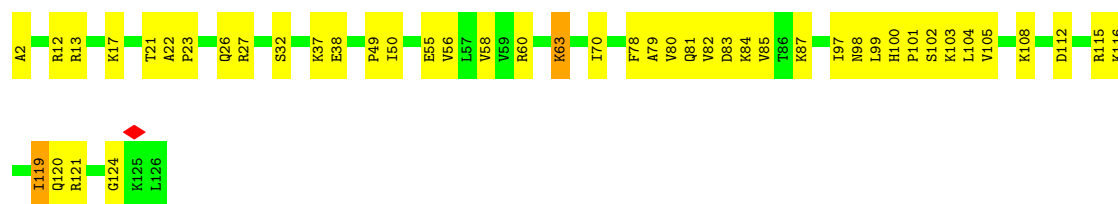
- Molecule 25: Large ribosomal subunit protein eL24A



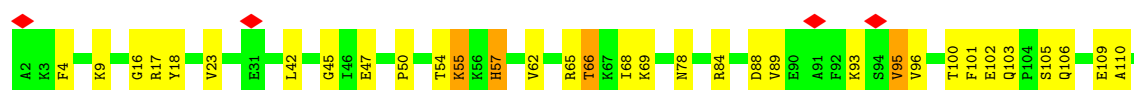
- Molecule 26: Large ribosomal subunit protein uL23



- Molecule 27: Large ribosomal subunit protein uL24A



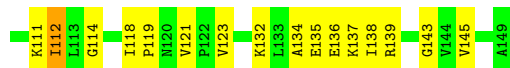
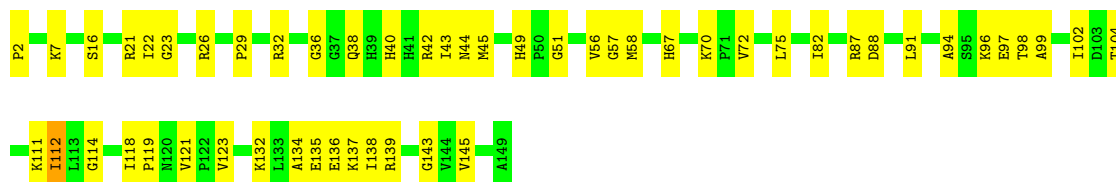
- Molecule 28: Large ribosomal subunit protein eL27A





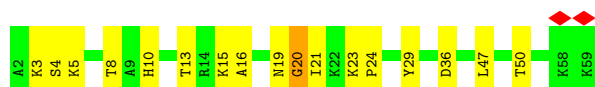
- Molecule 29: Large ribosomal subunit protein uL15

Chain Lc: 65% 34%



- Molecule 30: Large ribosomal subunit protein eL29

Chain Ld: 71% 28%



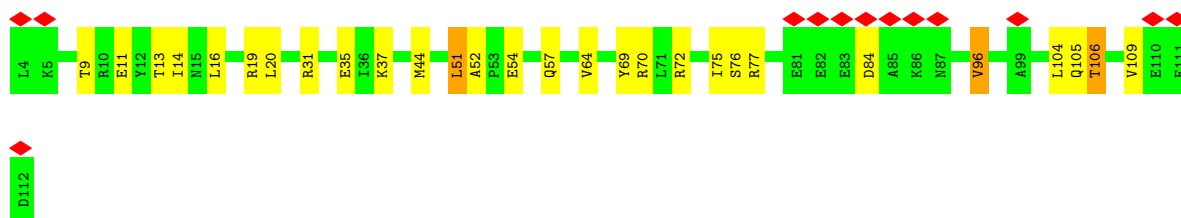
- Molecule 31: Large ribosomal subunit protein eL30

Chain Le: 72% 25%



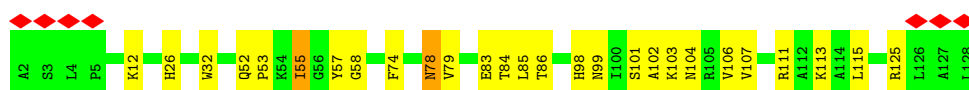
- Molecule 32: Large ribosomal subunit protein eL31A

Chain Lf: 12% 74% 23%




- Molecule 33: Large ribosomal subunit protein eL32

Chain Lg: 6% 79% 20%



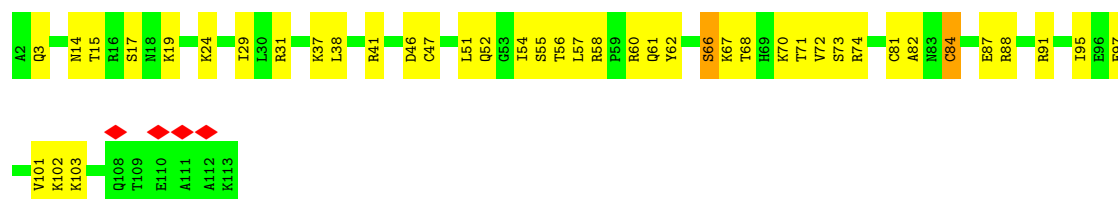
- Molecule 34: Large ribosomal subunit protein eL33A

Chain Lh:  82% 18%




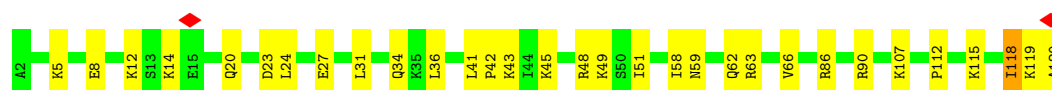
- Molecule 35: Large ribosomal subunit protein eL34A

Chain Li:  62% 36%



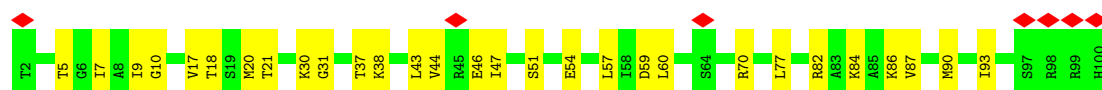
- Molecule 36: Large ribosomal subunit protein uL29A

Chain Lj:  74% 25%



- Molecule 37: Large ribosomal subunit protein eL36A

Chain Lk:  7% 71% 29%




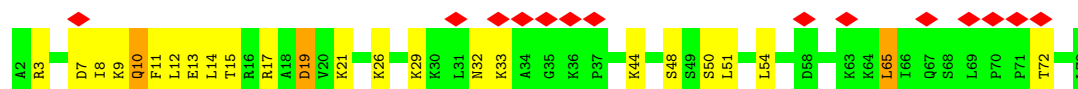
- Molecule 38: Large ribosomal subunit protein eL37A

Chain Ll:  65% 33%



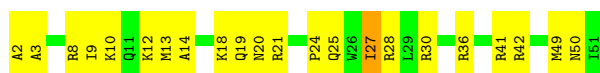
- Molecule 39: Large ribosomal subunit protein eL38

Chain Lm:  18% 69% 27%



- Molecule 40: Large ribosomal subunit protein eL39

Chain Ln:  56% 42%



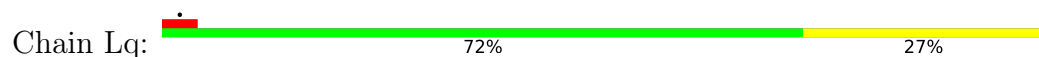
- Molecule 41: Large ribosomal subunit protein eL40A



- Molecule 42: Large ribosomal subunit protein eL41A



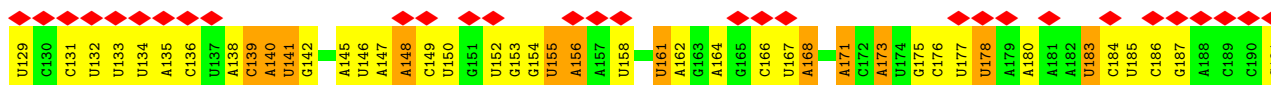
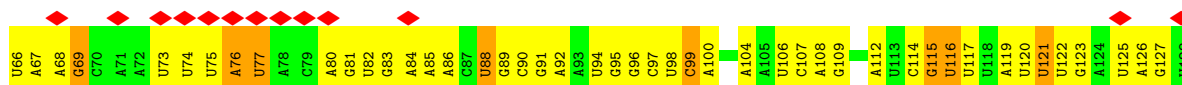
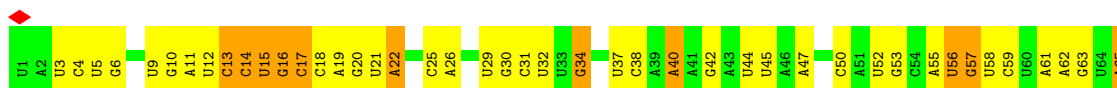
- Molecule 43: Large ribosomal subunit protein eL42A

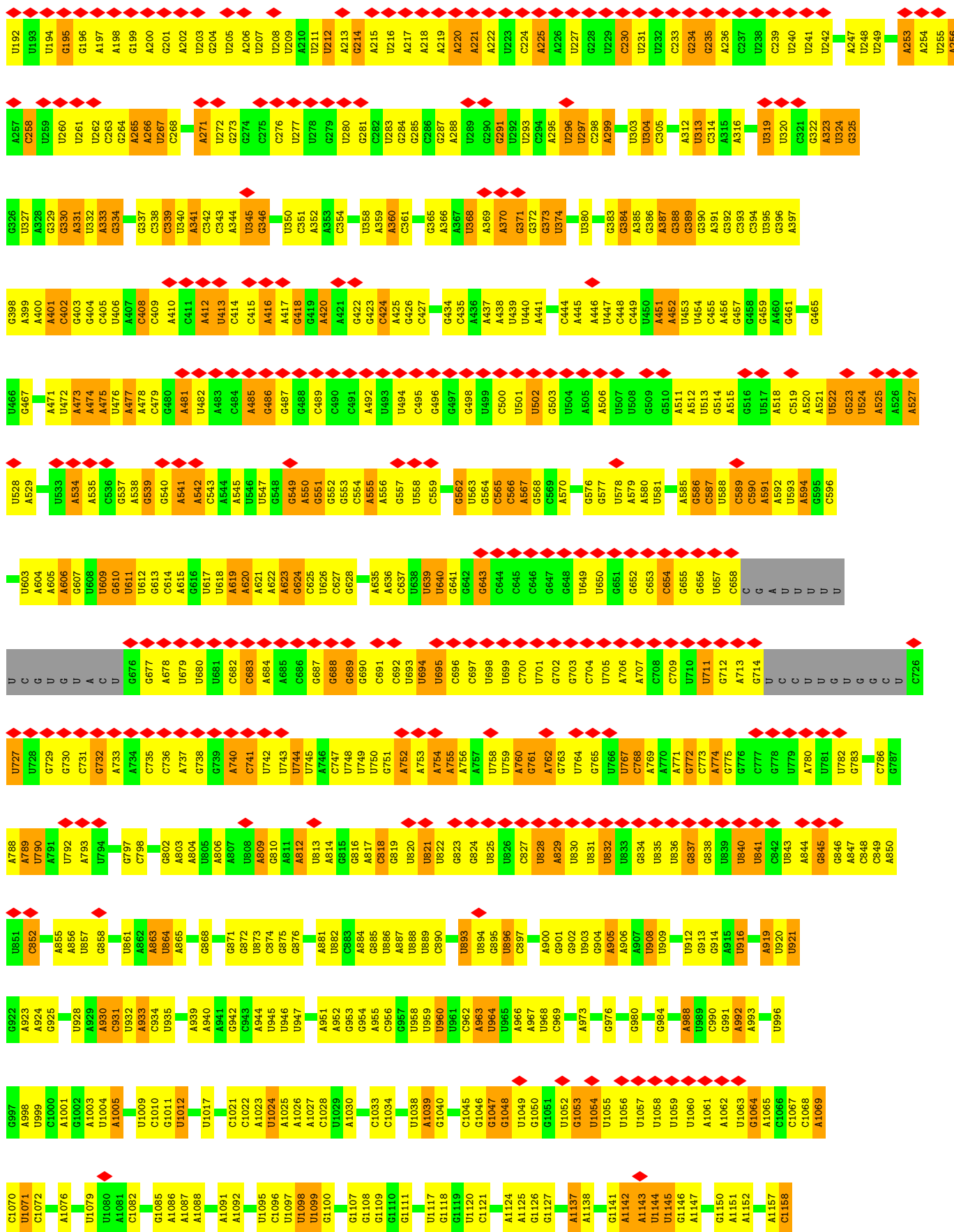


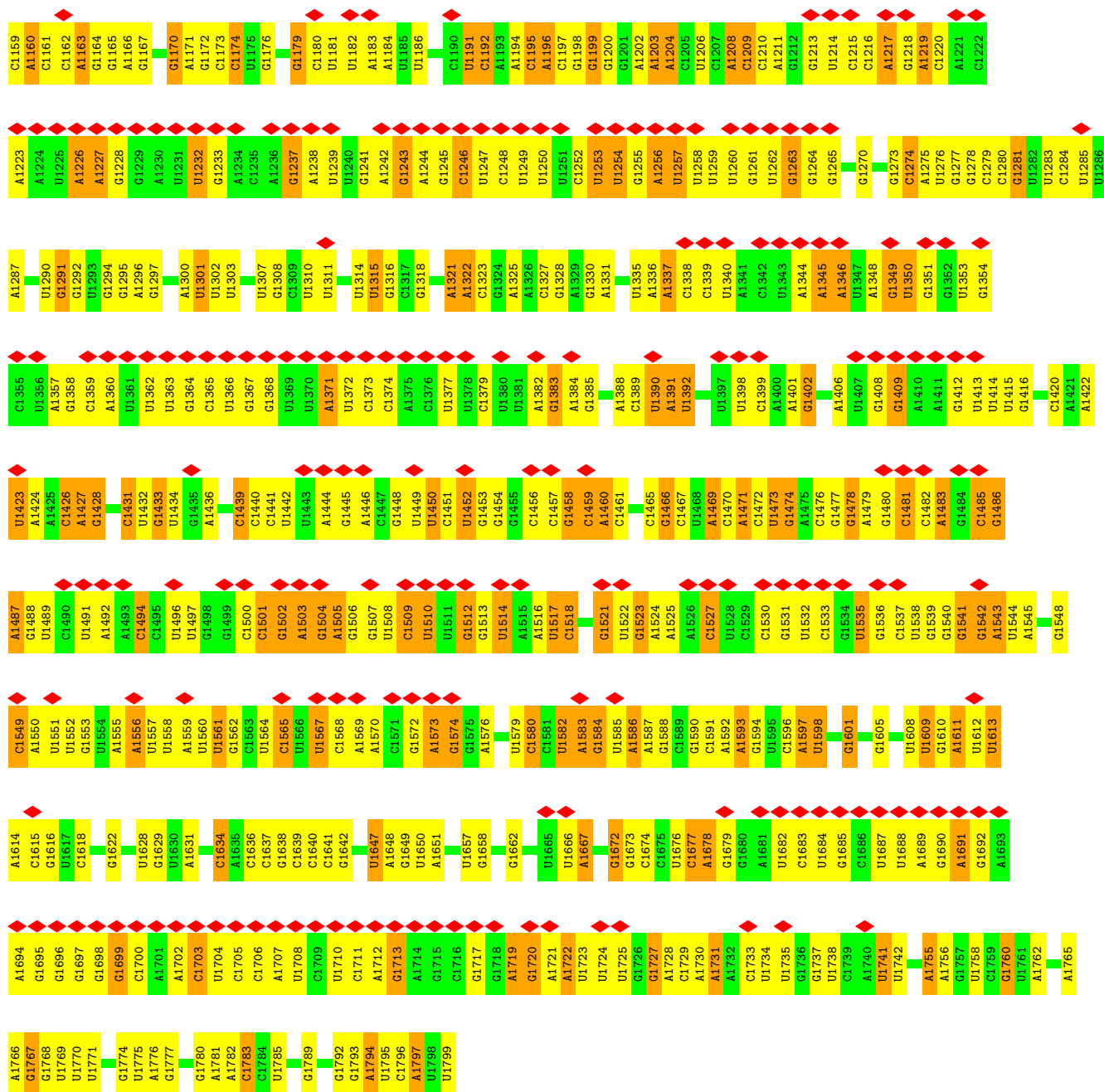
- Molecule 44: Large ribosomal subunit protein eL43A



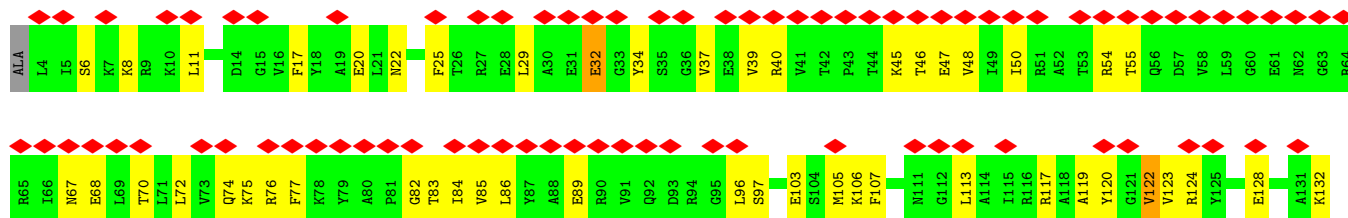
- Molecule 45: chain 2 18S rRNA (1799-MER)

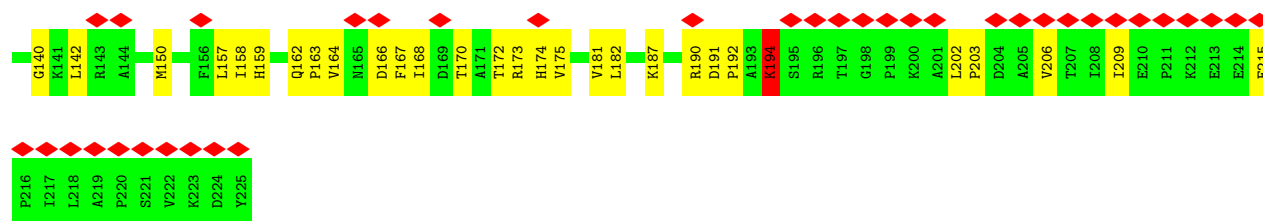




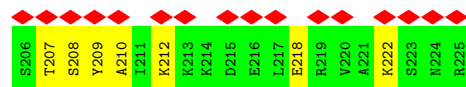
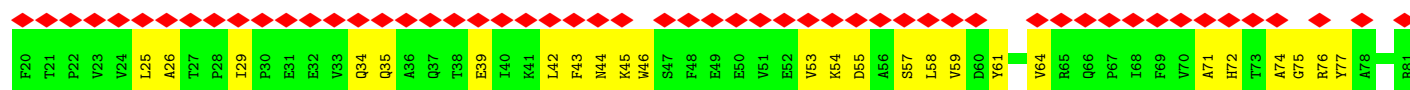
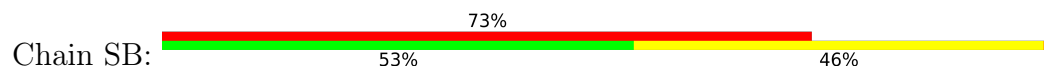


● Molecule 46: Small ribosomal subunit protein uS3

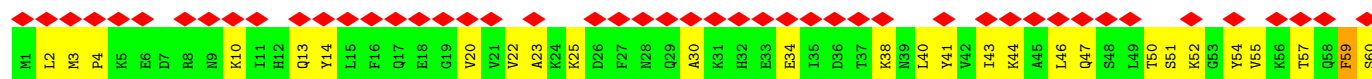
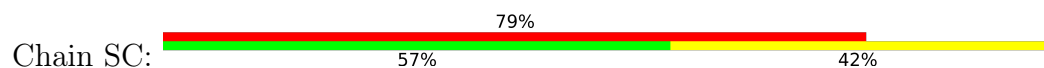




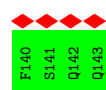
• Molecule 47: Small ribosomal subunit protein uS7



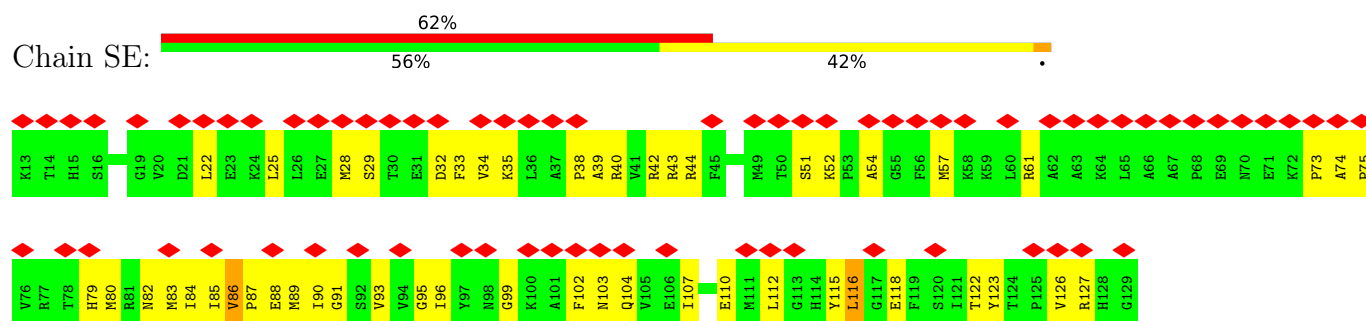
• Molecule 48: Small ribosomal subunit protein eS10A



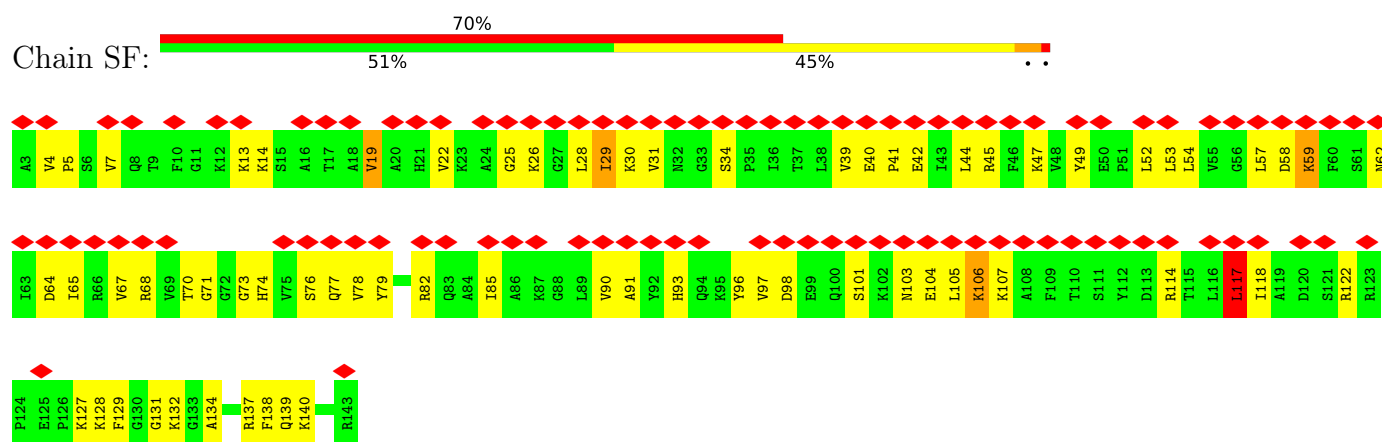
• Molecule 49: Small ribosomal subunit protein eS12



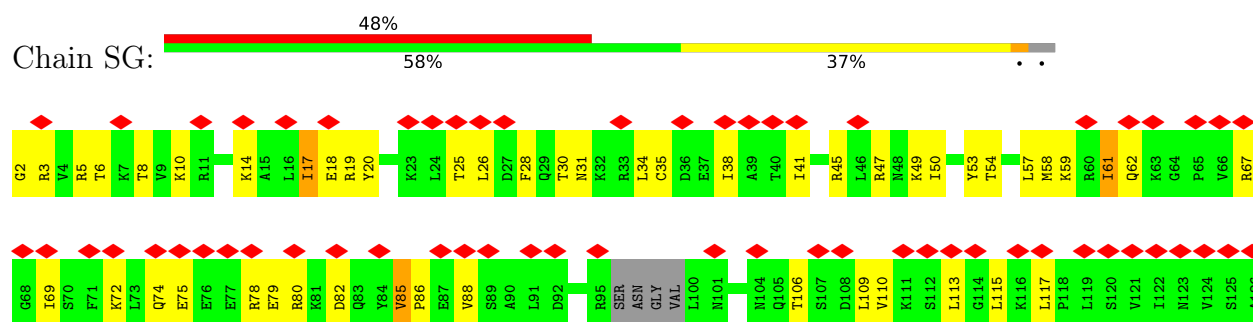
- Molecule 50: Small ribosomal subunit protein uS19



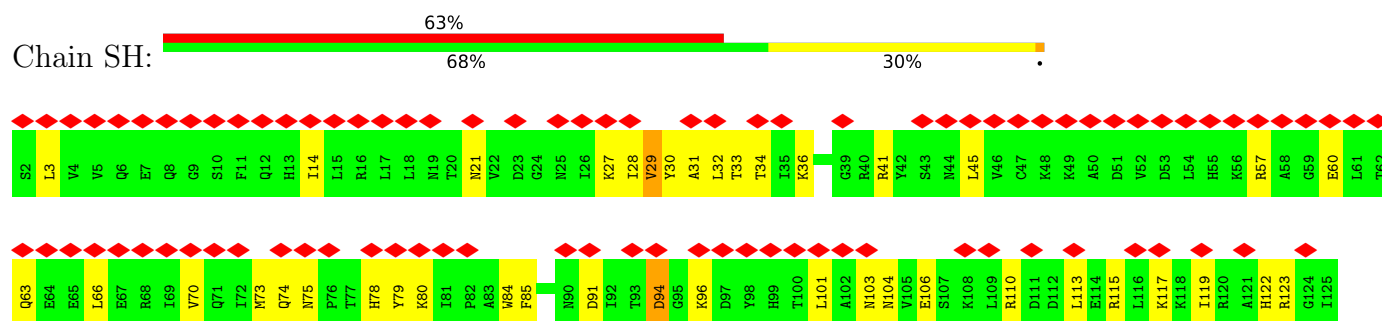
- Molecule 51: Small ribosomal subunit protein uS9A

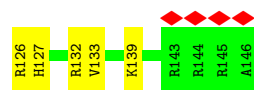


- Molecule 52: Small ribosomal subunit protein eS17A

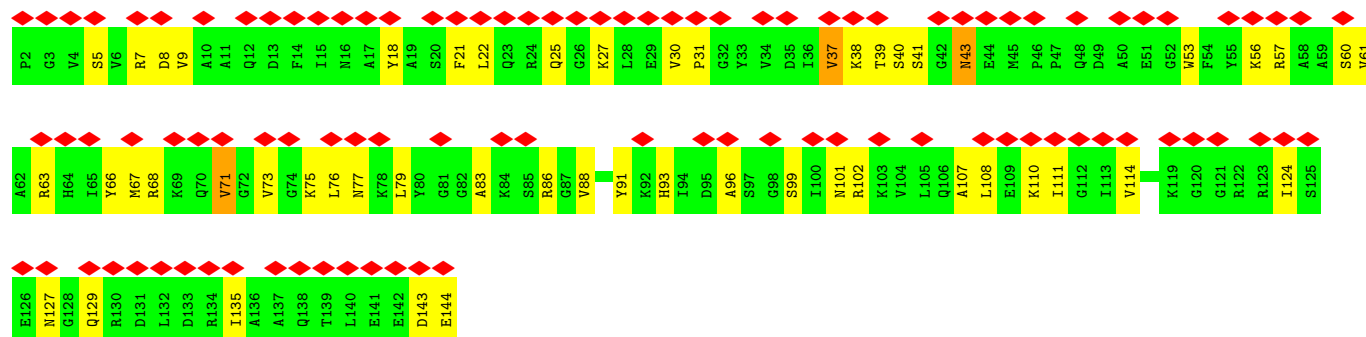


- Molecule 53: Small ribosomal subunit protein uS13A

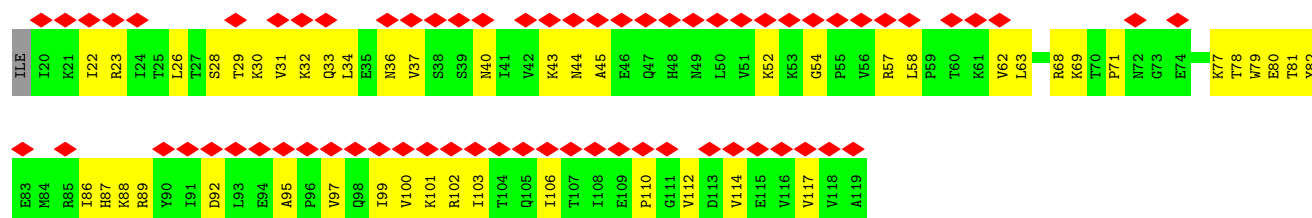




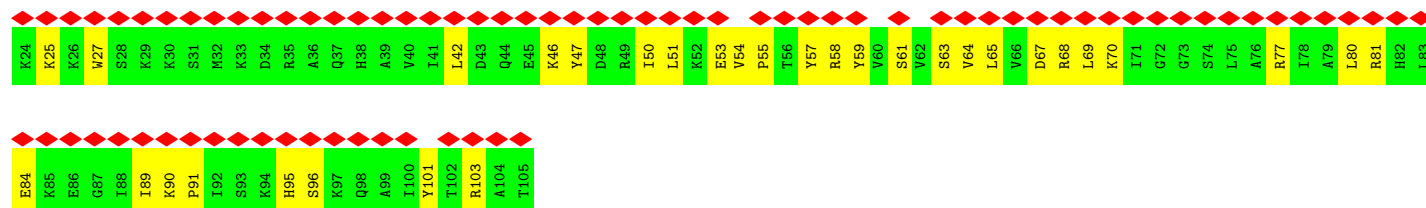
- Molecule 54: Small ribosomal subunit protein eS19A



- Molecule 55: Small ribosomal subunit protein uS10



- Molecule 56: Small ribosomal subunit protein eS25A

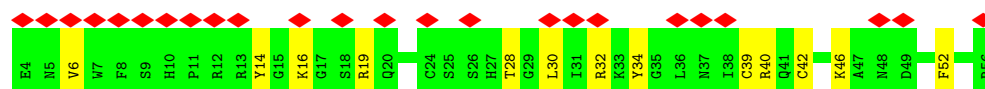
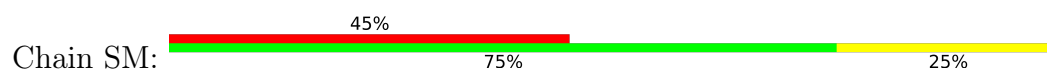


- Molecule 57: Small ribosomal subunit protein eS28A

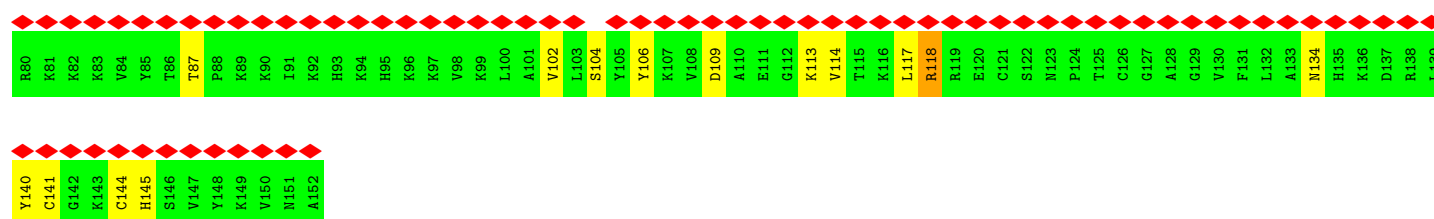
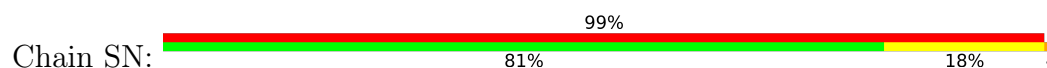




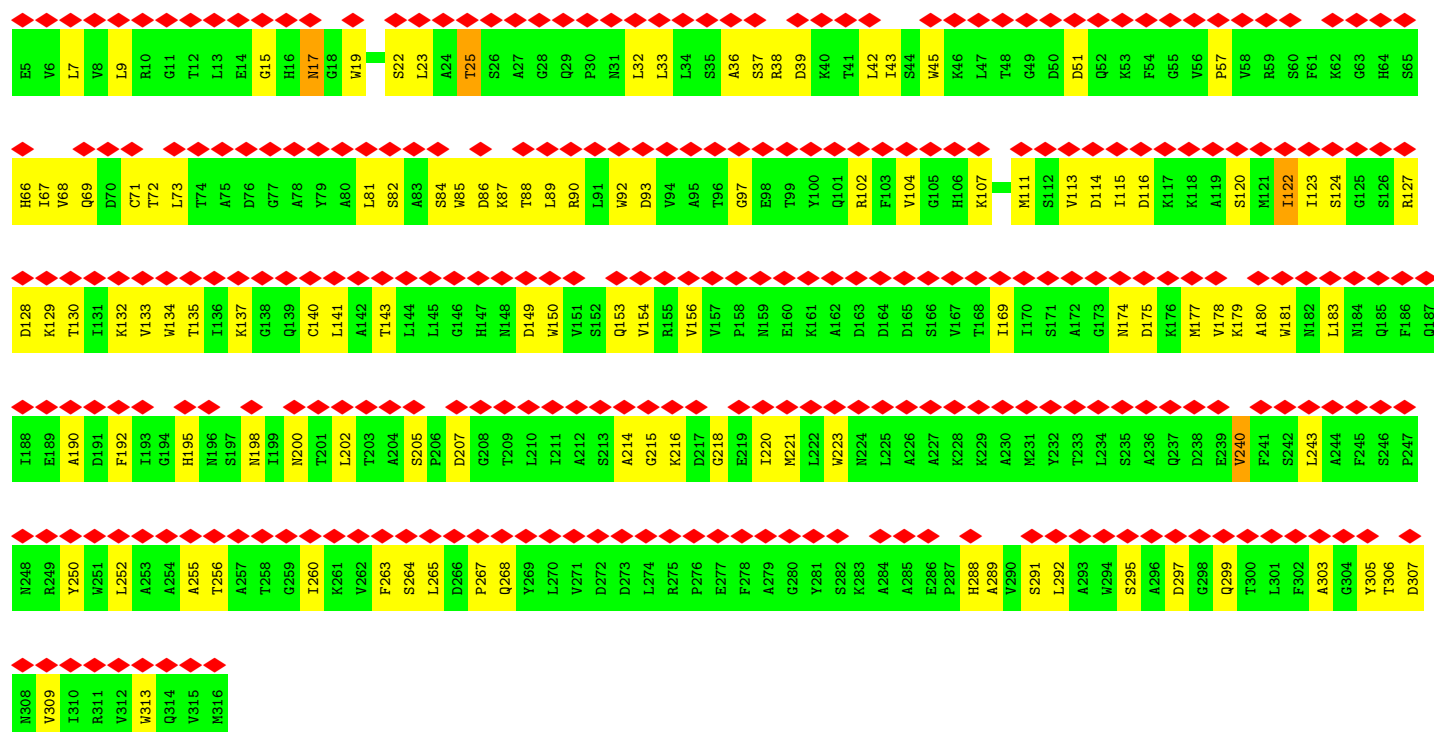
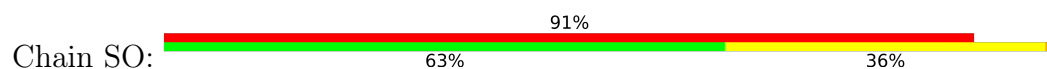
- Molecule 58: Small ribosomal subunit protein uS14A



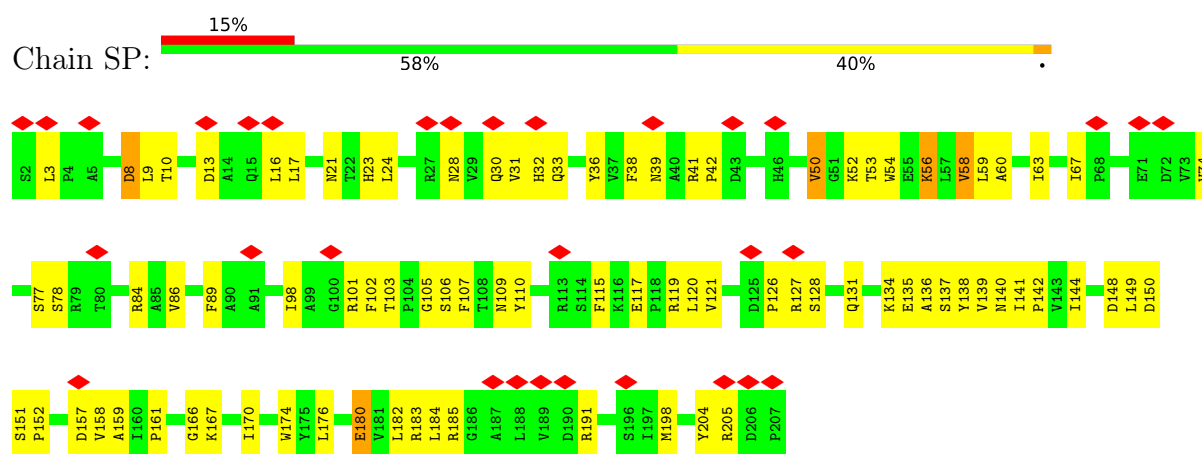
- Molecule 59: Small ribosomal subunit protein eS31



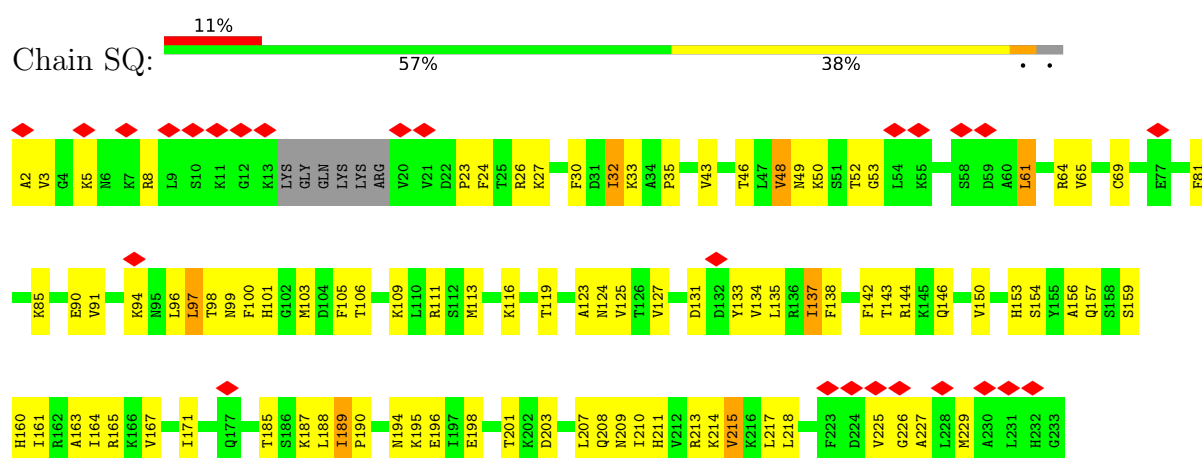
- Molecule 60: Small ribosomal subunit protein RACK1



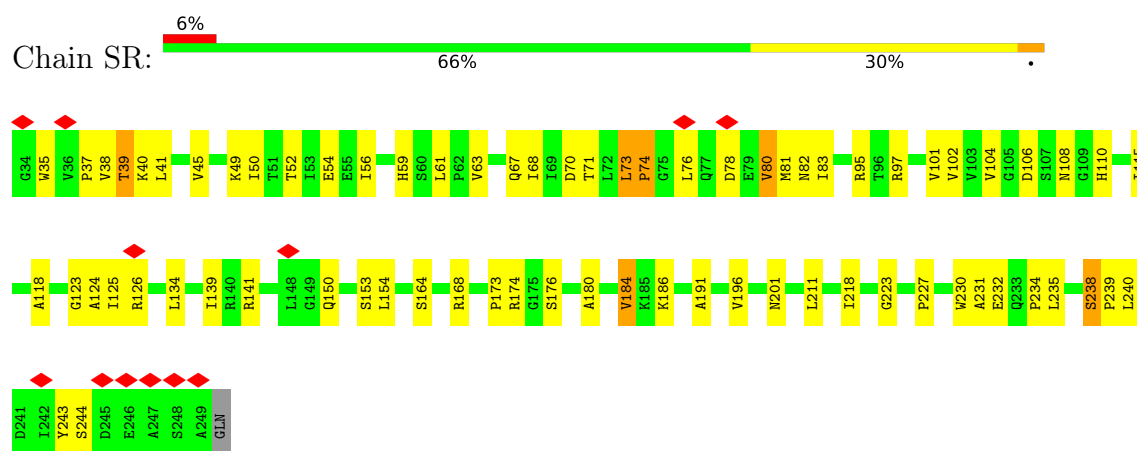
- Molecule 61: Small ribosomal subunit protein uS2A



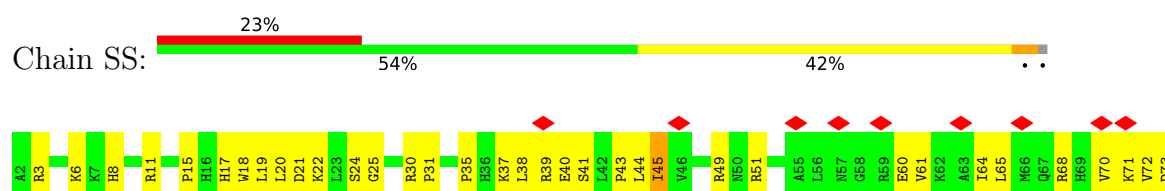
• Molecule 62: Small ribosomal subunit protein eS1A

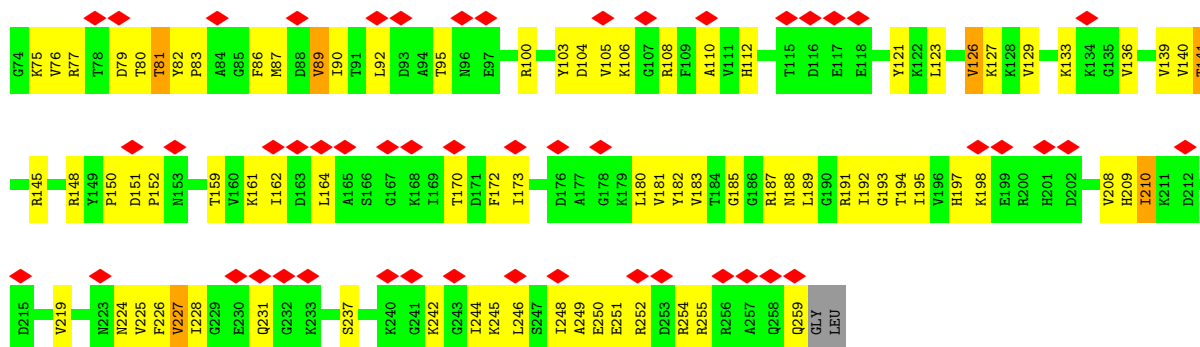


• Molecule 63: Small ribosomal subunit protein uS5

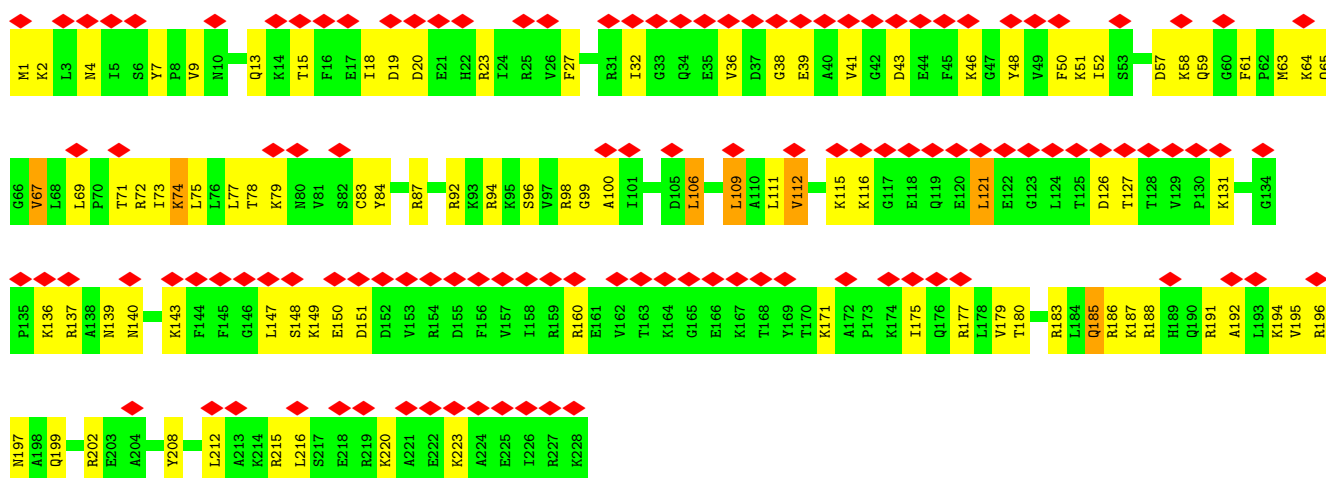


• Molecule 64: Small ribosomal subunit protein eS4A





• Molecule 65: Small ribosomal subunit protein eS6A

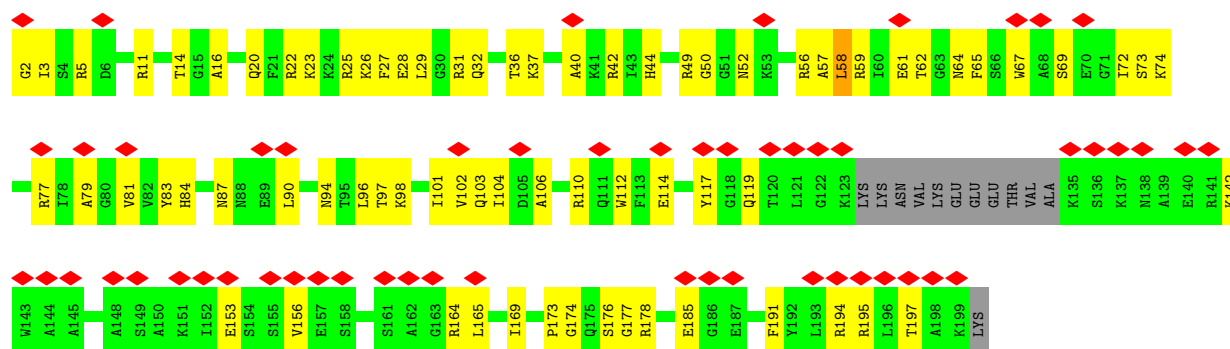


• Molecule 66: Small ribosomal subunit protein eS7A

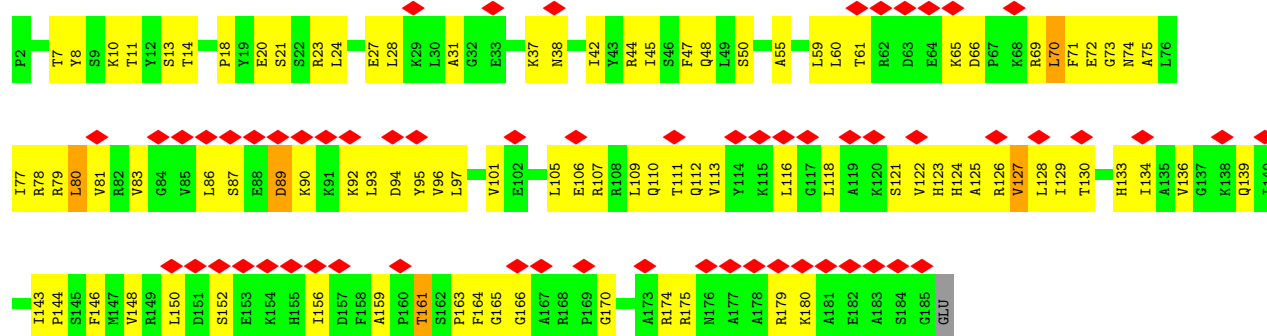


• Molecule 67: Small ribosomal subunit protein eS8A

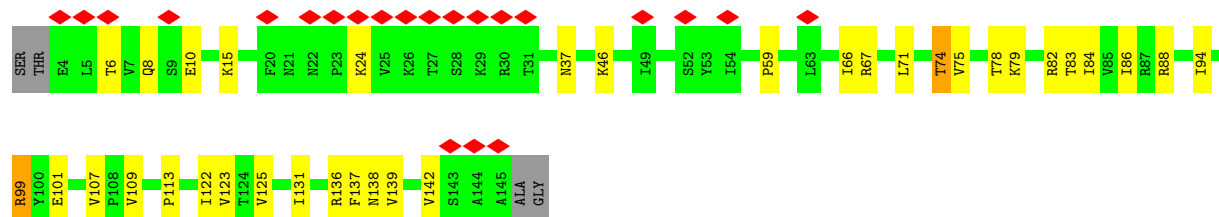
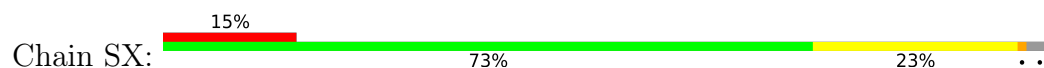




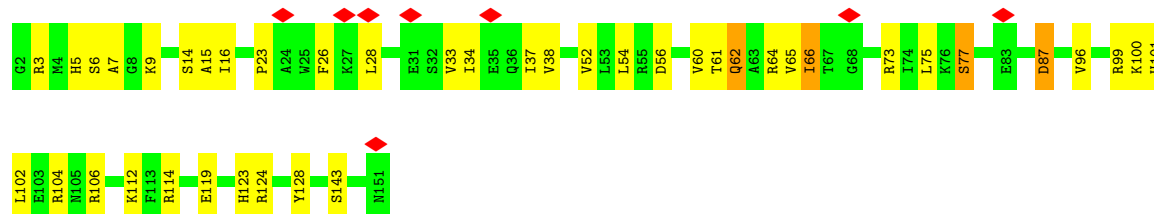
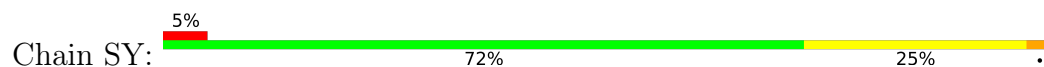
• Molecule 68: Small ribosomal subunit protein uS4A



• Molecule 69: Small ribosomal subunit protein uS17A

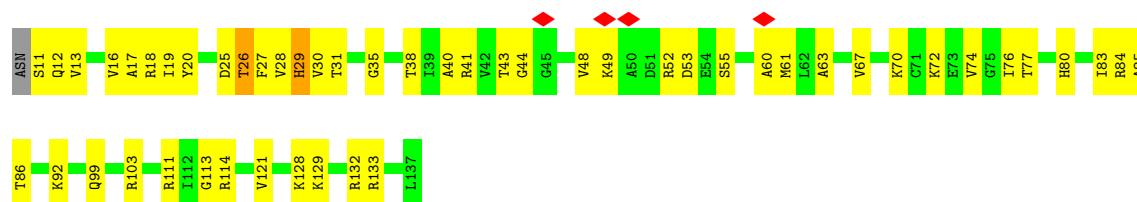


• Molecule 70: Small ribosomal subunit protein uS15



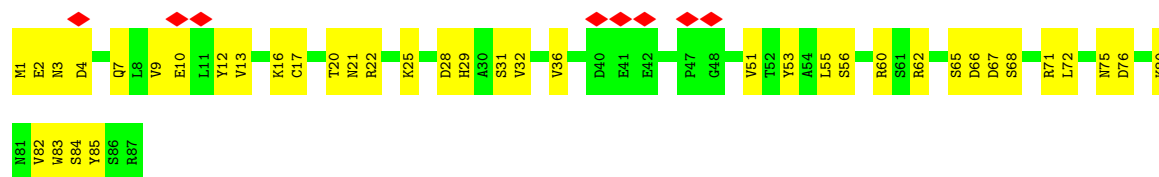
• Molecule 71: Small ribosomal subunit protein uS11B

Chain SZ:  59% 38%




- Molecule 72: Small ribosomal subunit protein eS21A

Chain Sa:  9% 55% 45%



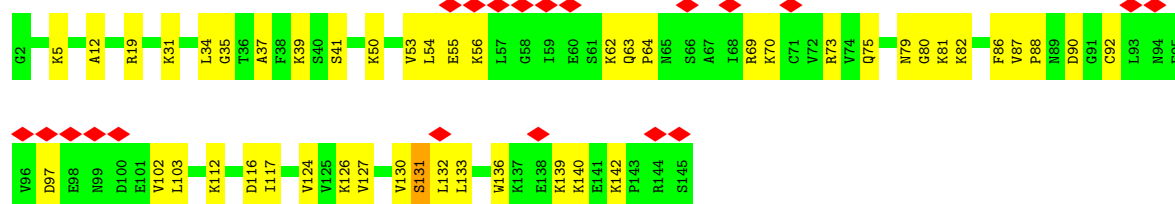
- Molecule 73: Small ribosomal subunit protein uS8A

Chain Sb:  74% 26%




- Molecule 74: Small ribosomal subunit protein uS12A

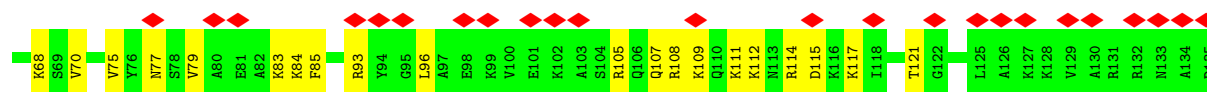
Chain Sc:  14% 67% 32%



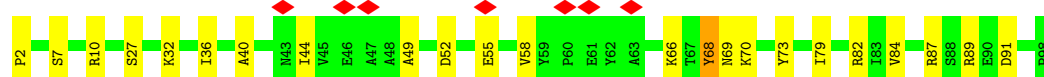
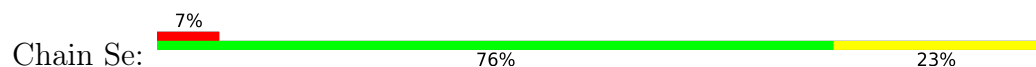
- Molecule 75: Small ribosomal subunit protein eS24A

Chain Sd:  39% 60% 38%

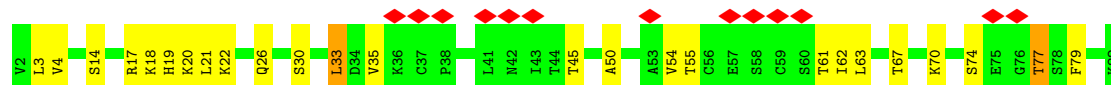




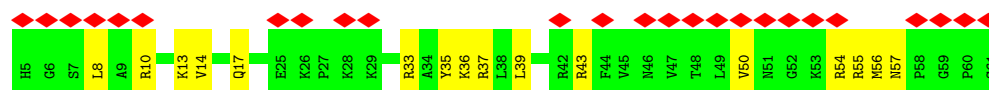
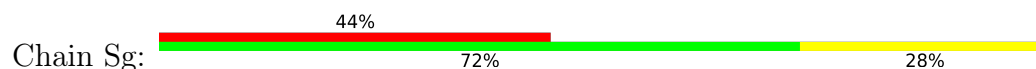
- Molecule 76: Small ribosomal subunit protein eS26B



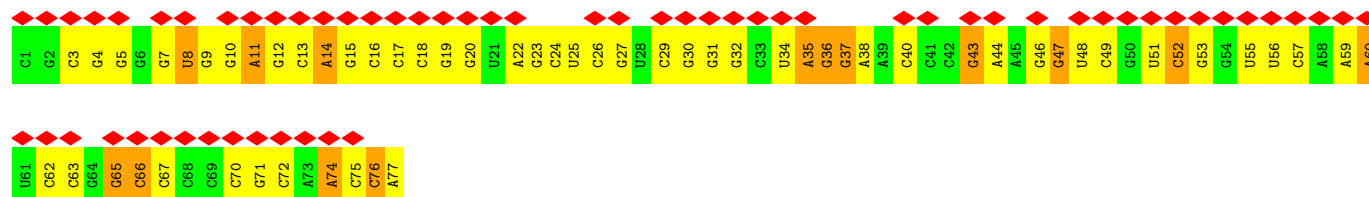
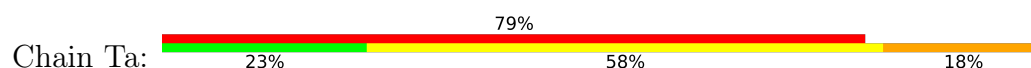
- Molecule 77: Small ribosomal subunit protein eS27A



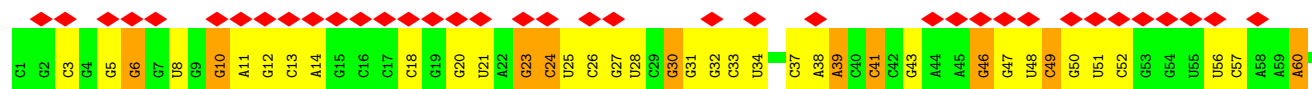
- Molecule 78: Small ribosomal subunit protein eS30A



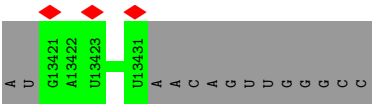
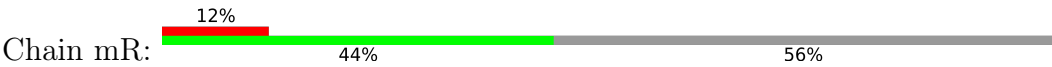
- Molecule 79: tRNA (77-MER)



- Molecule 80: tRNA (77-MER)



- Molecule 81: RNA (5'-R(P*GP*AP*UP*UP*GP*AP*CP*CP*CP*UP*U)-3')



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 84473 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | JEOL CRYO ARM 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 3.367 | Depositor |
| Minimum map value | -1.707 | Depositor |
| Average map value | -0.002 | Depositor |
| Map value standard deviation | 0.085 | Depositor |
| Recommended contour level | 0.26 | Depositor |
| Map size (\AA) | 570.0, 570.0, 570.0 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 0.95, 0.95, 0.95 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 | LA | 0.14 | 0/76214 | 0.32 | 0/118821 |
| 2 | LB | 0.13 | 0/2883 | 0.29 | 0/4491 |
| 3 | LC | 0.13 | 0/3746 | 0.30 | 0/5832 |
| 4 | LD | 0.17 | 0/1933 | 0.39 | 0/2598 |
| 5 | LE | 0.16 | 0/3146 | 0.38 | 0/4228 |
| 6 | LF | 0.17 | 0/2800 | 0.39 | 0/3790 |
| 7 | LG | 0.16 | 0/2400 | 0.40 | 1/3239 (0.0%) |
| 8 | LH | 0.16 | 0/1329 | 0.36 | 0/1794 |
| 9 | LI | 0.16 | 0/1821 | 0.37 | 0/2451 |
| 10 | LJ | 0.16 | 0/1836 | 0.39 | 0/2481 |
| 11 | LK | 0.20 | 0/1529 | 0.40 | 0/2060 |
| 12 | LL | 0.27 | 2/1801 (0.1%) | 0.43 | 2/2416 (0.1%) |
| 13 | LM | 0.17 | 0/1367 | 0.39 | 0/1834 |
| 14 | LN | 0.19 | 0/1568 | 0.40 | 0/2106 |
| 15 | LO | 0.30 | 1/1068 (0.1%) | 0.43 | 1/1438 (0.1%) |
| 16 | LP | 0.16 | 0/1757 | 0.38 | 0/2354 |
| 17 | LQ | 0.18 | 0/1585 | 0.37 | 0/2128 |
| 18 | LR | 0.15 | 0/1439 | 0.36 | 0/1938 |
| 19 | LS | 0.16 | 0/1465 | 0.38 | 0/1965 |
| 20 | LT | 0.17 | 0/1532 | 0.32 | 0/2043 |
| 21 | LU | 0.19 | 0/1473 | 0.37 | 0/1980 |
| 22 | LV | 0.17 | 0/1296 | 0.34 | 0/1739 |
| 23 | LW | 0.14 | 0/812 | 0.39 | 0/1099 |
| 24 | LX | 0.15 | 0/1018 | 0.36 | 0/1369 |
| 25 | LY | 0.14 | 0/540 | 0.31 | 0/717 |
| 26 | LZ | 0.14 | 0/979 | 0.34 | 0/1321 |
| 27 | La | 0.14 | 0/995 | 0.33 | 0/1329 |
| 28 | Lb | 0.17 | 0/1106 | 0.38 | 0/1485 |
| 29 | Lc | 0.17 | 0/1200 | 0.38 | 0/1607 |
| 30 | Ld | 0.19 | 0/473 | 0.38 | 0/629 |
| 31 | Le | 0.14 | 0/745 | 0.33 | 0/1001 |
| 32 | Lf | 0.25 | 1/890 (0.1%) | 0.34 | 0/1196 |
| 33 | Lg | 0.16 | 0/1038 | 0.34 | 0/1390 |
| 34 | Lh | 0.15 | 0/868 | 0.36 | 0/1168 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 35 | Li | 0.15 | 0/890 | 0.33 | 0/1189 |
| 36 | Lj | 0.17 | 0/978 | 0.41 | 1/1301 (0.1%) |
| 37 | Lk | 0.17 | 0/772 | 0.39 | 0/1026 |
| 38 | Ll | 0.18 | 0/660 | 0.37 | 0/875 |
| 39 | Lm | 0.15 | 0/618 | 0.42 | 1/826 (0.1%) |
| 40 | Ln | 0.18 | 0/443 | 0.33 | 0/588 |
| 41 | Lo | 0.13 | 0/416 | 0.34 | 0/553 |
| 42 | Lp | 0.14 | 0/230 | 0.35 | 0/296 |
| 43 | Lq | 0.52 | 2/836 (0.2%) | 0.52 | 1/1104 (0.1%) |
| 44 | Lr | 0.15 | 0/701 | 0.36 | 0/934 |
| 45 | S2 | 0.12 | 0/42211 | 0.31 | 0/65773 |
| 46 | SA | 0.28 | 0/1754 | 0.47 | 1/2361 (0.0%) |
| 47 | SB | 0.18 | 0/1625 | 0.44 | 0/2197 |
| 48 | SC | 0.12 | 0/769 | 0.36 | 0/1039 |
| 49 | SD | 0.26 | 0/883 | 0.61 | 0/1199 |
| 50 | SE | 0.15 | 0/936 | 0.39 | 0/1259 |
| 51 | SF | 0.24 | 0/1125 | 0.49 | 2/1510 (0.1%) |
| 52 | SG | 0.18 | 0/957 | 0.38 | 0/1283 |
| 53 | SH | 0.17 | 0/1207 | 0.38 | 0/1623 |
| 54 | SI | 0.17 | 0/1130 | 0.42 | 0/1517 |
| 55 | SJ | 0.15 | 0/807 | 0.40 | 0/1091 |
| 56 | SK | 0.20 | 0/661 | 0.41 | 0/888 |
| 57 | SL | 0.19 | 0/493 | 0.40 | 0/663 |
| 58 | SM | 0.10 | 0/452 | 0.28 | 0/600 |
| 59 | SN | 0.13 | 0/567 | 0.47 | 1/764 (0.1%) |
| 60 | SO | 0.18 | 0/2436 | 0.43 | 0/3318 |
| 61 | SP | 0.18 | 0/1644 | 0.42 | 0/2249 |
| 62 | SQ | 0.32 | 1/1823 (0.1%) | 0.48 | 1/2447 (0.0%) |
| 63 | SR | 0.28 | 0/1656 | 0.56 | 4/2251 (0.2%) |
| 64 | SS | 0.17 | 0/2097 | 0.43 | 0/2823 |
| 65 | ST | 0.15 | 0/1839 | 0.39 | 0/2460 |
| 66 | SU | 0.19 | 0/1498 | 0.45 | 0/2019 |
| 67 | SV | 0.17 | 0/1501 | 0.36 | 0/2006 |
| 68 | SW | 0.33 | 1/1504 (0.1%) | 0.59 | 4/2016 (0.2%) |
| 69 | SX | 0.15 | 0/1168 | 0.35 | 0/1575 |
| 70 | SY | 0.16 | 0/1215 | 0.39 | 0/1638 |
| 71 | SZ | 0.21 | 0/934 | 0.46 | 0/1257 |
| 72 | Sa | 0.15 | 0/682 | 0.37 | 0/921 |
| 73 | Sb | 0.18 | 0/1038 | 0.44 | 0/1395 |
| 74 | Sc | 0.16 | 0/1139 | 0.44 | 0/1518 |
| 75 | Sd | 0.15 | 0/1046 | 0.32 | 0/1401 |
| 76 | Se | 0.14 | 0/778 | 0.42 | 0/1042 |
| 77 | Sf | 0.15 | 0/620 | 0.37 | 0/838 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 78 | Sg | 0.15 | 0/459 | 0.38 | 0/611 |
| 79 | Ta | 0.13 | 0/1844 | 0.36 | 0/2873 |
| 80 | Tb | 0.11 | 0/1837 | 0.28 | 0/2861 |
| All | All | 0.16 | 8/217531 (0.0%) | 0.35 | 20/320015 (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 |
|-----|-------|---------------------|---------------------|
| 10 | LJ | 0 | 1 |
| 16 | LP | 0 | 1 |
| 30 | Ld | 0 | 1 |
| 73 | Sb | 0 | 1 |
| All | All | 0 | 4 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 43 | Lq | 55 | LYS | C-O | -9.04 | 1.16 | 1.24 |
| 62 | SQ | 189 | ILE | CA-CB | -7.25 | 1.50 | 1.54 |
| 12 | LL | 213 | PHE | C-O | 6.68 | 1.27 | 1.23 |
| 68 | SW | 159 | ALA | C-N | 6.08 | 1.39 | 1.33 |
| 32 | Lf | 51 | LEU | C-N | -5.79 | 1.24 | 1.33 |
| 43 | Lq | 57 | VAL | C-O | -5.65 | 1.18 | 1.24 |
| 15 | LO | 50 | LYS | CG-CD | -5.29 | 1.36 | 1.52 |
| 12 | LL | 214 | PRO | CG-CD | -5.16 | 1.33 | 1.50 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 12 | LL | 214 | PRO | N-CD-CG | -10.43 | 87.55 | 103.20 |
| 68 | SW | 166 | GLY | N-CA-C | 9.91 | 123.74 | 111.85 |
| 68 | SW | 165 | GLY | N-CA-C | -9.02 | 91.80 | 113.18 |
| 51 | SF | 117 | LEU | CB-CG-CD1 | -8.99 | 83.72 | 110.70 |
| 46 | SA | 194 | LYS | N-CA-C | -8.32 | 101.56 | 113.21 |
| 63 | SR | 74 | PRO | CA-N-CD | -7.12 | 102.04 | 112.00 |
| 36 | Lj | 118 | ILE | CG1-CB-CG2 | -6.52 | 91.14 | 110.70 |
| 43 | Lq | 56 | PRO | N-CA-C | 6.39 | 122.25 | 111.32 |
| 63 | SR | 234 | PRO | N-CA-C | 6.06 | 124.95 | 112.47 |
| 7 | LG | 84 | PRO | CA-N-CD | -5.76 | 103.93 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 15 | LO | 50 | LYS | CB-CG-CD | -5.67 | 98.27 | 111.30 |
| 12 | LL | 214 | PRO | CA-CB-CG | -5.64 | 93.77 | 104.50 |
| 68 | SW | 164 | PHE | N-CA-CB | 5.37 | 120.19 | 112.08 |
| 51 | SF | 106 | LYS | CD-CE-NZ | 5.26 | 128.72 | 111.90 |
| 63 | SR | 238 | SER | CA-C-N | -5.25 | 113.50 | 119.28 |
| 63 | SR | 238 | SER | C-N-CA | -5.25 | 113.50 | 119.28 |
| 68 | SW | 161 | THR | N-CA-C | -5.19 | 105.67 | 112.41 |
| 39 | Lm | 19 | ASP | N-CA-C | -5.11 | 108.07 | 114.56 |
| 62 | SQ | 226 | GLY | N-CA-C | 5.05 | 125.16 | 113.18 |
| 59 | SN | 118 | ARG | CA-CB-CG | 5.05 | 124.20 | 114.10 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 10 | LJ | 30 | THR | Peptide |
| 16 | LP | 75 | VAL | Peptide |
| 30 | Ld | 20 | GLY | Peptide |
| 73 | Sb | 54 | ASP | 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 | LA | 68091 | 0 | 34217 | 1099 | 0 |
| 2 | LB | 2579 | 0 | 1304 | 37 | 0 |
| 3 | LC | 3353 | 0 | 1695 | 73 | 0 |
| 4 | LD | 1899 | 0 | 1957 | 68 | 0 |
| 5 | LE | 3075 | 0 | 3142 | 86 | 0 |
| 6 | LF | 2748 | 0 | 2859 | 85 | 0 |
| 7 | LG | 2351 | 0 | 2294 | 74 | 0 |
| 8 | LH | 1307 | 0 | 1377 | 35 | 0 |
| 9 | LI | 1784 | 0 | 1862 | 52 | 0 |
| 10 | LJ | 1804 | 0 | 1877 | 51 | 0 |
| 11 | LK | 1508 | 0 | 1572 | 41 | 0 |
| 12 | LL | 1764 | 0 | 1804 | 57 | 0 |
| 13 | LM | 1346 | 0 | 1370 | 50 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | LN | 1543 | 0 | 1608 | 58 | 0 |
| 15 | LO | 1053 | 0 | 1149 | 53 | 0 |
| 16 | LP | 1720 | 0 | 1779 | 55 | 0 |
| 17 | LQ | 1555 | 0 | 1659 | 44 | 0 |
| 18 | LR | 1416 | 0 | 1433 | 36 | 0 |
| 19 | LS | 1441 | 0 | 1543 | 44 | 0 |
| 20 | LT | 1515 | 0 | 1606 | 34 | 0 |
| 21 | LU | 1437 | 0 | 1475 | 36 | 0 |
| 22 | LV | 1272 | 0 | 1312 | 42 | 0 |
| 23 | LW | 796 | 0 | 812 | 27 | 0 |
| 24 | LX | 1003 | 0 | 1048 | 23 | 0 |
| 25 | LY | 528 | 0 | 546 | 19 | 0 |
| 26 | LZ | 964 | 0 | 1025 | 28 | 0 |
| 27 | La | 984 | 0 | 1075 | 35 | 0 |
| 28 | Lb | 1080 | 0 | 1122 | 28 | 0 |
| 29 | Lc | 1169 | 0 | 1211 | 49 | 0 |
| 30 | Ld | 462 | 0 | 491 | 16 | 0 |
| 31 | Le | 737 | 0 | 792 | 19 | 0 |
| 32 | Lf | 876 | 0 | 912 | 22 | 0 |
| 33 | Lg | 1017 | 0 | 1081 | 25 | 0 |
| 34 | Lh | 850 | 0 | 880 | 18 | 0 |
| 35 | Li | 880 | 0 | 945 | 35 | 0 |
| 36 | Lj | 969 | 0 | 1078 | 31 | 0 |
| 37 | Lk | 766 | 0 | 844 | 23 | 0 |
| 38 | Ll | 645 | 0 | 649 | 29 | 0 |
| 39 | Lm | 612 | 0 | 682 | 18 | 0 |
| 40 | Ln | 436 | 0 | 475 | 19 | 0 |
| 41 | Lo | 410 | 0 | 446 | 15 | 0 |
| 42 | Lp | 229 | 0 | 273 | 9 | 0 |
| 43 | Lq | 824 | 0 | 892 | 22 | 0 |
| 44 | Lr | 694 | 0 | 738 | 21 | 0 |
| 45 | S2 | 37739 | 0 | 18988 | 798 | 0 |
| 46 | SA | 1729 | 0 | 1812 | 63 | 0 |
| 47 | SB | 1605 | 0 | 1669 | 101 | 0 |
| 48 | SC | 752 | 0 | 719 | 33 | 0 |
| 49 | SD | 875 | 0 | 878 | 33 | 0 |
| 50 | SE | 916 | 0 | 941 | 46 | 0 |
| 51 | SF | 1105 | 0 | 1166 | 61 | 0 |
| 52 | SG | 948 | 0 | 990 | 44 | 0 |
| 53 | SH | 1188 | 0 | 1218 | 44 | 0 |
| 54 | SI | 1112 | 0 | 1124 | 55 | 0 |
| 55 | SJ | 797 | 0 | 863 | 43 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56 | SK | 651 | 0 | 682 | 30 | 0 |
| 57 | SL | 491 | 0 | 524 | 35 | 0 |
| 58 | SM | 442 | 0 | 432 | 12 | 0 |
| 59 | SN | 556 | 0 | 549 | 11 | 0 |
| 60 | SO | 2383 | 0 | 2332 | 96 | 0 |
| 61 | SP | 1603 | 0 | 1610 | 64 | 0 |
| 62 | SQ | 1798 | 0 | 1890 | 99 | 0 |
| 63 | SR | 1626 | 0 | 1715 | 47 | 0 |
| 64 | SS | 2056 | 0 | 2140 | 103 | 0 |
| 65 | ST | 1815 | 0 | 1894 | 72 | 0 |
| 66 | SU | 1473 | 0 | 1555 | 72 | 0 |
| 67 | SV | 1476 | 0 | 1501 | 61 | 0 |
| 68 | SW | 1479 | 0 | 1556 | 81 | 0 |
| 69 | SX | 1142 | 0 | 1209 | 28 | 0 |
| 70 | SY | 1192 | 0 | 1255 | 33 | 0 |
| 71 | SZ | 923 | 0 | 948 | 54 | 0 |
| 72 | Sa | 673 | 0 | 662 | 30 | 0 |
| 73 | Sb | 1021 | 0 | 1060 | 30 | 0 |
| 74 | Sc | 1121 | 0 | 1196 | 37 | 0 |
| 75 | Sd | 1032 | 0 | 1044 | 46 | 0 |
| 76 | Se | 765 | 0 | 814 | 20 | 0 |
| 77 | Sf | 610 | 0 | 633 | 22 | 0 |
| 78 | Sg | 451 | 0 | 494 | 20 | 0 |
| 79 | Ta | 1650 | 0 | 838 | 21 | 0 |
| 80 | Tb | 1645 | 0 | 837 | 16 | 0 |
| 81 | mR | 230 | 0 | 0 | 0 | 0 |
| All | All | 202562 | 0 | 148649 | 4350 | 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 13.

All (4350) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 45:S2:752:A:N6 | 45:S2:797:G:H1 | 1.31 | 1.26 |
| 1:LA:3233:A:N6 | 1:LA:3252:G:H1 | 1.43 | 1.15 |
| 1:LA:1645:G:N2 | 1:LA:1808:A:H62 | 1.51 | 1.07 |
| 45:S2:220:A:N6 | 45:S2:841:U:H3 | 1.53 | 1.05 |
| 45:S2:761:G:N2 | 45:S2:789:A:H62 | 1.54 | 1.04 |
| 45:S2:1673:G:H1 | 45:S2:1728:A:H2 | 1.05 | 1.01 |
| 45:S2:1179:G:H21 | 45:S2:1460:A:N6 | 1.58 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:1645:G:H21 | 1:LA:1808:A:N6 | 1.59 | 0.99 |
| 56:SK:57:TYR:HE1 | 56:SK:68:ARG:HE | 1.07 | 0.99 |
| 45:S2:821:U:H3 | 45:S2:852:C:N4 | 1.59 | 0.98 |
| 1:LA:406:G:HO2' | 3:LC:16:G:N2 | 1.61 | 0.97 |
| 45:S2:1179:G:N2 | 45:S2:1460:A:H62 | 1.62 | 0.97 |
| 45:S2:761:G:H21 | 45:S2:789:A:H62 | 0.97 | 0.96 |
| 45:S2:761:G:H21 | 45:S2:789:A:N6 | 1.62 | 0.96 |
| 3:LC:121:U:H3 | 3:LC:132:G:H1 | 1.04 | 0.96 |
| 45:S2:1219:A:H62 | 45:S2:1264:G:N2 | 1.64 | 0.96 |
| 1:LA:1119:A:N6 | 1:LA:1137:U:C2 | 2.35 | 0.95 |
| 45:S2:1047:G:N2 | 45:S2:1071:U:O4 | 1.99 | 0.95 |
| 1:LA:541:G:H1 | 1:LA:548:U:H3 | 1.12 | 0.95 |
| 45:S2:1219:A:N6 | 45:S2:1264:G:H21 | 1.66 | 0.94 |
| 60:SO:240:VAL:HA | 60:SO:256:THR:HG22 | 1.49 | 0.94 |
| 1:LA:1121:U:N3 | 1:LA:1135:A:N6 | 2.14 | 0.94 |
| 1:LA:1625:U:H3 | 1:LA:1816:G:H1 | 1.07 | 0.94 |
| 1:LA:1384:C:HO2' | 8:LH:2:THR:N | 1.65 | 0.93 |
| 13:LM:85:LYS:NZ | 13:LM:89:TYR:OH | 2.01 | 0.93 |
| 47:SB:144:GLU:HB2 | 57:SL:57:MET:HE1 | 1.49 | 0.93 |
| 45:S2:1541:G:H21 | 45:S2:1570:A:H62 | 1.06 | 0.92 |
| 71:SZ:48:VAL:HG21 | 71:SZ:53:ASP:HB2 | 1.50 | 0.92 |
| 45:S2:220:A:N6 | 45:S2:841:U:N3 | 2.17 | 0.91 |
| 54:SI:63:ARG:HG2 | 54:SI:67:MET:HE3 | 1.51 | 0.91 |
| 1:LA:406:G:O2' | 3:LC:16:G:N2 | 2.03 | 0.90 |
| 45:S2:1402:G:P | 52:SG:5:ARG:HH12 | 1.95 | 0.90 |
| 12:LL:87:LEU:HD23 | 12:LL:138:VAL:HG22 | 1.54 | 0.90 |
| 1:LA:527:U:H3 | 1:LA:563:G:H1 | 1.19 | 0.89 |
| 30:Ld:16:ALA:O | 30:Ld:20:GLY:HA3 | 1.73 | 0.89 |
| 71:SZ:29:HIS:HB2 | 71:SZ:41:ARG:HA | 1.55 | 0.88 |
| 2:LB:75:G:N2 | 2:LB:103:A:N1 | 2.21 | 0.88 |
| 45:S2:1552:U:C2 | 45:S2:1556:A:N6 | 2.41 | 0.88 |
| 54:SI:66:TYR:HB2 | 54:SI:124:ILE:HD12 | 1.53 | 0.88 |
| 1:LA:1119:A:N6 | 1:LA:1137:U:O2 | 2.06 | 0.88 |
| 45:S2:1541:G:N2 | 45:S2:1570:A:H62 | 1.71 | 0.88 |
| 1:LA:2449:G:N2 | 1:LA:2495:C:O2 | 2.07 | 0.88 |
| 5:LE:205:VAL:HG21 | 5:LE:322:ILE:HD11 | 1.55 | 0.87 |
| 45:S2:1179:G:H21 | 45:S2:1460:A:H62 | 0.89 | 0.87 |
| 45:S2:1479:A:H5'' | 54:SI:60:SER:HB2 | 1.55 | 0.87 |
| 45:S2:387:A:H2' | 45:S2:402:C:H5' | 1.56 | 0.87 |
| 28:Lb:133:LYS:O | 28:Lb:135:ARG:NH1 | 2.07 | 0.86 |
| 10:LJ:190:VAL:HG23 | 10:LJ:192:GLN:HG3 | 1.56 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1471:A:N6 | 45:S2:1538:U:N3 | 2.23 | 0.85 |
| 45:S2:1483:A:N6 | 45:S2:1524:A:N7 | 2.25 | 0.85 |
| 45:S2:1616:G:O5' | 57:SL:18:ARG:NH2 | 2.10 | 0.85 |
| 57:SL:60:GLU:HG3 | 71:SZ:61:MET:HE2 | 1.57 | 0.85 |
| 60:SO:122:ILE:HG22 | 60:SO:134:TRP:HB2 | 1.59 | 0.85 |
| 1:LA:1723:U:H1' | 1:LA:1724:C:H5 | 1.39 | 0.85 |
| 1:LA:1121:U:H3 | 1:LA:1135:A:N6 | 1.72 | 0.85 |
| 46:SA:106:LYS:HE3 | 46:SA:173:ARG:HB3 | 1.59 | 0.85 |
| 1:LA:1645:G:H21 | 1:LA:1808:A:H62 | 0.85 | 0.84 |
| 1:LA:759:G:O2' | 1:LA:769:G:N2 | 2.09 | 0.84 |
| 45:S2:868:G:H1 | 45:S2:960:U:H3 | 1.26 | 0.84 |
| 1:LA:3382:G:H21 | 32:Lf:105:GLN:HG2 | 1.42 | 0.84 |
| 1:LA:1332:C:H5'' | 9:LI:110:ARG:HD3 | 1.58 | 0.83 |
| 73:Sb:81:VAL:O | 73:Sb:122:SER:OG | 1.96 | 0.83 |
| 45:S2:821:U:H3 | 45:S2:852:C:H42 | 0.86 | 0.83 |
| 66:SU:81:LEU:O | 66:SU:85:PHE:HB2 | 1.78 | 0.83 |
| 14:LN:119:TYR:O | 14:LN:123:ILE:HG23 | 1.78 | 0.83 |
| 45:S2:1471:A:N6 | 45:S2:1538:U:C2 | 2.47 | 0.82 |
| 45:S2:1219:A:N6 | 45:S2:1264:G:N2 | 2.24 | 0.82 |
| 45:S2:1728:A:H1' | 67:SV:32:GLN:HE22 | 1.44 | 0.82 |
| 45:S2:643:G:N2 | 45:S2:691:C:O2 | 2.13 | 0.81 |
| 4:LD:27:ALA:O | 4:LD:128:ARG:NH2 | 2.11 | 0.81 |
| 1:LA:406:G:HO2' | 3:LC:16:G:H22 | 1.17 | 0.81 |
| 47:SB:209:TYR:HA | 47:SB:212:LYS:HE2 | 1.63 | 0.81 |
| 45:S2:931:C:H5' | 62:SQ:116:LYS:HB3 | 1.63 | 0.81 |
| 23:LW:99:LYS:HG3 | 23:LW:102:GLU:HG3 | 1.60 | 0.81 |
| 53:SH:101:LEU:H | 53:SH:104:ASN:HB2 | 1.43 | 0.81 |
| 1:LA:1815:A:H2' | 1:LA:1816:G:H8 | 1.45 | 0.81 |
| 47:SB:144:GLU:HB2 | 57:SL:57:MET:CE | 2.10 | 0.81 |
| 60:SO:263:PHE:CE1 | 60:SO:268:GLN:HA | 2.16 | 0.81 |
| 3:LC:97:A:O2' | 36:Lj:59:ASN:OD1 | 1.99 | 0.81 |
| 71:SZ:72:LYS:HA | 71:SZ:72:LYS:HE3 | 1.62 | 0.80 |
| 1:LA:1393:A:N6 | 1:LA:1415:C:O2 | 2.14 | 0.80 |
| 1:LA:394:G:H22 | 1:LA:397:A:H5' | 1.47 | 0.80 |
| 13:LM:118:PRO:HD3 | 53:SH:103:ASN:HD21 | 1.44 | 0.80 |
| 53:SH:101:LEU:HD23 | 53:SH:103:ASN:H | 1.46 | 0.80 |
| 52:SG:35:CYS:HA | 52:SG:38:ILE:HG22 | 1.61 | 0.80 |
| 1:LA:791:G:H5'' | 29:Lc:2:PRO:HG3 | 1.62 | 0.80 |
| 46:SA:32:GLU:OE1 | 46:SA:32:GLU:N | 2.14 | 0.79 |
| 3:LC:14:C:H4' | 18:LR:123:PRO:HG3 | 1.64 | 0.79 |
| 45:S2:1047:G:H1 | 45:S2:1071:U:H3 | 1.29 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LN:3:ILE:HG21 | 29:Lc:45:MET:HE3 | 1.64 | 0.79 |
| 63:SR:95:ARG:NH1 | 63:SR:97:ARG:HH11 | 1.80 | 0.79 |
| 45:S2:1542:G:H22 | 45:S2:1568:C:H42 | 1.31 | 0.79 |
| 45:S2:893:U:H3 | 45:S2:919:A:N6 | 1.80 | 0.79 |
| 19:LS:170:ARG:HD2 | 29:Lc:57:GLY:HA3 | 1.63 | 0.79 |
| 51:SF:41:PRO:HD2 | 51:SF:45:ARG:HB2 | 1.65 | 0.79 |
| 1:LA:2355:A:H61 | 1:LA:2982:C:H5 | 1.29 | 0.78 |
| 22:LV:108:ARG:O | 22:LV:112:ASN:ND2 | 2.16 | 0.78 |
| 64:SS:191:ARG:HH21 | 64:SS:245:LYS:HB3 | 1.47 | 0.78 |
| 56:SK:65:LEU:O | 56:SK:69:LEU:HB2 | 1.83 | 0.78 |
| 67:SV:49:ARG:O | 67:SV:52:ASN:ND2 | 2.15 | 0.78 |
| 45:S2:1543:A:H62 | 45:S2:1567:U:H3 | 1.28 | 0.78 |
| 65:ST:50:PHE:HB3 | 65:ST:111:LEU:HD22 | 1.65 | 0.78 |
| 28:Lb:89:VAL:HG12 | 28:Lb:93:LYS:HE3 | 1.64 | 0.78 |
| 45:S2:1296:A:OP1 | 61:SP:138:TYR:OH | 2.00 | 0.78 |
| 45:S2:1673:G:O6 | 45:S2:1728:A:N1 | 2.17 | 0.78 |
| 45:S2:557:G:N2 | 45:S2:586:G:O6 | 2.16 | 0.78 |
| 45:S2:1585:U:H5'' | 45:S2:1610:G:H22 | 1.49 | 0.78 |
| 6:LF:126:ILE:O | 6:LF:129:THR:OG1 | 2.01 | 0.77 |
| 54:SI:38:LYS:O | 54:SI:43:ASN:ND2 | 2.17 | 0.77 |
| 60:SO:198:ASN:HD21 | 60:SO:216:LYS:NZ | 1.82 | 0.77 |
| 21:LU:48:LEU:HD12 | 22:LV:151:LEU:HD23 | 1.66 | 0.77 |
| 80:Tb:14:A:H61 | 80:Tb:23:G:H1 | 1.29 | 0.77 |
| 1:LA:234:G:N2 | 1:LA:235:A:N7 | 2.33 | 0.77 |
| 4:LD:39:GLY:HA2 | 4:LD:93:LYS:HG3 | 1.66 | 0.77 |
| 45:S2:1503:A:N6 | 45:S2:1564:U:O2' | 2.18 | 0.77 |
| 46:SA:39:VAL:HG22 | 46:SA:48:VAL:HG22 | 1.64 | 0.77 |
| 63:SR:81:MET:HG2 | 63:SR:211:LEU:HD11 | 1.66 | 0.77 |
| 46:SA:29:LEU:HA | 46:SA:32:GLU:OE2 | 1.85 | 0.77 |
| 5:LE:10:ARG:NH2 | 5:LE:263:SER:O | 2.18 | 0.76 |
| 45:S2:930:A:N3 | 62:SQ:111:ARG:NH2 | 2.34 | 0.76 |
| 52:SG:82:ASP:O | 61:SP:84:ARG:NH2 | 2.18 | 0.76 |
| 1:LA:3048:A:H5'' | 5:LE:53:MET:HB2 | 1.67 | 0.76 |
| 47:SB:208:SER:O | 47:SB:212:LYS:HG3 | 1.86 | 0.76 |
| 64:SS:60:GLU:OE2 | 64:SS:60:GLU:N | 2.14 | 0.76 |
| 5:LE:152:LYS:HG2 | 5:LE:192:VAL:HG11 | 1.68 | 0.76 |
| 61:SP:17:LEU:HD21 | 61:SP:176:LEU:HD11 | 1.66 | 0.76 |
| 66:SU:127:GLU:HG3 | 66:SU:135:ILE:HG13 | 1.67 | 0.76 |
| 10:LJ:98:ARG:NH1 | 10:LJ:188:THR:O | 2.16 | 0.75 |
| 46:SA:103:GLU:HG3 | 46:SA:107:PHE:CZ | 2.21 | 0.75 |
| 55:SJ:58:LEU:HD12 | 55:SJ:88:LYS:HB2 | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------------|--------------------------|-------------------|
| 11:LK:93:VAL:HG22 | 41:Lo:82:LEU:HG | 1.67 | 0.75 |
| 15:LO:135:LEU:HD21 | 17:LQ:178[A]:VAL:HG22 | 1.69 | 0.75 |
| 45:S2:1531:G:H5' | 56:SK:81:ARG:HH21 | 1.51 | 0.75 |
| 1:LA:3348:C:H42 | 1:LA:3355:G:H22 | 1.32 | 0.75 |
| 4:LD:80:GLU:HG3 | 4:LD:168:VAL:HG23 | 1.68 | 0.75 |
| 45:S2:992:A:O2' | 45:S2:1785:U:O2 | 2.02 | 0.75 |
| 45:S2:1047:G:OP2 | 62:SQ:157:GLN:NE2 | 2.19 | 0.75 |
| 1:LA:511:U:H3 | 1:LA:578:G:H1 | 1.33 | 0.75 |
| 9:LI:141:TYR:HD1 | 9:LI:189:ILE:HD13 | 1.52 | 0.75 |
| 64:SS:35:PRO:HD2 | 64:SS:83:PRO:HG2 | 1.67 | 0.75 |
| 45:S2:900:A:O2' | 45:S2:916:U:O2' | 2.04 | 0.75 |
| 1:LA:521:A:H62 | 1:LA:569:A:H61 | 1.34 | 0.74 |
| 1:LA:764:C:N4 | 14:LN:176:GLU:OE2 | 2.20 | 0.74 |
| 64:SS:104:ASP:OD1 | 64:SS:108:ARG:N | 2.18 | 0.74 |
| 71:SZ:99:GLN:NE2 | 76:Se:44:ILE:O | 2.19 | 0.74 |
| 1:LA:1173:G:HO2' | 17:LQ:21[A]:SER:HG | 1.34 | 0.74 |
| 6:LF:286:VAL:HG21 | 19:LS:28:LEU:HB3 | 1.68 | 0.74 |
| 45:S2:152:U:O2 | 65:ST:4:ASN:ND2 | 2.19 | 0.74 |
| 45:S2:1673:G:N1 | 45:S2:1728:A:C2 | 2.52 | 0.74 |
| 15:LO:38:ILE:HA | 15:LO:44:VAL:HG12 | 1.69 | 0.74 |
| 66:SU:61:PHE:HB3 | 66:SU:95:GLU:HG2 | 1.70 | 0.74 |
| 1:LA:2766:U:O2' | 43:Lq:30:ALA:O | 2.05 | 0.74 |
| 67:SV:58:LEU:O | 67:SV:59:ARG:HG2 | 1.87 | 0.74 |
| 1:LA:3233:A:N1 | 1:LA:3252:G:N2 | 2.32 | 0.74 |
| 45:S2:557:G:OP1 | 78:Sg:55:ARG:NH2 | 2.21 | 0.74 |
| 23:LW:22:PRO:HB2 | 23:LW:28:PHE:HB2 | 1.70 | 0.74 |
| 45:S2:1476:C:H2' | 45:S2:1477:G:H8 | 1.52 | 0.74 |
| 64:SS:250:GLU:O | 64:SS:254:ARG:NE | 2.21 | 0.74 |
| 1:LA:2149:G:O2' | 1:LA:2188:U:OP1 | 2.04 | 0.74 |
| 1:LA:2525:C:OP1 | 4:LD:37:ARG:NH1 | 2.22 | 0.73 |
| 45:S2:148:A:N6 | 45:S2:166:C:O2 | 2.20 | 0.73 |
| 45:S2:142:G:H1 | 45:S2:173:A:N6 | 1.85 | 0.73 |
| 13:LM:30:LEU:HD11 | 13:LM:47:GLN:HG2 | 1.69 | 0.73 |
| 33:Lg:98:HIS:O | 33:Lg:125:ARG:NH2 | 2.19 | 0.73 |
| 1:LA:654:C:H2' | 1:LA:655:A:H8 | 1.53 | 0.73 |
| 1:LA:735:A:C5 | 1:LA:736:G:H1' | 2.24 | 0.73 |
| 1:LA:2968:A:N7 | 4:LD:215:ASN:ND2 | 2.35 | 0.73 |
| 27:La:22:ALA:O | 27:La:27:ARG:NH1 | 2.21 | 0.73 |
| 43:Lq:36:PHE:O | 43:Lq:41:ARG:NH1 | 2.22 | 0.73 |
| 45:S2:1228:G:O2' | 59:SN:102:VAL:HG22 | 1.89 | 0.73 |
| 56:SK:57:TYR:HE1 | 56:SK:68:ARG:NE | 1.86 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 55:SJ:23:ARG:HB3 | 55:SJ:117:VAL:HG23 | 1.70 | 0.73 |
| 45:S2:1588:G:H1 | 45:S2:1608:U:H3 | 0.81 | 0.73 |
| 1:LA:617:C:OP1 | 18:LR:173:ARG:NH2 | 2.22 | 0.73 |
| 1:LA:814:G:OP2 | 38:Ll:31:LYS:NZ | 2.20 | 0.73 |
| 1:LA:1678:A:OP1 | 23:LW:94:ARG:NH1 | 2.22 | 0.73 |
| 43:Lq:65:THR:O | 43:Lq:87:ARG:NH1 | 2.22 | 0.73 |
| 62:SQ:201:THR:HG21 | 62:SQ:207:LEU:HD22 | 1.68 | 0.72 |
| 45:S2:1789:G:OP2 | 71:SZ:132:ARG:NH2 | 2.22 | 0.72 |
| 49:SD:32:LEU:HD21 | 49:SD:102:GLY:HA3 | 1.71 | 0.72 |
| 45:S2:1542:G:H4' | 45:S2:1543:A:H5' | 1.70 | 0.72 |
| 17:LQ:12[A]:LYS:HD3 | 17:LQ:37[A]:ARG:HH21 | 1.54 | 0.72 |
| 45:S2:167:U:OP1 | 65:ST:140:ASN:ND2 | 2.22 | 0.72 |
| 46:SA:132:LYS:HZ2 | 46:SA:192:PRO:HD2 | 1.53 | 0.72 |
| 15:LO:50:LYS:HD3 | 15:LO:50:LYS:N | 2.03 | 0.72 |
| 53:SH:70:VAL:HG13 | 53:SH:73:MET:HE3 | 1.70 | 0.72 |
| 1:LA:1808:A:OP1 | 28:Lb:65:ARG:NH1 | 2.22 | 0.72 |
| 61:SP:120:LEU:HD12 | 61:SP:142:PRO:HB2 | 1.71 | 0.72 |
| 63:SR:78:ASP:HB3 | 63:SR:104:VAL:HG22 | 1.72 | 0.72 |
| 1:LA:875:A:H5'' | 1:LA:1889:U:H5'' | 1.72 | 0.72 |
| 1:LA:3032:A:O2' | 11:LK:169:ASN:OD1 | 2.08 | 0.72 |
| 45:S2:643:G:N1 | 45:S2:691:C:N3 | 2.37 | 0.72 |
| 45:S2:1647:U:H2' | 45:S2:1648:A:C8 | 2.24 | 0.72 |
| 45:S2:563:U:O2' | 78:Sg:13:LYS:NZ | 2.22 | 0.72 |
| 77:Sf:67:THR:OG1 | 77:Sf:70:LYS:O | 2.07 | 0.72 |
| 1:LA:19:U:H4' | 16:LP:138:GLN:HG3 | 1.72 | 0.72 |
| 1:LA:1039:A:O2' | 1:LA:1040:U:O2 | 2.08 | 0.72 |
| 9:LI:168:ILE:O | 9:LI:172:ASN:ND2 | 2.22 | 0.72 |
| 62:SQ:207:LEU:O | 62:SQ:210:ILE:HD11 | 1.88 | 0.72 |
| 1:LA:2176:G:OP2 | 4:LD:128:ARG:NH1 | 2.23 | 0.71 |
| 1:LA:2837:A:OP1 | 12:LL:154:ARG:NH2 | 2.22 | 0.71 |
| 2:LB:7:G:OP1 | 7:LG:33:ARG:NH1 | 2.23 | 0.71 |
| 14:LN:48:PRO:HG2 | 36:Lj:115:LYS:HE3 | 1.71 | 0.71 |
| 24:LX:54:LEU:HD21 | 24:LX:119:GLY:HA3 | 1.70 | 0.71 |
| 45:S2:614:C:OP2 | 74:Sc:5:LYS:NZ | 2.23 | 0.71 |
| 45:S2:1158:C:H42 | 45:S2:1163:A:H61 | 1.36 | 0.71 |
| 64:SS:181:VAL:HA | 64:SS:227:VAL:HA | 1.72 | 0.71 |
| 67:SV:40:ALA:O | 67:SV:59:ARG:HG3 | 1.89 | 0.71 |
| 14:LN:172:LEU:O | 14:LN:176:GLU:HG2 | 1.90 | 0.71 |
| 31:Le:53:LYS:NZ | 31:Le:57:GLU:OE2 | 2.23 | 0.71 |
| 1:LA:1793:G:H4' | 4:LD:191:LEU:HD21 | 1.70 | 0.71 |
| 1:LA:3021:G:O2' | 1:LA:3030:G:O6 | 2.08 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:58:U:O2' | 45:S2:451:A:N1 | 2.22 | 0.71 |
| 45:S2:893:U:N3 | 45:S2:919:A:N6 | 2.37 | 0.71 |
| 45:S2:1467:C:O2' | 54:SI:88:VAL:O | 2.08 | 0.71 |
| 71:SZ:40:ALA:HB2 | 71:SZ:70:LYS:HG2 | 1.72 | 0.71 |
| 45:S2:550:A:N1 | 78:Sg:57:ASN:ND2 | 2.38 | 0.71 |
| 45:S2:900:A:H2' | 45:S2:901:G:H8 | 1.55 | 0.71 |
| 60:SO:135:THR:HG22 | 60:SO:137:LYS:H | 1.54 | 0.71 |
| 1:LA:405:U:O2' | 1:LA:1394:G:N2 | 2.23 | 0.71 |
| 1:LA:522:A:H62 | 1:LA:568:A:H2 | 1.37 | 0.71 |
| 1:LA:2513:U:OP2 | 1:LA:2585:G:N2 | 2.22 | 0.71 |
| 45:S2:752:A:N1 | 45:S2:797:G:N2 | 2.32 | 0.71 |
| 47:SB:143:ARG:HG2 | 57:SL:57:MET:HE2 | 1.73 | 0.71 |
| 54:SI:66:TYR:HD1 | 54:SI:124:ILE:HG21 | 1.55 | 0.71 |
| 54:SI:68:ARG:HE | 54:SI:68:ARG:HA | 1.56 | 0.71 |
| 1:LA:2269:A:H2' | 1:LA:2270:A:C8 | 2.25 | 0.71 |
| 8:LH:75:PRO:HA | 8:LH:138:GLN:HE22 | 1.55 | 0.71 |
| 60:SO:263:PHE:CZ | 60:SO:268:GLN:HA | 2.25 | 0.71 |
| 50:SE:44:ARG:HH22 | 50:SE:83:MET:HA | 1.55 | 0.71 |
| 4:LD:104:LEU:HD11 | 4:LD:158:ILE:HD11 | 1.71 | 0.71 |
| 45:S2:894:U:H2' | 45:S2:895:G:H8 | 1.56 | 0.71 |
| 69:SX:109:VAL:HG12 | 69:SX:137:PHE:HB2 | 1.71 | 0.71 |
| 1:LA:713:G:HO2' | 1:LA:752:C:HO2' | 1.37 | 0.70 |
| 7:LG:41:LYS:HE3 | 22:LV:93:VAL:HG11 | 1.73 | 0.70 |
| 1:LA:1625:U:O4 | 1:LA:1816:G:O6 | 2.09 | 0.70 |
| 66:SU:16:LEU:O | 66:SU:20:VAL:HG23 | 1.91 | 0.70 |
| 1:LA:2702:A:N6 | 7:LG:28:THR:O | 2.25 | 0.70 |
| 45:S2:959:U:H6 | 70:SY:61:THR:HG1 | 1.38 | 0.70 |
| 45:S2:1588:G:N2 | 45:S2:1608:U:O2 | 2.23 | 0.70 |
| 55:SJ:82:TYR:HB3 | 58:SM:52:PHE:HB3 | 1.73 | 0.70 |
| 6:LF:178:LEU:HD11 | 6:LF:222:VAL:HG12 | 1.73 | 0.70 |
| 67:SV:81:VAL:HG12 | 67:SV:102:VAL:HG12 | 1.73 | 0.70 |
| 1:LA:2879:U:OP1 | 24:LX:47:ASN:ND2 | 2.24 | 0.70 |
| 47:SB:182:ALA:O | 47:SB:186:ASN:ND2 | 2.25 | 0.70 |
| 74:Sc:75:GLN:NE2 | 74:Sc:80:GLY:O | 2.25 | 0.70 |
| 45:S2:271:A:N6 | 45:S2:285:G:C2 | 2.59 | 0.70 |
| 45:S2:475:A:OP2 | 68:SW:126:ARG:NH1 | 2.23 | 0.70 |
| 62:SQ:24:PHE:CE2 | 71:SZ:70:LYS:HE3 | 2.26 | 0.70 |
| 1:LA:1663:G:H1 | 1:LA:1784:U:H3 | 1.39 | 0.70 |
| 1:LA:3151:U:H5' | 1:LA:3292:U:H1' | 1.74 | 0.70 |
| 13:LM:116:TYR:HD1 | 53:SH:103:ASN:OD1 | 1.75 | 0.70 |
| 19:LS:99:THR:O | 19:LS:119:GLY:HA3 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:139:C:H42 | 45:S2:175:G:H21 | 1.37 | 0.70 |
| 1:LA:1900:A:O2' | 1:LA:2917:G:OP1 | 2.08 | 0.70 |
| 16:LP:96:ARG:NH2 | 16:LP:104:GLU:OE1 | 2.24 | 0.70 |
| 45:S2:142:G:N1 | 45:S2:173:A:N6 | 2.40 | 0.70 |
| 1:LA:1617:G:O2' | 3:LC:126:A:N1 | 2.24 | 0.69 |
| 1:LA:2184:G:O2' | 1:LA:2313:U:OP2 | 2.08 | 0.69 |
| 4:LD:147:ARG:HG2 | 4:LD:157:VAL:HG22 | 1.74 | 0.69 |
| 11:LK:92:TYR:HB2 | 11:LK:142:ASP:HB3 | 1.72 | 0.69 |
| 1:LA:2205:G:O2' | 1:LA:2207:A:N7 | 2.25 | 0.69 |
| 50:SE:39:ALA:HA | 50:SE:42:ARG:HD3 | 1.74 | 0.69 |
| 31:Le:18:ILE:HD11 | 31:Le:81:VAL:HG13 | 1.74 | 0.69 |
| 45:S2:1601:G:OP1 | 54:SI:86:ARG:NH1 | 2.24 | 0.69 |
| 47:SB:109:LYS:O | 47:SB:113:ILE:HD12 | 1.92 | 0.69 |
| 5:LE:304:THR:HG22 | 5:LE:306:THR:H | 1.54 | 0.69 |
| 45:S2:1471:A:H2 | 45:S2:1474:G:H21 | 1.41 | 0.69 |
| 64:SS:61:VAL:O | 64:SS:65:LEU:HD12 | 1.93 | 0.69 |
| 2:LB:64:A:N7 | 12:LL:209:ASN:ND2 | 2.40 | 0.69 |
| 63:SR:101:VAL:HG22 | 63:SR:115:ILE:HG12 | 1.73 | 0.69 |
| 75:Sd:15:ASN:HD21 | 75:Sd:20:ARG:NH1 | 1.89 | 0.69 |
| 1:LA:2652:C:O2' | 1:LA:2656:A:N1 | 2.22 | 0.69 |
| 45:S2:145:A:N6 | 45:S2:168:A:OP2 | 2.26 | 0.69 |
| 45:S2:399:A:H4' | 64:SS:3:ARG:HG2 | 1.75 | 0.69 |
| 56:SK:89:ILE:O | 56:SK:90:LYS:HE2 | 1.92 | 0.69 |
| 1:LA:696:A:HO2' | 1:LA:697:U:H6 | 1.38 | 0.69 |
| 7:LG:182:GLY:HA2 | 7:LG:194:LEU:HD23 | 1.75 | 0.69 |
| 45:S2:1483:A:H5'' | 51:SF:71:GLY:HA2 | 1.74 | 0.69 |
| 45:S2:1647:U:H2' | 45:S2:1648:A:H8 | 1.57 | 0.69 |
| 79:Ta:14:A:H62 | 79:Ta:23:G:H21 | 1.37 | 0.69 |
| 1:LA:895:A:H5'' | 4:LD:183:GLY:HA2 | 1.74 | 0.69 |
| 3:LC:43:A:H62 | 38:Ll:65:ARG:HH12 | 1.39 | 0.69 |
| 45:S2:1673:G:N1 | 45:S2:1728:A:H2 | 1.88 | 0.69 |
| 47:SB:162:VAL:HG13 | 57:SL:54:LEU:HD11 | 1.73 | 0.69 |
| 50:SE:61:ARG:NH1 | 50:SE:88:GLU:OE1 | 2.25 | 0.69 |
| 53:SH:75:ASN:HB3 | 53:SH:78:HIS:HB3 | 1.75 | 0.69 |
| 61:SP:21:ASN:HB3 | 61:SP:24:LEU:HD12 | 1.74 | 0.69 |
| 2:LB:77:G:N2 | 2:LB:102:A:OP2 | 2.22 | 0.69 |
| 13:LM:131:MET:HA | 13:LM:131:MET:HE2 | 1.74 | 0.69 |
| 47:SB:92:ARG:NH2 | 47:SB:169:ASN:OD1 | 2.22 | 0.69 |
| 1:LA:654:C:H2' | 1:LA:655:A:C8 | 2.28 | 0.68 |
| 45:S2:752:A:N6 | 45:S2:797:G:N1 | 2.12 | 0.68 |
| 64:SS:250:GLU:HB3 | 64:SS:254:ARG:NH2 | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:3311:U:H4' | 5:LE:25:ILE:HG12 | 1.75 | 0.68 |
| 7:LG:41:LYS:NZ | 22:LV:32:LYS:O | 2.26 | 0.68 |
| 19:LS:122:ILE:HG23 | 19:LS:126:GLN:HB2 | 1.74 | 0.68 |
| 28:Lb:50:PRO:HD3 | 28:Lb:68:ILE:HG12 | 1.75 | 0.68 |
| 40:Ln:27:ILE:HA | 40:Ln:30:ARG:HG3 | 1.75 | 0.68 |
| 45:S2:325:G:H4' | 69:SX:83:THR:HG21 | 1.73 | 0.68 |
| 45:S2:1142:A:H5'' | 76:Se:2:PRO:HB3 | 1.74 | 0.68 |
| 45:S2:1143:A:N6 | 45:S2:1631:A:OP2 | 2.25 | 0.68 |
| 45:S2:1541:G:H21 | 45:S2:1570:A:N6 | 1.87 | 0.68 |
| 62:SQ:105:PHE:HE1 | 62:SQ:109:LYS:CG | 2.06 | 0.68 |
| 31:Le:73:GLY:N | 31:Le:76:GLU:OE1 | 2.21 | 0.68 |
| 1:LA:439:C:H1' | 1:LA:493:G:H21 | 1.58 | 0.68 |
| 45:S2:956:C:O3' | 45:S2:1047:G:N2 | 2.26 | 0.68 |
| 66:SU:170:GLN:NE2 | 66:SU:181:ILE:O | 2.26 | 0.68 |
| 75:Sd:53:ASP:HB3 | 75:Sd:96:LEU:HD21 | 1.75 | 0.68 |
| 5:LE:17:LEU:HD11 | 5:LE:233:TRP:HH2 | 1.59 | 0.68 |
| 10:LJ:226:TYR:OH | 37:Lk:46:GLU:OE2 | 2.12 | 0.68 |
| 45:S2:1677:C:OP1 | 67:SV:42:ARG:NH1 | 2.25 | 0.68 |
| 47:SB:98:MET:HE1 | 47:SB:107:LYS:HG2 | 1.75 | 0.68 |
| 50:SE:86:VAL:HG23 | 50:SE:89:MET:HE1 | 1.76 | 0.68 |
| 60:SO:134:TRP:HD1 | 60:SO:140:CYS:HA | 1.58 | 0.68 |
| 71:SZ:72:LYS:NZ | 71:SZ:77:THR:HA | 2.08 | 0.68 |
| 1:LA:104:G:H4' | 1:LA:697:U:H3 | 1.57 | 0.68 |
| 1:LA:181:U:O2' | 38:Ll:75:LYS:NZ | 2.26 | 0.68 |
| 1:LA:1217:U:O2' | 1:LA:1222:A:OP1 | 2.10 | 0.68 |
| 1:LA:3270:G:C4 | 8:LH:108:LYS:HD2 | 2.29 | 0.68 |
| 45:S2:332:U:OP1 | 67:SV:31:ARG:NE | 2.25 | 0.68 |
| 66:SU:64:VAL:HG23 | 66:SU:67:LEU:HB2 | 1.75 | 0.68 |
| 1:LA:1342:A:H2' | 1:LA:1343:G:H8 | 1.59 | 0.68 |
| 2:LB:52:G:N2 | 13:LM:9:MET:SD | 2.66 | 0.68 |
| 45:S2:473:A:OP1 | 68:SW:44:ARG:NH1 | 2.27 | 0.68 |
| 45:S2:1755:A:O2' | 45:S2:1756:A:O4' | 2.11 | 0.68 |
| 47:SB:143:ARG:CG | 57:SL:57:MET:HE2 | 2.24 | 0.68 |
| 72:Sa:21:ASN:HB3 | 73:Sb:67:GLY:HA3 | 1.76 | 0.68 |
| 1:LA:2959:C:H2' | 1:LA:2960:G:C8 | 2.29 | 0.68 |
| 53:SH:113:LEU:HD12 | 53:SH:117:LYS:HZ1 | 1.58 | 0.68 |
| 1:LA:1655:A:OP2 | 35:Li:37:LYS:NZ | 2.26 | 0.67 |
| 26:LZ:29:SER:OG | 26:LZ:31:THR:OG1 | 2.10 | 0.67 |
| 28:Lb:57:HIS:HB2 | 28:Lb:62:VAL:HG23 | 1.76 | 0.67 |
| 68:SW:127:VAL:HA | 68:SW:130:THR:HG22 | 1.75 | 0.67 |
| 69:SX:94:ILE:HD11 | 69:SX:101:GLU:OE1 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:153:U:H4' | 1:LA:158:G:H4' | 1.76 | 0.67 |
| 1:LA:2571:C:H3' | 1:LA:2572:G:H4' | 1.76 | 0.67 |
| 29:Lc:104:THR:HG21 | 29:Lc:112:ILE:HD11 | 1.75 | 0.67 |
| 66:SU:90:VAL:O | 66:SU:91:ILE:HD13 | 1.94 | 0.67 |
| 1:LA:3041:U:OP2 | 1:LA:3091:C:N4 | 2.26 | 0.67 |
| 1:LA:3091:C:O2' | 1:LA:3093:A:OP2 | 2.11 | 0.67 |
| 45:S2:438:A:H1' | 45:S2:465:G:H22 | 1.59 | 0.67 |
| 45:S2:637:C:O2 | 66:SU:114:ARG:NH2 | 2.21 | 0.67 |
| 45:S2:990:C:H5'' | 71:SZ:129:LYS:HB2 | 1.75 | 0.67 |
| 45:S2:1315:U:OP1 | 45:S2:1328:G:N2 | 2.24 | 0.67 |
| 49:SD:60:VAL:HG22 | 49:SD:122:VAL:HG12 | 1.76 | 0.67 |
| 60:SO:263:PHE:CE2 | 60:SO:265:LEU:HA | 2.29 | 0.67 |
| 63:SR:223:GLY:HA3 | 72:Sa:25:LYS:HE3 | 1.77 | 0.67 |
| 66:SU:91:ILE:HG21 | 66:SU:129:LEU:HD12 | 1.76 | 0.67 |
| 1:LA:1660:G:H2' | 1:LA:1661:G:C8 | 2.29 | 0.67 |
| 1:LA:2895:A:OP1 | 41:Lo:102:ARG:NH1 | 2.28 | 0.67 |
| 3:LC:103:G:OP2 | 3:LC:105:A:O2' | 2.12 | 0.67 |
| 6:LF:114:ASN:HB2 | 6:LF:117:GLU:HG3 | 1.77 | 0.67 |
| 6:LF:300:ARG:O | 19:LS:39:ARG:NH1 | 2.27 | 0.67 |
| 13:LM:96:PHE:HB2 | 13:LM:156:LYS:HE2 | 1.76 | 0.67 |
| 19:LS:95:GLU:N | 19:LS:95:GLU:OE2 | 2.28 | 0.67 |
| 53:SH:123:ARG:HG3 | 53:SH:133:VAL:HG21 | 1.75 | 0.67 |
| 72:Sa:25:LYS:HB2 | 72:Sa:28:ASP:HB2 | 1.76 | 0.67 |
| 1:LA:271:C:O2 | 37:Lk:82:ARG:NH2 | 2.27 | 0.67 |
| 1:LA:768:G:O2' | 14:LN:168:ARG:NH1 | 2.27 | 0.67 |
| 13:LM:106:ILE:HG12 | 13:LM:127:PHE:HE1 | 1.57 | 0.67 |
| 45:S2:1452:U:H1' | 50:SE:79:HIS:HD2 | 1.60 | 0.67 |
| 64:SS:139:VAL:HG13 | 64:SS:150:PRO:HG3 | 1.74 | 0.67 |
| 10:LJ:162:LEU:HA | 16:LP:7:LEU:HD11 | 1.77 | 0.67 |
| 45:S2:1146:G:H2' | 45:S2:1147:A:C8 | 2.30 | 0.67 |
| 50:SE:54:ALA:HA | 50:SE:57:MET:HE2 | 1.75 | 0.67 |
| 65:ST:131:LYS:O | 65:ST:160:ARG:NH2 | 2.28 | 0.67 |
| 1:LA:663:U:H2' | 1:LA:664:A:C8 | 2.30 | 0.67 |
| 1:LA:1720:U:O2' | 1:LA:1722:A:N7 | 2.25 | 0.67 |
| 1:LA:2584:G:O6 | 10:LJ:47:SER:OG | 2.12 | 0.67 |
| 45:S2:435:C:H5'' | 74:Sc:50:LYS:HE3 | 1.76 | 0.67 |
| 9:LI:39:GLU:O | 9:LI:43:ILE:HG13 | 1.95 | 0.67 |
| 22:LV:84:TYR:HB2 | 30:Ld:24:PRO:HD3 | 1.75 | 0.67 |
| 67:SV:119:GLN:N | 67:SV:119:GLN:OE1 | 2.28 | 0.67 |
| 13:LM:54:VAL:HG13 | 13:LM:57:PHE:HB2 | 1.77 | 0.67 |
| 45:S2:610:G:OP2 | 74:Sc:19:ARG:NE | 2.28 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:818:C:N4 | 45:S2:819:G:O6 | 2.28 | 0.67 |
| 45:S2:1610:G:H5' | 47:SB:107:LYS:HG3 | 1.77 | 0.67 |
| 68:SW:20:GLU:O | 68:SW:24:LEU:HG | 1.95 | 0.67 |
| 68:SW:80:LEU:HD12 | 68:SW:86:LEU:HB2 | 1.77 | 0.67 |
| 1:LA:1665:G:H1 | 1:LA:1782:U:H3 | 1.43 | 0.67 |
| 25:LY:45:ASN:HB3 | 25:LY:48:ARG:HG3 | 1.77 | 0.67 |
| 45:S2:397:A:H4' | 67:SV:50:GLY:HA2 | 1.77 | 0.67 |
| 45:S2:871:G:H2' | 45:S2:872:G:C8 | 2.30 | 0.67 |
| 45:S2:1552:U:C2 | 45:S2:1556:A:C6 | 2.83 | 0.67 |
| 64:SS:195:ILE:HG22 | 64:SS:210:ILE:HD13 | 1.77 | 0.67 |
| 68:SW:75:ALA:O | 68:SW:79:ARG:HG3 | 1.94 | 0.67 |
| 6:LF:35:VAL:HG21 | 6:LF:244:LEU:HD21 | 1.77 | 0.66 |
| 45:S2:570:A:N6 | 74:Sc:116:ASP:OD1 | 2.28 | 0.66 |
| 65:ST:51:LYS:HB3 | 65:ST:112:VAL:HG13 | 1.77 | 0.66 |
| 68:SW:123:HIS:NE2 | 78:Sg:37:ARG:HG3 | 2.10 | 0.66 |
| 1:LA:1202:A:H2' | 1:LA:1203:A:C8 | 2.29 | 0.66 |
| 49:SD:73:LYS:HZ3 | 59:SN:109:ASP:H | 1.41 | 0.66 |
| 50:SE:96:ILE:HD11 | 50:SE:116:LEU:HG | 1.77 | 0.66 |
| 63:SR:45:VAL:HG21 | 63:SR:68:ILE:HG23 | 1.78 | 0.66 |
| 73:Sb:15:ASN:ND2 | 73:Sb:72:CYS:O | 2.28 | 0.66 |
| 1:LA:394:G:N1 | 1:LA:397:A:OP2 | 2.23 | 0.66 |
| 1:LA:2699:G:O2' | 1:LA:2704:A:N1 | 2.25 | 0.66 |
| 1:LA:2863:A:H5'' | 12:LL:114:GLY:HA2 | 1.78 | 0.66 |
| 21:LU:132:THR:HG22 | 21:LU:144:LEU:HD13 | 1.76 | 0.66 |
| 29:Lc:38:GLN:O | 29:Lc:42:ARG:NH1 | 2.29 | 0.66 |
| 47:SB:42:LEU:HD12 | 47:SB:43:PHE:H | 1.61 | 0.66 |
| 80:Tb:26:C:H2' | 80:Tb:27:G:H8 | 1.60 | 0.66 |
| 25:LY:6:ASP:OD2 | 25:LY:32:GLN:N | 2.21 | 0.66 |
| 26:LZ:50:ALA:HB1 | 36:Lj:66:VAL:HG11 | 1.76 | 0.66 |
| 61:SP:8:ASP:OD1 | 61:SP:8:ASP:N | 2.22 | 0.66 |
| 15:LO:48:GLY:HA3 | 15:LO:53:VAL:HB | 1.76 | 0.66 |
| 45:S2:932:U:O2 | 76:Se:32:LYS:NZ | 2.28 | 0.66 |
| 51:SF:31:VAL:HG12 | 51:SF:67:VAL:HB | 1.76 | 0.66 |
| 62:SQ:27:LYS:NZ | 62:SQ:49:ASN:OD1 | 2.27 | 0.66 |
| 64:SS:79:ASP:HB3 | 64:SS:82:TYR:HB2 | 1.77 | 0.66 |
| 1:LA:993:G:N2 | 1:LA:994:U:O4 | 2.22 | 0.66 |
| 1:LA:1119:A:N6 | 1:LA:1137:U:N3 | 2.38 | 0.66 |
| 54:SI:77:ASN:OD1 | 54:SI:101:ASN:ND2 | 2.25 | 0.66 |
| 65:ST:74:LYS:HE3 | 65:ST:96:SER:HB2 | 1.77 | 0.66 |
| 1:LA:1342:A:H2' | 1:LA:1343:G:C8 | 2.30 | 0.66 |
| 11:LK:41:ILE:HG21 | 11:LK:71:VAL:HG11 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1065:A:O2' | 62:SQ:146:GLN:NE2 | 2.28 | 0.66 |
| 66:SU:115:SER:OG | 66:SU:116:ARG:NH1 | 2.29 | 0.66 |
| 39:Lm:7:ASP:HB3 | 39:Lm:10:GLN:HB2 | 1.78 | 0.66 |
| 45:S2:299:A:OP1 | 64:SS:30:ARG:NH2 | 2.27 | 0.66 |
| 45:S2:1164:G:H2' | 45:S2:1165:G:H8 | 1.61 | 0.66 |
| 45:S2:1458:G:H21 | 50:SE:126:VAL:HG11 | 1.61 | 0.66 |
| 47:SB:173:ALA:O | 47:SB:177:ILE:HG13 | 1.95 | 0.66 |
| 64:SS:185:GLY:HA3 | 64:SS:224:ASN:ND2 | 2.10 | 0.66 |
| 1:LA:181:U:H4' | 38:Ll:75:LYS:HD3 | 1.77 | 0.66 |
| 32:Lf:44:MET:HE3 | 32:Lf:75:ILE:HB | 1.77 | 0.66 |
| 60:SO:179:LYS:HB3 | 60:SO:181:TRP:HE1 | 1.61 | 0.66 |
| 67:SV:69:SER:OG | 69:SX:24:LYS:NZ | 2.28 | 0.66 |
| 1:LA:2836:A:O2' | 1:LA:2849:G:N2 | 2.29 | 0.65 |
| 45:S2:1047:G:C5 | 45:S2:1048:G:H1' | 2.31 | 0.65 |
| 45:S2:1674:C:OP1 | 65:ST:92:ARG:NH1 | 2.26 | 0.65 |
| 46:SA:168:ILE:HD12 | 46:SA:187:LYS:HE2 | 1.76 | 0.65 |
| 10:LJ:169:LEU:HA | 37:Lk:43:LEU:HD11 | 1.78 | 0.65 |
| 56:SK:77:ARG:HB3 | 56:SK:81:ARG:HH12 | 1.61 | 0.65 |
| 1:LA:3296:U:H2' | 1:LA:3297:C:H6 | 1.61 | 0.65 |
| 45:S2:900:A:H2' | 45:S2:901:G:C8 | 2.30 | 0.65 |
| 45:S2:1346:A:O4' | 45:S2:1371:A:N6 | 2.29 | 0.65 |
| 65:ST:78:THR:HG23 | 65:ST:92:ARG:HD2 | 1.78 | 0.65 |
| 3:LC:154:C:H5'' | 10:LJ:181:LYS:HG2 | 1.79 | 0.65 |
| 12:LL:72:ALA:HB2 | 12:LL:155:ALA:HB2 | 1.79 | 0.65 |
| 45:S2:263:C:O2' | 45:S2:291:G:O2' | 2.13 | 0.65 |
| 45:S2:1303:U:O2' | 45:S2:1322:A:OP2 | 2.15 | 0.65 |
| 62:SQ:2:ALA:N | 71:SZ:49:LYS:O | 2.29 | 0.65 |
| 64:SS:129:VAL:HG13 | 64:SS:139:VAL:HG12 | 1.78 | 0.65 |
| 69:SX:78:THR:HA | 69:SX:84:ILE:HG22 | 1.79 | 0.65 |
| 71:SZ:20:TYR:HB3 | 71:SZ:27:PHE:HB2 | 1.79 | 0.65 |
| 1:LA:1723:U:H1' | 1:LA:1724:C:C5 | 2.28 | 0.65 |
| 38:Ll:25:ARG:HH12 | 40:Ln:50:ASN:HB3 | 1.60 | 0.65 |
| 45:S2:142:G:N2 | 45:S2:173:A:N1 | 2.45 | 0.65 |
| 45:S2:448:C:OP1 | 64:SS:49:ARG:NH2 | 2.25 | 0.65 |
| 68:SW:107:ARG:NH2 | 68:SW:150:LEU:HD23 | 2.12 | 0.65 |
| 1:LA:68:C:OP2 | 1:LA:301:G:N2 | 2.30 | 0.65 |
| 10:LJ:74:THR:O | 10:LJ:77:GLN:NE2 | 2.29 | 0.65 |
| 36:Lj:27:GLU:OE2 | 36:Lj:43:LYS:NZ | 2.30 | 0.65 |
| 45:S2:1085:G:N2 | 45:S2:1088:A:OP2 | 2.27 | 0.65 |
| 1:LA:1287:U:H2' | 1:LA:1288:G:C8 | 2.31 | 0.65 |
| 7:LG:85:ARG:NH2 | 7:LG:250:ASP:OD2 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:LT:136:ARG:O | 20:LT:140:GLU:HG3 | 1.97 | 0.65 |
| 34:Lh:14:LEU:HD11 | 34:Lh:31:LYS:HB3 | 1.78 | 0.65 |
| 45:S2:15:U:O2' | 45:S2:620:A:N6 | 2.30 | 0.65 |
| 68:SW:107:ARG:HH21 | 68:SW:150:LEU:HD23 | 1.61 | 0.65 |
| 45:S2:1215:C:N4 | 45:S2:1446:A:OP2 | 2.28 | 0.65 |
| 45:S2:1679:G:N2 | 45:S2:1722:A:C6 | 2.65 | 0.65 |
| 64:SS:80:THR:HG23 | 64:SS:81:THR:HG23 | 1.80 | 0.65 |
| 1:LA:876:C:O2' | 1:LA:879:G:O2' | 2.15 | 0.64 |
| 1:LA:2286:C:OP1 | 79:Ta:74:A:N6 | 2.29 | 0.64 |
| 13:LM:118:PRO:HD3 | 53:SH:103:ASN:ND2 | 2.12 | 0.64 |
| 55:SJ:69:LYS:HE2 | 55:SJ:80:GLU:HB3 | 1.78 | 0.64 |
| 60:SO:169:ILE:HD12 | 60:SO:181:TRP:CE3 | 2.32 | 0.64 |
| 71:SZ:92:LYS:HD2 | 71:SZ:121:VAL:HG22 | 1.79 | 0.64 |
| 1:LA:506:U:H2' | 1:LA:507:U:C6 | 2.32 | 0.64 |
| 1:LA:2795:G:N7 | 43:Lq:63:LYS:NZ | 2.41 | 0.64 |
| 10:LJ:74:THR:HG22 | 10:LJ:164:VAL:HG22 | 1.79 | 0.64 |
| 23:LW:18:ASP:HB3 | 23:LW:104:ARG:HB2 | 1.78 | 0.64 |
| 66:SU:63:PRO:HB2 | 66:SU:65:PRO:HD3 | 1.79 | 0.64 |
| 66:SU:64:VAL:HB | 66:SU:94:ALA:HB1 | 1.79 | 0.64 |
| 23:LW:99:LYS:HE3 | 23:LW:102:GLU:HG3 | 1.79 | 0.64 |
| 45:S2:424:C:O2' | 45:S2:426:G:OP1 | 2.12 | 0.64 |
| 45:S2:1383:G:OP1 | 55:SJ:89:ARG:NH2 | 2.31 | 0.64 |
| 47:SB:46:TRP:CD1 | 47:SB:129:PRO:HG2 | 2.32 | 0.64 |
| 18:LR:10:ASN:HD22 | 18:LR:13:LYS:HE2 | 1.61 | 0.64 |
| 22:LV:41:ASP:OD1 | 22:LV:61:THR:OG1 | 2.16 | 0.64 |
| 41:Lo:109:ASN:ND2 | 41:Lo:117:HIS:O | 2.30 | 0.64 |
| 61:SP:117:GLU:OE1 | 63:SR:40:LYS:HG3 | 1.97 | 0.64 |
| 63:SR:80:VAL:HG11 | 63:SR:125:ILE:HD12 | 1.79 | 0.64 |
| 67:SV:77:ARG:HG2 | 67:SV:77:ARG:HH11 | 1.62 | 0.64 |
| 68:SW:94:ASP:OD1 | 68:SW:95:TYR:N | 2.30 | 0.64 |
| 1:LA:2763:C:H42 | 80:Tb:77:A:H61 | 1.46 | 0.64 |
| 3:LC:62:C:OP1 | 36:Lj:48:ARG:NH2 | 2.29 | 0.64 |
| 60:SO:169:ILE:HG23 | 60:SO:183:LEU:HD22 | 1.80 | 0.64 |
| 1:LA:936:G:N2 | 1:LA:960:C:OP1 | 2.31 | 0.64 |
| 1:LA:1237:C:O2' | 1:LA:1238:C:OP1 | 2.16 | 0.64 |
| 1:LA:1824:G:H5'' | 39:Lm:48:SER:HB3 | 1.79 | 0.64 |
| 12:LL:102:MET:N | 12:LL:102:MET:SD | 2.70 | 0.64 |
| 36:Lj:58:ILE:HG22 | 36:Lj:62:GLN:NE2 | 2.11 | 0.64 |
| 44:Lr:46:THR:OG1 | 44:Lr:57:CYS:SG | 2.56 | 0.64 |
| 6:LF:187:LEU:HD22 | 6:LF:193:LYS:HD3 | 1.78 | 0.64 |
| 7:LG:83:LEU:HB3 | 7:LG:88:ILE:HB | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1241:G:OP1 | 50:SE:79:HIS:ND1 | 2.31 | 0.64 |
| 47:SB:134:VAL:O | 47:SB:138:THR:HG23 | 1.98 | 0.64 |
| 1:LA:594:G:H1 | 1:LA:608:G:H5'' | 1.63 | 0.64 |
| 1:LA:2405:C:H2' | 1:LA:2406:C:C6 | 2.33 | 0.64 |
| 20:LT:109:TYR:HB3 | 20:LT:115:ILE:HG12 | 1.80 | 0.64 |
| 26:LZ:96:LYS:HE2 | 26:LZ:107:VAL:HG22 | 1.80 | 0.64 |
| 31:Le:24:THR:HG23 | 31:Le:93:LEU:HD11 | 1.79 | 0.64 |
| 45:S2:1274:C:N4 | 79:Ta:35:A:N3 | 2.46 | 0.64 |
| 62:SQ:201:THR:HG21 | 62:SQ:207:LEU:HD13 | 1.79 | 0.64 |
| 63:SR:83:ILE:HD11 | 63:SR:125:ILE:HD11 | 1.80 | 0.64 |
| 67:SV:57:ALA:HB2 | 67:SV:177:GLY:HA2 | 1.79 | 0.64 |
| 1:LA:2536:U:O5' | 62:SQ:227:ALA:N | 2.31 | 0.64 |
| 4:LD:118:GLU:OE2 | 4:LD:156:LYS:NZ | 2.30 | 0.64 |
| 5:LE:29:VAL:HG22 | 5:LE:218:ILE:HD13 | 1.80 | 0.64 |
| 9:LI:239:LEU:O | 9:LI:243:MET:HG3 | 1.97 | 0.64 |
| 45:S2:761:G:H5'' | 68:SW:79:ARG:NH1 | 2.13 | 0.64 |
| 6:LF:129:THR:HG22 | 6:LF:246:ARG:O | 1.98 | 0.64 |
| 64:SS:87:MET:HE3 | 64:SS:123:LEU:HB2 | 1.79 | 0.64 |
| 64:SS:194:THR:OG1 | 64:SS:231:GLN:NE2 | 2.26 | 0.64 |
| 1:LA:3071:C:H2' | 1:LA:3072:A:O4' | 1.97 | 0.63 |
| 29:Lc:139:ARG:HH21 | 29:Lc:145:VAL:HG12 | 1.63 | 0.63 |
| 46:SA:45:LYS:NZ | 46:SA:82:GLY:O | 2.28 | 0.63 |
| 57:SL:13:ILE:HD13 | 57:SL:31:GLU:HB2 | 1.80 | 0.63 |
| 11:LK:113:GLU:OE1 | 11:LK:115:ARG:NH1 | 2.32 | 0.63 |
| 45:S2:405:C:O2' | 65:ST:92:ARG:O | 2.16 | 0.63 |
| 1:LA:2835:C:H5 | 1:LA:2851:C:H42 | 1.44 | 0.63 |
| 9:LI:118:LYS:HG3 | 9:LI:191:VAL:HG11 | 1.81 | 0.63 |
| 14:LN:105:ASN:ND2 | 14:LN:107:GLU:OE2 | 2.31 | 0.63 |
| 28:Lb:17:ARG:NH2 | 28:Lb:18:TYR:OH | 2.31 | 0.63 |
| 45:S2:422:G:H2' | 45:S2:423:G:H8 | 1.64 | 0.63 |
| 45:S2:1523:G:OP1 | 45:S2:1523:G:N2 | 2.30 | 0.63 |
| 46:SA:142:LEU:HD13 | 46:SA:150:MET:HE3 | 1.79 | 0.63 |
| 68:SW:70:LEU:O | 68:SW:74:ASN:ND2 | 2.29 | 0.63 |
| 1:LA:590:G:O2' | 8:LH:17:ALA:O | 2.16 | 0.63 |
| 1:LA:1221:G:N2 | 1:LA:1284:G:O2' | 2.32 | 0.63 |
| 1:LA:1777:G:O2' | 1:LA:1779:G:OP2 | 2.17 | 0.63 |
| 1:LA:1866:A:C2 | 1:LA:2118:A:H4' | 2.33 | 0.63 |
| 2:LB:112:G:H2' | 2:LB:113:C:C6 | 2.34 | 0.63 |
| 5:LE:85:VAL:HG22 | 5:LE:202:THR:HG22 | 1.79 | 0.63 |
| 23:LW:58:GLU:HG2 | 23:LW:60:GLY:H | 1.64 | 0.63 |
| 27:La:87:LYS:HB2 | 27:La:97:ILE:HD11 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 45:S2:1144:U:HO2' | 45:S2:1301:U:HO2' | 1.45 | 0.63 |
| 60:SO:252:LEU:HG | 60:SO:263:PHE:HB3 | 1.80 | 0.63 |
| 74:Sc:56:LYS:HG2 | 74:Sc:70:LYS:HE2 | 1.80 | 0.63 |
| 45:S2:1532:U:O2' | 53:SH:27:LYS:NZ | 2.32 | 0.63 |
| 46:SA:191:ASP:HB2 | 46:SA:194:LYS:HB2 | 1.81 | 0.63 |
| 47:SB:44:ASN:HB2 | 47:SB:45:LYS:HD3 | 1.81 | 0.63 |
| 54:SI:57:ARG:O | 54:SI:61:VAL:HG23 | 1.99 | 0.63 |
| 60:SO:214:ALA:HB1 | 60:SO:240:VAL:HG11 | 1.81 | 0.63 |
| 1:LA:238:A:H62 | 1:LA:239:G:H21 | 1.45 | 0.63 |
| 1:LA:2852:A:H5' | 12:LL:63:GLU:HB3 | 1.79 | 0.63 |
| 45:S2:304:U:OP1 | 69:SX:136:ARG:NE | 2.27 | 0.63 |
| 1:LA:2893:C:H2' | 1:LA:2894:G:H8 | 1.62 | 0.63 |
| 45:S2:16:G:H2' | 45:S2:17:C:C6 | 2.34 | 0.63 |
| 45:S2:701:U:O4 | 45:S2:732:G:N1 | 2.32 | 0.63 |
| 45:S2:1204:A:N6 | 58:SM:14:TYR:O | 2.32 | 0.63 |
| 45:S2:1218:G:H5'' | 45:S2:1219:A:H5' | 1.81 | 0.63 |
| 1:LA:899:G:H1' | 1:LA:1588:A:N6 | 2.13 | 0.63 |
| 17:LQ:12[A]:LYS:HD2 | 17:LQ:40[A]:GLU:HG2 | 1.80 | 0.63 |
| 27:La:116:LYS:O | 27:La:120:GLN:HG2 | 1.99 | 0.63 |
| 36:Lj:58:ILE:HG22 | 36:Lj:62:GLN:HE22 | 1.63 | 0.63 |
| 45:S2:924:A:H2' | 45:S2:925:G:C8 | 2.34 | 0.63 |
| 60:SO:111:MET:HE1 | 60:SO:127:ARG:HB2 | 1.81 | 0.63 |
| 1:LA:110:G:OP2 | 14:LN:73:ARG:NH1 | 2.23 | 0.62 |
| 1:LA:1387:U:O2' | 33:Lg:99:ASN:HB3 | 1.98 | 0.62 |
| 14:LN:92:THR:OG1 | 36:Lj:112:PRO:O | 2.15 | 0.62 |
| 45:S2:1034:C:HO2' | 73:Sb:2:THR:N | 1.97 | 0.62 |
| 46:SA:105:MET:HE1 | 46:SA:119:ALA:HA | 1.80 | 0.62 |
| 51:SF:127:LYS:NZ | 51:SF:131:GLY:O | 2.27 | 0.62 |
| 60:SO:218:GLY:HA2 | 60:SO:240:VAL:HG12 | 1.81 | 0.62 |
| 64:SS:197:HIS:CE1 | 64:SS:209:HIS:HD2 | 2.17 | 0.62 |
| 65:ST:67:VAL:HG13 | 65:ST:99:GLY:HA2 | 1.81 | 0.62 |
| 1:LA:1695:A:H2' | 1:LA:1696:A:C8 | 2.34 | 0.62 |
| 5:LE:102:LEU:HD21 | 5:LE:155:ALA:HB2 | 1.81 | 0.62 |
| 32:Lf:54:GLU:CD | 32:Lf:54:GLU:H | 2.07 | 0.62 |
| 45:S2:1450:U:O2' | 58:SM:6:VAL:O | 2.17 | 0.62 |
| 60:SO:180:ALA:HB3 | 60:SO:190:ALA:HB3 | 1.81 | 0.62 |
| 1:LA:618:A:OP1 | 18:LR:167:ARG:NH1 | 2.32 | 0.62 |
| 1:LA:964:A:H2 | 29:Lc:43:ILE:HD12 | 1.64 | 0.62 |
| 28:Lb:42:LEU:HD22 | 28:Lb:101:PHE:CE1 | 2.33 | 0.62 |
| 45:S2:615:A:O2' | 45:S2:621:A:N1 | 2.31 | 0.62 |
| 64:SS:45:ILE:HD12 | 64:SS:61:VAL:HG21 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:Sa:71:ARG:O | 72:Sa:75:ASN:ND2 | 2.33 | 0.62 |
| 3:LC:58:G:O6 | 38:Ll:63:ARG:NH1 | 2.33 | 0.62 |
| 4:LD:112:ILE:HG13 | 44:Lr:79:VAL:HG22 | 1.82 | 0.62 |
| 36:Lj:12:LYS:NZ | 36:Lj:20:GLN:OE1 | 2.31 | 0.62 |
| 45:S2:284:G:O6 | 65:ST:188:ARG:NH2 | 2.32 | 0.62 |
| 45:S2:873:U:O2' | 45:S2:1047:G:OP1 | 2.13 | 0.62 |
| 45:S2:967:A:OP2 | 70:SY:124:ARG:NH2 | 2.32 | 0.62 |
| 45:S2:1389:C:H6 | 52:SG:28:PHE:CE2 | 2.18 | 0.62 |
| 64:SS:250:GLU:C | 64:SS:254:ARG:HE | 2.07 | 0.62 |
| 1:LA:958:C:H41 | 1:LA:2800:A:H2' | 1.64 | 0.62 |
| 21:LU:44:PHE:O | 21:LU:48:LEU:HG | 1.99 | 0.62 |
| 45:S2:141:U:H5'' | 65:ST:179:VAL:HG21 | 1.80 | 0.62 |
| 45:S2:1488:G:O2' | 45:S2:1494:C:O2 | 2.13 | 0.62 |
| 45:S2:1609:U:OP2 | 51:SF:14:LYS:NZ | 2.25 | 0.62 |
| 47:SB:90:ILE:HG23 | 47:SB:114:ILE:HD11 | 1.80 | 0.62 |
| 66:SU:150:GLN:HB3 | 66:SU:181:ILE:HG22 | 1.79 | 0.62 |
| 1:LA:1476:A:OP1 | 1:LA:3074:G:O2' | 2.15 | 0.62 |
| 1:LA:2556:A:OP1 | 4:LD:69:TYR:OH | 2.15 | 0.62 |
| 1:LA:3207:G:H4' | 1:LA:3208:A:H5'' | 1.82 | 0.62 |
| 27:La:81:GLN:NE2 | 27:La:98:ASN:OD1 | 2.28 | 0.62 |
| 45:S2:30:G:H2' | 45:S2:31:C:C6 | 2.35 | 0.62 |
| 45:S2:874:C:H2' | 45:S2:875:G:C8 | 2.35 | 0.62 |
| 52:SG:50:ILE:O | 52:SG:54:THR:OG1 | 2.16 | 0.62 |
| 62:SQ:143:THR:HG21 | 62:SQ:156:ALA:HB2 | 1.80 | 0.62 |
| 50:SE:44:ARG:HH12 | 50:SE:84:ILE:H | 1.48 | 0.62 |
| 65:ST:64:LYS:NZ | 65:ST:83:CYS:SG | 2.67 | 0.62 |
| 65:ST:115:LYS:NZ | 65:ST:116:LYS:O | 2.33 | 0.62 |
| 68:SW:66:ASP:HB3 | 68:SW:69:ARG:HB3 | 1.80 | 0.62 |
| 1:LA:798:G:O2' | 14:LN:18:TRP:NE1 | 2.30 | 0.62 |
| 8:LH:69:PHE:N | 8:LH:142:ASP:OD2 | 2.33 | 0.62 |
| 16:LP:5:LYS:NZ | 16:LP:9:GLU:OE1 | 2.33 | 0.62 |
| 28:Lb:102:GLU:HG2 | 28:Lb:103:GLN:NE2 | 2.14 | 0.62 |
| 45:S2:840:U:H2' | 45:S2:841:U:H5 | 1.64 | 0.62 |
| 54:SI:114:VAL:HG22 | 54:SI:124:ILE:HA | 1.82 | 0.62 |
| 60:SO:111:MET:CE | 60:SO:127:ARG:HB2 | 2.30 | 0.62 |
| 1:LA:655:A:H2' | 1:LA:656:A:C8 | 2.35 | 0.62 |
| 4:LD:3:ARG:HB2 | 4:LD:207:VAL:HG22 | 1.80 | 0.62 |
| 45:S2:567:A:OP2 | 74:Sc:69:ARG:NH2 | 2.33 | 0.62 |
| 62:SQ:23:PRO:HB3 | 62:SQ:26:ARG:HH22 | 1.64 | 0.62 |
| 64:SS:68:ARG:HG3 | 64:SS:76:VAL:HG11 | 1.80 | 0.62 |
| 65:ST:32:ILE:HD13 | 65:ST:52:ILE:HG22 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 65:ST:199:GLN:OE1 | 65:ST:202:ARG:NH1 | 2.33 | 0.62 |
| 30:Ld:16:ALA:O | 30:Ld:20:GLY:CA | 2.47 | 0.62 |
| 49:SD:32:LEU:HD11 | 49:SD:102:GLY:H | 1.63 | 0.62 |
| 61:SP:139:VAL:HG23 | 61:SP:141:ILE:HG12 | 1.82 | 0.62 |
| 1:LA:1833:U:OP2 | 40:Ln:10:LYS:NZ | 2.32 | 0.61 |
| 4:LD:135:ILE:HB | 4:LD:149:ARG:HB3 | 1.82 | 0.61 |
| 45:S2:611:U:O2' | 69:SX:99:ARG:NH2 | 2.33 | 0.61 |
| 47:SB:95:ASN:O | 47:SB:98:MET:HG2 | 2.00 | 0.61 |
| 64:SS:71:LYS:HA | 64:SS:76:VAL:HA | 1.80 | 0.61 |
| 1:LA:1393:A:H4' | 1:LA:1419:C:H4' | 1.80 | 0.61 |
| 8:LH:42:LEU:O | 8:LH:49:GLY:N | 2.26 | 0.61 |
| 17:LQ:121[A]:PRO:HA | 17:LQ:124[A]:LEU:HD12 | 1.82 | 0.61 |
| 34:Lh:12:LYS:HB2 | 34:Lh:31:LYS:HG2 | 1.81 | 0.61 |
| 45:S2:127:G:H5' | 65:ST:194:LYS:HE2 | 1.81 | 0.61 |
| 45:S2:1027:A:OP1 | 45:S2:1789:G:O2' | 2.15 | 0.61 |
| 56:SK:89:ILE:HA | 56:SK:103:ARG:HA | 1.81 | 0.61 |
| 1:LA:1716:U:H2' | 1:LA:1717:G:C8 | 2.35 | 0.61 |
| 13:LM:60:ARG:HH21 | 43:Lq:104:LEU:H | 1.47 | 0.61 |
| 45:S2:837:G:H2' | 45:S2:838:G:C8 | 2.35 | 0.61 |
| 55:SJ:26:LEU:HB3 | 55:SJ:114:VAL:HG22 | 1.82 | 0.61 |
| 1:LA:648:A:OP2 | 1:LA:2867:U:O2' | 2.18 | 0.61 |
| 1:LA:3213:U:H3 | 15:LO:124:ARG:NH2 | 1.97 | 0.61 |
| 5:LE:166:ILE:HG12 | 5:LE:173:GLN:HB3 | 1.81 | 0.61 |
| 15:LO:40:ASP:OD1 | 15:LO:41:GLN:N | 2.31 | 0.61 |
| 45:S2:1551:U:OP2 | 50:SE:43:ARG:NH1 | 2.34 | 0.61 |
| 60:SO:169:ILE:HG12 | 60:SO:183:LEU:HD22 | 1.82 | 0.61 |
| 74:Sc:34:LEU:O | 74:Sc:39:LYS:NZ | 2.33 | 0.61 |
| 1:LA:361:A:O3' | 38:Ll:45:ARG:NH2 | 2.32 | 0.61 |
| 1:LA:1595:C:H2' | 1:LA:1596:C:C6 | 2.35 | 0.61 |
| 12:LL:171:TRP:O | 12:LL:174:THR:OG1 | 2.19 | 0.61 |
| 45:S2:298:C:H3' | 45:S2:299:A:H5'' | 1.82 | 0.61 |
| 56:SK:54:VAL:HG23 | 56:SK:55:PRO:HD3 | 1.81 | 0.61 |
| 60:SO:89:LEU:HD13 | 60:SO:113:VAL:HG21 | 1.83 | 0.61 |
| 67:SV:83:TYR:HB3 | 67:SV:101:ILE:HD12 | 1.83 | 0.61 |
| 71:SZ:28:VAL:HG22 | 71:SZ:67:VAL:HG11 | 1.82 | 0.61 |
| 31:Le:25:LEU:HD21 | 31:Le:81:VAL:HG11 | 1.80 | 0.61 |
| 35:Li:15:THR:HG22 | 35:Li:17:SER:H | 1.64 | 0.61 |
| 47:SB:209:TYR:HA | 47:SB:212:LYS:CE | 2.30 | 0.61 |
| 56:SK:77:ARG:HB3 | 56:SK:81:ARG:NH1 | 2.14 | 0.61 |
| 63:SR:180:ALA:HB1 | 63:SR:184:VAL:HG13 | 1.83 | 0.61 |
| 80:Tb:10:G:OP1 | 80:Tb:46:G:O2' | 2.17 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 5:LE:215:ILE:HD12 | 5:LE:338:LEU:HB3 | 1.81 | 0.61 |
| 17:LQ:74[A]:ARG:O | 17:LQ:142[A]:SER:OG | 2.18 | 0.61 |
| 27:La:55:GLU:HB2 | 27:La:108:LYS:HB3 | 1.83 | 0.61 |
| 45:S2:752:A:H61 | 45:S2:797:G:H1 | 0.66 | 0.61 |
| 1:LA:2114:G:H22 | 1:LA:2119:A:H1' | 1.65 | 0.61 |
| 5:LE:291:GLU:HB3 | 5:LE:302:LYS:HE3 | 1.82 | 0.61 |
| 6:LF:234:ASN:HB3 | 6:LF:237:GLN:OE1 | 2.00 | 0.61 |
| 46:SA:40:ARG:HB3 | 46:SA:47:GLU:HB3 | 1.81 | 0.61 |
| 1:LA:1470:U:OP1 | 20:LT:5:ARG:NH1 | 2.34 | 0.61 |
| 1:LA:1810:G:O2' | 1:LA:1811:G:O4' | 2.13 | 0.61 |
| 1:LA:3382:G:N2 | 32:Lf:105:GLN:HG2 | 2.15 | 0.61 |
| 2:LB:119:U:OP2 | 7:LG:258:LYS:NZ | 2.34 | 0.61 |
| 13:LM:118:PRO:CD | 53:SH:103:ASN:HD21 | 2.12 | 0.61 |
| 45:S2:1420:C:OP1 | 55:SJ:69:LYS:NZ | 2.33 | 0.61 |
| 61:SP:134:LYS:O | 61:SP:137:SER:OG | 2.19 | 0.61 |
| 1:LA:2495:C:H2' | 1:LA:2496:U:H5 | 1.65 | 0.61 |
| 45:S2:14:C:O5' | 63:SR:164:SER:OG | 2.16 | 0.61 |
| 60:SO:200:ASN:H | 60:SO:215:GLY:HA2 | 1.65 | 0.61 |
| 61:SP:63:ILE:HG12 | 72:Sa:36:VAL:HG22 | 1.82 | 0.61 |
| 14:LN:74:GLY:O | 14:LN:101:ARG:NH1 | 2.34 | 0.60 |
| 45:S2:333:A:OP1 | 67:SV:31:ARG:NH2 | 2.34 | 0.60 |
| 47:SB:130:ILE:O | 47:SB:134:VAL:HG13 | 2.01 | 0.60 |
| 50:SE:123:TYR:OH | 53:SH:122:HIS:NE2 | 2.28 | 0.60 |
| 54:SI:63:ARG:O | 54:SI:67:MET:HG2 | 2.00 | 0.60 |
| 62:SQ:61:LEU:HD21 | 62:SQ:96:LEU:HD23 | 1.83 | 0.60 |
| 68:SW:81:VAL:HG12 | 68:SW:86:LEU:HB3 | 1.82 | 0.60 |
| 68:SW:125:ALA:O | 68:SW:129:ILE:HD12 | 1.99 | 0.60 |
| 1:LA:2110:G:H5'' | 25:LY:48:ARG:CZ | 2.30 | 0.60 |
| 1:LA:3312:U:H4' | 5:LE:173:GLN:HG3 | 1.82 | 0.60 |
| 1:LA:3348:C:H42 | 1:LA:3355:G:N2 | 2.00 | 0.60 |
| 71:SZ:29:HIS:CE1 | 71:SZ:31:THR:HG22 | 2.37 | 0.60 |
| 79:Ta:8:U:H3 | 79:Ta:16:C:H42 | 1.47 | 0.60 |
| 1:LA:407:A:C2 | 3:LC:17:A:H1' | 2.36 | 0.60 |
| 1:LA:1239:A:H8 | 1:LA:1240:U:H4' | 1.66 | 0.60 |
| 1:LA:1638:C:H5' | 35:Li:52:GLN:HG3 | 1.83 | 0.60 |
| 1:LA:3229:G:H4' | 15:LO:132:LYS:HE3 | 1.82 | 0.60 |
| 6:LF:234:ASN:HD21 | 6:LF:236:LEU:HB2 | 1.66 | 0.60 |
| 52:SG:14:LYS:HG3 | 52:SG:69:ILE:CG1 | 2.31 | 0.60 |
| 55:SJ:71:PRO:O | 58:SM:40:ARG:NH2 | 2.34 | 0.60 |
| 1:LA:12:A:H2' | 1:LA:13:A:C8 | 2.36 | 0.60 |
| 1:LA:196:G:N1 | 1:LA:199:A:OP2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:LA:2356:A:H2' | 1:LA:2357:A:C8 | 2.36 | 0.60 |
| 1:LA:2609:G:H5'' | 16:LP:81:TYR:HA | 1.82 | 0.60 |
| 45:S2:905:A:O2' | 71:SZ:52:ARG:NH1 | 2.34 | 0.60 |
| 45:S2:1048:G:H2' | 45:S2:1048:G:N3 | 2.17 | 0.60 |
| 1:LA:3032:A:H3' | 1:LA:3033:C:H5'' | 1.82 | 0.60 |
| 2:LB:2:G:H4' | 7:LG:273:ARG:HH21 | 1.67 | 0.60 |
| 7:LG:39:GLN:NE2 | 7:LG:46:THR:O | 2.33 | 0.60 |
| 13:LM:82:ARG:NH1 | 13:LM:112:LEU:O | 2.32 | 0.60 |
| 23:LW:77:LYS:O | 23:LW:81:LYS:HG3 | 2.02 | 0.60 |
| 45:S2:1679:G:N2 | 45:S2:1722:A:C5 | 2.69 | 0.60 |
| 61:SP:157:ASP:OD1 | 72:Sa:60:ARG:NH1 | 2.34 | 0.60 |
| 61:SP:198:MET:SD | 61:SP:198:MET:N | 2.65 | 0.60 |
| 62:SQ:61:LEU:HD21 | 62:SQ:96:LEU:CD2 | 2.31 | 0.60 |
| 64:SS:37:LYS:HB2 | 64:SS:40:GLU:HG2 | 1.83 | 0.60 |
| 23:LW:37:LEU:O | 23:LW:41:ILE:HG12 | 2.01 | 0.60 |
| 39:Lm:19:ASP:O | 39:Lm:21:LYS:HE2 | 2.01 | 0.60 |
| 45:S2:1488:G:H21 | 45:S2:1512:G:H21 | 1.48 | 0.60 |
| 54:SI:40:SER:HB3 | 54:SI:43:ASN:HD21 | 1.66 | 0.60 |
| 60:SO:263:PHE:HE1 | 60:SO:268:GLN:HA | 1.63 | 0.60 |
| 79:Ta:23:G:N7 | 79:Ta:47:G:N2 | 2.49 | 0.60 |
| 1:LA:2736:C:O2' | 30:Ld:36:ASP:OD1 | 2.17 | 0.60 |
| 1:LA:3018:U:O2' | 1:LA:3019:U:O5' | 2.14 | 0.60 |
| 7:LG:129:TYR:OH | 7:LG:175:HIS:O | 2.16 | 0.60 |
| 45:S2:1328:G:OP1 | 46:SA:159:HIS:N | 2.34 | 0.60 |
| 46:SA:166:ASP:OD1 | 46:SA:167:PHE:N | 2.33 | 0.60 |
| 52:SG:19:ARG:HG3 | 52:SG:20:TYR:CE1 | 2.37 | 0.60 |
| 61:SP:67:ILE:HD11 | 61:SP:119:ARG:HB2 | 1.84 | 0.60 |
| 62:SQ:109:LYS:O | 62:SQ:113:MET:HG2 | 2.01 | 0.60 |
| 62:SQ:133:TYR:HD2 | 62:SQ:217:LEU:HD11 | 1.65 | 0.60 |
| 66:SU:168:SER:O | 66:SU:172:VAL:HG13 | 2.01 | 0.60 |
| 67:SV:20:GLN:NE2 | 67:SV:22:ARG:O | 2.35 | 0.60 |
| 71:SZ:16:VAL:HG12 | 71:SZ:18:ARG:HG2 | 1.84 | 0.60 |
| 1:LA:815:A:H5' | 1:LA:905:A:H61 | 1.67 | 0.60 |
| 1:LA:2382:C:OP2 | 17:LQ:85[A]:ARG:NH2 | 2.34 | 0.60 |
| 7:LG:64:ILE:HG13 | 7:LG:109:THR:HG21 | 1.83 | 0.60 |
| 23:LW:16:THR:HG22 | 23:LW:102:GLU:HA | 1.84 | 0.60 |
| 68:SW:44:ARG:HG2 | 68:SW:45:ILE:HD12 | 1.84 | 0.60 |
| 71:SZ:72:LYS:HA | 71:SZ:72:LYS:CE | 2.28 | 0.60 |
| 1:LA:2212:A:H2' | 1:LA:2213:A:C8 | 2.37 | 0.60 |
| 1:LA:2630:U:OP2 | 22:LV:4:SER:OG | 2.18 | 0.60 |
| 1:LA:3150:U:H4' | 1:LA:3293:A:H1' | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:3378:C:O2' | 1:LA:3379:U:O5' | 2.20 | 0.60 |
| 4:LD:33:ASP:O | 4:LD:37:ARG:NH2 | 2.34 | 0.60 |
| 12:LL:170:LYS:HA | 12:LL:177:ASP:HA | 1.83 | 0.60 |
| 15:LO:50:LYS:HE3 | 15:LO:82:SER:HA | 1.83 | 0.60 |
| 17:LQ:54[A]:TYR:OH | 17:LQ:73[A]:PHE:O | 2.19 | 0.60 |
| 41:Lo:103:LEU:HD12 | 41:Lo:121:LEU:HD11 | 1.83 | 0.60 |
| 45:S2:1650:U:H2' | 45:S2:1651:A:C8 | 2.37 | 0.60 |
| 47:SB:58:LEU:HD12 | 47:SB:138:THR:HG22 | 1.83 | 0.60 |
| 50:SE:54:ALA:HA | 50:SE:57:MET:CE | 2.31 | 0.60 |
| 54:SI:71:VAL:HG23 | 54:SI:75:LYS:HB2 | 1.82 | 0.60 |
| 61:SP:167:LYS:NZ | 61:SP:204:TYR:O | 2.35 | 0.60 |
| 74:Sc:54:LEU:HD11 | 74:Sc:75:GLN:HB2 | 1.84 | 0.60 |
| 1:LA:2947:C:OP1 | 5:LE:244:ARG:NH2 | 2.33 | 0.59 |
| 45:S2:69:G:H1 | 45:S2:82:U:H3 | 1.50 | 0.59 |
| 47:SB:71:ALA:O | 47:SB:91:GLU:HG3 | 2.01 | 0.59 |
| 64:SS:136:VAL:HG21 | 64:SS:148:ARG:HH21 | 1.65 | 0.59 |
| 1:LA:1603:G:H4' | 1:LA:1834:A:H4' | 1.84 | 0.59 |
| 6:LF:326:ARG:O | 9:LI:41:ARG:NH1 | 2.35 | 0.59 |
| 45:S2:1364:G:H2' | 45:S2:1365:C:C6 | 2.37 | 0.59 |
| 45:S2:1459:C:H41 | 53:SH:139:LYS:HE3 | 1.68 | 0.59 |
| 45:S2:1641:C:H2' | 45:S2:1642:G:C8 | 2.37 | 0.59 |
| 47:SB:123:VAL:HG23 | 47:SB:124:LEU:HD12 | 1.83 | 0.59 |
| 52:SG:41:ILE:O | 52:SG:47:ARG:NH2 | 2.34 | 0.59 |
| 1:LA:358:G:N2 | 1:LA:361:A:OP2 | 2.31 | 0.59 |
| 1:LA:1646:A:H62 | 1:LA:1807:G:H21 | 1.48 | 0.59 |
| 1:LA:3033:C:C2 | 11:LK:120:ASP:HB2 | 2.37 | 0.59 |
| 8:LH:170:LYS:HB3 | 8:LH:172:HIS:CE1 | 2.37 | 0.59 |
| 18:LR:126:ARG:HD3 | 18:LR:140:GLU:OE2 | 2.02 | 0.59 |
| 32:Lf:72:ARG:HD3 | 32:Lf:104:LEU:HD13 | 1.84 | 0.59 |
| 45:S2:264:G:H5'' | 45:S2:265:A:H5'' | 1.83 | 0.59 |
| 53:SH:28:ILE:O | 53:SH:32:LEU:HG | 2.02 | 0.59 |
| 55:SJ:23:ARG:HB2 | 55:SJ:92:ASP:OD1 | 2.01 | 0.59 |
| 64:SS:162:ILE:HG22 | 64:SS:164:LEU:H | 1.66 | 0.59 |
| 65:ST:20:ASP:O | 65:ST:23:ARG:HG3 | 2.01 | 0.59 |
| 66:SU:91:ILE:HD11 | 66:SU:169:PHE:HE1 | 1.68 | 0.59 |
| 19:LS:111:ARG:HD3 | 19:LS:121:CYS:SG | 2.42 | 0.59 |
| 45:S2:1628:U:H2' | 45:S2:1629:G:C8 | 2.37 | 0.59 |
| 62:SQ:210:ILE:HG22 | 62:SQ:210:ILE:O | 2.03 | 0.59 |
| 63:SR:150:GLN:O | 63:SR:174:ARG:NH2 | 2.34 | 0.59 |
| 1:LA:1939:G:H21 | 1:LA:3361:A:H8 | 1.48 | 0.59 |
| 1:LA:3358:A:H2' | 1:LA:3359:C:O4' | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:LI:24:GLU:HG2 | 9:LI:26:VAL:H | 1.68 | 0.59 |
| 10:LJ:85:ASN:O | 10:LJ:89:GLU:HG3 | 2.03 | 0.59 |
| 45:S2:790:U:H5' | 64:SS:187:ARG:NH2 | 2.18 | 0.59 |
| 45:S2:1724:U:H2' | 45:S2:1725:U:H5 | 1.67 | 0.59 |
| 47:SB:174:LEU:HD22 | 47:SB:210:ALA:HA | 1.85 | 0.59 |
| 53:SH:14:ILE:HD11 | 53:SH:21:ASN:HB3 | 1.84 | 0.59 |
| 8:LH:83:TYR:OH | 34:Lh:48:ARG:NH2 | 2.34 | 0.59 |
| 28:Lb:47:GLU:HB3 | 28:Lb:69:LYS:HD2 | 1.85 | 0.59 |
| 45:S2:740:A:O2' | 45:S2:741:C:OP1 | 2.20 | 0.59 |
| 45:S2:754:A:H5'' | 45:S2:755:A:H5' | 1.83 | 0.59 |
| 45:S2:1164:G:H2' | 45:S2:1165:G:C8 | 2.37 | 0.59 |
| 52:SG:20:TYR:CD2 | 52:SG:38:ILE:HD11 | 2.38 | 0.59 |
| 72:Sa:9:VAL:O | 72:Sa:10:GLU:HG3 | 2.03 | 0.59 |
| 5:LE:140:ASP:OD1 | 5:LE:140:ASP:N | 2.34 | 0.59 |
| 45:S2:354:C:H5'' | 67:SV:16:ALA:HB2 | 1.85 | 0.59 |
| 45:S2:374:U:O2' | 45:S2:603:U:OP1 | 2.21 | 0.59 |
| 47:SB:45:LYS:HE2 | 47:SB:46:TRP:CH2 | 2.37 | 0.59 |
| 75:Sd:8:ARG:HH12 | 75:Sd:10:ARG:CZ | 2.16 | 0.59 |
| 1:LA:1228:G:C2 | 1:LA:1229:G:N2 | 2.71 | 0.59 |
| 1:LA:1614:C:H2' | 1:LA:1615:U:C6 | 2.38 | 0.59 |
| 1:LA:1694:U:O2' | 1:LA:1748:A:N1 | 2.29 | 0.59 |
| 4:LD:44:ILE:HD11 | 4:LD:85:GLY:HA2 | 1.85 | 0.59 |
| 6:LF:113:VAL:HB | 6:LF:118:LYS:HE3 | 1.85 | 0.59 |
| 6:LF:169:LEU:HG | 6:LF:174:ALA:HB3 | 1.85 | 0.59 |
| 17:LQ:61[A]:ALA:HA | 17:LQ:70[A]:PRO:HD2 | 1.85 | 0.59 |
| 44:Lr:78:THR:O | 44:Lr:82:THR:HG22 | 2.03 | 0.59 |
| 46:SA:32:GLU:CD | 46:SA:32:GLU:H | 2.11 | 0.59 |
| 55:SJ:28:SER:OG | 55:SJ:29:THR:N | 2.36 | 0.59 |
| 64:SS:250:GLU:HB3 | 64:SS:254:ARG:HH21 | 1.66 | 0.59 |
| 73:Sb:6:VAL:HG13 | 73:Sb:29:PRO:HD2 | 1.83 | 0.59 |
| 1:LA:1175:C:H2' | 1:LA:1176:G:N2 | 2.18 | 0.59 |
| 1:LA:1898:G:O2' | 1:LA:2333:U:O4 | 2.16 | 0.59 |
| 1:LA:2565:C:H2' | 1:LA:2566:C:C6 | 2.38 | 0.59 |
| 3:LC:143:U:OP1 | 16:LP:38:ARG:NH2 | 2.33 | 0.59 |
| 33:Lg:111:ARG:HE | 33:Lg:115:LEU:CD2 | 2.16 | 0.59 |
| 45:S2:947:U:OP1 | 62:SQ:165:ARG:NH1 | 2.36 | 0.59 |
| 68:SW:107:ARG:HH22 | 68:SW:148:VAL:HG23 | 1.68 | 0.59 |
| 1:LA:1388:G:OP1 | 33:Lg:104:ASN:ND2 | 2.35 | 0.59 |
| 1:LA:2521:G:O6 | 4:LD:72:ARG:NH2 | 2.36 | 0.59 |
| 1:LA:2959:C:H2' | 1:LA:2960:G:H8 | 1.68 | 0.59 |
| 1:LA:3323:C:OP1 | 32:Lf:19:ARG:NH1 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:LL:91:VAL:HG12 | 12:LL:133:GLN:HE21 | 1.66 | 0.59 |
| 21:LU:70:THR:C | 21:LU:71:LYS:HD3 | 2.27 | 0.59 |
| 48:SC:23:ALA:O | 48:SC:64:TYR:HB2 | 2.03 | 0.59 |
| 67:SV:56:ARG:NH1 | 67:SV:174:GLY:O | 2.36 | 0.59 |
| 13:LM:133:ARG:NH2 | 13:LM:158:ASP:OD2 | 2.36 | 0.58 |
| 23:LW:83:TYR:O | 23:LW:87:ASN:ND2 | 2.35 | 0.58 |
| 47:SB:189:THR:O | 47:SB:193:THR:HG23 | 2.03 | 0.58 |
| 52:SG:14:LYS:HG3 | 52:SG:69:ILE:HG13 | 1.84 | 0.58 |
| 1:LA:2900:G:O2' | 1:LA:3023:A:N1 | 2.36 | 0.58 |
| 5:LE:166:ILE:HD11 | 5:LE:171:LEU:HB2 | 1.84 | 0.58 |
| 15:LO:92:GLU:CD | 15:LO:92:GLU:H | 2.10 | 0.58 |
| 45:S2:1392:U:OP1 | 52:SG:59:LYS:NZ | 2.29 | 0.58 |
| 71:SZ:111:ARG:HB3 | 76:Se:58:VAL:HG23 | 1.85 | 0.58 |
| 1:LA:2217:G:H2' | 1:LA:2218:A:H8 | 1.67 | 0.58 |
| 1:LA:2427:U:H2' | 1:LA:2428:G:H8 | 1.68 | 0.58 |
| 24:LX:40:LYS:HG3 | 24:LX:57:MET:SD | 2.42 | 0.58 |
| 32:Lf:52:ALA:HB1 | 32:Lf:54:GLU:OE1 | 2.03 | 0.58 |
| 41:Lo:93:LYS:HD3 | 41:Lo:102:ARG:HD2 | 1.84 | 0.58 |
| 68:SW:90:LYS:HB3 | 68:SW:92:LYS:HD2 | 1.86 | 0.58 |
| 1:LA:296:A:N3 | 1:LA:299:G:O2' | 2.34 | 0.58 |
| 1:LA:924:A:N6 | 4:LD:2:GLY:O | 2.28 | 0.58 |
| 1:LA:2534:A:H3' | 1:LA:2535:A:H4' | 1.85 | 0.58 |
| 1:LA:2669:G:H2' | 1:LA:2670:A:C8 | 2.39 | 0.58 |
| 5:LE:375:GLU:OE2 | 25:LY:14:TYR:OH | 2.16 | 0.58 |
| 14:LN:4:SER:O | 29:Lc:44:ASN:ND2 | 2.37 | 0.58 |
| 45:S2:1408:G:H1' | 60:SO:17:ASN:ND2 | 2.18 | 0.58 |
| 63:SR:70:ASP:O | 63:SR:74:PRO:HD3 | 2.04 | 0.58 |
| 71:SZ:103:ARG:HE | 76:Se:49:ALA:HB2 | 1.68 | 0.58 |
| 1:LA:516:G:OP1 | 9:LI:60:ARG:NH2 | 2.36 | 0.58 |
| 1:LA:1033:U:H2' | 1:LA:1034:G:O4' | 2.04 | 0.58 |
| 1:LA:1083:A:H2' | 1:LA:1084:A:C8 | 2.39 | 0.58 |
| 1:LA:1596:C:H5' | 1:LA:1695:A:H1' | 1.85 | 0.58 |
| 12:LL:75:TYR:O | 12:LL:79:VAL:HG22 | 2.03 | 0.58 |
| 31:Le:34:LEU:HD13 | 31:Le:59:TYR:HB3 | 1.85 | 0.58 |
| 45:S2:175:G:H1 | 45:S2:266:A:H5' | 1.69 | 0.58 |
| 46:SA:132:LYS:NZ | 46:SA:192:PRO:HD2 | 2.17 | 0.58 |
| 1:LA:269:G:N2 | 1:LA:295:A:OP2 | 2.22 | 0.58 |
| 1:LA:1480:A:H62 | 1:LA:1871:C:H5 | 1.50 | 0.58 |
| 3:LC:142:C:OP1 | 16:LP:38:ARG:NH1 | 2.34 | 0.58 |
| 45:S2:1473:U:O2' | 47:SB:103:ASN:OD1 | 2.17 | 0.58 |
| 45:S2:1481:C:C4 | 54:SI:79:LEU:HD11 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:SC:52:LYS:HE3 | 48:SC:54:TYR:HE2 | 1.68 | 0.58 |
| 61:SP:121:VAL:HG23 | 61:SP:141:ILE:HG21 | 1.86 | 0.58 |
| 61:SP:136:ALA:HB1 | 61:SP:141:ILE:HB | 1.86 | 0.58 |
| 63:SR:231:ALA:O | 72:Sa:16:LYS:NZ | 2.32 | 0.58 |
| 65:ST:148:SER:HB2 | 65:ST:151:ASP:HB2 | 1.85 | 0.58 |
| 70:SY:99:ARG:NH2 | 70:SY:119:GLU:OE1 | 2.36 | 0.58 |
| 1:LA:1445:A:H5'' | 18:LR:65:SER:OG | 2.04 | 0.58 |
| 5:LE:383:LEU:HD13 | 5:LE:385:LYS:HE2 | 1.85 | 0.58 |
| 6:LF:234:ASN:ND2 | 6:LF:236:LEU:HB2 | 2.18 | 0.58 |
| 45:S2:341:A:H2' | 45:S2:342:C:C6 | 2.39 | 0.58 |
| 45:S2:586:G:C6 | 45:S2:587:C:H1' | 2.39 | 0.58 |
| 45:S2:1171:A:H2' | 45:S2:1172:G:C8 | 2.39 | 0.58 |
| 50:SE:102:PHE:O | 50:SE:104:GLN:NE2 | 2.37 | 0.58 |
| 60:SO:132:LYS:HE3 | 60:SO:134:TRP:CZ2 | 2.38 | 0.58 |
| 63:SR:50:ILE:HD11 | 63:SR:239:PRO:HB3 | 1.84 | 0.58 |
| 67:SV:3:ILE:H | 67:SV:3:ILE:HD12 | 1.67 | 0.58 |
| 1:LA:144:A:OP1 | 10:LJ:193:LYS:NZ | 2.34 | 0.58 |
| 1:LA:937:C:OP2 | 29:Lc:26:ARG:NH1 | 2.36 | 0.58 |
| 1:LA:3017:C:OP1 | 1:LA:3020:A:N6 | 2.37 | 0.58 |
| 6:LF:289:ILE:O | 6:LF:292:SER:OG | 2.21 | 0.58 |
| 45:S2:760:A:O2' | 68:SW:72:GLU:OE2 | 2.17 | 0.58 |
| 70:SY:96:VAL:HG12 | 70:SY:100:LYS:HE3 | 1.86 | 0.58 |
| 1:LA:3257:U:O2' | 1:LA:3259:G:OP1 | 2.22 | 0.58 |
| 6:LF:6:VAL:N | 6:LF:20:LEU:O | 2.35 | 0.58 |
| 6:LF:281:ILE:HA | 19:LS:123:THR:HG21 | 1.84 | 0.58 |
| 7:LG:34:LYS:HA | 22:LV:27:LEU:HD11 | 1.86 | 0.58 |
| 45:S2:256:A:O2' | 67:SV:72:ILE:HD12 | 2.03 | 0.58 |
| 45:S2:885:G:H2' | 45:S2:886:U:C6 | 2.39 | 0.58 |
| 47:SB:72:HIS:O | 51:SF:47:LYS:NZ | 2.37 | 0.58 |
| 50:SE:85:ILE:HG22 | 50:SE:112:LEU:HD23 | 1.86 | 0.58 |
| 52:SG:18:GLU:OE2 | 52:SG:19:ARG:NH1 | 2.36 | 0.58 |
| 71:SZ:72:LYS:HZ2 | 71:SZ:77:THR:HA | 1.68 | 0.58 |
| 74:Sc:130:VAL:HG23 | 74:Sc:140:LYS:HD2 | 1.84 | 0.58 |
| 74:Sc:133:LEU:HA | 74:Sc:136:TRP:HB3 | 1.85 | 0.58 |
| 1:LA:2681:C:H1' | 1:LA:2682:U:C5 | 2.38 | 0.58 |
| 1:LA:2996:G:H1' | 1:LA:3394:G:H4' | 1.85 | 0.58 |
| 5:LE:169:THR:HG22 | 5:LE:171:LEU:HG | 1.86 | 0.58 |
| 7:LG:294:ALA:HB1 | 12:LL:217:PHE:HB3 | 1.85 | 0.58 |
| 31:Le:24:THR:OG1 | 31:Le:91:SER:OG | 2.19 | 0.58 |
| 45:S2:1206:U:H1' | 58:SM:16:LYS:HG3 | 1.85 | 0.58 |
| 45:S2:1727:G:H2' | 45:S2:1728:A:C8 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 46:SA:55:THR:HG21 | 46:SA:89:GLU:C | 2.29 | 0.58 |
| 52:SG:25:THR:O | 52:SG:31:ASN:ND2 | 2.36 | 0.58 |
| 70:SY:62:GLN:HG3 | 70:SY:65:VAL:HG13 | 1.86 | 0.58 |
| 1:LA:1798:A:H2' | 1:LA:1799:A:C8 | 2.39 | 0.57 |
| 45:S2:1724:U:H2' | 45:S2:1725:U:C5 | 2.38 | 0.57 |
| 49:SD:130:THR:O | 49:SD:133:LEU:HD23 | 2.03 | 0.57 |
| 63:SR:81:MET:HE1 | 63:SR:186:LYS:HG2 | 1.85 | 0.57 |
| 75:Sd:3:ASP:H | 75:Sd:32:ARG:HH22 | 1.52 | 0.57 |
| 1:LA:3110:U:OP1 | 11:LK:184:LYS:NZ | 2.36 | 0.57 |
| 5:LE:356:LEU:HD23 | 5:LE:359:ILE:HD11 | 1.85 | 0.57 |
| 12:LL:53:VAL:HG21 | 12:LL:166:ILE:HD12 | 1.86 | 0.57 |
| 17:LQ:84[A]:LEU:HD22 | 17:LQ:102[A]:LEU:HD22 | 1.86 | 0.57 |
| 27:La:99:LEU:HD11 | 27:La:104:LEU:HD21 | 1.86 | 0.57 |
| 50:SE:95:GLY:HA2 | 50:SE:103:ASN:O | 2.03 | 0.57 |
| 60:SO:90:ARG:HH21 | 60:SO:102:ARG:HH21 | 1.51 | 0.57 |
| 1:LA:1127:U:OP1 | 12:LL:4:ARG:NH1 | 2.31 | 0.57 |
| 9:LI:151:ARG:HD2 | 9:LI:207:LEU:HD23 | 1.86 | 0.57 |
| 11:LK:120:ASP:OD2 | 11:LK:124:ARG:NH2 | 2.37 | 0.57 |
| 12:LL:54:SER:HB3 | 12:LL:135:ILE:HD11 | 1.86 | 0.57 |
| 45:S2:1415:U:H2' | 45:S2:1416:G:H8 | 1.69 | 0.57 |
| 45:S2:1512:G:O2' | 45:S2:1513:G:O4' | 2.13 | 0.57 |
| 61:SP:182:LEU:HD23 | 61:SP:185:ARG:HH12 | 1.68 | 0.57 |
| 64:SS:72:VAL:N | 64:SS:75:LYS:O | 2.37 | 0.57 |
| 64:SS:112:HIS:NE2 | 64:SS:237:SER:O | 2.31 | 0.57 |
| 1:LA:196:G:H22 | 1:LA:199:A:H5' | 1.69 | 0.57 |
| 1:LA:992:G:N3 | 1:LA:2636:A:H2' | 2.19 | 0.57 |
| 1:LA:1823:U:C2 | 1:LA:1824:G:C8 | 2.93 | 0.57 |
| 1:LA:2635:A:H5' | 1:LA:2636:A:C5' | 2.34 | 0.57 |
| 1:LA:2696:A:H2' | 1:LA:2697:G:C8 | 2.39 | 0.57 |
| 45:S2:319:U:H1' | 45:S2:323:A:H62 | 1.70 | 0.57 |
| 45:S2:388:G:H2' | 45:S2:389:G:C8 | 2.39 | 0.57 |
| 46:SA:162:GLN:NE2 | 46:SA:166:ASP:OD2 | 2.38 | 0.57 |
| 60:SO:81:LEU:HD13 | 60:SO:122:ILE:HD11 | 1.85 | 0.57 |
| 66:SU:139:ARG:HH12 | 73:Sb:53:ILE:HG23 | 1.69 | 0.57 |
| 67:SV:79:ALA:HB3 | 67:SV:103:GLN:HB2 | 1.84 | 0.57 |
| 69:SX:82:ARG:HE | 69:SX:113:PRO:HG3 | 1.68 | 0.57 |
| 75:Sd:21:LYS:HB3 | 75:Sd:75:VAL:HG12 | 1.86 | 0.57 |
| 1:LA:405:U:H4' | 1:LA:1415:C:H4' | 1.87 | 0.57 |
| 1:LA:497:A:O2' | 1:LA:3272:A:N1 | 2.33 | 0.57 |
| 1:LA:1440:G:H4' | 3:LC:15:G:H4' | 1.85 | 0.57 |
| 1:LA:2405:C:H2' | 1:LA:2406:C:H6 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|----------------------|--------------------------|-------------------|
| 45:S2:112:A:O2' | 69:SX:67:ARG:NH1 | 2.37 | 0.57 |
| 45:S2:370:A:N7 | 68:SW:61:THR:OG1 | 2.33 | 0.57 |
| 45:S2:1389:C:N4 | 45:S2:1391:A:O4' | 2.38 | 0.57 |
| 45:S2:1591:C:H2' | 45:S2:1592:A:H8 | 1.69 | 0.57 |
| 77:Sf:33:LEU:HD13 | 77:Sf:35:VAL:HG13 | 1.86 | 0.57 |
| 1:LA:3118:U:H4' | 41:Lo:104:PRO:HG2 | 1.85 | 0.57 |
| 7:LG:153:THR:HG23 | 7:LG:160:PHE:HZ | 1.69 | 0.57 |
| 31:Le:40:LYS:HB3 | 31:Le:101:LEU:HD13 | 1.86 | 0.57 |
| 45:S2:230:C:O2 | 45:S2:230:C:H2' | 2.04 | 0.57 |
| 45:S2:1442:U:O2' | 45:S2:1446:A:H1' | 2.05 | 0.57 |
| 60:SO:260:ILE:HD12 | 60:SO:260:ILE:O | 2.04 | 0.57 |
| 63:SR:49:LYS:HB3 | 63:SR:243:TYR:CD2 | 2.39 | 0.57 |
| 65:ST:7:TYR:HE2 | 65:ST:116:LYS:HB2 | 1.69 | 0.57 |
| 75:Sd:111:LYS:HA | 75:Sd:114:ARG:HD2 | 1.85 | 0.57 |
| 1:LA:1260:G:H4' | 1:LA:1277:A:N1 | 2.19 | 0.57 |
| 1:LA:1686:U:H5'' | 1:LA:1687:U:H5'' | 1.85 | 0.57 |
| 10:LJ:75:ILE:HD11 | 16:LP:18:VAL:HG23 | 1.85 | 0.57 |
| 21:LU:109:ASP:OD1 | 21:LU:113:ARG:HD2 | 2.04 | 0.57 |
| 45:S2:5:U:H2' | 45:S2:6:G:H8 | 1.70 | 0.57 |
| 45:S2:472:U:H2' | 45:S2:473:A:C8 | 2.39 | 0.57 |
| 45:S2:809:A:H2' | 45:S2:810:G:C8 | 2.40 | 0.57 |
| 45:S2:894:U:H2' | 45:S2:895:G:C8 | 2.39 | 0.57 |
| 45:S2:1552:U:N3 | 45:S2:1556:A:N6 | 2.51 | 0.57 |
| 45:S2:1573:A:H4' | 45:S2:1574:G:OP2 | 2.05 | 0.57 |
| 45:S2:1613:U:OP1 | 47:SB:84:LYS:NZ | 2.32 | 0.57 |
| 45:S2:1712:A:N6 | 45:S2:1713:G:O6 | 2.37 | 0.57 |
| 65:ST:149:LYS:HD2 | 65:ST:150:GLU:HB3 | 1.87 | 0.57 |
| 17:LQ:143[A]:THR:HG21 | 17:LQ:150[A]:GLU:OE1 | 2.05 | 0.57 |
| 40:Ln:14:ALA:O | 40:Ln:18:LYS:HG3 | 2.05 | 0.57 |
| 45:S2:884:A:H2' | 45:S2:885:G:H8 | 1.70 | 0.57 |
| 45:S2:1552:U:N3 | 45:S2:1556:A:C6 | 2.72 | 0.57 |
| 53:SH:57:ARG:NE | 53:SH:60:GLU:OE1 | 2.37 | 0.57 |
| 55:SJ:31:VAL:HG22 | 55:SJ:87:HIS:CE1 | 2.40 | 0.57 |
| 65:ST:69:LEU:HG | 65:ST:73:ILE:HD11 | 1.86 | 0.57 |
| 1:LA:3305:U:O2' | 1:LA:3307:C:OP2 | 2.20 | 0.57 |
| 35:Li:47:CYS:HA | 44:Lr:61:LYS:HE3 | 1.86 | 0.57 |
| 45:S2:1171:A:H1' | 45:S2:1570:A:N3 | 2.20 | 0.57 |
| 45:S2:1345:A:OP1 | 55:SJ:54:GLY:N | 2.30 | 0.57 |
| 45:S2:1525:A:H4' | 54:SI:83:ALA:HB2 | 1.86 | 0.57 |
| 45:S2:1673:G:C6 | 45:S2:1728:A:N1 | 2.73 | 0.57 |
| 52:SG:10:LYS:HG2 | 52:SG:53:TYR:CE2 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:94:G:H2' | 1:LA:95:A:C8 | 2.40 | 0.57 |
| 1:LA:429:U:H2' | 1:LA:430:U:C6 | 2.39 | 0.57 |
| 1:LA:839:C:H5'' | 1:LA:1723:U:H5 | 1.70 | 0.57 |
| 1:LA:2893:C:H2' | 1:LA:2894:G:C8 | 2.40 | 0.57 |
| 1:LA:3033:C:O2 | 11:LK:122:LYS:N | 2.37 | 0.57 |
| 1:LA:3213:U:H3 | 15:LO:124:ARG:HH22 | 1.53 | 0.57 |
| 1:LA:3308:G:H1' | 18:LR:69:ARG:HD2 | 1.87 | 0.57 |
| 6:LF:317:PRO:C | 6:LF:319:LYS:H | 2.11 | 0.57 |
| 13:LM:10:ARG:NH2 | 13:LM:151:SER:O | 2.34 | 0.57 |
| 45:S2:344:A:H2' | 45:S2:345:U:H4' | 1.87 | 0.57 |
| 63:SR:139:ILE:HD12 | 63:SR:218:ILE:HB | 1.86 | 0.57 |
| 70:SY:60:VAL:HG13 | 70:SY:66:ILE:HD13 | 1.86 | 0.57 |
| 80:Tb:26:C:H2' | 80:Tb:27:G:C8 | 2.40 | 0.57 |
| 1:LA:838:C:H4' | 1:LA:1723:U:H2' | 1.86 | 0.56 |
| 1:LA:2552:U:O2' | 35:Li:91:ARG:NH1 | 2.31 | 0.56 |
| 20:LT:47:ASN:ND2 | 20:LT:47:ASN:O | 2.38 | 0.56 |
| 45:S2:44:U:OP2 | 45:S2:437:A:N6 | 2.30 | 0.56 |
| 45:S2:1158:C:N4 | 45:S2:1163:A:H61 | 2.01 | 0.56 |
| 47:SB:103:ASN:HA | 47:SB:106:LYS:HD2 | 1.87 | 0.56 |
| 54:SI:143:ASP:OD1 | 54:SI:144:GLU:N | 2.37 | 0.56 |
| 65:ST:180:THR:HG23 | 65:ST:183:ARG:H | 1.68 | 0.56 |
| 1:LA:309:U:P | 37:Lk:84:LYS:NZ | 2.78 | 0.56 |
| 39:Lm:7:ASP:OD1 | 39:Lm:9:LYS:NZ | 2.38 | 0.56 |
| 45:S2:812:A:H62 | 45:S2:858:G:H2' | 1.70 | 0.56 |
| 45:S2:980:G:H4' | 45:S2:1776:A:H4' | 1.86 | 0.56 |
| 45:S2:1003:A:O2' | 45:S2:1005:A:N7 | 2.33 | 0.56 |
| 45:S2:1466:G:OP1 | 51:SF:132:LYS:NZ | 2.38 | 0.56 |
| 56:SK:84:GLU:OE2 | 56:SK:84:GLU:HA | 2.05 | 0.56 |
| 57:SL:25:VAL:HA | 57:SL:44:VAL:O | 2.04 | 0.56 |
| 76:Se:66:LYS:HG3 | 76:Se:68:TYR:CE1 | 2.40 | 0.56 |
| 1:LA:1647:A:H2' | 1:LA:1648:U:O4' | 2.06 | 0.56 |
| 1:LA:2205:G:N1 | 1:LA:2235:G:O6 | 2.39 | 0.56 |
| 1:LA:2343:U:H2' | 1:LA:2344:A:C8 | 2.41 | 0.56 |
| 1:LA:2561:A:H1' | 10:LJ:30:THR:HB | 1.87 | 0.56 |
| 1:LA:3348:C:N4 | 1:LA:3355:G:H22 | 2.01 | 0.56 |
| 4:LD:65:ASP:OD2 | 4:LD:72:ARG:NE | 2.38 | 0.56 |
| 6:LF:157:GLU:HG3 | 6:LF:251:THR:HG21 | 1.87 | 0.56 |
| 9:LI:121:LYS:HB2 | 22:LV:133:ALA:HB3 | 1.86 | 0.56 |
| 10:LJ:195:SER:OG | 10:LJ:197:VAL:O | 2.23 | 0.56 |
| 15:LO:19:ARG:NH1 | 15:LO:66:THR:O | 2.33 | 0.56 |
| 45:S2:1218:G:H4' | 45:S2:1220:C:H41 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1402:G:P | 52:SG:5:ARG:NH1 | 2.73 | 0.56 |
| 45:S2:1583:A:H62 | 47:SB:76:ARG:HA | 1.71 | 0.56 |
| 57:SL:49:ARG:NH1 | 57:SL:52:ASP:OD2 | 2.39 | 0.56 |
| 60:SO:15:GLY:HA3 | 60:SO:45:TRP:HH2 | 1.70 | 0.56 |
| 61:SP:101:ARG:HG2 | 61:SP:101:ARG:HH11 | 1.69 | 0.56 |
| 64:SS:191:ARG:NH2 | 64:SS:245:LYS:HB3 | 2.16 | 0.56 |
| 65:ST:192:ALA:O | 65:ST:196:ARG:HG2 | 2.04 | 0.56 |
| 70:SY:23:PRO:HD2 | 70:SY:26:PHE:HB3 | 1.86 | 0.56 |
| 72:Sa:53:TYR:OH | 72:Sa:76:ASP:OD2 | 2.19 | 0.56 |
| 11:LK:129:ARG:H | 11:LK:157:ASN:HD21 | 1.52 | 0.56 |
| 14:LN:122:LYS:HE3 | 36:Lj:120:ALA:HA | 1.88 | 0.56 |
| 28:Lb:106:GLN:O | 28:Lb:109:GLU:HG3 | 2.05 | 0.56 |
| 45:S2:513:U:H2' | 45:S2:514:G:H8 | 1.70 | 0.56 |
| 45:S2:744:U:H2' | 45:S2:745:U:O4' | 2.04 | 0.56 |
| 45:S2:1125:A:O2' | 45:S2:1776:A:OP1 | 2.15 | 0.56 |
| 45:S2:1503:A:H5' | 54:SI:99:SER:HB3 | 1.88 | 0.56 |
| 67:SV:194:ARG:HA | 67:SV:197:THR:HG22 | 1.86 | 0.56 |
| 1:LA:626:U:H2' | 1:LA:627:A:C8 | 2.39 | 0.56 |
| 1:LA:1866:A:H2 | 1:LA:2118:A:H4' | 1.71 | 0.56 |
| 34:Lh:16:TYR:OH | 34:Lh:89:LEU:O | 2.17 | 0.56 |
| 46:SA:75:LYS:NZ | 48:SC:20:VAL:O | 2.38 | 0.56 |
| 76:Se:87:ARG:HB3 | 76:Se:91:ASP:OD1 | 2.05 | 0.56 |
| 1:LA:927:C:H2' | 1:LA:928:A:C8 | 2.39 | 0.56 |
| 1:LA:1157:A:OP2 | 9:LI:90:LYS:NZ | 2.34 | 0.56 |
| 12:LL:109:ASP:N | 12:LL:109:ASP:OD1 | 2.39 | 0.56 |
| 22:LV:136:ARG:HG2 | 22:LV:136:ARG:HH11 | 1.70 | 0.56 |
| 26:LZ:81:ILE:HG12 | 26:LZ:125:ARG:HB2 | 1.88 | 0.56 |
| 40:Ln:25:GLN:HE22 | 40:Ln:28:ARG:NH1 | 2.04 | 0.56 |
| 45:S2:1034:C:OP1 | 70:SY:9:LYS:NZ | 2.35 | 0.56 |
| 45:S2:1527:C:OP1 | 47:SB:109:LYS:NZ | 2.37 | 0.56 |
| 47:SB:45:LYS:HE2 | 47:SB:46:TRP:CZ2 | 2.40 | 0.56 |
| 62:SQ:207:LEU:HD23 | 62:SQ:210:ILE:HD11 | 1.87 | 0.56 |
| 1:LA:785:A:H4' | 1:LA:786:G:H5' | 1.87 | 0.56 |
| 1:LA:2536:U:H5'' | 62:SQ:229:MET:HG2 | 1.87 | 0.56 |
| 1:LA:2695:A:H2' | 1:LA:2696:A:C8 | 2.41 | 0.56 |
| 1:LA:2915:U:H1' | 24:LX:44:SER:HB3 | 1.88 | 0.56 |
| 4:LD:201:GLY:HA2 | 4:LD:204:MET:HG3 | 1.87 | 0.56 |
| 19:LS:67:ILE:HG23 | 19:LS:81:VAL:HG11 | 1.88 | 0.56 |
| 24:LX:59:MET:HE3 | 24:LX:73:VAL:HG12 | 1.87 | 0.56 |
| 28:Lb:78:ASN:OD1 | 31:Le:35:ARG:NH2 | 2.39 | 0.56 |
| 45:S2:639:U:OP1 | 66:SU:112:ARG:NH2 | 2.37 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 45:S2:959:U:H6 | 70:SY:61:THR:OG1 | 1.89 | 0.56 |
| 47:SB:110:ALA:O | 47:SB:114:ILE:HG22 | 2.06 | 0.56 |
| 48:SC:46:LEU:O | 48:SC:50:THR:HG23 | 2.06 | 0.56 |
| 58:SM:19:ARG:HH12 | 58:SM:32:ARG:HB2 | 1.71 | 0.56 |
| 62:SQ:135:LEU:HD23 | 62:SQ:217:LEU:HA | 1.88 | 0.56 |
| 75:Sd:3:ASP:N | 75:Sd:32:ARG:HH22 | 2.02 | 0.56 |
| 1:LA:417:A:H2' | 1:LA:418:A:C8 | 2.40 | 0.56 |
| 1:LA:2591:G:H4' | 1:LA:2593:C:C2 | 2.41 | 0.56 |
| 3:LC:41:A:H4' | 38:Ll:59:THR:HG23 | 1.88 | 0.56 |
| 45:S2:412:A:C8 | 45:S2:413:U:H5 | 2.24 | 0.56 |
| 45:S2:477:A:O2' | 78:Sg:33:ARG:NH2 | 2.37 | 0.56 |
| 45:S2:790:U:H5' | 64:SS:187:ARG:HH22 | 1.68 | 0.56 |
| 45:S2:884:A:H2' | 45:S2:885:G:C8 | 2.40 | 0.56 |
| 45:S2:1045:C:OP1 | 62:SQ:153:HIS:CE1 | 2.59 | 0.56 |
| 46:SA:76:ARG:NH1 | 46:SA:76:ARG:O | 2.37 | 0.56 |
| 64:SS:38:LEU:HG | 64:SS:39:ARG:HD2 | 1.87 | 0.56 |
| 71:SZ:80:HIS:HA | 71:SZ:113:GLY:O | 2.06 | 0.56 |
| 1:LA:371:G:N1 | 1:LA:374:A:OP2 | 2.35 | 0.56 |
| 1:LA:3005:A:H2' | 1:LA:3006:U:O4' | 2.06 | 0.56 |
| 3:LC:55:U:O4 | 3:LC:62:C:N3 | 2.39 | 0.56 |
| 10:LJ:239:GLY:O | 10:LJ:243:GLN:HG2 | 2.06 | 0.56 |
| 16:LP:60:VAL:HG22 | 16:LP:134:LEU:HB2 | 1.88 | 0.56 |
| 40:Ln:21:ARG:HH21 | 40:Ln:24:PRO:HG3 | 1.70 | 0.56 |
| 45:S2:342:C:H2' | 45:S2:343:C:C6 | 2.41 | 0.56 |
| 45:S2:772:G:OP1 | 68:SW:7:THR:OG1 | 2.21 | 0.56 |
| 45:S2:1171:A:H2' | 45:S2:1172:G:H8 | 1.71 | 0.56 |
| 45:S2:1191:U:H2' | 45:S2:1192:C:C6 | 2.41 | 0.56 |
| 73:Sb:93:LEU:HD13 | 73:Sb:128:PHE:CD1 | 2.41 | 0.56 |
| 1:LA:1202:A:H2' | 1:LA:1203:A:H8 | 1.70 | 0.56 |
| 1:LA:3027:G:H2' | 1:LA:3028:A:C8 | 2.41 | 0.56 |
| 17:LQ:18[A]:ARG:NH1 | 17:LQ:128[A]:ARG:HH21 | 2.04 | 0.56 |
| 43:Lq:25:VAL:HG22 | 43:Lq:72:LEU:HD22 | 1.88 | 0.56 |
| 45:S2:40:A:H62 | 45:S2:467:G:H21 | 1.54 | 0.56 |
| 45:S2:333:A:N6 | 67:SV:27:PHE:HB2 | 2.21 | 0.56 |
| 45:S2:434:G:N1 | 45:S2:437:A:OP2 | 2.36 | 0.56 |
| 45:S2:844:A:N6 | 45:S2:845:G:O6 | 2.38 | 0.56 |
| 62:SQ:119:THR:HG21 | 62:SQ:161:ILE:HD11 | 1.87 | 0.56 |
| 63:SR:95:ARG:HH12 | 63:SR:97:ARG:HH11 | 1.53 | 0.56 |
| 64:SS:11:ARG:HH11 | 64:SS:20:LEU:HD13 | 1.71 | 0.56 |
| 71:SZ:26:THR:HG21 | 71:SZ:60:ALA:HB2 | 1.87 | 0.56 |
| 75:Sd:18:LEU:HD12 | 75:Sd:20:ARG:NH1 | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:400:G:H4' | 1:LA:401:U:H5' | 1.89 | 0.55 |
| 1:LA:1785:G:H2' | 1:LA:1786:A:C8 | 2.41 | 0.55 |
| 36:Lj:31:LEU:HD11 | 36:Lj:43:LYS:HG3 | 1.88 | 0.55 |
| 45:S2:594:A:P | 68:SW:38:ASN:HD21 | 2.29 | 0.55 |
| 45:S2:1476:C:H2' | 45:S2:1477:G:C8 | 2.38 | 0.55 |
| 53:SH:3:LEU:HD23 | 53:SH:3:LEU:H | 1.71 | 0.55 |
| 55:SJ:40:ASN:HA | 55:SJ:43:LYS:HG2 | 1.88 | 0.55 |
| 57:SL:15:VAL:HA | 57:SL:28:VAL:HG12 | 1.87 | 0.55 |
| 64:SS:11:ARG:NH2 | 64:SS:24:SER:O | 2.38 | 0.55 |
| 65:ST:67:VAL:CG1 | 65:ST:99:GLY:HA2 | 2.36 | 0.55 |
| 68:SW:112:GLN:O | 68:SW:116:LEU:HG | 2.06 | 0.55 |
| 1:LA:661:U:H2' | 1:LA:662:C:C6 | 2.42 | 0.55 |
| 1:LA:696:A:O2' | 1:LA:697:U:H6 | 1.89 | 0.55 |
| 1:LA:760:A:H2' | 1:LA:761:U:C6 | 2.40 | 0.55 |
| 1:LA:1136:C:H2' | 1:LA:1137:U:H5' | 1.88 | 0.55 |
| 4:LD:137:ILE:HD11 | 4:LD:149:ARG:HB2 | 1.87 | 0.55 |
| 14:LN:106:GLN:NE2 | 14:LN:110:ASP:OD1 | 2.39 | 0.55 |
| 32:Lf:11:GLU:O | 32:Lf:106:THR:HA | 2.07 | 0.55 |
| 33:Lg:86:THR:HG22 | 33:Lg:115:LEU:HG | 1.87 | 0.55 |
| 45:S2:123:G:OP1 | 64:SS:77:ARG:NH2 | 2.35 | 0.55 |
| 60:SO:198:ASN:HD21 | 60:SO:216:LYS:CE | 2.18 | 0.55 |
| 61:SP:50:VAL:O | 61:SP:53:THR:HG22 | 2.06 | 0.55 |
| 64:SS:18:TRP:C | 64:SS:51:ARG:HH22 | 2.14 | 0.55 |
| 66:SU:44:LYS:HG3 | 66:SU:63:PRO:HG3 | 1.87 | 0.55 |
| 1:LA:2159:G:H2' | 1:LA:2160:G:H8 | 1.71 | 0.55 |
| 5:LE:77:THR:HG21 | 5:LE:328:ILE:HG12 | 1.87 | 0.55 |
| 6:LF:181:VAL:HG11 | 6:LF:224:GLY:HA3 | 1.89 | 0.55 |
| 7:LG:125:VAL:O | 7:LG:196:ARG:NH1 | 2.40 | 0.55 |
| 13:LM:49:LYS:HB3 | 13:LM:62:ASN:HA | 1.89 | 0.55 |
| 19:LS:74:GLU:OE2 | 19:LS:74:GLU:N | 2.26 | 0.55 |
| 27:La:63:LYS:NZ | 27:La:97:ILE:HD12 | 2.21 | 0.55 |
| 45:S2:1318:G:H5' | 52:SG:67:ARG:HH12 | 1.71 | 0.55 |
| 45:S2:1426:C:H3' | 45:S2:1427:A:H4' | 1.88 | 0.55 |
| 45:S2:1485:C:H3' | 45:S2:1486:G:H5' | 1.87 | 0.55 |
| 47:SB:174:LEU:HA | 47:SB:177:ILE:HD11 | 1.87 | 0.55 |
| 55:SJ:68:ARG:HH12 | 55:SJ:77:LYS:HA | 1.71 | 0.55 |
| 1:LA:669:C:OP1 | 19:LS:147:ARG:NH2 | 2.40 | 0.55 |
| 1:LA:2418:A:H2' | 1:LA:2419:C:C6 | 2.41 | 0.55 |
| 1:LA:3333:U:H4' | 1:LA:3334:A:H5' | 1.88 | 0.55 |
| 1:LA:3349:C:O2' | 1:LA:3350:U:OP1 | 2.22 | 0.55 |
| 3:LC:128:U:OP1 | 3:LC:129:C:N4 | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:LN:76:THR:HG22 | 14:LN:78:ALA:H | 1.71 | 0.55 |
| 22:LV:17:ARG:HG2 | 22:LV:22:HIS:HA | 1.86 | 0.55 |
| 52:SG:109:LEU:HA | 61:SP:38:PHE:HE2 | 1.71 | 0.55 |
| 65:ST:32:ILE:HD11 | 65:ST:63:MET:HE1 | 1.88 | 0.55 |
| 72:Sa:1:MET:HG3 | 72:Sa:10:GLU:HG2 | 1.88 | 0.55 |
| 1:LA:2175:U:OP1 | 4:LD:54:ARG:NH2 | 2.36 | 0.55 |
| 11:LK:67:ALA:O | 11:LK:71:VAL:HG13 | 2.07 | 0.55 |
| 13:LM:10:ARG:O | 13:LM:133:ARG:NH1 | 2.39 | 0.55 |
| 27:La:17:LYS:O | 27:La:21:THR:OG1 | 2.23 | 0.55 |
| 66:SU:51:VAL:HG12 | 66:SU:53:GLY:H | 1.71 | 0.55 |
| 1:LA:77:A:N7 | 14:LN:73:ARG:NH2 | 2.55 | 0.55 |
| 1:LA:736:G:H2' | 1:LA:737:A:H8 | 1.70 | 0.55 |
| 1:LA:1599:U:OP1 | 20:LT:42:ARG:NH1 | 2.40 | 0.55 |
| 1:LA:1837:G:H5'' | 1:LA:1838:A:H5' | 1.88 | 0.55 |
| 1:LA:3106:U:H2' | 1:LA:3107:G:H8 | 1.71 | 0.55 |
| 3:LC:57:C:H4' | 3:LC:63:G:N7 | 2.21 | 0.55 |
| 45:S2:1321:A:H4' | 45:S2:1322:A:H5' | 1.89 | 0.55 |
| 45:S2:1357:A:H2' | 45:S2:1358:G:C8 | 2.41 | 0.55 |
| 48:SC:59:PHE:HD1 | 48:SC:62:GLN:HA | 1.72 | 0.55 |
| 49:SD:131:ASP:OD1 | 49:SD:131:ASP:N | 2.37 | 0.55 |
| 64:SS:60:GLU:O | 64:SS:64:ILE:HD13 | 2.06 | 0.55 |
| 74:Sc:55:GLU:O | 74:Sc:70:LYS:NZ | 2.33 | 0.55 |
| 1:LA:1597:G:OP2 | 35:Li:31:ARG:NH2 | 2.39 | 0.55 |
| 1:LA:2406:C:H2' | 1:LA:2407:U:C6 | 2.42 | 0.55 |
| 1:LA:2880:C:H2' | 1:LA:2881:U:C6 | 2.41 | 0.55 |
| 45:S2:30:G:O2' | 74:Sc:133:LEU:HD21 | 2.06 | 0.55 |
| 45:S2:372:G:H4' | 45:S2:612:U:H3 | 1.70 | 0.55 |
| 45:S2:1203:A:H2' | 45:S2:1204:A:H5'' | 1.88 | 0.55 |
| 45:S2:1252:C:H1' | 59:SN:140:TYR:HE2 | 1.71 | 0.55 |
| 49:SD:34:THR:HA | 49:SD:37:VAL:HG22 | 1.88 | 0.55 |
| 64:SS:248:ILE:HA | 64:SS:251:GLU:HG3 | 1.88 | 0.55 |
| 1:LA:744:C:H2' | 1:LA:745:A:H8 | 1.71 | 0.55 |
| 1:LA:1815:A:H2' | 1:LA:1816:G:C8 | 2.35 | 0.55 |
| 1:LA:2406:C:H2' | 1:LA:2407:U:H6 | 1.72 | 0.55 |
| 1:LA:2659:G:OP1 | 1:LA:2749:U:O2' | 2.24 | 0.55 |
| 3:LC:69:U:H2' | 3:LC:70:G:O4' | 2.07 | 0.55 |
| 8:LH:152:THR:OG1 | 8:LH:155:LEU:HB2 | 2.07 | 0.55 |
| 11:LK:174:LYS:HB2 | 41:Lo:127:LEU:HD11 | 1.88 | 0.55 |
| 45:S2:1776:A:H2' | 45:S2:1777:G:C8 | 2.42 | 0.55 |
| 65:ST:19:ASP:H | 65:ST:23:ARG:HH21 | 1.54 | 0.55 |
| 66:SU:44:LYS:N | 66:SU:61:PHE:O | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:SX:74:THR:HG22 | 69:SX:122:ILE:HG12 | 1.88 | 0.55 |
| 1:LA:500:A:H2' | 1:LA:501:U:C6 | 2.41 | 0.55 |
| 1:LA:3072:A:H2' | 1:LA:3073:G:O4' | 2.07 | 0.55 |
| 3:LC:12:A:OP1 | 18:LR:3:ARG:NE | 2.40 | 0.55 |
| 11:LK:90:MET:HE1 | 11:LK:161:LEU:CD2 | 2.37 | 0.55 |
| 39:Lm:14:LEU:HD23 | 39:Lm:17:ARG:HD3 | 1.88 | 0.55 |
| 45:S2:155:U:H2' | 45:S2:156:A:H8 | 1.72 | 0.55 |
| 45:S2:415:C:O2' | 45:S2:416:A:H2' | 2.07 | 0.55 |
| 45:S2:525:A:H5' | 75:Sd:93:ARG:HH21 | 1.72 | 0.55 |
| 45:S2:893:U:H2' | 45:S2:894:U:C6 | 2.42 | 0.55 |
| 51:SF:22:VAL:HG13 | 51:SF:65:ILE:HG12 | 1.89 | 0.55 |
| 51:SF:29:ILE:HD13 | 51:SF:65:ILE:HB | 1.88 | 0.55 |
| 61:SP:52:LYS:HE2 | 72:Sa:82:VAL:HA | 1.87 | 0.55 |
| 67:SV:194:ARG:NH1 | 67:SV:194:ARG:HB2 | 2.22 | 0.55 |
| 70:SY:56:ASP:OD1 | 77:Sf:50:ALA:HA | 2.06 | 0.55 |
| 73:Sb:81:VAL:HG21 | 73:Sb:125:ILE:HB | 1.89 | 0.55 |
| 1:LA:973:G:H2' | 1:LA:974:C:C6 | 2.42 | 0.55 |
| 5:LE:108:GLU:HG3 | 5:LE:137:TYR:CG | 2.42 | 0.55 |
| 45:S2:478:A:OP1 | 78:Sg:37:ARG:NH2 | 2.40 | 0.55 |
| 45:S2:1039:A:H2' | 45:S2:1040:G:O4' | 2.07 | 0.55 |
| 45:S2:1596:C:O2' | 45:S2:1598:U:OP2 | 2.22 | 0.55 |
| 45:S2:1729:C:H2' | 45:S2:1730:A:O4' | 2.07 | 0.55 |
| 48:SC:25:LYS:HD2 | 48:SC:62:GLN:HB2 | 1.89 | 0.55 |
| 1:LA:1540:G:H1' | 1:LA:1556:A:C5 | 2.42 | 0.54 |
| 1:LA:2221:A:H2' | 1:LA:2222:A:C8 | 2.42 | 0.54 |
| 1:LA:3294:A:OP1 | 5:LE:119:TYR:OH | 2.18 | 0.54 |
| 4:LD:188:LYS:O | 4:LD:192:LYS:HG3 | 2.06 | 0.54 |
| 29:Lc:96:LYS:O | 29:Lc:97:GLU:HG3 | 2.07 | 0.54 |
| 45:S2:1181:U:N3 | 45:S2:1458:G:C6 | 2.75 | 0.54 |
| 46:SA:72:LEU:HD22 | 48:SC:20:VAL:HG21 | 1.87 | 0.54 |
| 63:SR:56:ILE:HG12 | 63:SR:61:LEU:HD12 | 1.88 | 0.54 |
| 64:SS:244:ILE:HD11 | 64:SS:246:LEU:HB3 | 1.90 | 0.54 |
| 69:SX:109:VAL:HG21 | 69:SX:125:VAL:HG11 | 1.90 | 0.54 |
| 1:LA:516:G:P | 9:LI:60:ARG:HH22 | 2.30 | 0.54 |
| 1:LA:1039:A:O2' | 1:LA:1040:U:H5'' | 2.07 | 0.54 |
| 1:LA:2151:A:HO2' | 1:LA:2242:A:HO2' | 1.51 | 0.54 |
| 1:LA:2258:A:H5' | 1:LA:2259:U:C5 | 2.42 | 0.54 |
| 45:S2:17:C:O2' | 45:S2:1137:A:N1 | 2.39 | 0.54 |
| 45:S2:253:A:H2' | 45:S2:254:A:C8 | 2.42 | 0.54 |
| 45:S2:1297:G:N2 | 45:S2:1300:A:OP2 | 2.31 | 0.54 |
| 51:SF:58:ASP:OD2 | 51:SF:59:LYS:NZ | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:SJ:28:SER:HB3 | 55:SJ:34:LEU:HD12 | 1.90 | 0.54 |
| 55:SJ:33:GLN:HA | 55:SJ:36:ASN:HD21 | 1.72 | 0.54 |
| 60:SO:169:ILE:CD1 | 60:SO:181:TRP:HE3 | 2.20 | 0.54 |
| 1:LA:1533:A:H2' | 1:LA:1534:A:C8 | 2.42 | 0.54 |
| 1:LA:2879:U:H1' | 5:LE:250:ALA:HB3 | 1.90 | 0.54 |
| 19:LS:94:PHE:CZ | 29:Lc:119:PRO:HD3 | 2.43 | 0.54 |
| 22:LV:102:ARG:O | 22:LV:106:LEU:HG | 2.07 | 0.54 |
| 45:S2:62:A:H1' | 45:S2:287:G:H21 | 1.72 | 0.54 |
| 45:S2:1001:A:OP1 | 80:Tb:39:A:O2' | 2.16 | 0.54 |
| 60:SO:183:LEU:HD23 | 60:SO:183:LEU:H | 1.72 | 0.54 |
| 63:SR:67:GLN:O | 63:SR:71:THR:HG22 | 2.07 | 0.54 |
| 65:ST:69:LEU:O | 65:ST:99:GLY:HA3 | 2.08 | 0.54 |
| 68:SW:45:ILE:HG13 | 68:SW:48:GLN:HE21 | 1.71 | 0.54 |
| 1:LA:180:C:O2 | 1:LA:236:G:N2 | 2.41 | 0.54 |
| 1:LA:505:U:H2' | 1:LA:506:U:O4' | 2.07 | 0.54 |
| 1:LA:908:G:OP1 | 16:LP:77:LYS:HA | 2.08 | 0.54 |
| 1:LA:1360:U:OP1 | 6:LF:309:ARG:HG2 | 2.07 | 0.54 |
| 1:LA:1693:U:H4' | 35:Li:24:LYS:HD3 | 1.90 | 0.54 |
| 1:LA:2552:U:H3' | 1:LA:2553:A:H5'' | 1.89 | 0.54 |
| 8:LH:102:ASN:ND2 | 8:LH:104:GLU:HG2 | 2.23 | 0.54 |
| 11:LK:120:ASP:OD1 | 11:LK:120:ASP:N | 2.36 | 0.54 |
| 45:S2:1025:A:H5' | 45:S2:1774:G:H4' | 1.90 | 0.54 |
| 46:SA:40:ARG:HA | 55:SJ:110:PRO:HB3 | 1.89 | 0.54 |
| 47:SB:144:GLU:HB3 | 47:SB:218:GLU:OE2 | 2.08 | 0.54 |
| 55:SJ:97:VAL:HG22 | 55:SJ:101:LYS:HD2 | 1.88 | 0.54 |
| 71:SZ:44:GLY:O | 71:SZ:48:VAL:HG12 | 2.07 | 0.54 |
| 72:Sa:9:VAL:HG22 | 72:Sa:10:GLU:H | 1.73 | 0.54 |
| 1:LA:530:G:H2' | 1:LA:531:A:C8 | 2.42 | 0.54 |
| 1:LA:1224:A:H61 | 1:LA:1284:G:N2 | 2.05 | 0.54 |
| 1:LA:1612:A:OP1 | 39:Lm:51:LEU:N | 2.40 | 0.54 |
| 1:LA:2412:A:H2' | 1:LA:2413:G:H8 | 1.72 | 0.54 |
| 1:LA:3294:A:H2' | 1:LA:3295:A:C8 | 2.43 | 0.54 |
| 3:LC:70:G:OP1 | 27:La:121:ARG:NH2 | 2.41 | 0.54 |
| 4:LD:133:TYR:HB3 | 4:LD:168:VAL:HG12 | 1.90 | 0.54 |
| 16:LP:155:VAL:O | 16:LP:162:ARG:NH2 | 2.36 | 0.54 |
| 21:LU:8:GLN:HB3 | 21:LU:64:ILE:HD11 | 1.88 | 0.54 |
| 29:Lc:75:LEU:HB3 | 29:Lc:118:ILE:HG23 | 1.89 | 0.54 |
| 45:S2:97:C:H2' | 45:S2:98:U:C6 | 2.42 | 0.54 |
| 45:S2:1452:U:H5'' | 50:SE:80:MET:HE1 | 1.88 | 0.54 |
| 62:SQ:24:PHE:CG | 71:SZ:74:VAL:HG22 | 2.42 | 0.54 |
| 66:SU:163:ASP:OD1 | 66:SU:163:ASP:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 68:SW:18:PRO:O | 68:SW:23:ARG:NH2 | 2.39 | 0.54 |
| 1:LA:20:A:H2' | 1:LA:21:G:C8 | 2.41 | 0.54 |
| 1:LA:2427:U:H2' | 1:LA:2428:G:C8 | 2.42 | 0.54 |
| 2:LB:118:A:H5'' | 7:LG:253:PHE:HZ | 1.72 | 0.54 |
| 20:LT:139:VAL:O | 20:LT:143:ILE:HD13 | 2.07 | 0.54 |
| 45:S2:1047:G:C2 | 45:S2:1071:U:O4 | 2.60 | 0.54 |
| 45:S2:1214:U:H5' | 45:S2:1246:C:H1' | 1.88 | 0.54 |
| 1:LA:1192:A:OP1 | 17:LQ:49[A]:ARG:NH2 | 2.40 | 0.54 |
| 1:LA:1570:A:H2' | 1:LA:1571:U:H4' | 1.89 | 0.54 |
| 1:LA:1830:U:O2' | 3:LC:114:G:OP1 | 2.17 | 0.54 |
| 1:LA:3260:C:OP1 | 15:LO:126:GLN:NE2 | 2.36 | 0.54 |
| 3:LC:47:C:H1' | 3:LC:61:A:H2' | 1.88 | 0.54 |
| 6:LF:234:ASN:OD1 | 6:LF:236:LEU:N | 2.31 | 0.54 |
| 16:LP:99:ARG:O | 16:LP:103:GLU:HG2 | 2.08 | 0.54 |
| 20:LT:23:TRP:CE3 | 20:LT:51:VAL:HG12 | 2.43 | 0.54 |
| 45:S2:395:U:H2' | 45:S2:396:G:O4' | 2.07 | 0.54 |
| 45:S2:1556:A:OP1 | 50:SE:115:TYR:OH | 2.24 | 0.54 |
| 45:S2:1576:A:HO2' | 80:Tb:41:C:HO2' | 1.44 | 0.54 |
| 45:S2:1593:A:H2' | 45:S2:1594:G:H8 | 1.73 | 0.54 |
| 66:SU:126:LEU:HD21 | 66:SU:152:VAL:HG21 | 1.88 | 0.54 |
| 67:SV:77:ARG:HG2 | 67:SV:77:ARG:NH1 | 2.23 | 0.54 |
| 71:SZ:63:ALA:O | 71:SZ:67:VAL:HG12 | 2.08 | 0.54 |
| 1:LA:1133:G:O2' | 1:LA:2641:A:N3 | 2.33 | 0.54 |
| 1:LA:1244:A:H3' | 1:LA:1245:G:H5'' | 1.90 | 0.54 |
| 9:LI:89:ILE:HD12 | 9:LI:214:TRP:CH2 | 2.43 | 0.54 |
| 15:LO:79:ALA:O | 15:LO:82:SER:OG | 2.20 | 0.54 |
| 45:S2:221:A:N7 | 45:S2:832:U:N3 | 2.55 | 0.54 |
| 45:S2:939:A:H2' | 45:S2:940:A:C8 | 2.43 | 0.54 |
| 55:SJ:34:LEU:HD13 | 55:SJ:87:HIS:HB2 | 1.89 | 0.54 |
| 64:SS:100:ARG:NH1 | 64:SS:121:TYR:O | 2.37 | 0.54 |
| 75:Sd:27:VAL:HG23 | 75:Sd:29:HIS:CD2 | 2.42 | 0.54 |
| 1:LA:2716:U:H4' | 43:Lq:13:LYS:HD3 | 1.90 | 0.54 |
| 3:LC:21:C:OP1 | 6:LF:193:LYS:NZ | 2.36 | 0.54 |
| 14:LN:27:ASP:O | 14:LN:31:LYS:HB2 | 2.08 | 0.54 |
| 14:LN:87:ALA:O | 14:LN:91:ARG:HG3 | 2.07 | 0.54 |
| 22:LV:84:TYR:CE1 | 30:Ld:21:ILE:HG22 | 2.43 | 0.54 |
| 23:LW:61:THR:HG23 | 23:LW:62:VAL:HG13 | 1.90 | 0.54 |
| 29:Lc:36:GLY:HA3 | 29:Lc:40:HIS:CE1 | 2.43 | 0.54 |
| 45:S2:1095:U:O2' | 73:Sb:19:LYS:NZ | 2.41 | 0.54 |
| 45:S2:1173:C:H5' | 45:S2:1543:A:O2' | 2.08 | 0.54 |
| 45:S2:1486:G:H2' | 45:S2:1487:A:C8 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:LA:75:G:H1' | 14:LN:61:PRO:HG3 | 1.90 | 0.54 |
| 1:LA:1826:C:H2' | 1:LA:1827:A:C8 | 2.44 | 0.54 |
| 1:LA:3293:A:H5' | 5:LE:128:LYS:HG3 | 1.89 | 0.54 |
| 2:LB:89:G:H4' | 21:LU:84:ARG:HD3 | 1.88 | 0.54 |
| 9:LI:163:LEU:O | 9:LI:168:ILE:HD11 | 2.08 | 0.54 |
| 27:La:70:ILE:HD13 | 27:La:82:VAL:HG22 | 1.90 | 0.54 |
| 41:Lo:124:LYS:O | 41:Lo:126:LYS:NZ | 2.39 | 0.54 |
| 45:S2:65:A:O2' | 45:S2:67:A:OP2 | 2.24 | 0.54 |
| 45:S2:1069:A:OP1 | 61:SP:28:ASN:ND2 | 2.40 | 0.54 |
| 46:SA:74:GLN:HE22 | 46:SA:84:ILE:H | 1.56 | 0.54 |
| 51:SF:34:SER:HB2 | 54:SI:7:ARG:HB3 | 1.90 | 0.54 |
| 54:SI:61:VAL:HG13 | 54:SI:76:LEU:HD11 | 1.90 | 0.54 |
| 66:SU:173:TYR:CD2 | 66:SU:181:ILE:HD13 | 2.43 | 0.54 |
| 76:Se:89:ARG:HG2 | 76:Se:89:ARG:HH11 | 1.72 | 0.54 |
| 78:Sg:50:VAL:HG12 | 78:Sg:54:ARG:HG2 | 1.90 | 0.54 |
| 1:LA:47:C:OP2 | 1:LA:48:A:O2' | 2.22 | 0.53 |
| 1:LA:1665:G:H2' | 1:LA:1666:A:H8 | 1.73 | 0.53 |
| 1:LA:3049:U:O2' | 25:LY:16:GLY:O | 2.27 | 0.53 |
| 1:LA:3180:C:H2' | 1:LA:3181:G:H5'' | 1.90 | 0.53 |
| 3:LC:106:C:H4' | 3:LC:107:G:H5'' | 1.90 | 0.53 |
| 31:Le:17:VAL:HG23 | 31:Le:95:ALA:HA | 1.88 | 0.53 |
| 45:S2:127:G:H1' | 45:S2:178:U:H3 | 1.73 | 0.53 |
| 45:S2:390:G:OP2 | 45:S2:390:G:N2 | 2.35 | 0.53 |
| 45:S2:953:G:H2' | 45:S2:954:G:H8 | 1.74 | 0.53 |
| 45:S2:1390:U:OP2 | 52:SG:49:LYS:NZ | 2.41 | 0.53 |
| 45:S2:1402:G:OP1 | 52:SG:5:ARG:NH1 | 2.40 | 0.53 |
| 68:SW:106:GLU:HA | 68:SW:111:THR:HG21 | 1.89 | 0.53 |
| 75:Sd:68:LYS:NZ | 75:Sd:70:VAL:HG22 | 2.23 | 0.53 |
| 1:LA:49:A:N7 | 16:LP:187:ARG:HD3 | 2.23 | 0.53 |
| 1:LA:727:G:H5'' | 19:LS:43:PRO:HB2 | 1.90 | 0.53 |
| 1:LA:2111:U:H4' | 1:LA:2112:A:OP2 | 2.07 | 0.53 |
| 1:LA:2375:G:H2' | 1:LA:2376:G:C8 | 2.44 | 0.53 |
| 1:LA:3163:C:N4 | 1:LA:3283:G:O6 | 2.42 | 0.53 |
| 7:LG:278:SER:OG | 7:LG:280:GLU:OE1 | 2.22 | 0.53 |
| 16:LP:45:PRO:O | 16:LP:49:ARG:HG3 | 2.08 | 0.53 |
| 51:SF:13:LYS:HG3 | 51:SF:14:LYS:H | 1.73 | 0.53 |
| 60:SO:107:LYS:N | 60:SO:128:ASP:OD2 | 2.41 | 0.53 |
| 1:LA:68:C:O3' | 16:LP:177:GLY:HA2 | 2.07 | 0.53 |
| 1:LA:1377:U:H2' | 1:LA:1378:G:H8 | 1.73 | 0.53 |
| 4:LD:180:LEU:HD22 | 44:Lr:18:TYR:HB3 | 1.91 | 0.53 |
| 31:Le:43:ILE:HB | 31:Le:90:VAL:HG13 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:803:A:HO2' | 45:S2:804:A:H8 | 1.56 | 0.53 |
| 47:SB:161:ASP:OD1 | 57:SL:42:ARG:NH1 | 2.42 | 0.53 |
| 51:SF:30:LYS:NZ | 54:SI:8:ASP:OD1 | 2.40 | 0.53 |
| 60:SO:205:SER:OG | 60:SO:207:ASP:OD1 | 2.24 | 0.53 |
| 60:SO:264:SER:O | 60:SO:267:PRO:HD2 | 2.09 | 0.53 |
| 64:SS:192:ILE:HD13 | 64:SS:242:LYS:O | 2.09 | 0.53 |
| 74:Sc:86:PHE:CE2 | 74:Sc:88:PRO:HA | 2.42 | 0.53 |
| 78:Sg:14:VAL:HA | 78:Sg:17:GLN:HE21 | 1.73 | 0.53 |
| 1:LA:308:A:C6 | 1:LA:309:U:H1' | 2.43 | 0.53 |
| 1:LA:760:A:C2 | 1:LA:770:A:H1' | 2.44 | 0.53 |
| 1:LA:2915:U:H5 | 1:LA:2934:U:HO2' | 1.57 | 0.53 |
| 1:LA:3267:A:H3' | 1:LA:3268:U:H2' | 1.90 | 0.53 |
| 15:LO:112:LEU:HD12 | 15:LO:116:GLU:HB3 | 1.90 | 0.53 |
| 18:LR:29:THR:HB | 18:LR:119:VAL:HG21 | 1.90 | 0.53 |
| 29:Lc:22:ILE:HD12 | 29:Lc:22:ILE:H | 1.72 | 0.53 |
| 33:Lg:111:ARG:HE | 33:Lg:115:LEU:HD21 | 1.72 | 0.53 |
| 45:S2:88:U:H4' | 45:S2:171:A:H5'' | 1.90 | 0.53 |
| 45:S2:1120:U:H2' | 45:S2:1121:C:C6 | 2.44 | 0.53 |
| 45:S2:1454:G:H4' | 50:SE:122:THR:HG21 | 1.91 | 0.53 |
| 56:SK:61:SER:H | 56:SK:64:VAL:HB | 1.73 | 0.53 |
| 75:Sd:114:ARG:HA | 75:Sd:117:LYS:HE3 | 1.90 | 0.53 |
| 1:LA:3106:U:H2' | 1:LA:3107:G:C8 | 2.42 | 0.53 |
| 1:LA:3174:U:H5' | 34:Lh:10:LYS:HE2 | 1.90 | 0.53 |
| 3:LC:9:A:H2' | 3:LC:10:A:C8 | 2.43 | 0.53 |
| 7:LG:261:THR:HG22 | 7:LG:263:GLU:H | 1.73 | 0.53 |
| 9:LI:116:PHE:O | 9:LI:199:ASN:ND2 | 2.42 | 0.53 |
| 10:LJ:81:THR:HG21 | 10:LJ:181:LYS:HD3 | 1.90 | 0.53 |
| 30:Ld:5:LYS:HE3 | 30:Ld:8:THR:HB | 1.91 | 0.53 |
| 32:Lf:11:GLU:OE1 | 32:Lf:96:VAL:HG21 | 2.09 | 0.53 |
| 43:Lq:25:VAL:HG22 | 43:Lq:72:LEU:CD2 | 2.38 | 0.53 |
| 45:S2:415:C:H2' | 45:S2:416:A:H5'' | 1.90 | 0.53 |
| 45:S2:639:U:H4' | 45:S2:640:U:O5' | 2.08 | 0.53 |
| 45:S2:1211:A:O2' | 50:SE:99:GLY:O | 2.15 | 0.53 |
| 47:SB:53:VAL:HG13 | 47:SB:55:ASP:H | 1.74 | 0.53 |
| 47:SB:205:SER:OG | 47:SB:207:THR:OG1 | 2.23 | 0.53 |
| 60:SO:153:GLN:OE1 | 60:SO:202:LEU:N | 2.42 | 0.53 |
| 61:SP:140:ASN:ND2 | 72:Sa:31:SER:O | 2.42 | 0.53 |
| 65:ST:74:LYS:CE | 65:ST:96:SER:HB2 | 2.38 | 0.53 |
| 65:ST:137:ARG:HB3 | 65:ST:140:ASN:HB2 | 1.91 | 0.53 |
| 70:SY:101:HIS:HA | 70:SY:104:ARG:NH2 | 2.24 | 0.53 |
| 1:LA:820:U:H2' | 1:LA:821:G:H8 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:915:G:H5' | 1:LA:916:A:OP1 | 2.09 | 0.53 |
| 1:LA:2882:U:H2' | 1:LA:2883:C:C6 | 2.43 | 0.53 |
| 1:LA:3297:C:C2 | 1:LA:3298:A:C8 | 2.97 | 0.53 |
| 5:LE:37:ARG:HH12 | 5:LE:191:LYS:HZ1 | 1.56 | 0.53 |
| 12:LL:207:GLU:OE1 | 12:LL:207:GLU:N | 2.33 | 0.53 |
| 15:LO:108:ARG:O | 15:LO:112:LEU:HD22 | 2.07 | 0.53 |
| 23:LW:101:ASN:HA | 23:LW:103:TYR:CZ | 2.44 | 0.53 |
| 33:Lg:74:PHE:CG | 33:Lg:85:LEU:HD11 | 2.44 | 0.53 |
| 45:S2:126:A:OP2 | 65:ST:197:ASN:ND2 | 2.31 | 0.53 |
| 45:S2:1262:U:H2' | 45:S2:1263:G:C8 | 2.43 | 0.53 |
| 47:SB:161:ASP:HB2 | 47:SB:162:VAL:HG23 | 1.90 | 0.53 |
| 54:SI:66:TYR:CD1 | 54:SI:124:ILE:HG21 | 2.41 | 0.53 |
| 60:SO:90:ARG:HB3 | 60:SO:92:TRP:CZ3 | 2.44 | 0.53 |
| 70:SY:87:ASP:OD1 | 70:SY:87:ASP:N | 2.40 | 0.53 |
| 1:LA:1645:G:N2 | 1:LA:1808:A:N6 | 2.33 | 0.53 |
| 1:LA:2616:U:H3' | 30:Ld:3:LYS:HD2 | 1.90 | 0.53 |
| 12:LL:52:LEU:HB3 | 12:LL:136:PHE:HB2 | 1.89 | 0.53 |
| 12:LL:182:LEU:HD12 | 12:LL:185:ARG:HH21 | 1.74 | 0.53 |
| 13:LM:54:VAL:CG2 | 13:LM:56:THR:HG22 | 2.39 | 0.53 |
| 45:S2:1087:A:H2' | 45:S2:1088:A:C8 | 2.43 | 0.53 |
| 46:SA:17:PHE:HA | 46:SA:20:GLU:HG3 | 1.91 | 0.53 |
| 66:SU:38:LEU:HA | 66:SU:41:LEU:HG | 1.90 | 0.53 |
| 1:LA:253:A:O2' | 1:LA:254:A:OP1 | 2.22 | 0.53 |
| 1:LA:398:A:O2' | 1:LA:1415:C:OP1 | 2.23 | 0.53 |
| 1:LA:1860:G:O2' | 1:LA:3065:U:OP1 | 2.26 | 0.53 |
| 1:LA:2780:U:O2' | 14:LN:185:LYS:HD3 | 2.09 | 0.53 |
| 7:LG:187:THR:OG1 | 7:LG:189:GLU:OE1 | 2.25 | 0.53 |
| 12:LL:182:LEU:O | 12:LL:186:GLU:HG2 | 2.09 | 0.53 |
| 45:S2:1543:A:N6 | 45:S2:1567:U:H3 | 2.02 | 0.53 |
| 51:SF:7:VAL:HG12 | 51:SF:22:VAL:HB | 1.91 | 0.53 |
| 51:SF:132:LYS:HG3 | 51:SF:138:PHE:HE1 | 1.73 | 0.53 |
| 55:SJ:37:VAL:HA | 55:SJ:40:ASN:HD21 | 1.74 | 0.53 |
| 61:SP:103:THR:O | 61:SP:106:SER:OG | 2.27 | 0.53 |
| 64:SS:104:ASP:OD2 | 64:SS:108:ARG:NH2 | 2.35 | 0.53 |
| 1:LA:309:U:O4 | 1:LA:2779:A:N6 | 2.40 | 0.53 |
| 1:LA:1210:U:H2' | 1:LA:1211:A:C8 | 2.43 | 0.53 |
| 1:LA:1341:C:H2' | 1:LA:1342:A:C8 | 2.44 | 0.53 |
| 1:LA:2963:G:N2 | 1:LA:2966:A:OP2 | 2.35 | 0.53 |
| 2:LB:90:U:H2' | 2:LB:91:G:O4' | 2.09 | 0.53 |
| 5:LE:204:ALA:O | 5:LE:207:SER:OG | 2.25 | 0.53 |
| 11:LK:90:MET:HE1 | 11:LK:161:LEU:HD22 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:LR:122:ALA:HB3 | 18:LR:143:PRO:HB2 | 1.91 | 0.53 |
| 26:LZ:129:ASP:OD1 | 26:LZ:129:ASP:N | 2.41 | 0.53 |
| 27:La:23:PRO:HG2 | 27:La:26:GLN:HG3 | 1.89 | 0.53 |
| 45:S2:17:C:H2' | 45:S2:18:C:C6 | 2.44 | 0.53 |
| 45:S2:592:A:H2' | 45:S2:593:U:O4' | 2.09 | 0.53 |
| 45:S2:1564:U:OP1 | 54:SI:38:LYS:NZ | 2.30 | 0.53 |
| 48:SC:73:VAL:HG13 | 48:SC:77:ARG:HH21 | 1.74 | 0.53 |
| 1:LA:401:U:O2' | 40:Ln:36:ARG:NH2 | 2.42 | 0.53 |
| 1:LA:3293:A:H2' | 1:LA:3294:A:O4' | 2.09 | 0.53 |
| 3:LC:150:G:OP1 | 26:LZ:27:ARG:NH2 | 2.42 | 0.53 |
| 10:LJ:183:LYS:HB2 | 10:LJ:194:THR:HG23 | 1.91 | 0.53 |
| 15:LO:73:PRO:HG2 | 15:LO:76:ALA:HB2 | 1.90 | 0.53 |
| 27:La:63:LYS:HD2 | 27:La:85:VAL:HG13 | 1.90 | 0.53 |
| 44:Lr:36:ARG:HG3 | 44:Lr:48:LYS:HD3 | 1.90 | 0.53 |
| 45:S2:108:A:H2' | 45:S2:109:G:C8 | 2.44 | 0.53 |
| 45:S2:1335:U:H3 | 45:S2:1416:G:H1 | 1.57 | 0.53 |
| 67:SV:67:TRP:HB3 | 67:SV:72:ILE:HG22 | 1.90 | 0.53 |
| 71:SZ:13:VAL:HG23 | 71:SZ:76:ILE:HA | 1.91 | 0.53 |
| 1:LA:2417:G:N3 | 80:Tb:73:A:N6 | 2.56 | 0.52 |
| 3:LC:142:C:H2' | 3:LC:143:U:C6 | 2.44 | 0.52 |
| 15:LO:49:PRO:HB3 | 15:LO:78:THR:HG23 | 1.91 | 0.52 |
| 27:La:79:ALA:HB1 | 27:La:98:ASN:HB3 | 1.90 | 0.52 |
| 28:Lb:106:GLN:NE2 | 28:Lb:109:GLU:OE1 | 2.42 | 0.52 |
| 45:S2:683:C:OP1 | 45:S2:684:A:N6 | 2.39 | 0.52 |
| 46:SA:120:TYR:HA | 46:SA:123:VAL:HG12 | 1.91 | 0.52 |
| 52:SG:75:GLU:HA | 52:SG:78:ARG:HG2 | 1.92 | 0.52 |
| 54:SI:40:SER:OG | 54:SI:41:SER:N | 2.42 | 0.52 |
| 56:SK:53:GLU:HG2 | 56:SK:57:TYR:HE2 | 1.73 | 0.52 |
| 60:SO:116:ASP:OD1 | 60:SO:120:SER:N | 2.42 | 0.52 |
| 79:Ta:10:G:O6 | 79:Ta:25:U:O2 | 2.27 | 0.52 |
| 79:Ta:76:C:H2' | 79:Ta:77:A:C8 | 2.43 | 0.52 |
| 1:LA:1870:U:H2' | 1:LA:1871:C:O2 | 2.09 | 0.52 |
| 6:LF:358:THR:HG21 | 22:LV:148:PRO:HG2 | 1.92 | 0.52 |
| 10:LJ:97:TYR:OH | 10:LJ:204:ARG:N | 2.29 | 0.52 |
| 15:LO:65:LEU:HD11 | 21:LU:152:LEU:HD12 | 1.91 | 0.52 |
| 23:LW:81:LYS:HZ3 | 23:LW:90:ARG:CZ | 2.23 | 0.52 |
| 45:S2:187:G:N2 | 45:S2:197:A:H61 | 2.06 | 0.52 |
| 45:S2:1452:U:O2' | 50:SE:79:HIS:HB3 | 2.10 | 0.52 |
| 45:S2:1573:A:H62 | 47:SB:181:GLU:HA | 1.74 | 0.52 |
| 48:SC:30:ALA:HA | 48:SC:38:LYS:HG2 | 1.90 | 0.52 |
| 50:SE:32:ASP:HA | 50:SE:35:LYS:HG2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:SE:38:PRO:O | 50:SE:42:ARG:HG3 | 2.10 | 0.52 |
| 54:SI:5:SER:O | 54:SI:9:VAL:HG23 | 2.09 | 0.52 |
| 62:SQ:113:MET:HE3 | 62:SQ:142:PHE:HE2 | 1.74 | 0.52 |
| 62:SQ:144:ARG:HB3 | 62:SQ:208:GLN:HB3 | 1.92 | 0.52 |
| 65:ST:64:LYS:HG3 | 65:ST:83:CYS:SG | 2.49 | 0.52 |
| 68:SW:71:PHE:CD1 | 68:SW:71:PHE:C | 2.87 | 0.52 |
| 68:SW:136:VAL:O | 68:SW:152:SER:OG | 2.27 | 0.52 |
| 1:LA:1316:A:O2' | 1:LA:1317:A:H3' | 2.09 | 0.52 |
| 1:LA:1481:A:OP2 | 1:LA:1857:A:O2' | 2.28 | 0.52 |
| 1:LA:2159:G:H2' | 1:LA:2160:G:C8 | 2.43 | 0.52 |
| 1:LA:2673:A:C2 | 13:LM:124:GLY:HA3 | 2.44 | 0.52 |
| 1:LA:2708:C:H2' | 1:LA:2709:C:C6 | 2.44 | 0.52 |
| 40:Ln:25:GLN:HE22 | 40:Ln:28:ARG:HH11 | 1.57 | 0.52 |
| 45:S2:323:A:H5'' | 67:SV:11:ARG:HD2 | 1.92 | 0.52 |
| 46:SA:70:THR:HB | 46:SA:86:LEU:HB2 | 1.91 | 0.52 |
| 47:SB:26:ALA:HB3 | 51:SF:26:LYS:NZ | 2.24 | 0.52 |
| 75:Sd:29:HIS:HB2 | 75:Sd:32:ARG:HG3 | 1.91 | 0.52 |
| 79:Ta:16:C:H5' | 79:Ta:17:C:H5 | 1.74 | 0.52 |
| 1:LA:2217:G:H2' | 1:LA:2218:A:C8 | 2.44 | 0.52 |
| 1:LA:2412:A:H2' | 1:LA:2413:G:C8 | 2.45 | 0.52 |
| 6:LF:106:TRP:CZ2 | 14:LN:19:GLN:HG2 | 2.44 | 0.52 |
| 6:LF:215:ILE:HD12 | 6:LF:219:LEU:HD23 | 1.91 | 0.52 |
| 7:LG:266:ALA:O | 7:LG:270:LYS:HB2 | 2.09 | 0.52 |
| 9:LI:116:PHE:CE1 | 9:LI:144:ILE:HG12 | 2.45 | 0.52 |
| 45:S2:107:C:H2' | 45:S2:108:A:H8 | 1.73 | 0.52 |
| 45:S2:340:U:H2' | 45:S2:341:A:C8 | 2.45 | 0.52 |
| 45:S2:358:U:O2' | 45:S2:360:A:OP1 | 2.21 | 0.52 |
| 45:S2:764:U:O2 | 45:S2:772:G:O6 | 2.26 | 0.52 |
| 51:SF:93:HIS:HD2 | 51:SF:105:LEU:HD22 | 1.74 | 0.52 |
| 55:SJ:36:ASN:O | 55:SJ:40:ASN:ND2 | 2.42 | 0.52 |
| 61:SP:30:GLN:HE22 | 61:SP:149:LEU:HB3 | 1.73 | 0.52 |
| 62:SQ:24:PHE:HE2 | 71:SZ:70:LYS:HE3 | 1.71 | 0.52 |
| 62:SQ:96:LEU:O | 62:SQ:96:LEU:HD12 | 2.10 | 0.52 |
| 70:SY:33:VAL:HG21 | 70:SY:66:ILE:HG21 | 1.91 | 0.52 |
| 1:LA:524:C:H2' | 1:LA:525:C:H6 | 1.73 | 0.52 |
| 1:LA:2838:G:O6 | 1:LA:2844:A:O2' | 2.20 | 0.52 |
| 6:LF:260:GLN:OE1 | 6:LF:260:GLN:N | 2.43 | 0.52 |
| 8:LH:60:ASP:OD1 | 8:LH:62:THR:OG1 | 2.26 | 0.52 |
| 9:LI:180:SER:OG | 9:LI:183:ASP:OD1 | 2.26 | 0.52 |
| 28:Lb:106:GLN:HA | 28:Lb:109:GLU:CG | 2.39 | 0.52 |
| 45:S2:107:C:H2' | 45:S2:108:A:C8 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1181:U:N3 | 45:S2:1458:G:N1 | 2.57 | 0.52 |
| 73:Sb:29:PRO:HB2 | 73:Sb:58:SER:HB3 | 1.91 | 0.52 |
| 10:LJ:111:LYS:HD2 | 10:LJ:111:LYS:C | 2.35 | 0.52 |
| 16:LP:16:SER:O | 16:LP:20:ARG:HG3 | 2.10 | 0.52 |
| 45:S2:183:U:H2' | 45:S2:184:C:C6 | 2.45 | 0.52 |
| 45:S2:1592:A:H2' | 45:S2:1593:A:C8 | 2.44 | 0.52 |
| 48:SC:50:THR:HG22 | 48:SC:55:VAL:HG13 | 1.90 | 0.52 |
| 52:SG:106:THR:O | 52:SG:110:VAL:HG23 | 2.10 | 0.52 |
| 60:SO:43:ILE:HD11 | 60:SO:57:PRO:HB3 | 1.92 | 0.52 |
| 64:SS:191:ARG:NH2 | 64:SS:244:ILE:O | 2.42 | 0.52 |
| 1:LA:619:U:H1' | 34:Lh:60:ARG:HH22 | 1.75 | 0.52 |
| 1:LA:815:A:H5' | 1:LA:905:A:N6 | 2.23 | 0.52 |
| 1:LA:1314:U:OP2 | 17:LQ:44[A]:SER:OG | 2.20 | 0.52 |
| 1:LA:2991:U:OP1 | 1:LA:3309:A:O2' | 2.12 | 0.52 |
| 7:LG:41:LYS:HB2 | 22:LV:68:THR:O | 2.10 | 0.52 |
| 19:LS:152:HIS:ND1 | 19:LS:162:ALA:O | 2.32 | 0.52 |
| 24:LX:15:LEU:HD13 | 24:LX:51:ALA:HB3 | 1.92 | 0.52 |
| 45:S2:502:U:H2' | 45:S2:503:G:H8 | 1.74 | 0.52 |
| 45:S2:804:A:OP1 | 66:SU:101:LYS:NZ | 2.41 | 0.52 |
| 46:SA:162:GLN:N | 46:SA:163:PRO:HD2 | 2.25 | 0.52 |
| 47:SB:166:ARG:HH12 | 57:SL:45:LYS:HE2 | 1.74 | 0.52 |
| 49:SD:75:VAL:HA | 49:SD:78:LEU:HG | 1.92 | 0.52 |
| 50:SE:22:LEU:HA | 50:SE:25:LEU:HG | 1.92 | 0.52 |
| 62:SQ:3:VAL:HG22 | 71:SZ:49:LYS:HA | 1.91 | 0.52 |
| 63:SR:41:LEU:HD11 | 63:SR:56:ILE:HD11 | 1.91 | 0.52 |
| 67:SV:74:LYS:NZ | 67:SV:112:TRP:HE3 | 2.07 | 0.52 |
| 1:LA:266:A:N6 | 37:Lk:30:LYS:HA | 2.25 | 0.52 |
| 1:LA:688:U:O4 | 6:LF:209:TYR:OH | 2.20 | 0.52 |
| 10:LJ:143:ILE:HG23 | 10:LJ:175:VAL:HG11 | 1.92 | 0.52 |
| 11:LK:90:MET:HE3 | 11:LK:144:ILE:HG23 | 1.92 | 0.52 |
| 12:LL:140:THR:HG21 | 12:LL:148:VAL:HG21 | 1.92 | 0.52 |
| 28:Lb:121:ARG:HD2 | 28:Lb:127:ASN:ND2 | 2.25 | 0.52 |
| 45:S2:834:G:N2 | 45:S2:835:U:O4 | 2.43 | 0.52 |
| 50:SE:34:VAL:O | 50:SE:42:ARG:HG2 | 2.09 | 0.52 |
| 51:SF:26:LYS:HG3 | 51:SF:28:LEU:HD23 | 1.91 | 0.52 |
| 65:ST:220:LYS:HA | 65:ST:223:LYS:HE2 | 1.91 | 0.52 |
| 68:SW:127:VAL:HA | 68:SW:130:THR:CG2 | 2.40 | 0.52 |
| 75:Sd:83:LYS:HE2 | 75:Sd:96:LEU:HB3 | 1.91 | 0.52 |
| 1:LA:1109:U:H2' | 1:LA:1110:U:C6 | 2.44 | 0.52 |
| 1:LA:2914:U:C5 | 5:LE:7:GLU:HG2 | 2.45 | 0.52 |
| 6:LF:295:ILE:O | 6:LF:299:ILE:HD13 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:LM:32:ARG:NH1 | 13:LM:119:SER:O | 2.42 | 0.52 |
| 33:Lg:83:GLU:O | 33:Lg:86:THR:OG1 | 2.21 | 0.52 |
| 45:S2:551:G:H2' | 45:S2:552:G:H8 | 1.75 | 0.52 |
| 45:S2:904:G:H2' | 45:S2:905:A:H5'' | 1.91 | 0.52 |
| 45:S2:1794:A:H1' | 76:Se:79:ILE:HD13 | 1.92 | 0.52 |
| 46:SA:40:ARG:HH12 | 46:SA:46:THR:HA | 1.75 | 0.52 |
| 53:SH:29:VAL:O | 53:SH:33:THR:HG23 | 2.09 | 0.52 |
| 61:SP:107:PHE:HB3 | 61:SP:139:VAL:HG21 | 1.92 | 0.52 |
| 64:SS:182:TYR:N | 64:SS:226:PHE:O | 2.29 | 0.52 |
| 66:SU:150:GLN:O | 66:SU:181:ILE:HA | 2.10 | 0.52 |
| 72:Sa:60:ARG:HG2 | 72:Sa:60:ARG:HH11 | 1.75 | 0.52 |
| 73:Sb:6:VAL:HG12 | 73:Sb:34:ILE:HD11 | 1.91 | 0.52 |
| 77:Sf:19:HIS:HB3 | 77:Sf:22:LYS:HG3 | 1.92 | 0.52 |
| 1:LA:190:U:H2' | 27:La:60:ARG:NH2 | 2.24 | 0.52 |
| 1:LA:258:G:H2' | 1:LA:258:G:N3 | 2.25 | 0.52 |
| 1:LA:393:U:H2' | 1:LA:394:G:O4' | 2.10 | 0.52 |
| 1:LA:791:G:H2' | 1:LA:792:C:C6 | 2.45 | 0.52 |
| 1:LA:1720:U:OP2 | 20:LT:124:TYR:OH | 2.27 | 0.52 |
| 1:LA:3010:A:N1 | 1:LA:3042:C:O2' | 2.38 | 0.52 |
| 6:LF:362:ASP:HA | 21:LU:28:ARG:HH11 | 1.75 | 0.52 |
| 45:S2:623:A:H3' | 45:S2:624:G:H5'' | 1.92 | 0.52 |
| 45:S2:754:A:N6 | 45:S2:793:A:OP2 | 2.43 | 0.52 |
| 45:S2:821:U:N3 | 45:S2:852:C:N4 | 2.35 | 0.52 |
| 47:SB:75:GLY:HA3 | 47:SB:77:TYR:CZ | 2.45 | 0.52 |
| 61:SP:31:VAL:HG12 | 61:SP:33:GLN:H | 1.74 | 0.52 |
| 62:SQ:52:THR:OG1 | 62:SQ:53:GLY:N | 2.42 | 0.52 |
| 65:ST:139:ASN:O | 65:ST:143:LYS:HG3 | 2.09 | 0.52 |
| 71:SZ:17:ALA:HB1 | 71:SZ:19:ILE:HD11 | 1.92 | 0.52 |
| 1:LA:353:G:O6 | 38:Ll:55:ARG:NH2 | 2.43 | 0.51 |
| 1:LA:422:A:C2 | 1:LA:2362:A:H4' | 2.45 | 0.51 |
| 1:LA:642:U:O2' | 1:LA:1152:A:N1 | 2.29 | 0.51 |
| 1:LA:780:G:OP1 | 19:LS:151:ARG:NH1 | 2.43 | 0.51 |
| 1:LA:1638:C:OP2 | 35:Li:74:ARG:NH1 | 2.41 | 0.51 |
| 1:LA:1803:A:H2' | 1:LA:1804:C:C6 | 2.45 | 0.51 |
| 1:LA:1947:G:H2' | 1:LA:1948:G:H8 | 1.73 | 0.51 |
| 3:LC:94:C:OP1 | 38:Ll:75:LYS:NZ | 2.38 | 0.51 |
| 45:S2:1480:G:H3' | 45:S2:1481:C:C6 | 2.45 | 0.51 |
| 45:S2:1544:U:H5'' | 53:SH:132:ARG:HE | 1.74 | 0.51 |
| 47:SB:143:ARG:HG2 | 57:SL:57:MET:CE | 2.39 | 0.51 |
| 69:SX:75:VAL:HG12 | 69:SX:84:ILE:HD13 | 1.91 | 0.51 |
| 74:Sc:62:LYS:HG2 | 74:Sc:63:GLN:H | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 1:LA:262:U:H2' | 1:LA:263:C:O4' | 2.09 | 0.51 |
| 1:LA:973:G:H2' | 1:LA:974:C:H6 | 1.75 | 0.51 |
| 1:LA:1806:G:H8 | 1:LA:1806:G:OP2 | 1.92 | 0.51 |
| 1:LA:1912:A:N3 | 1:LA:2119:A:H2' | 2.25 | 0.51 |
| 1:LA:2283:C:O2' | 1:LA:2284:C:OP1 | 2.27 | 0.51 |
| 1:LA:2351:A:H5'' | 18:LR:83:TRP:O | 2.09 | 0.51 |
| 1:LA:2566:C:H2' | 1:LA:2567:C:H6 | 1.75 | 0.51 |
| 11:LK:94:TYR:HA | 11:LK:177:ASP:OD1 | 2.10 | 0.51 |
| 17:LQ:116[A]:LYS:NZ | 21:LU:165:TYR:O | 2.30 | 0.51 |
| 24:LX:5:GLY:HA3 | 24:LX:106:LYS:O | 2.10 | 0.51 |
| 45:S2:607:G:H5' | 45:S2:613:G:N2 | 2.25 | 0.51 |
| 45:S2:837:G:P | 45:S2:837:G:H8 | 2.33 | 0.51 |
| 45:S2:1373:C:H2' | 45:S2:1374:C:C6 | 2.46 | 0.51 |
| 46:SA:8:LYS:HE2 | 55:SJ:63:LEU:HD22 | 1.92 | 0.51 |
| 52:SG:110:VAL:HG11 | 52:SG:117:LEU:HD21 | 1.92 | 0.51 |
| 64:SS:121:TYR:CG | 64:SS:161:LYS:HE3 | 2.45 | 0.51 |
| 67:SV:37:LYS:H | 67:SV:59:ARG:H | 1.57 | 0.51 |
| 67:SV:61:GLU:HG3 | 67:SV:62:THR:HG23 | 1.93 | 0.51 |
| 1:LA:506:U:H2' | 1:LA:507:U:H6 | 1.74 | 0.51 |
| 1:LA:524:C:OP2 | 15:LO:77:ARG:NH1 | 2.44 | 0.51 |
| 1:LA:1119:A:N6 | 1:LA:1137:U:H3 | 2.06 | 0.51 |
| 1:LA:2356:A:H2' | 1:LA:2357:A:H8 | 1.74 | 0.51 |
| 1:LA:2372:A:N3 | 1:LA:2823:G:O2' | 2.30 | 0.51 |
| 1:LA:2827:G:O2' | 12:LL:4:ARG:NH2 | 2.42 | 0.51 |
| 7:LG:235:SER:O | 7:LG:239:ILE:HG23 | 2.09 | 0.51 |
| 10:LJ:33:ASN:HD22 | 10:LJ:38:GLN:HG3 | 1.73 | 0.51 |
| 13:LM:32:ARG:CZ | 13:LM:119:SER:O | 2.58 | 0.51 |
| 15:LO:120:VAL:HG23 | 17:LQ:197[A]:LEU:HD23 | 1.92 | 0.51 |
| 36:Lj:5:LYS:O | 36:Lj:8:GLU:HG2 | 2.10 | 0.51 |
| 36:Lj:31:LEU:HA | 36:Lj:34:GLN:HG3 | 1.93 | 0.51 |
| 45:S2:140:A:OP1 | 65:ST:187:LYS:NZ | 2.40 | 0.51 |
| 45:S2:456:A:H2' | 45:S2:457:G:C8 | 2.46 | 0.51 |
| 45:S2:1262:U:H2' | 45:S2:1263:G:H8 | 1.75 | 0.51 |
| 45:S2:1579:U:O3' | 51:SF:140:LYS:HB2 | 2.09 | 0.51 |
| 54:SI:73:VAL:O | 54:SI:77:ASN:ND2 | 2.43 | 0.51 |
| 66:SU:99:LEU:HD13 | 66:SU:116:ARG:HG2 | 1.92 | 0.51 |
| 75:Sd:29:HIS:CE1 | 75:Sd:34:ASN:HA | 2.45 | 0.51 |
| 1:LA:628:U:H2' | 1:LA:629:A:C8 | 2.45 | 0.51 |
| 1:LA:639:U:H2' | 1:LA:640:C:C6 | 2.46 | 0.51 |
| 1:LA:2785:G:N2 | 29:Lc:58:MET:SD | 2.79 | 0.51 |
| 3:LC:25:G:N7 | 27:La:13:ARG:NH1 | 2.54 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 4:LD:19:HIS:ND1 | 4:LD:190:ARG:O | 2.36 | 0.51 |
| 6:LF:104:LYS:HD2 | 6:LF:106:TRP:CZ2 | 2.46 | 0.51 |
| 6:LF:203:ARG:NE | 6:LF:226:GLU:OE2 | 2.42 | 0.51 |
| 9:LI:116:PHE:CZ | 9:LI:144:ILE:HG12 | 2.44 | 0.51 |
| 9:LI:147:LEU:HD21 | 9:LI:207:LEU:HD21 | 1.92 | 0.51 |
| 15:LO:10:SER:HB2 | 15:LO:12:TRP:HZ3 | 1.75 | 0.51 |
| 31:Le:74:ASN:OD1 | 31:Le:74:ASN:N | 2.42 | 0.51 |
| 43:Lq:72:LEU:HG | 43:Lq:83:LEU:HD21 | 1.92 | 0.51 |
| 50:SE:89:MET:SD | 50:SE:89:MET:N | 2.81 | 0.51 |
| 60:SO:303:ALA:HB3 | 60:SO:313:TRP:HZ3 | 1.75 | 0.51 |
| 62:SQ:30:PHE:CD2 | 62:SQ:94:LYS:HA | 2.46 | 0.51 |
| 5:LE:94:GLU:HG3 | 17:LQ:152[A]:VAL:HG13 | 1.92 | 0.51 |
| 7:LG:257:GLU:N | 7:LG:257:GLU:OE2 | 2.44 | 0.51 |
| 27:La:56:VAL:HG21 | 27:La:104:LEU:HD13 | 1.93 | 0.51 |
| 45:S2:513:U:H2' | 45:S2:514:G:C8 | 2.45 | 0.51 |
| 45:S2:654:C:N4 | 45:S2:678:A:N7 | 2.58 | 0.51 |
| 48:SC:54:TYR:CD1 | 48:SC:72:GLY:HA2 | 2.45 | 0.51 |
| 50:SE:118:GLU:O | 53:SH:122:HIS:N | 2.44 | 0.51 |
| 54:SI:108:LEU:HB3 | 54:SI:114:VAL:HB | 1.92 | 0.51 |
| 60:SO:175:ASP:HB3 | 60:SO:177:MET:HG2 | 1.93 | 0.51 |
| 3:LC:8:C:H2' | 3:LC:9:A:C8 | 2.46 | 0.51 |
| 4:LD:102:LEU:HD13 | 4:LD:166:ILE:HD11 | 1.92 | 0.51 |
| 5:LE:44:THR:OG1 | 5:LE:182:GLN:O | 2.29 | 0.51 |
| 10:LJ:157:VAL:HG21 | 10:LJ:163:VAL:HG22 | 1.92 | 0.51 |
| 12:LL:55:ASN:OD1 | 12:LL:164:LYS:HE2 | 2.10 | 0.51 |
| 15:LO:32:LEU:HD11 | 15:LO:94:TRP:CG | 2.46 | 0.51 |
| 18:LR:20:SER:HB3 | 18:LR:21:TYR:CD1 | 2.45 | 0.51 |
| 28:Lb:23:VAL:HG12 | 28:Lb:45:GLY:HA3 | 1.92 | 0.51 |
| 45:S2:372:G:H5'' | 45:S2:373:G:OP2 | 2.10 | 0.51 |
| 45:S2:385:A:H5'' | 67:SV:22:ARG:HG2 | 1.93 | 0.51 |
| 45:S2:1322:A:H2' | 45:S2:1323:C:C6 | 2.45 | 0.51 |
| 45:S2:1471:A:N6 | 45:S2:1538:U:H3 | 2.06 | 0.51 |
| 47:SB:92:ARG:HG2 | 47:SB:92:ARG:HH11 | 1.76 | 0.51 |
| 69:SX:123:VAL:HG12 | 69:SX:142:VAL:HA | 1.93 | 0.51 |
| 1:LA:509:G:H1 | 1:LA:580:U:H3 | 1.57 | 0.51 |
| 1:LA:1925:C:H5'' | 44:Lr:7:LYS:HD3 | 1.92 | 0.51 |
| 9:LI:102:VAL:HG13 | 9:LI:126:LEU:HG | 1.92 | 0.51 |
| 15:LO:109:ARG:HA | 15:LO:112:LEU:CD2 | 2.41 | 0.51 |
| 17:LQ:56[A]:ASP:OD1 | 17:LQ:59[A]:ARG:NH2 | 2.44 | 0.51 |
| 45:S2:331:A:H2' | 45:S2:332:U:C6 | 2.45 | 0.51 |
| 45:S2:1469:A:O2' | 45:S2:1540:G:N2 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:SB:99:MET:O | 47:SB:103:ASN:HB2 | 2.11 | 0.51 |
| 64:SS:248:ILE:HG13 | 68:SW:71:PHE:HE2 | 1.75 | 0.51 |
| 71:SZ:40:ALA:HB3 | 71:SZ:67:VAL:HG23 | 1.92 | 0.51 |
| 1:LA:430:U:H2' | 1:LA:431:U:C6 | 2.45 | 0.51 |
| 5:LE:50:LYS:HG2 | 5:LE:332:ARG:HA | 1.92 | 0.51 |
| 6:LF:23:PRO:HD2 | 6:LF:26:PHE:CD2 | 2.46 | 0.51 |
| 12:LL:30:LYS:HG2 | 12:LL:63:GLU:HG3 | 1.93 | 0.51 |
| 14:LN:89:TYR:O | 14:LN:92:THR:HG22 | 2.11 | 0.51 |
| 24:LX:35:TYR:CE1 | 24:LX:37:ILE:HG22 | 2.45 | 0.51 |
| 45:S2:5:U:H2' | 45:S2:6:G:C8 | 2.46 | 0.51 |
| 45:S2:112:A:C2 | 45:S2:303:U:H1' | 2.46 | 0.51 |
| 51:SF:49:TYR:HB3 | 51:SF:53:LEU:HG | 1.93 | 0.51 |
| 57:SL:39:THR:O | 57:SL:40:ILE:HD13 | 2.10 | 0.51 |
| 60:SO:33:LEU:HD23 | 60:SO:45:TRP:CD1 | 2.46 | 0.51 |
| 60:SO:66:HIS:CG | 60:SO:67:ILE:H | 2.28 | 0.51 |
| 60:SO:123:ILE:HD12 | 60:SO:154:VAL:CG1 | 2.41 | 0.51 |
| 63:SR:35:TRP:C | 63:SR:35:TRP:CD1 | 2.89 | 0.51 |
| 1:LA:177:U:C4 | 1:LA:241:G:O6 | 2.64 | 0.51 |
| 1:LA:309:U:H2' | 1:LA:310:U:C5 | 2.45 | 0.51 |
| 1:LA:830:G:O2' | 1:LA:1863:A:N3 | 2.38 | 0.51 |
| 1:LA:1348:G:H22 | 1:LA:1352:U:P | 2.34 | 0.51 |
| 1:LA:2102:U:H2' | 1:LA:2103:A:C8 | 2.46 | 0.51 |
| 1:LA:2337:C:H5'' | 24:LX:47:ASN:O | 2.11 | 0.51 |
| 1:LA:2522:A:OP1 | 26:LZ:31:THR:HG22 | 2.09 | 0.51 |
| 16:LP:68:ARG:HD3 | 16:LP:128:LYS:HG3 | 1.92 | 0.51 |
| 19:LS:116:LYS:NZ | 29:Lc:88:ASP:OD2 | 2.43 | 0.51 |
| 23:LW:27:VAL:HG22 | 23:LW:89:LEU:HD11 | 1.92 | 0.51 |
| 28:Lb:105:SER:O | 28:Lb:109:GLU:HG2 | 2.11 | 0.51 |
| 45:S2:959:U:O2 | 77:Sf:30:SER:OG | 2.28 | 0.51 |
| 45:S2:1608:U:H2' | 45:S2:1609:U:C6 | 2.46 | 0.51 |
| 47:SB:128:ASN:HB3 | 47:SB:131:GLN:HB3 | 1.92 | 0.51 |
| 49:SD:135:MET:O | 49:SD:138:GLU:HG3 | 2.11 | 0.51 |
| 51:SF:127:LYS:HA | 51:SF:134:ALA:HA | 1.92 | 0.51 |
| 74:Sc:90:ASP:HB3 | 74:Sc:136:TRP:CZ3 | 2.46 | 0.51 |
| 1:LA:2256:C:N4 | 45:S2:1647:U:OP1 | 2.44 | 0.51 |
| 1:LA:2946:G:C2 | 5:LE:250:ALA:HB1 | 2.46 | 0.51 |
| 13:LM:96:PHE:CB | 13:LM:156:LYS:HE2 | 2.41 | 0.51 |
| 32:Lf:14:ILE:HG12 | 32:Lf:16:LEU:HD22 | 1.92 | 0.51 |
| 44:Lr:21:SER:O | 44:Lr:25:GLN:HG3 | 2.11 | 0.51 |
| 45:S2:900:A:N7 | 62:SQ:5:LYS:NZ | 2.56 | 0.51 |
| 45:S2:1196:A:H4' | 45:S2:1197:C:H5'' | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:SH:30:TYR:O | 53:SH:34:THR:HG23 | 2.11 | 0.51 |
| 63:SR:153:SER:OG | 63:SR:154:LEU:N | 2.43 | 0.51 |
| 1:LA:618:A:H5'' | 1:LA:619:U:OP1 | 2.11 | 0.50 |
| 1:LA:1107:U:H2' | 1:LA:1108:U:C6 | 2.46 | 0.50 |
| 1:LA:1665:G:H2' | 1:LA:1666:A:C8 | 2.46 | 0.50 |
| 6:LF:315:LYS:HB2 | 6:LF:323:VAL:HG21 | 1.93 | 0.50 |
| 10:LJ:134:TYR:HB3 | 10:LJ:190:VAL:HG11 | 1.93 | 0.50 |
| 13:LM:132:ASN:HA | 13:LM:154:THR:HG21 | 1.93 | 0.50 |
| 17:LQ:73[A]:PHE:HB3 | 17:LQ:78[A]:ARG:HB3 | 1.93 | 0.50 |
| 19:LS:174:ARG:O | 29:Lc:56:VAL:HG11 | 2.11 | 0.50 |
| 40:Ln:20:ASN:ND2 | 40:Ln:42:ARG:O | 2.39 | 0.50 |
| 45:S2:643:G:O6 | 45:S2:692:C:N4 | 2.44 | 0.50 |
| 46:SA:68:GLU:OE2 | 48:SC:67:THR:HG23 | 2.12 | 0.50 |
| 54:SI:25:GLN:HB3 | 54:SI:27:LYS:HD3 | 1.92 | 0.50 |
| 54:SI:107:ALA:O | 54:SI:111:ILE:HG12 | 2.10 | 0.50 |
| 62:SQ:85:LYS:HB3 | 62:SQ:101:HIS:HB3 | 1.93 | 0.50 |
| 62:SQ:90:GLU:OE1 | 62:SQ:225:VAL:HG23 | 2.11 | 0.50 |
| 64:SS:159:THR:HG21 | 64:SS:227:VAL:O | 2.10 | 0.50 |
| 72:Sa:32:VAL:HG22 | 72:Sa:60:ARG:HD2 | 1.93 | 0.50 |
| 1:LA:309:U:P | 37:Lk:84:LYS:HZ1 | 2.34 | 0.50 |
| 1:LA:944:C:H2' | 1:LA:945:U:C6 | 2.46 | 0.50 |
| 1:LA:1276:C:O2' | 1:LA:1277:A:O5' | 2.25 | 0.50 |
| 1:LA:1377:U:H2' | 1:LA:1378:G:C8 | 2.46 | 0.50 |
| 1:LA:1496:C:H2' | 1:LA:1497:A:C8 | 2.46 | 0.50 |
| 1:LA:1835:C:O2' | 1:LA:1841:A:N1 | 2.35 | 0.50 |
| 1:LA:2306:G:O2' | 1:LA:2309:U:OP2 | 2.22 | 0.50 |
| 1:LA:2882:U:H2' | 1:LA:2883:C:H6 | 1.76 | 0.50 |
| 11:LK:36:LYS:HB2 | 11:LK:78:MET:SD | 2.51 | 0.50 |
| 13:LM:93:ASP:HB2 | 13:LM:156:LYS:HZ1 | 1.75 | 0.50 |
| 18:LR:120:ASN:N | 18:LR:120:ASN:OD1 | 2.43 | 0.50 |
| 19:LS:83:VAL:O | 19:LS:103:ALA:HA | 2.12 | 0.50 |
| 28:Lb:133:LYS:O | 28:Lb:135:ARG:CZ | 2.59 | 0.50 |
| 45:S2:502:U:H2' | 45:S2:503:G:C8 | 2.47 | 0.50 |
| 1:LA:370:U:H4' | 1:LA:404:G:H5' | 1.93 | 0.50 |
| 1:LA:499:C:H5'' | 8:LH:82:ARG:HG3 | 1.92 | 0.50 |
| 1:LA:1311:C:O2' | 17:LQ:83[A]:ALA:O | 2.30 | 0.50 |
| 1:LA:2496:U:O2' | 1:LA:2497:U:OP1 | 2.25 | 0.50 |
| 1:LA:2766:U:H2' | 1:LA:2767:U:C6 | 2.46 | 0.50 |
| 1:LA:3314:G:P | 5:LE:116:ARG:HH22 | 2.34 | 0.50 |
| 9:LI:47:ARG:HH22 | 9:LI:179:LEU:HD12 | 1.77 | 0.50 |
| 12:LL:51:HIS:HB3 | 12:LL:134:ILE:HD12 | 1.91 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:LU:8:GLN:HG3 | 21:LU:8:GLN:O | 2.10 | 0.50 |
| 32:Lf:31:ARG:O | 32:Lf:35:GLU:HG2 | 2.11 | 0.50 |
| 35:Li:71:THR:OG1 | 35:Li:72:VAL:N | 2.44 | 0.50 |
| 43:Lq:45:ARG:O | 43:Lq:48:SER:OG | 2.28 | 0.50 |
| 45:S2:1216:C:O2' | 45:S2:1217:A:H8 | 1.95 | 0.50 |
| 62:SQ:135:LEU:HD21 | 62:SQ:217:LEU:HD12 | 1.92 | 0.50 |
| 65:ST:188:ARG:HA | 65:ST:191:ARG:HG3 | 1.92 | 0.50 |
| 74:Sc:103:LEU:HB3 | 74:Sc:126:LYS:HB2 | 1.93 | 0.50 |
| 1:LA:169:U:H2' | 1:LA:170:G:C8 | 2.46 | 0.50 |
| 1:LA:1639:G:O6 | 35:Li:73:SER:OG | 2.29 | 0.50 |
| 1:LA:2764:C:O3' | 43:Lq:39:GLY:HA3 | 2.11 | 0.50 |
| 1:LA:3379:U:O2' | 1:LA:3381:U:OP1 | 2.27 | 0.50 |
| 18:LR:60:PHE:HB3 | 18:LR:64:ASN:HB3 | 1.94 | 0.50 |
| 30:Ld:16:ALA:HB1 | 30:Ld:21:ILE:HD11 | 1.93 | 0.50 |
| 30:Ld:47:LEU:HA | 30:Ld:50:THR:HG22 | 1.93 | 0.50 |
| 31:Le:86:ARG:NH1 | 44:Lr:44:LYS:HE3 | 2.26 | 0.50 |
| 35:Li:81:CYS:SG | 35:Li:82:ALA:N | 2.84 | 0.50 |
| 45:S2:478:A:H5'' | 78:Sg:37:ARG:NH2 | 2.26 | 0.50 |
| 47:SB:74:ALA:N | 51:SF:79:TYR:OH | 2.41 | 0.50 |
| 54:SI:18:TYR:HD1 | 54:SI:135:ILE:HG13 | 1.76 | 0.50 |
| 56:SK:57:TYR:OH | 56:SK:68:ARG:HG2 | 2.11 | 0.50 |
| 60:SO:220:ILE:HD11 | 60:SO:243:LEU:HD22 | 1.93 | 0.50 |
| 60:SO:295:SER:OG | 60:SO:297:ASP:OD1 | 2.29 | 0.50 |
| 63:SR:108:ASN:HB2 | 63:SR:141:ARG:HH22 | 1.77 | 0.50 |
| 1:LA:1465:G:N2 | 1:LA:1509:G:H5'' | 2.26 | 0.50 |
| 1:LA:1649:G:H5'' | 4:LD:70:ARG:HD3 | 1.93 | 0.50 |
| 1:LA:1666:A:H2' | 1:LA:1667:G:C8 | 2.46 | 0.50 |
| 1:LA:2723:U:OP1 | 22:LV:78:LYS:NZ | 2.42 | 0.50 |
| 1:LA:3067:U:OP2 | 20:LT:62:ARG:NH2 | 2.33 | 0.50 |
| 1:LA:3206:U:O4 | 21:LU:159:SER:OG | 2.22 | 0.50 |
| 5:LE:111:SER:O | 5:LE:114:VAL:HG12 | 2.11 | 0.50 |
| 12:LL:140:THR:OG1 | 12:LL:141:LYS:N | 2.44 | 0.50 |
| 24:LX:81:GLN:HG2 | 24:LX:83:LYS:H | 1.76 | 0.50 |
| 29:Lc:132:LYS:O | 29:Lc:136:GLU:HG3 | 2.11 | 0.50 |
| 45:S2:369:A:H3' | 45:S2:369:A:N3 | 2.26 | 0.50 |
| 45:S2:628:G:OP1 | 70:SY:124:ARG:NH1 | 2.38 | 0.50 |
| 45:S2:1797:A:N6 | 76:Se:84:VAL:HB | 2.27 | 0.50 |
| 47:SB:123:VAL:O | 56:SK:58:ARG:NH1 | 2.42 | 0.50 |
| 64:SS:21:ASP:OD2 | 64:SS:24:SER:OG | 2.27 | 0.50 |
| 65:ST:98:ARG:HE | 65:ST:106:LEU:HG | 1.75 | 0.50 |
| 68:SW:45:ILE:HG22 | 68:SW:101:VAL:HG23 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:LA:201:A:OP1 | 1:LA:220:G:O2' | 2.30 | 0.50 |
| 1:LA:1384:C:OP1 | 6:LF:141:ARG:NH2 | 2.40 | 0.50 |
| 1:LA:2558:U:H5' | 1:LA:2560:A:H5' | 1.93 | 0.50 |
| 1:LA:2712:U:H3' | 43:Lq:9:LYS:O | 2.10 | 0.50 |
| 5:LE:167:ARG:HG2 | 5:LE:167:ARG:HH11 | 1.76 | 0.50 |
| 14:LN:122:LYS:HE3 | 36:Lj:120:ALA:CA | 2.42 | 0.50 |
| 16:LP:114:ARG:NH1 | 16:LP:151:ILE:O | 2.45 | 0.50 |
| 28:Lb:96:VAL:HG22 | 28:Lb:110:ALA:HB1 | 1.93 | 0.50 |
| 37:Lk:44:VAL:HA | 37:Lk:47:ILE:HG22 | 1.94 | 0.50 |
| 37:Lk:90:MET:HE2 | 37:Lk:93:ILE:HD12 | 1.93 | 0.50 |
| 40:Ln:18:LYS:HB2 | 40:Ln:18:LYS:NZ | 2.27 | 0.50 |
| 1:LA:269:G:OP1 | 16:LP:47:LYS:NZ | 2.44 | 0.50 |
| 1:LA:948:C:O2' | 1:LA:970:G:OP1 | 2.23 | 0.50 |
| 1:LA:1092:A:H1' | 1:LA:1093:U:C2 | 2.47 | 0.50 |
| 1:LA:1770:C:H2' | 1:LA:1771:U:O4' | 2.11 | 0.50 |
| 1:LA:2272:G:N2 | 1:LA:2310:G:H2' | 2.27 | 0.50 |
| 1:LA:2767:U:H2' | 1:LA:2768:A:H8 | 1.77 | 0.50 |
| 1:LA:3203:C:H2' | 1:LA:3204:G:C8 | 2.47 | 0.50 |
| 2:LB:5:G:OP1 | 13:LM:143:ARG:NH2 | 2.26 | 0.50 |
| 7:LG:22:ARG:HB3 | 7:LG:28:THR:HG23 | 1.93 | 0.50 |
| 11:LK:92:TYR:OH | 11:LK:101:VAL:HG21 | 2.12 | 0.50 |
| 18:LR:16:SER:O | 18:LR:101:ASN:ND2 | 2.42 | 0.50 |
| 37:Lk:51:SER:OG | 37:Lk:54:GLU:OE2 | 2.28 | 0.50 |
| 45:S2:1531:G:H5' | 56:SK:81:ARG:NH2 | 2.21 | 0.50 |
| 54:SI:39:THR:HG22 | 54:SI:53:TRP:CZ3 | 2.47 | 0.50 |
| 60:SO:113:VAL:HG12 | 60:SO:124:SER:HB2 | 1.94 | 0.50 |
| 1:LA:964:A:C2 | 29:Lc:43:ILE:HD12 | 2.44 | 0.50 |
| 1:LA:2381:G:N7 | 17:LQ:91[A]:LYS:NZ | 2.54 | 0.50 |
| 1:LA:2557:U:H1' | 4:LD:69:TYR:CG | 2.47 | 0.50 |
| 1:LA:2896:A:H2' | 1:LA:2898:C:O5' | 2.12 | 0.50 |
| 13:LM:116:TYR:CD1 | 53:SH:103:ASN:OD1 | 2.59 | 0.50 |
| 14:LN:45:LYS:HG2 | 14:LN:46:ILE:HG23 | 1.92 | 0.50 |
| 15:LO:24:LYS:HE2 | 15:LO:64:VAL:HG22 | 1.94 | 0.50 |
| 15:LO:98:SER:HA | 15:LO:101:LYS:HB2 | 1.94 | 0.50 |
| 16:LP:9:GLU:HB3 | 37:Lk:44:VAL:HG21 | 1.94 | 0.50 |
| 17:LQ:173[A]:ALA:HA | 17:LQ:176[A]:LYS:HD3 | 1.92 | 0.50 |
| 17:LQ:189[A]:ASP:O | 17:LQ:193[A]:GLN:HG3 | 2.12 | 0.50 |
| 29:Lc:70:LYS:HD3 | 29:Lc:111:LYS:HB2 | 1.94 | 0.50 |
| 45:S2:187:G:H22 | 45:S2:197:A:H61 | 1.58 | 0.50 |
| 45:S2:475:A:H2' | 45:S2:476:U:O4' | 2.12 | 0.50 |
| 45:S2:485:A:N6 | 45:S2:486:G:N3 | 2.59 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:895:G:H4' | 62:SQ:27:LYS:HZ1 | 1.77 | 0.50 |
| 46:SA:164:VAL:O | 46:SA:168:ILE:HB | 2.11 | 0.50 |
| 47:SB:25:LEU:HD13 | 51:SF:57:LEU:HD13 | 1.94 | 0.50 |
| 47:SB:218:GLU:OE2 | 47:SB:218:GLU:HA | 2.11 | 0.50 |
| 54:SI:77:ASN:HA | 54:SI:96:ALA:HB3 | 1.93 | 0.50 |
| 56:SK:67:ASP:OD1 | 56:SK:68:ARG:N | 2.45 | 0.50 |
| 62:SQ:207:LEU:O | 62:SQ:207:LEU:HD23 | 2.12 | 0.50 |
| 64:SS:73:ASP:OD2 | 64:SS:145:ARG:NH2 | 2.45 | 0.50 |
| 77:Sf:70:LYS:H | 77:Sf:70:LYS:CD | 2.25 | 0.50 |
| 1:LA:654:C:H5'' | 33:Lg:26:HIS:HB3 | 1.94 | 0.50 |
| 1:LA:1634:G:N2 | 1:LA:1637:A:OP2 | 2.34 | 0.50 |
| 1:LA:2946:G:N3 | 5:LE:250:ALA:HB1 | 2.26 | 0.50 |
| 1:LA:3392:U:H2' | 1:LA:3393:U:C6 | 2.47 | 0.50 |
| 6:LF:316:ASN:HD22 | 6:LF:319:LYS:HE3 | 1.76 | 0.50 |
| 11:LK:5:GLN:OE1 | 11:LK:58:HIS:ND1 | 2.44 | 0.50 |
| 22:LV:39:ILE:HD12 | 22:LV:102:ARG:HD3 | 1.92 | 0.50 |
| 28:Lb:88:ASP:O | 28:Lb:121:ARG:NH2 | 2.45 | 0.50 |
| 45:S2:415:C:O2 | 45:S2:418:G:O6 | 2.30 | 0.50 |
| 45:S2:919:A:H5' | 45:S2:920:U:OP2 | 2.12 | 0.50 |
| 45:S2:1592:A:H2' | 45:S2:1593:A:H8 | 1.77 | 0.50 |
| 47:SB:117:THR:HG21 | 47:SB:194:LEU:HD13 | 1.94 | 0.50 |
| 51:SF:42:GLU:OE1 | 51:SF:45:ARG:NH2 | 2.45 | 0.50 |
| 59:SN:104:SER:HB2 | 59:SN:106:TYR:CE1 | 2.46 | 0.50 |
| 60:SO:123:ILE:HD12 | 60:SO:154:VAL:HG11 | 1.94 | 0.50 |
| 68:SW:133:HIS:C | 68:SW:134:ILE:HD12 | 2.37 | 0.50 |
| 71:SZ:13:VAL:HG22 | 71:SZ:77:THR:HG22 | 1.94 | 0.50 |
| 1:LA:70:A:H2 | 1:LA:72:C:H42 | 1.60 | 0.49 |
| 1:LA:100:A:H2' | 1:LA:101:G:N3 | 2.27 | 0.49 |
| 1:LA:672:U:H2' | 1:LA:673:G:C8 | 2.47 | 0.49 |
| 1:LA:1418:A:H5'' | 6:LF:193:LYS:HE2 | 1.93 | 0.49 |
| 1:LA:1790:C:H2' | 1:LA:1791:C:C6 | 2.46 | 0.49 |
| 1:LA:1806:G:H2' | 1:LA:1807:G:N3 | 2.28 | 0.49 |
| 1:LA:1806:G:H2' | 1:LA:1807:G:C4 | 2.47 | 0.49 |
| 1:LA:2166:A:H2' | 1:LA:2167:A:C8 | 2.47 | 0.49 |
| 1:LA:3233:A:H61 | 1:LA:3252:G:H1 | 0.64 | 0.49 |
| 7:LG:86:TYR:OH | 7:LG:250:ASP:O | 2.27 | 0.49 |
| 9:LI:66:LYS:HG3 | 9:LI:76:TYR:HD2 | 1.75 | 0.49 |
| 18:LR:33:ALA:HB1 | 18:LR:117:ILE:HG12 | 1.94 | 0.49 |
| 26:LZ:62:VAL:HA | 26:LZ:87:SER:HB3 | 1.94 | 0.49 |
| 27:La:83:ASP:OD1 | 27:La:84:LYS:NZ | 2.45 | 0.49 |
| 45:S2:1160:A:H2' | 45:S2:1161:C:C6 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:S2:1184:A:N3 | 45:S2:1210:C:O2' | 2.45 | 0.49 |
| 47:SB:99:MET:HB2 | 47:SB:180:ARG:NH2 | 2.26 | 0.49 |
| 53:SH:63:GLN:O | 53:SH:66:LEU:HG | 2.12 | 0.49 |
| 62:SQ:32:ILE:HA | 62:SQ:96:LEU:HD12 | 1.94 | 0.49 |
| 64:SS:126:VAL:HA | 64:SS:141:THR:HA | 1.92 | 0.49 |
| 66:SU:90:VAL:C | 66:SU:91:ILE:HD13 | 2.36 | 0.49 |
| 70:SY:101:HIS:HA | 70:SY:104:ARG:HH22 | 1.77 | 0.49 |
| 1:LA:19:U:H2' | 1:LA:20:A:C8 | 2.47 | 0.49 |
| 1:LA:209:A:O2' | 1:LA:211:A:OP2 | 2.27 | 0.49 |
| 1:LA:1721:U:O4' | 20:LT:96:ILE:HD13 | 2.11 | 0.49 |
| 1:LA:3158:C:H5' | 1:LA:3394:G:C5 | 2.46 | 0.49 |
| 3:LC:43:A:H62 | 38:LI:65:ARG:NH1 | 2.09 | 0.49 |
| 12:LL:51:HIS:HD2 | 12:LL:137:SER:HB3 | 1.78 | 0.49 |
| 13:LM:19:LEU:HD21 | 13:LM:79:ILE:HG21 | 1.94 | 0.49 |
| 14:LN:167:PHE:CD2 | 29:Lc:132:LYS:HG3 | 2.47 | 0.49 |
| 15:LO:50:LYS:CE | 15:LO:82:SER:HA | 2.42 | 0.49 |
| 16:LP:73:ARG:NH1 | 16:LP:88:GLY:O | 2.46 | 0.49 |
| 27:La:50:ILE:HD13 | 27:La:80:VAL:HG11 | 1.93 | 0.49 |
| 35:Li:46:ASP:HB2 | 35:Li:84:CYS:SG | 2.52 | 0.49 |
| 45:S2:334:G:O6 | 67:SV:5:ARG:NH2 | 2.45 | 0.49 |
| 45:S2:702:G:N7 | 45:S2:732:G:N2 | 2.60 | 0.49 |
| 48:SC:54:TYR:HD1 | 48:SC:72:GLY:HA2 | 1.77 | 0.49 |
| 1:LA:314:U:H2' | 1:LA:315:C:C6 | 2.47 | 0.49 |
| 1:LA:577:A:N6 | 9:LI:141:TYR:OH | 2.45 | 0.49 |
| 1:LA:615:G:H2' | 1:LA:616:G:C8 | 2.47 | 0.49 |
| 1:LA:1642:A:H2' | 1:LA:1643:C:C2 | 2.46 | 0.49 |
| 1:LA:1683:U:O2 | 1:LA:1683:U:H2' | 2.12 | 0.49 |
| 1:LA:1823:U:H2' | 1:LA:1824:G:H8 | 1.78 | 0.49 |
| 1:LA:2266:C:H2' | 1:LA:2267:U:C6 | 2.47 | 0.49 |
| 1:LA:2368:G:H2' | 1:LA:2369:G:C8 | 2.46 | 0.49 |
| 1:LA:3194:U:H2' | 1:LA:3196:G:H21 | 1.77 | 0.49 |
| 4:LD:144:ASN:HB2 | 4:LD:160:SER:HB2 | 1.93 | 0.49 |
| 8:LH:102:ASN:HD21 | 8:LH:104:GLU:HG2 | 1.75 | 0.49 |
| 10:LJ:33:ASN:ND2 | 10:LJ:38:GLN:HG3 | 2.28 | 0.49 |
| 13:LM:23:VAL:HG11 | 13:LM:29:ARG:HB3 | 1.92 | 0.49 |
| 14:LN:162:ASN:ND2 | 14:LN:164:GLU:OE1 | 2.45 | 0.49 |
| 26:LZ:131:ASP:HB3 | 26:LZ:134:ASP:HB3 | 1.95 | 0.49 |
| 45:S2:523:G:H5'' | 75:Sd:59:GLY:HA2 | 1.93 | 0.49 |
| 45:S2:1349:G:H2' | 45:S2:1350:U:C6 | 2.47 | 0.49 |
| 47:SB:163:SER:HB3 | 47:SB:166:ARG:HB3 | 1.93 | 0.49 |
| 68:SW:77:ILE:HG23 | 68:SW:86:LEU:HD23 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:Se:40:ALA:HB3 | 76:Se:69:ASN:OD1 | 2.13 | 0.49 |
| 1:LA:327:A:OP2 | 14:LN:31:LYS:NZ | 2.42 | 0.49 |
| 1:LA:2143:A:H1' | 1:LA:2280:A:N6 | 2.27 | 0.49 |
| 1:LA:2277:C:OP1 | 42:Lp:23:ARG:NH2 | 2.45 | 0.49 |
| 2:LB:12:U:OP2 | 2:LB:68:C:O2' | 2.31 | 0.49 |
| 8:LH:43:LEU:HD21 | 8:LH:85:ILE:HD12 | 1.93 | 0.49 |
| 27:La:100:HIS:ND1 | 27:La:102:SER:OG | 2.37 | 0.49 |
| 36:Lj:59:ASN:HD21 | 36:Lj:63:ARG:HD2 | 1.77 | 0.49 |
| 37:Lk:20:MET:HE3 | 37:Lk:20:MET:HA | 1.95 | 0.49 |
| 38:Ll:25:ARG:NH1 | 40:Ln:50:ASN:HB3 | 2.27 | 0.49 |
| 45:S2:235:G:H2' | 45:S2:235:G:N3 | 2.26 | 0.49 |
| 45:S2:247:A:O2' | 69:SX:37:ASN:O | 2.25 | 0.49 |
| 45:S2:478:A:H5'' | 78:Sg:37:ARG:HH22 | 1.76 | 0.49 |
| 45:S2:1556:A:H5'' | 50:SE:40:ARG:HD2 | 1.95 | 0.49 |
| 45:S2:1567:U:H4' | 53:SH:36:LYS:HD2 | 1.93 | 0.49 |
| 46:SA:124:ARG:O | 46:SA:128:GLU:HG2 | 2.12 | 0.49 |
| 49:SD:84:ASN:O | 49:SD:86:VAL:HG23 | 2.12 | 0.49 |
| 61:SP:148:ASP:OD1 | 61:SP:149:LEU:N | 2.45 | 0.49 |
| 61:SP:180:GLU:O | 61:SP:184:LEU:HD22 | 2.11 | 0.49 |
| 62:SQ:24:PHE:HE2 | 71:SZ:70:LYS:CE | 2.25 | 0.49 |
| 64:SS:18:TRP:HH2 | 64:SS:31:PRO:HD3 | 1.77 | 0.49 |
| 68:SW:37:LYS:O | 78:Sg:36:LYS:HD2 | 2.11 | 0.49 |
| 1:LA:946:G:H2' | 1:LA:947:C:C6 | 2.47 | 0.49 |
| 1:LA:951:A:H4' | 1:LA:967:G:N2 | 2.28 | 0.49 |
| 1:LA:1143:U:OP1 | 1:LA:1366:G:O2' | 2.25 | 0.49 |
| 1:LA:1682:A:H3' | 1:LA:1682:A:N3 | 2.28 | 0.49 |
| 1:LA:3120:U:H1' | 1:LA:3121:A:H5'' | 1.95 | 0.49 |
| 1:LA:3272:A:OP2 | 8:LH:77:ARG:NH2 | 2.37 | 0.49 |
| 1:LA:3321:A:H2' | 1:LA:3322:A:C8 | 2.47 | 0.49 |
| 2:LB:87:G:O2' | 21:LU:119:ARG:NH2 | 2.43 | 0.49 |
| 5:LE:284:ARG:NH1 | 5:LE:293:ASN:O | 2.45 | 0.49 |
| 9:LI:130:ILE:HD12 | 9:LI:134:VAL:HG11 | 1.94 | 0.49 |
| 45:S2:393:C:H2' | 45:S2:394:C:C6 | 2.47 | 0.49 |
| 45:S2:893:U:H2' | 45:S2:894:U:C5 | 2.47 | 0.49 |
| 45:S2:1636:C:O2 | 45:S2:1765:A:N6 | 2.45 | 0.49 |
| 53:SH:94:ASP:HB3 | 53:SH:96:LYS:HG2 | 1.94 | 0.49 |
| 62:SQ:125:VAL:HG12 | 62:SQ:127:VAL:HG12 | 1.94 | 0.49 |
| 64:SS:183:VAL:HG11 | 64:SS:188:ASN:HB2 | 1.94 | 0.49 |
| 66:SU:43:PHE:C | 66:SU:43:PHE:CD1 | 2.91 | 0.49 |
| 75:Sd:18:LEU:HD12 | 75:Sd:20:ARG:HH12 | 1.77 | 0.49 |
| 75:Sd:29:HIS:HE1 | 75:Sd:34:ASN:HA | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:354:U:H5 | 1:LA:365:A:N7 | 2.10 | 0.49 |
| 1:LA:758:U:H2' | 1:LA:759:G:O4' | 2.13 | 0.49 |
| 1:LA:2635:A:H5' | 1:LA:2636:A:H5'' | 1.94 | 0.49 |
| 1:LA:3065:U:H2' | 1:LA:3066:C:C6 | 2.48 | 0.49 |
| 4:LD:36:GLU:HA | 4:LD:91:GLY:HA2 | 1.94 | 0.49 |
| 32:Lf:44:MET:HB3 | 32:Lf:77:ARG:HD3 | 1.95 | 0.49 |
| 42:Lp:2:ARG:HB3 | 42:Lp:5:TRP:CD1 | 2.48 | 0.49 |
| 45:S2:195:G:H2' | 45:S2:196:G:C8 | 2.47 | 0.49 |
| 45:S2:1071:U:OP1 | 45:S2:1071:U:H4' | 2.11 | 0.49 |
| 47:SB:194:LEU:HD23 | 47:SB:198:LEU:HD23 | 1.93 | 0.49 |
| 49:SD:81:ASP:O | 49:SD:83:GLU:N | 2.38 | 0.49 |
| 50:SE:28:MET:HE3 | 50:SE:32:ASP:CG | 2.37 | 0.49 |
| 52:SG:57:LEU:O | 52:SG:61:ILE:HG22 | 2.13 | 0.49 |
| 60:SO:81:LEU:HB3 | 60:SO:89:LEU:HD11 | 1.95 | 0.49 |
| 65:ST:43:ASP:OD1 | 65:ST:46:LYS:NZ | 2.43 | 0.49 |
| 73:Sb:101:TYR:HB3 | 73:Sb:112:ASP:HB2 | 1.94 | 0.49 |
| 75:Sd:19:ALA:HB1 | 75:Sd:77:ASN:ND2 | 2.28 | 0.49 |
| 1:LA:341:G:O2' | 3:LC:22:U:O4 | 2.28 | 0.49 |
| 1:LA:1646:A:H62 | 1:LA:1807:G:N2 | 2.10 | 0.49 |
| 1:LA:2222:A:OP2 | 1:LA:2222:A:H8 | 1.95 | 0.49 |
| 1:LA:2875:C:H2' | 1:LA:2876:G:O4' | 2.13 | 0.49 |
| 1:LA:3149:A:H2' | 1:LA:3150:U:O4' | 2.13 | 0.49 |
| 2:LB:23:A:H2' | 2:LB:24:A:C8 | 2.48 | 0.49 |
| 3:LC:151:C:H5 | 26:LZ:24:LEU:HD11 | 1.76 | 0.49 |
| 6:LF:351:PRO:HA | 9:LI:71:ALA:HA | 1.95 | 0.49 |
| 11:LK:112:ILE:HB | 11:LK:126:VAL:HG13 | 1.94 | 0.49 |
| 26:LZ:131:ASP:O | 26:LZ:135:ILE:HD13 | 2.13 | 0.49 |
| 45:S2:391:A:OP2 | 67:SV:23:LYS:NZ | 2.46 | 0.49 |
| 45:S2:1067:C:H5'' | 62:SQ:150:VAL:HG23 | 1.93 | 0.49 |
| 45:S2:1648:A:H2' | 45:S2:1649:G:C8 | 2.46 | 0.49 |
| 46:SA:40:ARG:HH22 | 46:SA:45:LYS:HG3 | 1.76 | 0.49 |
| 54:SI:71:VAL:HG22 | 54:SI:76:LEU:HD22 | 1.94 | 0.49 |
| 65:ST:7:TYR:HE1 | 65:ST:9:VAL:HB | 1.77 | 0.49 |
| 65:ST:39:GLU:HB2 | 65:ST:46:LYS:HE3 | 1.94 | 0.49 |
| 78:Sg:39:LEU:O | 78:Sg:43:ARG:HB2 | 2.12 | 0.49 |
| 1:LA:619:U:H5' | 18:LR:167:ARG:NH2 | 2.27 | 0.49 |
| 1:LA:1276:C:O2' | 1:LA:1277:A:H8 | 1.94 | 0.49 |
| 1:LA:2628:U:O4 | 22:LV:2:GLY:N | 2.45 | 0.49 |
| 1:LA:3001:C:O2' | 5:LE:180:GLU:OE2 | 2.22 | 0.49 |
| 1:LA:3296:U:H2' | 1:LA:3297:C:C6 | 2.45 | 0.49 |
| 3:LC:63:G:H22 | 3:LC:97:A:H2 | 1.61 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:LC:67:U:H2' | 3:LC:68:G:H8 | 1.78 | 0.49 |
| 5:LE:105:VAL:HG21 | 5:LE:148:LEU:HD13 | 1.95 | 0.49 |
| 5:LE:377:HIS:HD1 | 5:LE:377:HIS:C | 2.19 | 0.49 |
| 8:LH:43:LEU:HD11 | 8:LH:85:ILE:HG13 | 1.95 | 0.49 |
| 14:LN:42:ARG:HG2 | 14:LN:51:LEU:HD11 | 1.95 | 0.49 |
| 25:LY:33:ASN:HD22 | 25:LY:33:ASN:N | 2.11 | 0.49 |
| 45:S2:953:G:H2' | 45:S2:954:G:C8 | 2.48 | 0.49 |
| 47:SB:35:GLN:O | 47:SB:39:GLU:HG2 | 2.11 | 0.49 |
| 60:SO:69:GLN:HB2 | 60:SO:85:TRP:CD1 | 2.48 | 0.49 |
| 64:SS:151:ASP:HB2 | 65:ST:215:ARG:HH12 | 1.78 | 0.49 |
| 64:SS:248:ILE:HD12 | 64:SS:251:GLU:HB2 | 1.94 | 0.49 |
| 68:SW:133:HIS:O | 68:SW:134:ILE:HD12 | 2.12 | 0.49 |
| 72:Sa:66:ASP:OD1 | 72:Sa:67:ASP:N | 2.46 | 0.49 |
| 1:LA:584:A:H2' | 1:LA:585:C:C6 | 2.47 | 0.49 |
| 1:LA:588:A:H1' | 1:LA:1336:A:H5'' | 1.95 | 0.49 |
| 1:LA:895:A:H5'' | 4:LD:183:GLY:CA | 2.42 | 0.49 |
| 1:LA:1652:G:H2' | 1:LA:1653:A:H8 | 1.77 | 0.49 |
| 1:LA:1658:U:H2' | 1:LA:1659:C:C6 | 2.48 | 0.49 |
| 1:LA:2813:G:OP1 | 6:LF:73:ARG:NH1 | 2.34 | 0.49 |
| 1:LA:2960:G:H2' | 1:LA:2961:U:C6 | 2.48 | 0.49 |
| 4:LD:33:ASP:OD1 | 4:LD:33:ASP:N | 2.31 | 0.49 |
| 6:LF:20:LEU:HD11 | 6:LF:252:GLU:HG3 | 1.95 | 0.49 |
| 6:LF:302:ALA:HB2 | 19:LS:39:ARG:CZ | 2.43 | 0.49 |
| 12:LL:53:VAL:HG22 | 12:LL:134:ILE:CD1 | 2.43 | 0.49 |
| 15:LO:50:LYS:HE2 | 15:LO:82:SER:HB2 | 1.94 | 0.49 |
| 19:LS:19:PRO:HD3 | 19:LS:53:PHE:CD1 | 2.48 | 0.49 |
| 25:LY:52:THR:O | 25:LY:56:ARG:HG3 | 2.13 | 0.49 |
| 26:LZ:34:LEU:HD12 | 26:LZ:35:PRO:HD2 | 1.95 | 0.49 |
| 45:S2:207:U:H5' | 67:SV:176:SER:HB3 | 1.95 | 0.49 |
| 45:S2:371:G:N7 | 45:S2:372:G:N2 | 2.61 | 0.49 |
| 45:S2:1336:A:N6 | 45:S2:1416:G:O6 | 2.46 | 0.49 |
| 46:SA:40:ARG:NH2 | 46:SA:47:GLU:HB2 | 2.28 | 0.49 |
| 46:SA:105:MET:CE | 46:SA:119:ALA:HA | 2.42 | 0.49 |
| 61:SP:60:ALA:HB1 | 61:SP:144:ILE:HD13 | 1.94 | 0.49 |
| 66:SU:79:ARG:O | 66:SU:79:ARG:HD3 | 2.13 | 0.49 |
| 80:Tb:13:C:H2' | 80:Tb:14:A:C5 | 2.48 | 0.49 |
| 1:LA:29:C:H4' | 1:LA:62:A:H4' | 1.95 | 0.49 |
| 1:LA:2630:U:OP1 | 1:LA:2756:U:O2' | 2.25 | 0.49 |
| 1:LA:2698:G:H5' | 22:LV:16:GLN:HG3 | 1.95 | 0.49 |
| 1:LA:3274:U:O2' | 34:Lh:99:ARG:NH1 | 2.46 | 0.49 |
| 7:LG:108:ARG:CZ | 7:LG:253:PHE:HB2 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:LI:163:LEU:O | 9:LI:165:ASP:N | 2.46 | 0.49 |
| 45:S2:95:G:H3' | 45:S2:96:G:H8 | 1.77 | 0.49 |
| 45:S2:1208:A:H2 | 45:S2:1209:C:C6 | 2.31 | 0.49 |
| 45:S2:1311:U:O2 | 52:SG:2:GLY:N | 2.46 | 0.49 |
| 45:S2:1502:G:C8 | 54:SI:99:SER:HB2 | 2.48 | 0.49 |
| 55:SJ:33:GLN:HA | 55:SJ:36:ASN:ND2 | 2.28 | 0.49 |
| 62:SQ:32:ILE:HD12 | 62:SQ:43:VAL:HG23 | 1.95 | 0.49 |
| 62:SQ:35:PRO:HG3 | 62:SQ:99:ASN:HA | 1.94 | 0.49 |
| 1:LA:1474:A:H4' | 32:Lf:57:GLN:HG2 | 1.95 | 0.48 |
| 1:LA:3175:G:N2 | 1:LA:3212:A:H1' | 2.28 | 0.48 |
| 1:LA:3379:U:H2' | 1:LA:3380:U:C2 | 2.48 | 0.48 |
| 5:LE:296:THR:OG1 | 5:LE:297:SER:N | 2.45 | 0.48 |
| 6:LF:269:SER:C | 6:LF:271:LYS:H | 2.21 | 0.48 |
| 14:LN:158:ALA:HA | 29:Lc:97:GLU:HA | 1.95 | 0.48 |
| 26:LZ:57:LEU:HG | 26:LZ:62:VAL:HG12 | 1.93 | 0.48 |
| 45:S2:17:C:H2' | 45:S2:18:C:H6 | 1.78 | 0.48 |
| 45:S2:323:A:H2' | 45:S2:324:U:C5 | 2.47 | 0.48 |
| 45:S2:627:C:H5'' | 70:SY:5:HIS:HD2 | 1.77 | 0.48 |
| 45:S2:817:A:H2' | 45:S2:818:C:C6 | 2.47 | 0.48 |
| 45:S2:1433:G:N2 | 58:SM:42:CYS:SG | 2.74 | 0.48 |
| 45:S2:1648:A:H2' | 45:S2:1649:G:H8 | 1.77 | 0.48 |
| 47:SB:61:TYR:OH | 57:SL:49:ARG:NH1 | 2.46 | 0.48 |
| 52:SG:57:LEU:HD12 | 52:SG:69:ILE:HD13 | 1.95 | 0.48 |
| 67:SV:25:ARG:HB2 | 67:SV:28:GLU:HG2 | 1.95 | 0.48 |
| 72:Sa:85:TYR:HE1 | 77:Sf:4:VAL:HG12 | 1.77 | 0.48 |
| 1:LA:243:G:H2' | 1:LA:244:G:C8 | 2.49 | 0.48 |
| 1:LA:744:C:H2' | 1:LA:745:A:C8 | 2.48 | 0.48 |
| 1:LA:986:U:H2' | 1:LA:987:U:C6 | 2.49 | 0.48 |
| 1:LA:1792:C:OP2 | 44:Lr:49:ARG:NH2 | 2.44 | 0.48 |
| 1:LA:2723:U:OP2 | 1:LA:2725:C:N4 | 2.47 | 0.48 |
| 1:LA:2726:A:C2 | 29:Lc:43:ILE:HG23 | 2.48 | 0.48 |
| 6:LF:313:LEU:HD23 | 6:LF:315:LYS:HE2 | 1.94 | 0.48 |
| 24:LX:18:PRO:HA | 24:LX:51:ALA:HA | 1.95 | 0.48 |
| 29:Lc:139:ARG:HH21 | 29:Lc:145:VAL:CG1 | 2.25 | 0.48 |
| 30:Ld:23:LYS:HE3 | 30:Ld:24:PRO:HD2 | 1.94 | 0.48 |
| 32:Lf:84:ASP:OD1 | 32:Lf:84:ASP:N | 2.44 | 0.48 |
| 40:Ln:8:ARG:O | 40:Ln:12:LYS:HG2 | 2.13 | 0.48 |
| 44:Lr:84:ARG:NH2 | 45:S2:882:U:H5'' | 2.28 | 0.48 |
| 45:S2:340:U:H2' | 45:S2:341:A:H8 | 1.78 | 0.48 |
| 45:S2:1426:C:HO2' | 45:S2:1428:G:H8 | 1.61 | 0.48 |
| 45:S2:1512:G:H2' | 45:S2:1513:G:C8 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1561:U:H2' | 45:S2:1562:G:H8 | 1.78 | 0.48 |
| 47:SB:177:ILE:HD12 | 47:SB:178:GLY:N | 2.28 | 0.48 |
| 48:SC:55:VAL:HB | 48:SC:68:LEU:HD12 | 1.94 | 0.48 |
| 53:SH:115:ARG:O | 53:SH:119:ILE:HG12 | 2.12 | 0.48 |
| 60:SO:86:ASP:C | 60:SO:87:LYS:HD3 | 2.38 | 0.48 |
| 62:SQ:81:PHE:HD1 | 62:SQ:105:PHE:CZ | 2.31 | 0.48 |
| 64:SS:86:PHE:CE2 | 64:SS:87:MET:HG2 | 2.48 | 0.48 |
| 66:SU:34:LEU:HD12 | 66:SU:38:LEU:HD23 | 1.95 | 0.48 |
| 67:SV:36:THR:HG21 | 67:SV:173:PRO:HB2 | 1.95 | 0.48 |
| 75:Sd:5:VAL:HG13 | 75:Sd:32:ARG:HH21 | 1.78 | 0.48 |
| 1:LA:968:C:OP1 | 30:Ld:19:ASN:ND2 | 2.44 | 0.48 |
| 1:LA:1065:G:H2' | 1:LA:1066:U:C6 | 2.48 | 0.48 |
| 1:LA:1202:A:H61 | 1:LA:1299:G:H2' | 1.77 | 0.48 |
| 1:LA:1346:U:H5'' | 6:LF:303:GLY:H | 1.79 | 0.48 |
| 1:LA:2535:A:C4 | 62:SQ:227:ALA:HB3 | 2.49 | 0.48 |
| 1:LA:2696:A:H2' | 1:LA:2697:G:H8 | 1.78 | 0.48 |
| 1:LA:3217:A:H5'' | 1:LA:3218:G:C5 | 2.48 | 0.48 |
| 1:LA:3379:U:H2' | 1:LA:3380:U:O2 | 2.13 | 0.48 |
| 2:LB:113:C:H2' | 2:LB:114:U:O4' | 2.13 | 0.48 |
| 9:LI:184:LEU:HD12 | 9:LI:198:ALA:HB1 | 1.95 | 0.48 |
| 10:LJ:140:VAL:HG22 | 10:LJ:166:LEU:HD21 | 1.95 | 0.48 |
| 12:LL:86:HIS:HB3 | 12:LL:139:ARG:HG3 | 1.95 | 0.48 |
| 22:LV:75:ILE:HD11 | 22:LV:88:ARG:HH21 | 1.78 | 0.48 |
| 27:La:27:ARG:HG2 | 27:La:78:PHE:CE1 | 2.47 | 0.48 |
| 45:S2:76:A:H8 | 45:S2:77:U:H4' | 1.78 | 0.48 |
| 45:S2:1365:C:H2' | 45:S2:1366:U:C6 | 2.48 | 0.48 |
| 45:S2:1450:U:O2 | 45:S2:1450:U:H2' | 2.12 | 0.48 |
| 47:SB:55:ASP:O | 47:SB:59:VAL:HG13 | 2.13 | 0.48 |
| 60:SO:123:ILE:HD13 | 60:SO:169:ILE:HD13 | 1.95 | 0.48 |
| 66:SU:139:ARG:NH1 | 73:Sb:53:ILE:HG23 | 2.27 | 0.48 |
| 71:SZ:31:THR:OG1 | 71:SZ:35:GLY:HA2 | 2.13 | 0.48 |
| 74:Sc:87:VAL:HB | 74:Sc:92:CYS:SG | 2.53 | 0.48 |
| 77:Sf:17:ARG:CZ | 77:Sf:17:ARG:HB2 | 2.43 | 0.48 |
| 1:LA:2680:U:O2' | 13:LM:22:SER:HB3 | 2.13 | 0.48 |
| 1:LA:3266:A:H2' | 8:LH:69:PHE:CZ | 2.49 | 0.48 |
| 12:LL:44:ASP:OD1 | 12:LL:185:ARG:NH1 | 2.45 | 0.48 |
| 15:LO:25:LYS:HE2 | 15:LO:62:GLN:HG3 | 1.95 | 0.48 |
| 19:LS:34:THR:HG23 | 19:LS:49:LEU:HD11 | 1.96 | 0.48 |
| 23:LW:42:LYS:HG2 | 23:LW:47:VAL:HG13 | 1.95 | 0.48 |
| 29:Lc:91:LEU:HA | 29:Lc:121:VAL:HG21 | 1.94 | 0.48 |
| 45:S2:56:U:OP1 | 45:S2:403:G:N1 | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1327:C:H5'' | 46:SA:157:LEU:O | 2.12 | 0.48 |
| 45:S2:1415:U:H2' | 45:S2:1416:G:C8 | 2.48 | 0.48 |
| 45:S2:1471:A:H2 | 45:S2:1474:G:N2 | 2.09 | 0.48 |
| 52:SG:115:LEU:HD11 | 61:SP:9:LEU:HD23 | 1.95 | 0.48 |
| 60:SO:88:THR:HG22 | 60:SO:104:VAL:HG23 | 1.95 | 0.48 |
| 62:SQ:81:PHE:CD1 | 62:SQ:105:PHE:CZ | 3.01 | 0.48 |
| 64:SS:64:ILE:HD12 | 75:Sd:18:LEU:HD21 | 1.94 | 0.48 |
| 64:SS:81:THR:O | 64:SS:81:THR:OG1 | 2.29 | 0.48 |
| 65:ST:185:GLN:HG3 | 65:ST:186:ARG:N | 2.27 | 0.48 |
| 73:Sb:3:ARG:NH1 | 73:Sb:29:PRO:HD3 | 2.29 | 0.48 |
| 74:Sc:37:ALA:O | 74:Sc:41:SER:OG | 2.23 | 0.48 |
| 1:LA:93:C:OP2 | 1:LA:2763:C:O2' | 2.28 | 0.48 |
| 1:LA:735:A:C4 | 1:LA:736:G:H1' | 2.48 | 0.48 |
| 1:LA:3095:C:H2' | 1:LA:3096:C:C6 | 2.48 | 0.48 |
| 3:LC:40:A:OP2 | 3:LC:103:G:N1 | 2.34 | 0.48 |
| 11:LK:126:VAL:HG11 | 11:LK:161:LEU:HD12 | 1.96 | 0.48 |
| 45:S2:30:G:H2' | 45:S2:31:C:H6 | 1.75 | 0.48 |
| 45:S2:772:G:H5' | 64:SS:22:LYS:HE3 | 1.96 | 0.48 |
| 45:S2:803:A:O2' | 45:S2:804:A:H8 | 1.95 | 0.48 |
| 45:S2:1591:C:H2' | 45:S2:1592:A:C8 | 2.48 | 0.48 |
| 47:SB:35:GLN:NE2 | 47:SB:39:GLU:OE2 | 2.33 | 0.48 |
| 57:SL:35:ASP:O | 57:SL:38:ARG:HB3 | 2.13 | 0.48 |
| 64:SS:185:GLY:N | 64:SS:189:LEU:HD12 | 2.28 | 0.48 |
| 71:SZ:13:VAL:H | 71:SZ:77:THR:HG22 | 1.79 | 0.48 |
| 1:LA:241:G:H1' | 14:LN:45:LYS:HG3 | 1.96 | 0.48 |
| 1:LA:914:A:H8 | 1:LA:2135:C:O2' | 1.97 | 0.48 |
| 1:LA:1480:A:N6 | 1:LA:1871:C:H5 | 2.12 | 0.48 |
| 1:LA:2561:A:O3' | 28:Lb:54:THR:HG22 | 2.14 | 0.48 |
| 1:LA:3191:U:H2' | 1:LA:3192:C:C6 | 2.48 | 0.48 |
| 4:LD:117:GLU:HG2 | 4:LD:122:ASP:OD1 | 2.13 | 0.48 |
| 6:LF:234:ASN:OD1 | 6:LF:235:LEU:N | 2.47 | 0.48 |
| 12:LL:184:LYS:HE3 | 12:LL:189:GLU:OE2 | 2.14 | 0.48 |
| 19:LS:157:PRO:HA | 19:LS:186:VAL:HG12 | 1.95 | 0.48 |
| 19:LS:170:ARG:O | 19:LS:171:LYS:HG2 | 2.14 | 0.48 |
| 33:Lg:12:LYS:NZ | 33:Lg:58:GLY:O | 2.41 | 0.48 |
| 39:Lm:29:LYS:HG2 | 39:Lm:29:LYS:O | 2.14 | 0.48 |
| 45:S2:119:A:H2' | 45:S2:120:U:O4' | 2.13 | 0.48 |
| 45:S2:212:U:H2' | 45:S2:213:A:H8 | 1.78 | 0.48 |
| 45:S2:472:U:H1' | 45:S2:769:A:H2 | 1.79 | 0.48 |
| 47:SB:44:ASN:HB2 | 47:SB:45:LYS:CD | 2.44 | 0.48 |
| 60:SO:9:LEU:HG | 60:SO:313:TRP:NE1 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:SP:41:ARG:HG2 | 61:SP:42:PRO:O | 2.14 | 0.48 |
| 62:SQ:48:VAL:HB | 62:SQ:61:LEU:HD13 | 1.95 | 0.48 |
| 62:SQ:157:GLN:C | 62:SQ:159:SER:H | 2.21 | 0.48 |
| 64:SS:172:PHE:O | 64:SS:173:ILE:HD13 | 2.14 | 0.48 |
| 71:SZ:72:LYS:HZ1 | 71:SZ:77:THR:HA | 1.78 | 0.48 |
| 71:SZ:128:LYS:HE3 | 76:Se:27:SER:HB3 | 1.96 | 0.48 |
| 1:LA:1645:G:C2 | 1:LA:1808:A:N6 | 2.79 | 0.48 |
| 1:LA:1712:G:O6 | 31:Le:28:LYS:HE2 | 2.14 | 0.48 |
| 1:LA:1862:G:N1 | 1:LA:1865:C:OP2 | 2.43 | 0.48 |
| 1:LA:1926:G:C8 | 44:Lr:16:VAL:HG12 | 2.49 | 0.48 |
| 1:LA:2584:G:N3 | 1:LA:2584:G:H2' | 2.29 | 0.48 |
| 2:LB:118:A:H5'' | 7:LG:253:PHE:CZ | 2.49 | 0.48 |
| 3:LC:14:C:H2' | 3:LC:15:G:H5' | 1.93 | 0.48 |
| 4:LD:47:GLN:HA | 4:LD:84:THR:HG22 | 1.94 | 0.48 |
| 5:LE:238:LEU:HD12 | 5:LE:246:LEU:HA | 1.95 | 0.48 |
| 14:LN:144:THR:HG23 | 14:LN:145:PHE:CD2 | 2.48 | 0.48 |
| 14:LN:157:ARG:HG2 | 14:LN:158:ALA:H | 1.79 | 0.48 |
| 20:LT:15:VAL:HG23 | 20:LT:17:VAL:HG22 | 1.96 | 0.48 |
| 23:LW:81:LYS:NZ | 23:LW:90:ARG:CZ | 2.77 | 0.48 |
| 24:LX:17:LEU:HB2 | 24:LX:52:ALA:HB3 | 1.95 | 0.48 |
| 27:La:101:PRO:HA | 27:La:104:LEU:HD12 | 1.95 | 0.48 |
| 29:Lc:96:LYS:C | 29:Lc:98:THR:H | 2.21 | 0.48 |
| 36:Lj:24:LEU:HB3 | 36:Lj:51:ILE:HG12 | 1.96 | 0.48 |
| 45:S2:271:A:C6 | 45:S2:285:G:C2 | 3.02 | 0.48 |
| 45:S2:1699:G:H22 | 45:S2:1703:C:N4 | 2.11 | 0.48 |
| 68:SW:101:VAL:O | 68:SW:105:LEU:HD13 | 2.13 | 0.48 |
| 1:LA:38:U:H2' | 1:LA:39:A:O4' | 2.13 | 0.48 |
| 1:LA:541:G:N2 | 1:LA:548:U:O2 | 2.35 | 0.48 |
| 1:LA:594:G:N1 | 1:LA:608:G:H5'' | 2.28 | 0.48 |
| 1:LA:1659:C:H2' | 1:LA:1660:G:C8 | 2.49 | 0.48 |
| 1:LA:3315:A:OP2 | 5:LE:123:TYR:HB2 | 2.14 | 0.48 |
| 5:LE:57:VAL:HG22 | 5:LE:73:VAL:HG22 | 1.96 | 0.48 |
| 7:LG:153:THR:HG23 | 7:LG:160:PHE:CZ | 2.48 | 0.48 |
| 8:LH:152:THR:OG1 | 8:LH:155:LEU:HD12 | 2.14 | 0.48 |
| 13:LM:95:ASN:ND2 | 13:LM:103:GLY:O | 2.42 | 0.48 |
| 31:Le:14:LEU:O | 31:Le:17:VAL:HG12 | 2.13 | 0.48 |
| 33:Lg:32:TRP:CH2 | 33:Lg:52:GLN:HG2 | 2.49 | 0.48 |
| 35:Li:103:LYS:HE3 | 35:Li:103:LYS:HB3 | 1.53 | 0.48 |
| 45:S2:21:U:H2' | 45:S2:22:A:C8 | 2.49 | 0.48 |
| 45:S2:459:G:H5' | 45:S2:461:G:O6 | 2.14 | 0.48 |
| 45:S2:939:A:OP1 | 70:SY:114:ARG:NH2 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:1331:A:OP1 | 52:SG:45:ARG:NH2 | 2.46 | 0.48 |
| 51:SF:103:ASN:O | 51:SF:107:LYS:HG2 | 2.14 | 0.48 |
| 59:SN:113:LYS:NZ | 59:SN:114:VAL:O | 2.43 | 0.48 |
| 72:Sa:20:THR:OG1 | 72:Sa:22:ARG:HG2 | 2.14 | 0.48 |
| 74:Sc:35:GLY:O | 74:Sc:39:LYS:HD3 | 2.14 | 0.48 |
| 1:LA:429:U:H2' | 1:LA:430:U:H6 | 1.79 | 0.48 |
| 1:LA:1326:C:O2' | 34:Lh:76:GLY:HA2 | 2.14 | 0.48 |
| 1:LA:3056:U:H5' | 1:LA:3085:A:H61 | 1.79 | 0.48 |
| 1:LA:3192:C:H2' | 1:LA:3193:C:C6 | 2.49 | 0.48 |
| 7:LG:236:LEU:O | 7:LG:239:ILE:HG12 | 2.14 | 0.48 |
| 21:LU:129:ILE:HG12 | 21:LU:134:ASP:HB3 | 1.96 | 0.48 |
| 27:La:112:ASP:N | 27:La:112:ASP:OD1 | 2.46 | 0.48 |
| 33:Lg:32:TRP:CZ2 | 33:Lg:53:PRO:HD2 | 2.49 | 0.48 |
| 33:Lg:32:TRP:HH2 | 33:Lg:52:GLN:HG2 | 1.77 | 0.48 |
| 45:S2:702:G:O2' | 45:S2:703:G:O4' | 2.27 | 0.48 |
| 45:S2:923:A:H2' | 45:S2:924:A:C8 | 2.49 | 0.48 |
| 45:S2:1727:G:H21 | 67:SV:32:GLN:CD | 2.21 | 0.48 |
| 47:SB:126:ASP:CG | 56:SK:58:ARG:HH12 | 2.22 | 0.48 |
| 48:SC:3:MET:HE3 | 48:SC:4:PRO:HD2 | 1.95 | 0.48 |
| 51:SF:39:VAL:HG23 | 51:SF:41:PRO:HD3 | 1.95 | 0.48 |
| 60:SO:128:ASP:OD1 | 60:SO:130:THR:HG22 | 2.14 | 0.48 |
| 62:SQ:210:ILE:HD12 | 62:SQ:210:ILE:N | 2.29 | 0.48 |
| 64:SS:19:LEU:HD21 | 64:SS:108:ARG:HD2 | 1.96 | 0.48 |
| 67:SV:106:ALA:HB2 | 67:SV:165:LEU:HG | 1.94 | 0.48 |
| 69:SX:94:ILE:HD12 | 74:Sc:12:ALA:HB1 | 1.96 | 0.48 |
| 80:Tb:5:G:C6 | 80:Tb:6:G:H1' | 2.49 | 0.48 |
| 1:LA:309:U:H2' | 1:LA:310:U:H5 | 1.79 | 0.48 |
| 1:LA:596:G:H2' | 1:LA:597:A:H8 | 1.79 | 0.48 |
| 1:LA:1462:U:H2' | 1:LA:1463:G:O4' | 2.14 | 0.48 |
| 1:LA:1521:U:OP1 | 26:LZ:123:TYR:OH | 2.30 | 0.48 |
| 1:LA:1799:A:H3' | 1:LA:1800:U:O2 | 2.14 | 0.48 |
| 1:LA:2713:G:OP2 | 43:Lq:10:THR:OG1 | 2.31 | 0.48 |
| 4:LD:10:LYS:HA | 4:LD:16:PHE:CD2 | 2.49 | 0.48 |
| 5:LE:58:ARG:HD2 | 5:LE:354:VAL:HG13 | 1.96 | 0.48 |
| 6:LF:138:ARG:HD3 | 6:LF:245:GLY:C | 2.38 | 0.48 |
| 8:LH:102:ASN:H | 8:LH:105:TYR:HB3 | 1.79 | 0.48 |
| 14:LN:5:LYS:H | 14:LN:5:LYS:HD2 | 1.79 | 0.48 |
| 27:La:37:LYS:HG3 | 27:La:38:GLU:N | 2.28 | 0.48 |
| 45:S2:329:G:H5'' | 67:SV:98:LYS:HB3 | 1.95 | 0.48 |
| 45:S2:1039:A:H5'' | 72:Sa:62:ARG:NH2 | 2.29 | 0.48 |
| 45:S2:1509:C:H2' | 45:S2:1510:U:O4' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:S2:1521:G:H21 | 51:SF:70:THR:HG23 | 1.78 | 0.48 |
| 51:SF:19:VAL:HG23 | 51:SF:68:ARG:HB3 | 1.96 | 0.48 |
| 52:SG:54:THR:O | 52:SG:58:MET:HG2 | 2.14 | 0.48 |
| 62:SQ:69:CYS:SG | 71:SZ:114:ARG:NH1 | 2.86 | 0.48 |
| 65:ST:61:PHE:HD2 | 65:ST:72:ARG:HG2 | 1.78 | 0.48 |
| 68:SW:28:LEU:HD22 | 78:Sg:43:ARG:HD2 | 1.95 | 0.48 |
| 75:Sd:60:PHE:HA | 75:Sd:70:VAL:O | 2.14 | 0.48 |
| 76:Se:36:ILE:HB | 76:Se:73:TYR:HB2 | 1.95 | 0.48 |
| 1:LA:92:G:H5' | 1:LA:93:C:H5'' | 1.96 | 0.47 |
| 1:LA:655:A:H2' | 1:LA:656:A:H8 | 1.78 | 0.47 |
| 1:LA:2151:A:H2' | 1:LA:2152:U:H6 | 1.78 | 0.47 |
| 1:LA:2506:C:H2' | 1:LA:2507:U:C6 | 2.49 | 0.47 |
| 1:LA:2633:U:O3' | 12:LL:15:LYS:NZ | 2.48 | 0.47 |
| 1:LA:3312:U:H5' | 5:LE:175:LYS:HD3 | 1.95 | 0.47 |
| 2:LB:106:U:H5' | 2:LB:107:C:OP2 | 2.14 | 0.47 |
| 3:LC:40:A:H2' | 3:LC:41:A:C8 | 2.49 | 0.47 |
| 6:LF:16:THR:OG1 | 6:LF:17:ALA:N | 2.47 | 0.47 |
| 7:LG:129:TYR:CG | 7:LG:177:GLU:HB3 | 2.49 | 0.47 |
| 24:LX:120:LYS:HD3 | 24:LX:124:ASP:OD1 | 2.14 | 0.47 |
| 28:Lb:84:ARG:NH1 | 35:Li:97:GLU:OE1 | 2.47 | 0.47 |
| 36:Lj:45:LYS:HE3 | 36:Lj:49:LYS:CE | 2.44 | 0.47 |
| 45:S2:31:C:H2' | 45:S2:32:U:O4' | 2.14 | 0.47 |
| 45:S2:297:U:H4' | 64:SS:37:LYS:HD3 | 1.95 | 0.47 |
| 45:S2:553:G:OP2 | 45:S2:554:C:O2' | 2.26 | 0.47 |
| 45:S2:861:U:O2' | 73:Sb:56:HIS:O | 2.32 | 0.47 |
| 45:S2:968:U:H2' | 45:S2:969:C:O4' | 2.14 | 0.47 |
| 45:S2:1776:A:H2' | 45:S2:1777:G:H8 | 1.79 | 0.47 |
| 54:SI:127:ASN:OD1 | 54:SI:127:ASN:N | 2.47 | 0.47 |
| 60:SO:23:LEU:HB2 | 60:SO:33:LEU:HD11 | 1.95 | 0.47 |
| 63:SR:173:PRO:O | 63:SR:176:SER:OG | 2.21 | 0.47 |
| 66:SU:142:TYR:O | 73:Sb:42:GLN:NE2 | 2.46 | 0.47 |
| 67:SV:117:TYR:HB3 | 67:SV:119:GLN:OE1 | 2.14 | 0.47 |
| 68:SW:110:GLN:OE1 | 68:SW:126:ARG:HD3 | 2.14 | 0.47 |
| 1:LA:340:C:H2' | 1:LA:341:G:O4' | 2.14 | 0.47 |
| 1:LA:1721:U:OP1 | 20:LT:100:ARG:NE | 2.36 | 0.47 |
| 1:LA:2136:U:OP2 | 1:LA:2141:A:N6 | 2.34 | 0.47 |
| 1:LA:2343:U:H2' | 1:LA:2344:A:H8 | 1.79 | 0.47 |
| 1:LA:3067:U:H3' | 1:LA:3068:G:C5' | 2.44 | 0.47 |
| 1:LA:3213:U:N3 | 15:LO:124:ARG:NH2 | 2.62 | 0.47 |
| 1:LA:3304:A:H2' | 1:LA:3305:U:O4' | 2.14 | 0.47 |
| 7:LG:264:GLN:O | 7:LG:268:GLU:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:LH:64:LEU:HD11 | 8:LH:76:LEU:HD22 | 1.97 | 0.47 |
| 13:LM:137:ARG:O | 13:LM:141:ARG:HG2 | 2.14 | 0.47 |
| 20:LT:105:LEU:HD13 | 20:LT:135:LYS:HG2 | 1.96 | 0.47 |
| 23:LW:81:LYS:HZ3 | 23:LW:90:ARG:NH2 | 2.12 | 0.47 |
| 25:LY:18:GLY:HA3 | 25:LY:31:PHE:O | 2.14 | 0.47 |
| 38:LI:25:ARG:O | 38:LI:25:ARG:HD3 | 2.13 | 0.47 |
| 45:S2:121:U:H2' | 45:S2:122:U:C6 | 2.49 | 0.47 |
| 45:S2:304:U:H5' | 45:S2:305:C:OP2 | 2.13 | 0.47 |
| 45:S2:401:A:O2' | 45:S2:402:C:H4' | 2.13 | 0.47 |
| 45:S2:549:G:N2 | 45:S2:589:C:O2 | 2.47 | 0.47 |
| 45:S2:711:U:OP2 | 45:S2:727:U:N3 | 2.47 | 0.47 |
| 47:SB:112:ARG:HD2 | 47:SB:116:HIS:NE2 | 2.28 | 0.47 |
| 52:SG:26:LEU:HD21 | 52:SG:62:GLN:HG3 | 1.95 | 0.47 |
| 62:SQ:23:PRO:HA | 62:SQ:26:ARG:NH1 | 2.29 | 0.47 |
| 73:Sb:69:LEU:HD11 | 73:Sb:72:CYS:HB3 | 1.95 | 0.47 |
| 79:Ta:11:A:H3' | 79:Ta:12:G:H8 | 1.79 | 0.47 |
| 1:LA:38:U:H4' | 29:Lc:32:ARG:HD3 | 1.96 | 0.47 |
| 1:LA:962:G:O2' | 29:Lc:29:PRO:O | 2.28 | 0.47 |
| 2:LB:6:C:O2' | 7:LG:72:ASP:OD2 | 2.29 | 0.47 |
| 6:LF:177:ASP:HB3 | 6:LF:205:PRO:HD3 | 1.96 | 0.47 |
| 7:LG:65:ILE:HG21 | 7:LG:72:ASP:HB3 | 1.97 | 0.47 |
| 9:LI:83:LEU:HD21 | 9:LI:144:ILE:HD11 | 1.96 | 0.47 |
| 11:LK:47:LYS:H | 15:LO:7:VAL:HG11 | 1.78 | 0.47 |
| 14:LN:106:GLN:O | 14:LN:110:ASP:OD1 | 2.32 | 0.47 |
| 14:LN:161:ASP:OD1 | 29:Lc:139:ARG:NH1 | 2.47 | 0.47 |
| 18:LR:128:ARG:HD2 | 18:LR:136:ILE:HG21 | 1.96 | 0.47 |
| 38:LI:19:CYS:HB3 | 38:LI:22:CYS:O | 2.15 | 0.47 |
| 39:Lm:32:ASN:OD1 | 39:Lm:33:LYS:N | 2.48 | 0.47 |
| 45:S2:888:U:O2 | 45:S2:988:A:O2' | 2.30 | 0.47 |
| 45:S2:1219:A:C6 | 45:S2:1264:G:N2 | 2.78 | 0.47 |
| 45:S2:1514:U:O2' | 46:SA:6:SER:HA | 2.14 | 0.47 |
| 45:S2:1582:U:O2' | 45:S2:1583:A:OP2 | 2.29 | 0.47 |
| 45:S2:1649:G:H2' | 45:S2:1650:U:C6 | 2.49 | 0.47 |
| 1:LA:1459:A:H2' | 1:LA:1460:A:C8 | 2.49 | 0.47 |
| 1:LA:1590:G:H5'' | 35:Li:37:LYS:HZ1 | 1.80 | 0.47 |
| 1:LA:2154:G:OP1 | 4:LD:241:ARG:HG3 | 2.15 | 0.47 |
| 5:LE:346:THR:OG1 | 5:LE:347:SER:N | 2.46 | 0.47 |
| 7:LG:223:PHE:HD1 | 7:LG:226:TYR:HD2 | 1.61 | 0.47 |
| 8:LH:171:PRO:HA | 8:LH:174:LEU:HB2 | 1.96 | 0.47 |
| 10:LJ:24:ASN:HB3 | 10:LJ:25:PRO:HD3 | 1.96 | 0.47 |
| 19:LS:76:ALA:HA | 19:LS:79:LYS:HD2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 19:LS:180:ARG:HG2 | 19:LS:180:ARG:HH11 | 1.79 | 0.47 |
| 23:LW:32:SER:OG | 23:LW:83:TYR:OH | 2.29 | 0.47 |
| 45:S2:963:A:H4' | 70:SY:128:TYR:OH | 2.14 | 0.47 |
| 45:S2:1440:C:H2' | 45:S2:1441:C:C6 | 2.49 | 0.47 |
| 63:SR:38:VAL:O | 63:SR:39:THR:HG23 | 2.15 | 0.47 |
| 68:SW:79:ARG:O | 68:SW:83:VAL:HG23 | 2.13 | 0.47 |
| 68:SW:124:HIS:CE1 | 68:SW:128:LEU:HD11 | 2.49 | 0.47 |
| 73:Sb:31:SER:H | 73:Sb:34:ILE:HD12 | 1.80 | 0.47 |
| 74:Sc:97:ASP:OD2 | 74:Sc:142:LYS:NZ | 2.47 | 0.47 |
| 1:LA:1649:G:N1 | 1:LA:1805:A:N6 | 2.63 | 0.47 |
| 1:LA:3213:U:O4 | 15:LO:124:ARG:NH2 | 2.32 | 0.47 |
| 3:LC:72:A:N3 | 3:LC:88:A:O2' | 2.47 | 0.47 |
| 4:LD:52:SER:HB3 | 4:LD:191:LEU:HD22 | 1.97 | 0.47 |
| 9:LI:110:ARG:HH12 | 9:LI:206:LYS:NZ | 2.11 | 0.47 |
| 10:LJ:54:GLU:O | 10:LJ:58:VAL:HG23 | 2.15 | 0.47 |
| 11:LK:23:ARG:C | 11:LK:24:ILE:HD13 | 2.39 | 0.47 |
| 11:LK:146:LEU:CD1 | 11:LK:157:ASN:HB3 | 2.45 | 0.47 |
| 15:LO:32:LEU:HB3 | 15:LO:85:TRP:HH2 | 1.78 | 0.47 |
| 32:Lf:20:LEU:HD23 | 32:Lf:31:ARG:HG2 | 1.96 | 0.47 |
| 45:S2:177:U:O4 | 65:ST:191:ARG:NH2 | 2.47 | 0.47 |
| 45:S2:609:U:H4' | 45:S2:610:G:O5' | 2.15 | 0.47 |
| 45:S2:886:U:C2 | 45:S2:887:A:C8 | 3.03 | 0.47 |
| 45:S2:920:U:H2' | 45:S2:921:U:O4' | 2.14 | 0.47 |
| 52:SG:19:ARG:HG3 | 52:SG:20:TYR:CD1 | 2.50 | 0.47 |
| 56:SK:95:HIS:ND1 | 56:SK:96:SER:O | 2.45 | 0.47 |
| 62:SQ:137:ILE:HG23 | 62:SQ:215:VAL:HB | 1.95 | 0.47 |
| 66:SU:95:GLU:OE1 | 66:SU:95:GLU:HA | 2.14 | 0.47 |
| 69:SX:125:VAL:HG12 | 69:SX:139:VAL:HA | 1.96 | 0.47 |
| 1:LA:954:U:H2' | 1:LA:955:U:C6 | 2.49 | 0.47 |
| 1:LA:1855:C:H2' | 1:LA:1856:C:H6 | 1.79 | 0.47 |
| 1:LA:2128:U:H2' | 1:LA:2129:G:C8 | 2.50 | 0.47 |
| 1:LA:2191:C:O2' | 1:LA:2311:A:N1 | 2.43 | 0.47 |
| 1:LA:2596:U:H2' | 1:LA:2597:G:H8 | 1.79 | 0.47 |
| 1:LA:3349:C:O2' | 1:LA:3350:U:H2' | 2.14 | 0.47 |
| 3:LC:26:U:H2' | 3:LC:27:U:C6 | 2.49 | 0.47 |
| 14:LN:140:SER:O | 14:LN:144:THR:HG22 | 2.14 | 0.47 |
| 17:LQ:109[A]:PRO:HB2 | 17:LQ:111[A]:PRO:HD2 | 1.96 | 0.47 |
| 45:S2:30:G:H4' | 74:Sc:131:SER:HB2 | 1.95 | 0.47 |
| 45:S2:810:G:N2 | 66:SU:109:VAL:O | 2.47 | 0.47 |
| 45:S2:1294:G:O2' | 61:SP:109:ASN:HB2 | 2.14 | 0.47 |
| 46:SA:105:MET:HE3 | 46:SA:122:VAL:HB | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 50:SE:44:ARG:HH12 | 50:SE:84:ILE:N | 2.13 | 0.47 |
| 51:SF:129:PHE:HB2 | 55:SJ:79:TRP:HD1 | 1.80 | 0.47 |
| 52:SG:72:LYS:O | 52:SG:75:GLU:HG3 | 2.15 | 0.47 |
| 53:SH:84:TRP:CZ3 | 53:SH:85:PHE:CE1 | 3.03 | 0.47 |
| 61:SP:38:PHE:C | 61:SP:38:PHE:CD1 | 2.93 | 0.47 |
| 64:SS:31:PRO:HG3 | 64:SS:43:PRO:HG3 | 1.96 | 0.47 |
| 64:SS:37:LYS:O | 64:SS:41:SER:OG | 2.24 | 0.47 |
| 65:ST:77:LEU:HD13 | 65:ST:84:TYR:HB2 | 1.96 | 0.47 |
| 66:SU:34:LEU:HD12 | 66:SU:38:LEU:CD2 | 2.44 | 0.47 |
| 77:Sf:70:LYS:H | 77:Sf:70:LYS:HE2 | 1.79 | 0.47 |
| 79:Ta:65:G:H4' | 79:Ta:66:C:OP2 | 2.14 | 0.47 |
| 1:LA:407:A:H5' | 1:LA:1395:C:HO2' | 1.80 | 0.47 |
| 1:LA:829:A:H2' | 1:LA:830:G:O4' | 2.14 | 0.47 |
| 1:LA:838:C:H4' | 1:LA:1723:U:H5' | 1.97 | 0.47 |
| 1:LA:984:U:H2' | 1:LA:985:U:H6 | 1.78 | 0.47 |
| 1:LA:1225:G:H2' | 1:LA:1226:C:C6 | 2.50 | 0.47 |
| 1:LA:1524:G:H5' | 1:LA:1829:G:OP2 | 2.15 | 0.47 |
| 1:LA:1621:U:H2' | 1:LA:1622:G:H8 | 1.79 | 0.47 |
| 1:LA:1795:G:H5' | 4:LD:22:LEU:HD12 | 1.97 | 0.47 |
| 1:LA:1883:A:OP1 | 32:Lf:31:ARG:NH2 | 2.47 | 0.47 |
| 1:LA:2418:A:H2' | 1:LA:2419:C:H6 | 1.78 | 0.47 |
| 2:LB:7:G:H8 | 7:LG:22:ARG:NH1 | 2.12 | 0.47 |
| 2:LB:20:A:H2' | 2:LB:21:G:C8 | 2.49 | 0.47 |
| 7:LG:197:SER:O | 7:LG:202:GLY:N | 2.37 | 0.47 |
| 8:LH:69:PHE:HB2 | 8:LH:138:GLN:NE2 | 2.30 | 0.47 |
| 14:LN:42:ARG:O | 14:LN:46:ILE:HG12 | 2.15 | 0.47 |
| 15:LO:23:ILE:O | 15:LO:30:GLY:N | 2.48 | 0.47 |
| 15:LO:79:ALA:HA | 15:LO:82:SER:OG | 2.15 | 0.47 |
| 16:LP:15:GLN:HB3 | 37:Lk:51:SER:HB3 | 1.97 | 0.47 |
| 16:LP:31:ARG:NH1 | 16:LP:124:ASP:OD2 | 2.46 | 0.47 |
| 17:LQ:176[A]:LYS:HG2 | 17:LQ:177[A]:LYS:N | 2.29 | 0.47 |
| 19:LS:120:GLU:OE1 | 19:LS:130:ARG:NH1 | 2.48 | 0.47 |
| 23:LW:19:VAL:HG21 | 23:LW:30:PRO:HB3 | 1.97 | 0.47 |
| 32:Lf:16:LEU:HA | 32:Lf:19:ARG:HB2 | 1.97 | 0.47 |
| 44:Lr:27:LYS:O | 44:Lr:31:ILE:HG12 | 2.14 | 0.47 |
| 45:S2:29:U:H2' | 45:S2:30:G:H8 | 1.80 | 0.47 |
| 45:S2:82:U:H2' | 45:S2:83:G:O4' | 2.15 | 0.47 |
| 45:S2:112:A:H1' | 69:SX:67:ARG:NH1 | 2.30 | 0.47 |
| 45:S2:388:G:O6 | 45:S2:408:C:N4 | 2.47 | 0.47 |
| 45:S2:609:U:O2 | 74:Sc:19:ARG:NH1 | 2.48 | 0.47 |
| 45:S2:1226:A:O2' | 45:S2:1227:A:OP1 | 2.27 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------------|--------------------------|-------------------|
| 45:S2:1241:G:H21 | 45:S2:1241:G:P | 2.37 | 0.47 |
| 45:S2:1402:G:OP2 | 52:SG:5:ARG:NH1 | 2.33 | 0.47 |
| 53:SH:79:TYR:O | 53:SH:80:LYS:HG2 | 2.15 | 0.47 |
| 57:SL:10:ALA:O | 57:SL:54:LEU:CB | 2.62 | 0.47 |
| 60:SO:9:LEU:HG | 60:SO:313:TRP:HE1 | 1.79 | 0.47 |
| 60:SO:178:VAL:HB | 60:SO:192:PHE:HB2 | 1.95 | 0.47 |
| 61:SP:56:LYS:HD3 | 61:SP:159:ALA:O | 2.15 | 0.47 |
| 64:SS:255:ARG:CZ | 64:SS:259:GLN:HA | 2.44 | 0.47 |
| 66:SU:91:ILE:CD1 | 66:SU:169:PHE:HE1 | 2.26 | 0.47 |
| 67:SV:36:THR:HG23 | 67:SV:96:LEU:HB2 | 1.96 | 0.47 |
| 67:SV:58:LEU:C | 67:SV:59:ARG:HG2 | 2.39 | 0.47 |
| 70:SY:102:LEU:HD11 | 70:SY:112:LYS:HA | 1.95 | 0.47 |
| 71:SZ:19:ILE:HB | 71:SZ:83:ILE:HD13 | 1.96 | 0.47 |
| 73:Sb:51:GLU:O | 73:Sb:61:ILE:HA | 2.14 | 0.47 |
| 77:Sf:70:LYS:H | 77:Sf:70:LYS:CE | 2.28 | 0.47 |
| 78:Sg:43:ARG:NE | 78:Sg:56:MET:HE1 | 2.29 | 0.47 |
| 1:LA:2549:U:H5 | 4:LD:40:TYR:O | 1.98 | 0.47 |
| 5:LE:316:GLU:OE1 | 5:LE:316:GLU:N | 2.48 | 0.47 |
| 10:LJ:78:PHE:O | 10:LJ:79:GLN:HG2 | 2.15 | 0.47 |
| 10:LJ:86:THR:O | 10:LJ:90:THR:OG1 | 2.33 | 0.47 |
| 15:LO:100:ALA:HA | 15:LO:103:ILE:HD12 | 1.97 | 0.47 |
| 45:S2:622:A:H4' | 45:S2:623:A:O5' | 2.15 | 0.47 |
| 45:S2:931:C:H5' | 62:SQ:116:LYS:CB | 2.41 | 0.47 |
| 45:S2:1439:C:H2' | 45:S2:1440:C:C6 | 2.50 | 0.47 |
| 49:SD:33:ARG:O | 49:SD:37:VAL:HG13 | 2.15 | 0.47 |
| 60:SO:37:SER:OG | 60:SO:39:ASP:OD1 | 2.23 | 0.47 |
| 1:LA:1388:G:H5'' | 33:Lg:101:SER:HB3 | 1.97 | 0.47 |
| 1:LA:1652:G:H2' | 1:LA:1653:A:C8 | 2.49 | 0.47 |
| 1:LA:2366:A:H2' | 1:LA:2367:A:C8 | 2.50 | 0.47 |
| 1:LA:2614:G:H2' | 1:LA:2615:C:H6 | 1.79 | 0.47 |
| 1:LA:3251:G:H2' | 1:LA:3252:G:H8 | 1.80 | 0.47 |
| 5:LE:108:GLU:HG3 | 5:LE:137:TYR:CD1 | 2.50 | 0.47 |
| 5:LE:284:ARG:HB3 | 5:LE:323:MET:HE2 | 1.97 | 0.47 |
| 17:LQ:108[A]:ILE:N | 17:LQ:108[A]:ILE:HD12 | 2.30 | 0.47 |
| 20:LT:159:ALA:HB1 | 20:LT:163:ARG:NH2 | 2.30 | 0.47 |
| 33:Lg:103:LYS:O | 33:Lg:107:VAL:HG23 | 2.14 | 0.47 |
| 45:S2:1176:G:O2' | 45:S2:1195:C:O2' | 2.25 | 0.47 |
| 51:SF:22:VAL:HG22 | 51:SF:65:ILE:HG23 | 1.96 | 0.47 |
| 54:SI:63:ARG:CG | 54:SI:67:MET:HE3 | 2.35 | 0.47 |
| 59:SN:104:SER:HB2 | 59:SN:106:TYR:HE1 | 1.80 | 0.47 |
| 63:SR:67:GLN:HA | 63:SR:70:ASP:OD2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 64:SS:255:ARG:O | 64:SS:255:ARG:HD2 | 2.15 | 0.47 |
| 66:SU:39:ARG:HG3 | 66:SU:40:PRO:HD3 | 1.97 | 0.47 |
| 1:LA:663:U:H5' | 6:LF:107:ARG:HA | 1.97 | 0.47 |
| 1:LA:1039:A:N6 | 7:LG:9:SER:HB2 | 2.29 | 0.47 |
| 1:LA:1459:A:H2' | 1:LA:1460:A:H8 | 1.80 | 0.47 |
| 1:LA:1885:A:O2' | 5:LE:226:PHE:O | 2.31 | 0.47 |
| 1:LA:1894:A:O2' | 1:LA:3052:G:H4' | 2.15 | 0.47 |
| 1:LA:3350:U:O2' | 1:LA:3351:U:H5' | 2.15 | 0.47 |
| 10:LJ:56:VAL:O | 10:LJ:60:ARG:HD2 | 2.15 | 0.47 |
| 29:Lc:94:ALA:HB2 | 29:Lc:121:VAL:HG22 | 1.95 | 0.47 |
| 29:Lc:134:ALA:O | 29:Lc:138:ILE:HG13 | 2.15 | 0.47 |
| 38:Ll:39:TYR:CD1 | 38:Ll:40:PRO:HA | 2.50 | 0.47 |
| 45:S2:90:C:H1' | 45:S2:451:A:H1' | 1.97 | 0.47 |
| 45:S2:928:U:O2' | 45:S2:945:U:H5' | 2.15 | 0.47 |
| 45:S2:1588:G:O6 | 45:S2:1608:U:O4 | 2.32 | 0.47 |
| 64:SS:112:HIS:HE2 | 64:SS:237:SER:C | 2.20 | 0.47 |
| 67:SV:64:ASN:C | 67:SV:65:PHE:HD1 | 2.23 | 0.47 |
| 67:SV:87:ASN:HB3 | 67:SV:90:LEU:HG | 1.97 | 0.47 |
| 68:SW:113:VAL:HA | 68:SW:118:LEU:HD13 | 1.96 | 0.47 |
| 69:SX:71:LEU:HG | 69:SX:88:ARG:CZ | 2.45 | 0.47 |
| 70:SY:26:PHE:CZ | 70:SY:28:LEU:HB3 | 2.50 | 0.47 |
| 1:LA:839:C:H5'' | 1:LA:1723:U:C5 | 2.50 | 0.46 |
| 1:LA:1301:A:N7 | 1:LA:2856:C:O2' | 2.43 | 0.46 |
| 1:LA:1359:C:H2' | 1:LA:1360:U:O4' | 2.16 | 0.46 |
| 1:LA:1621:U:C2 | 1:LA:1622:G:C8 | 3.03 | 0.46 |
| 1:LA:1663:G:H2' | 1:LA:1664:C:C6 | 2.50 | 0.46 |
| 1:LA:2139:U:H1' | 1:LA:2977:U:H5' | 1.97 | 0.46 |
| 1:LA:2281:U:OP1 | 1:LA:2972:G:O2' | 2.20 | 0.46 |
| 4:LD:127:ALA:HB2 | 4:LD:134:VAL:HG23 | 1.97 | 0.46 |
| 5:LE:62:ARG:HG3 | 5:LE:65:SER:HB3 | 1.97 | 0.46 |
| 5:LE:292:ALA:HB2 | 5:LE:302:LYS:HA | 1.97 | 0.46 |
| 7:LG:40:HIS:CE1 | 7:LG:42:ALA:HB3 | 2.50 | 0.46 |
| 7:LG:108:ARG:NE | 7:LG:253:PHE:HB2 | 2.30 | 0.46 |
| 7:LG:286:VAL:HG13 | 12:LL:206:LEU:HD11 | 1.95 | 0.46 |
| 8:LH:140:VAL:O | 8:LH:143:LYS:HG3 | 2.15 | 0.46 |
| 12:LL:48:LEU:O | 12:LL:139:ARG:HA | 2.16 | 0.46 |
| 14:LN:60:ALA:HB3 | 14:LN:65:TYR:O | 2.15 | 0.46 |
| 19:LS:148:GLU:O | 19:LS:151:ARG:HG2 | 2.15 | 0.46 |
| 32:Lf:9:THR:HG23 | 32:Lf:76:SER:HB3 | 1.97 | 0.46 |
| 33:Lg:78:ASN:N | 33:Lg:78:ASN:OD1 | 2.46 | 0.46 |
| 45:S2:50:C:OP2 | 45:S2:423:G:N2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:S2:566:C:HO2' | 45:S2:567:A:P | 2.38 | 0.46 |
| 45:S2:625:C:H2' | 45:S2:626:U:C6 | 2.50 | 0.46 |
| 45:S2:863:A:O5' | 73:Sb:57:ARG:HD2 | 2.15 | 0.46 |
| 45:S2:908:U:H1' | 45:S2:996:U:O2' | 2.14 | 0.46 |
| 48:SC:75:TYR:O | 48:SC:78:GLU:HG3 | 2.15 | 0.46 |
| 51:SF:101:SER:O | 51:SF:104:GLU:HG3 | 2.14 | 0.46 |
| 53:SH:31:ALA:O | 53:SH:34:THR:OG1 | 2.29 | 0.46 |
| 55:SJ:44:ASN:OD1 | 55:SJ:45:ALA:N | 2.48 | 0.46 |
| 57:SL:42:ARG:NH2 | 57:SL:58:GLU:O | 2.48 | 0.46 |
| 60:SO:169:ILE:HD12 | 60:SO:181:TRP:HE3 | 1.75 | 0.46 |
| 62:SQ:105:PHE:HE1 | 62:SQ:109:LYS:HG3 | 1.78 | 0.46 |
| 63:SR:101:VAL:HG11 | 63:SR:211:LEU:HD12 | 1.97 | 0.46 |
| 65:ST:57:ASP:HA | 65:ST:106:LEU:HA | 1.96 | 0.46 |
| 1:LA:210:U:C2 | 1:LA:230:U:H4' | 2.51 | 0.46 |
| 1:LA:275:U:H2' | 1:LA:276:U:C6 | 2.50 | 0.46 |
| 1:LA:396:A:O2' | 1:LA:399:A:OP1 | 2.30 | 0.46 |
| 1:LA:502:C:H2' | 1:LA:503:A:H8 | 1.80 | 0.46 |
| 1:LA:1497:A:H2' | 1:LA:1498:C:C6 | 2.50 | 0.46 |
| 1:LA:1659:C:H2' | 1:LA:1660:G:H8 | 1.79 | 0.46 |
| 1:LA:2283:C:HO2' | 1:LA:2284:C:P | 2.39 | 0.46 |
| 1:LA:2680:U:OP1 | 13:LM:50:ALA:HA | 2.14 | 0.46 |
| 1:LA:2710:C:O2' | 1:LA:2743:U:OP1 | 2.32 | 0.46 |
| 2:LB:45:A:H2' | 2:LB:46:A:C8 | 2.51 | 0.46 |
| 4:LD:77:ILE:HD13 | 4:LD:128:ARG:HB3 | 1.98 | 0.46 |
| 6:LF:304:GLN:C | 6:LF:306:THR:H | 2.23 | 0.46 |
| 6:LF:333:VAL:O | 6:LF:337:GLU:HG3 | 2.16 | 0.46 |
| 28:Lb:4:PHE:O | 28:Lb:9:LYS:HD2 | 2.15 | 0.46 |
| 34:Lh:67:MET:HE2 | 34:Lh:89:LEU:HD23 | 1.97 | 0.46 |
| 45:S2:234:G:H3' | 45:S2:234:G:N3 | 2.30 | 0.46 |
| 45:S2:296:U:H1' | 64:SS:127:LYS:NZ | 2.31 | 0.46 |
| 45:S2:539:G:O2' | 45:S2:540:G:O4' | 2.34 | 0.46 |
| 45:S2:694:U:N3 | 66:SU:96:ARG:O | 2.46 | 0.46 |
| 45:S2:1584:G:C8 | 51:SF:122:ARG:HB2 | 2.50 | 0.46 |
| 45:S2:1672:G:H2' | 45:S2:1673:G:C8 | 2.51 | 0.46 |
| 45:S2:1728:A:H1' | 67:SV:32:GLN:NE2 | 2.22 | 0.46 |
| 50:SE:22:LEU:HD23 | 50:SE:25:LEU:HD21 | 1.97 | 0.46 |
| 51:SF:26:LYS:HE3 | 51:SF:28:LEU:HB3 | 1.97 | 0.46 |
| 53:SH:36:LYS:NZ | 53:SH:106:GLU:OE2 | 2.42 | 0.46 |
| 53:SH:70:VAL:O | 53:SH:74:GLN:HG3 | 2.14 | 0.46 |
| 60:SO:69:GLN:HE22 | 60:SO:111:MET:HA | 1.81 | 0.46 |
| 64:SS:249:ALA:O | 64:SS:252:ARG:HG3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 1:LA:786:G:H2' | 1:LA:787:C:C6 | 2.49 | 0.46 |
| 1:LA:975:U:H2' | 1:LA:976:C:O4' | 2.16 | 0.46 |
| 1:LA:1614:C:H2' | 1:LA:1615:U:H6 | 1.78 | 0.46 |
| 1:LA:2422:U:H2' | 1:LA:2423:A:C8 | 2.50 | 0.46 |
| 1:LA:3213:U:C4 | 15:LO:124:ARG:NH2 | 2.83 | 0.46 |
| 2:LB:20:A:H2' | 2:LB:21:G:H8 | 1.80 | 0.46 |
| 2:LB:75:G:N2 | 2:LB:104:A:N6 | 2.64 | 0.46 |
| 7:LG:8:LYS:HD2 | 7:LG:12:TYR:CE2 | 2.50 | 0.46 |
| 7:LG:160:PHE:HA | 7:LG:163:LEU:HB3 | 1.97 | 0.46 |
| 7:LG:273:ARG:HD3 | 7:LG:273:ARG:HA | 1.63 | 0.46 |
| 10:LJ:149:LYS:N | 10:LJ:200:LEU:O | 2.47 | 0.46 |
| 14:LN:126:PHE:HZ | 14:LN:134:GLU:HA | 1.80 | 0.46 |
| 16:LP:14:LYS:HE2 | 16:LP:14:LYS:HB2 | 1.73 | 0.46 |
| 17:LQ:37[A]:ARG:HG2 | 17:LQ:108[A]:ILE:HD11 | 1.97 | 0.46 |
| 26:LZ:58:ASP:O | 26:LZ:62:VAL:HG13 | 2.15 | 0.46 |
| 38:LI:54:LYS:O | 38:LI:58:THR:HB | 2.15 | 0.46 |
| 45:S2:968:U:OP1 | 45:S2:1033:C:O2' | 2.33 | 0.46 |
| 45:S2:1159:C:H4' | 45:S2:1580:C:OP1 | 2.16 | 0.46 |
| 49:SD:79:ALA:HB1 | 49:SD:86:VAL:HG22 | 1.97 | 0.46 |
| 53:SH:73:MET:SD | 53:SH:74:GLN:N | 2.87 | 0.46 |
| 56:SK:25:LYS:HG3 | 56:SK:27:TRP:H | 1.79 | 0.46 |
| 57:SL:38:ARG:HG3 | 57:SL:38:ARG:O | 2.15 | 0.46 |
| 62:SQ:157:GLN:O | 62:SQ:159:SER:N | 2.48 | 0.46 |
| 63:SR:106:ASP:OD2 | 63:SR:110:HIS:HB2 | 2.15 | 0.46 |
| 65:ST:126:ASP:OD1 | 65:ST:127:THR:N | 2.49 | 0.46 |
| 72:Sa:12:TYR:CG | 72:Sa:12:TYR:O | 2.68 | 0.46 |
| 72:Sa:17:CYS:HB2 | 72:Sa:56:SER:HB2 | 1.95 | 0.46 |
| 74:Sc:73:ARG:HG2 | 74:Sc:82:LYS:HE2 | 1.96 | 0.46 |
| 75:Sd:37:LYS:HB3 | 75:Sd:57:VAL:HG23 | 1.98 | 0.46 |
| 76:Se:89:ARG:HG2 | 76:Se:89:ARG:NH1 | 2.30 | 0.46 |
| 1:LA:593:U:H2' | 1:LA:608:G:O6 | 2.15 | 0.46 |
| 1:LA:2165:A:H5' | 16:LP:76:PRO:HG3 | 1.98 | 0.46 |
| 9:LI:142:SER:O | 9:LI:146:GLN:HG3 | 2.14 | 0.46 |
| 9:LI:234:GLU:O | 9:LI:237:ASN:ND2 | 2.39 | 0.46 |
| 35:Li:87:GLU:OE2 | 35:Li:91:ARG:NH2 | 2.49 | 0.46 |
| 39:Lm:11:PHE:C | 39:Lm:11:PHE:CD1 | 2.94 | 0.46 |
| 45:S2:116:U:H2' | 45:S2:117:U:C6 | 2.50 | 0.46 |
| 45:S2:1011:G:H2' | 45:S2:1012:U:C5 | 2.50 | 0.46 |
| 45:S2:1242:A:H2' | 45:S2:1243:G:H21 | 1.80 | 0.46 |
| 45:S2:1767:G:OP1 | 45:S2:1770:U:H4' | 2.15 | 0.46 |
| 49:SD:66:VAL:HG23 | 49:SD:67:THR:H | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 1:LA:208:C:H2' | 1:LA:209:A:O4' | 2.16 | 0.46 |
| 1:LA:364:G:OP2 | 38:Ll:52:LYS:NZ | 2.42 | 0.46 |
| 1:LA:670:U:H2' | 1:LA:671:A:H8 | 1.80 | 0.46 |
| 1:LA:1320:G:N2 | 21:LU:112:ALA:HB2 | 2.31 | 0.46 |
| 1:LA:1596:C:H2' | 1:LA:1597:G:C8 | 2.50 | 0.46 |
| 1:LA:2546:A:H3' | 1:LA:2547:C:H5'' | 1.98 | 0.46 |
| 1:LA:2940:A:H8 | 1:LA:2940:A:OP2 | 1.98 | 0.46 |
| 1:LA:3331:U:H2' | 1:LA:3332:G:O4' | 2.16 | 0.46 |
| 1:LA:3336:G:H2' | 1:LA:3337:C:C6 | 2.51 | 0.46 |
| 3:LC:94:C:H5'' | 38:Ll:76:ASN:ND2 | 2.30 | 0.46 |
| 6:LF:191:LYS:HG2 | 6:LF:194:TYR:OH | 2.15 | 0.46 |
| 38:Ll:21:ARG:NH1 | 38:Ll:41:ALA:O | 2.38 | 0.46 |
| 45:S2:15:U:H1' | 45:S2:619:A:C5 | 2.51 | 0.46 |
| 45:S2:34:G:C2 | 45:S2:475:A:C8 | 3.04 | 0.46 |
| 45:S2:522:U:H5'' | 75:Sd:37:LYS:HE2 | 1.97 | 0.46 |
| 45:S2:1097:U:O4 | 63:SR:201:ASN:ND2 | 2.48 | 0.46 |
| 45:S2:1590:G:OP1 | 54:Sl:91:TYR:HB2 | 2.16 | 0.46 |
| 55:SJ:28:SER:HB2 | 55:SJ:112:VAL:HA | 1.97 | 0.46 |
| 60:SO:68:VAL:HA | 60:SO:84:SER:HA | 1.95 | 0.46 |
| 62:SQ:185:THR:O | 62:SQ:189:ILE:HG13 | 2.16 | 0.46 |
| 65:ST:7:TYR:CE2 | 65:ST:116:LYS:HB2 | 2.50 | 0.46 |
| 66:SU:124:LYS:HD3 | 66:SU:124:LYS:HA | 1.73 | 0.46 |
| 68:SW:86:LEU:HD12 | 68:SW:87:SER:H | 1.80 | 0.46 |
| 1:LA:910:C:OP1 | 4:LD:14:SER:OG | 2.31 | 0.46 |
| 1:LA:1294:G:OP1 | 21:LU:84:ARG:HG3 | 2.16 | 0.46 |
| 1:LA:2277:C:P | 42:Lp:23:ARG:NH2 | 2.89 | 0.46 |
| 1:LA:2528:A:H2' | 1:LA:2528:A:N3 | 2.29 | 0.46 |
| 3:LC:8:C:H2' | 3:LC:9:A:H8 | 1.81 | 0.46 |
| 9:LI:120:THR:H | 9:LI:123:THR:HB | 1.81 | 0.46 |
| 10:LJ:43:LYS:HE2 | 10:LJ:43:LYS:HB2 | 1.69 | 0.46 |
| 15:LO:36:VAL:HG21 | 15:LO:47:ASP:HB2 | 1.97 | 0.46 |
| 17:LQ:77[A]:SER:HB2 | 17:LQ:104[A]:VAL:HG22 | 1.97 | 0.46 |
| 22:LV:91:LEU:HD12 | 22:LV:96:ILE:HD11 | 1.98 | 0.46 |
| 26:LZ:90:ALA:O | 26:LZ:120:LYS:NZ | 2.47 | 0.46 |
| 38:Ll:27:PHE:HA | 38:Ll:34:CYS:HA | 1.96 | 0.46 |
| 45:S2:473:A:H2' | 45:S2:474:A:O4' | 2.16 | 0.46 |
| 45:S2:908:U:O4 | 45:S2:1009:U:O2' | 2.18 | 0.46 |
| 45:S2:1579:U:H2' | 45:S2:1580:C:C6 | 2.51 | 0.46 |
| 60:SO:198:ASN:HD21 | 60:SO:216:LYS:HZ3 | 1.61 | 0.46 |
| 60:SO:263:PHE:CZ | 60:SO:265:LEU:HA | 2.50 | 0.46 |
| 61:SP:54:TRP:HZ3 | 61:SP:176:LEU:HD22 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 75:Sd:37:LYS:NZ | 75:Sd:93:ARG:HD3 | 2.31 | 0.46 |
| 80:Tb:49:C:O2' | 80:Tb:60:A:O2' | 2.33 | 0.46 |
| 1:LA:168:U:H2' | 1:LA:169:U:H4' | 1.98 | 0.46 |
| 1:LA:599:G:H22 | 1:LA:601:A:N6 | 2.13 | 0.46 |
| 1:LA:846:A:H5' | 70:SY:123:HIS:CE1 | 2.51 | 0.46 |
| 1:LA:1142:A:H5' | 1:LA:1367:U:H1' | 1.98 | 0.46 |
| 1:LA:1380:A:H2' | 1:LA:1381:G:H8 | 1.81 | 0.46 |
| 1:LA:2525:C:H2' | 1:LA:2526:G:C8 | 2.51 | 0.46 |
| 1:LA:2635:A:H5' | 1:LA:2636:A:H5' | 1.97 | 0.46 |
| 9:LI:149:TYR:OH | 9:LI:182:ASP:OD1 | 2.29 | 0.46 |
| 12:LL:53:VAL:CG2 | 12:LL:166:ILE:HD12 | 2.45 | 0.46 |
| 20:LT:68:GLN:NE2 | 20:LT:72:GLU:OE2 | 2.48 | 0.46 |
| 37:Lk:70:ARG:HE | 37:Lk:87:VAL:HB | 1.79 | 0.46 |
| 39:Lm:12:LEU:O | 39:Lm:15:THR:HG22 | 2.15 | 0.46 |
| 45:S2:392:G:OP1 | 45:S2:1729:C:O2' | 2.32 | 0.46 |
| 45:S2:427:C:H1' | 45:S2:459:G:H1' | 1.97 | 0.46 |
| 45:S2:1388:A:H5' | 45:S2:1389:C:C6 | 2.50 | 0.46 |
| 45:S2:1486:G:H2' | 45:S2:1487:A:H8 | 1.80 | 0.46 |
| 45:S2:1585:U:O2' | 51:SF:134:ALA:HB3 | 2.15 | 0.46 |
| 47:SB:174:LEU:O | 47:SB:177:ILE:HD12 | 2.16 | 0.46 |
| 50:SE:33:PHE:CE2 | 50:SE:86:VAL:HG12 | 2.51 | 0.46 |
| 58:SM:42:CYS:O | 58:SM:46:LYS:HG2 | 2.15 | 0.46 |
| 66:SU:177:THR:OG1 | 66:SU:179:LYS:HG2 | 2.16 | 0.46 |
| 68:SW:175:ARG:CZ | 68:SW:175:ARG:HB2 | 2.46 | 0.46 |
| 74:Sc:88:PRO:HG2 | 74:Sc:132:LEU:HD22 | 1.98 | 0.46 |
| 77:Sf:55:THR:HB | 77:Sf:62:ILE:HA | 1.97 | 0.46 |
| 1:LA:806:A:H61 | 1:LA:933:G:H22 | 1.62 | 0.46 |
| 1:LA:1024:A:H2' | 1:LA:1025:A:H5'' | 1.98 | 0.46 |
| 1:LA:2179:G:H2' | 1:LA:2180:C:C6 | 2.51 | 0.46 |
| 1:LA:2862:G:OP1 | 12:LL:107:GLY:HA2 | 2.16 | 0.46 |
| 2:LB:11:A:N6 | 7:LG:16:PHE:O | 2.49 | 0.46 |
| 3:LC:21:C:C2' | 3:LC:22:U:H5' | 2.46 | 0.46 |
| 3:LC:78:G:H1' | 36:Lj:42:PRO:HG2 | 1.98 | 0.46 |
| 4:LD:206:PRO:HD3 | 4:LD:213:GLY:CA | 2.46 | 0.46 |
| 11:LK:18:VAL:HG13 | 11:LK:27:VAL:HG22 | 1.98 | 0.46 |
| 12:LL:207:GLU:O | 12:LL:211:ARG:HG3 | 2.14 | 0.46 |
| 18:LR:35:ALA:HB2 | 18:LR:58:ILE:HG23 | 1.98 | 0.46 |
| 33:Lg:103:LYS:O | 33:Lg:106:VAL:HG22 | 2.15 | 0.46 |
| 45:S2:323:A:O2' | 45:S2:324:U:O5' | 2.34 | 0.46 |
| 45:S2:409:C:N4 | 45:S2:423:G:O6 | 2.49 | 0.46 |
| 45:S2:1273:G:H5'' | 45:S2:1274:C:H3' | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:SA:29:LEU:HB3 | 46:SA:34:TYR:HB2 | 1.98 | 0.46 |
| 47:SB:124:LEU:HD11 | 56:SK:59:TYR:HB2 | 1.97 | 0.46 |
| 52:SG:79:GLU:HG3 | 52:SG:80:ARG:N | 2.31 | 0.46 |
| 63:SR:35:TRP:NE1 | 63:SR:37:PRO:HB3 | 2.30 | 0.46 |
| 66:SU:23:ALA:O | 66:SU:26:GLU:HG2 | 2.16 | 0.46 |
| 69:SX:59:PRO:HG3 | 69:SX:138:ASN:HB3 | 1.97 | 0.46 |
| 70:SY:73:ARG:O | 70:SY:77:SER:OG | 2.31 | 0.46 |
| 1:LA:820:U:H2' | 1:LA:821:G:C8 | 2.51 | 0.46 |
| 1:LA:1496:C:O2' | 1:LA:1601:A:N3 | 2.46 | 0.46 |
| 1:LA:1679:G:H2' | 1:LA:1680:U:H6 | 1.81 | 0.46 |
| 1:LA:1719:U:OP2 | 20:LT:120:TYR:OH | 2.26 | 0.46 |
| 1:LA:1798:A:H2' | 1:LA:1799:A:H8 | 1.81 | 0.46 |
| 1:LA:2281:U:O2 | 1:LA:2309:U:H4' | 2.15 | 0.46 |
| 1:LA:2672:A:OP1 | 13:LM:95:ASN:HA | 2.15 | 0.46 |
| 1:LA:3391:U:H2' | 1:LA:3392:U:C6 | 2.50 | 0.46 |
| 2:LB:35:C:N3 | 2:LB:45:A:O2' | 2.40 | 0.46 |
| 7:LG:178:ASN:HA | 7:LG:183:TRP:CD2 | 2.51 | 0.46 |
| 13:LM:96:PHE:O | 13:LM:156:LYS:HE3 | 2.16 | 0.46 |
| 23:LW:19:VAL:O | 23:LW:22:PRO:HD2 | 2.16 | 0.46 |
| 35:Li:29:ILE:HD11 | 35:Li:31:ARG:HE | 1.81 | 0.46 |
| 45:S2:220:A:OP2 | 45:S2:831:U:O2' | 2.29 | 0.46 |
| 46:SA:37:VAL:HG12 | 46:SA:50:ILE:HG12 | 1.97 | 0.46 |
| 51:SF:73:GLY:O | 51:SF:77:GLN:HG3 | 2.15 | 0.46 |
| 57:SL:42:ARG:HH21 | 57:SL:59:SER:HA | 1.80 | 0.46 |
| 57:SL:54:LEU:HD12 | 57:SL:54:LEU:HA | 1.74 | 0.46 |
| 62:SQ:208:GLN:HG3 | 62:SQ:209:ASN:HB2 | 1.97 | 0.46 |
| 65:ST:1:MET:CE | 65:ST:109:LEU:HD12 | 2.46 | 0.46 |
| 66:SU:104:ARG:H | 66:SU:104:ARG:HD2 | 1.80 | 0.46 |
| 70:SY:37:ILE:HG12 | 70:SY:54:LEU:HD11 | 1.97 | 0.46 |
| 1:LA:1808:A:H2' | 1:LA:1808:A:N3 | 2.30 | 0.46 |
| 1:LA:2555:C:H2' | 1:LA:2556:A:O4' | 2.15 | 0.46 |
| 1:LA:2609:G:C5' | 16:LP:81:TYR:HA | 2.46 | 0.46 |
| 8:LH:132:THR:HA | 8:LH:135:VAL:HG12 | 1.98 | 0.46 |
| 15:LO:94:TRP:CE2 | 15:LO:100:ALA:HB2 | 2.51 | 0.46 |
| 18:LR:31:GLU:OE1 | 18:LR:31:GLU:HA | 2.16 | 0.46 |
| 22:LV:73:GLY:HA2 | 22:LV:89:LEU:O | 2.16 | 0.46 |
| 45:S2:256:A:O2' | 67:SV:73:SER:N | 2.49 | 0.46 |
| 45:S2:258:C:O2 | 67:SV:178:ARG:NH1 | 2.49 | 0.46 |
| 45:S2:564:G:N2 | 45:S2:577:G:OP1 | 2.49 | 0.46 |
| 45:S2:1053:G:H5' | 45:S2:1054:U:OP2 | 2.15 | 0.46 |
| 45:S2:1233:G:H21 | 59:SN:145:HIS:HE1 | 1.64 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:S2:1503:A:O2' | 54:SI:41:SER:HB2 | 2.16 | 0.46 |
| 48:SC:14:TYR:OH | 48:SC:34:GLU:OE1 | 2.34 | 0.46 |
| 61:SP:166:GLY:O | 61:SP:170:ILE:HG13 | 2.16 | 0.46 |
| 62:SQ:46:THR:OG1 | 62:SQ:64:ARG:NH1 | 2.49 | 0.46 |
| 66:SU:32:PRO:HA | 66:SU:35:LYS:HE3 | 1.97 | 0.46 |
| 68:SW:10:LYS:HE3 | 68:SW:10:LYS:HB3 | 1.76 | 0.46 |
| 71:SZ:11:SER:OG | 71:SZ:12:GLN:N | 2.48 | 0.46 |
| 75:Sd:38:ASP:OD1 | 75:Sd:39:GLU:N | 2.49 | 0.46 |
| 75:Sd:43:LYS:O | 75:Sd:47:VAL:HG13 | 2.16 | 0.46 |
| 75:Sd:105:ARG:O | 75:Sd:109:LYS:HG3 | 2.15 | 0.46 |
| 1:LA:26:A:H2' | 1:LA:27:C:H6 | 1.81 | 0.45 |
| 1:LA:161:G:H2' | 1:LA:162:G:O4' | 2.15 | 0.45 |
| 1:LA:407:A:H5' | 1:LA:1395:C:O2' | 2.15 | 0.45 |
| 1:LA:775:U:H5 | 1:LA:2718:U:O2 | 1.99 | 0.45 |
| 1:LA:1477:C:H2' | 1:LA:1478:U:C6 | 2.52 | 0.45 |
| 1:LA:1874:G:O6 | 20:LT:20:ARG:NH1 | 2.49 | 0.45 |
| 1:LA:2147:U:H2' | 1:LA:2148:A:C5 | 2.50 | 0.45 |
| 1:LA:2228:A:H2' | 1:LA:2229:C:C6 | 2.51 | 0.45 |
| 1:LA:2561:A:N6 | 1:LA:2578:G:O2' | 2.47 | 0.45 |
| 15:LO:17:VAL:HG11 | 15:LO:74:ARG:HA | 1.98 | 0.45 |
| 18:LR:138:LYS:NZ | 18:LR:140:GLU:HG3 | 2.30 | 0.45 |
| 21:LU:14:LEU:HD11 | 22:LV:136:ARG:NH2 | 2.31 | 0.45 |
| 21:LU:66:GLU:OE2 | 21:LU:98:SER:HA | 2.15 | 0.45 |
| 22:LV:80:VAL:O | 22:LV:83:ARG:NH1 | 2.49 | 0.45 |
| 26:LZ:107:VAL:HA | 26:LZ:126:LEU:HA | 1.97 | 0.45 |
| 28:Lb:95:VAL:HG11 | 28:Lb:113:VAL:HG11 | 1.98 | 0.45 |
| 45:S2:514:G:H2' | 45:S2:515:A:H8 | 1.80 | 0.45 |
| 45:S2:821:U:C4 | 45:S2:852:C:N4 | 2.79 | 0.45 |
| 45:S2:1219:A:C5 | 45:S2:1264:G:N2 | 2.84 | 0.45 |
| 45:S2:1273:G:N7 | 45:S2:1431:C:H5' | 2.31 | 0.45 |
| 45:S2:1544:U:H5' | 53:SH:132:ARG:HH21 | 1.80 | 0.45 |
| 46:SA:105:MET:HE1 | 46:SA:119:ALA:CA | 2.46 | 0.45 |
| 50:SE:28:MET:HG3 | 50:SE:29:SER:H | 1.81 | 0.45 |
| 52:SG:17:ILE:HD13 | 52:SG:17:ILE:HA | 1.73 | 0.45 |
| 56:SK:42:LEU:HD11 | 56:SK:47:TYR:HD2 | 1.81 | 0.45 |
| 60:SO:221:MET:HB3 | 60:SO:223:TRP:HE1 | 1.80 | 0.45 |
| 61:SP:59:LEU:O | 61:SP:63:ILE:HG13 | 2.17 | 0.45 |
| 68:SW:116:LEU:HB2 | 68:SW:118:LEU:HD11 | 1.98 | 0.45 |
| 79:Ta:35:A:H2' | 79:Ta:36:G:N2 | 2.31 | 0.45 |
| 1:LA:215:G:H5'' | 27:La:12:ARG:HG3 | 1.98 | 0.45 |
| 1:LA:1221:G:H21 | 1:LA:1222:A:N6 | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:LA:1494:U:H5 | 1:LA:1834:A:N1 | 2.15 | 0.45 |
| 1:LA:2655:A:H4' | 43:Lq:98:LYS:HE3 | 1.97 | 0.45 |
| 2:LB:64:A:H8 | 12:LL:204:GLY:O | 2.00 | 0.45 |
| 3:LC:95:G:N3 | 38:Ll:79:GLN:HG3 | 2.31 | 0.45 |
| 7:LG:85:ARG:NH1 | 7:LG:86:TYR:OH | 2.49 | 0.45 |
| 22:LV:125:ALA:O | 22:LV:127:GLN:HG2 | 2.16 | 0.45 |
| 25:LY:25:ASP:OD1 | 25:LY:25:ASP:N | 2.46 | 0.45 |
| 26:LZ:105:VAL:HG11 | 26:LZ:135:ILE:HG12 | 1.98 | 0.45 |
| 29:Lc:139:ARG:HD3 | 29:Lc:139:ARG:HA | 1.78 | 0.45 |
| 45:S2:298:C:O2' | 64:SS:30:ARG:NH1 | 2.48 | 0.45 |
| 45:S2:895:G:H2' | 45:S2:896:U:C6 | 2.51 | 0.45 |
| 45:S2:1280:C:H4' | 55:SJ:69:LYS:HB3 | 1.98 | 0.45 |
| 55:SJ:28:SER:HB2 | 55:SJ:112:VAL:HG13 | 1.97 | 0.45 |
| 61:SP:126:PRO:HG2 | 61:SP:151:SER:HB3 | 1.97 | 0.45 |
| 61:SP:140:ASN:ND2 | 72:Sa:29:HIS:O | 2.48 | 0.45 |
| 64:SS:44:LEU:HD23 | 64:SS:82:TYR:HB3 | 1.98 | 0.45 |
| 66:SU:129:LEU:HD11 | 66:SU:172:VAL:HG21 | 1.97 | 0.45 |
| 67:SV:153:GLU:HG3 | 67:SV:156:VAL:HG22 | 1.97 | 0.45 |
| 68:SW:170:GLY:O | 68:SW:174:ARG:HG2 | 2.16 | 0.45 |
| 1:LA:397:A:H5'' | 1:LA:399:A:OP1 | 2.16 | 0.45 |
| 1:LA:1221:G:H21 | 1:LA:1222:A:H62 | 1.65 | 0.45 |
| 1:LA:1389:A:N6 | 1:LA:1417:A:O2' | 2.44 | 0.45 |
| 1:LA:2759:C:N3 | 43:Lq:63:LYS:HE3 | 2.31 | 0.45 |
| 1:LA:3094:U:H2' | 1:LA:3095:C:C6 | 2.51 | 0.45 |
| 3:LC:142:C:H2' | 3:LC:143:U:H6 | 1.81 | 0.45 |
| 4:LD:80:GLU:HG2 | 4:LD:170:ALA:HA | 1.98 | 0.45 |
| 16:LP:110:ALA:HB1 | 16:LP:113:LEU:HD12 | 1.99 | 0.45 |
| 17:LQ:19[A]:LEU:HD23 | 17:LQ:41[A]:LEU:HD21 | 1.97 | 0.45 |
| 19:LS:180:ARG:HG2 | 19:LS:180:ARG:NH1 | 2.31 | 0.45 |
| 24:LX:96:GLU:OE2 | 25:LY:24:GLY:N | 2.49 | 0.45 |
| 25:LY:56:ARG:HB3 | 25:LY:61:LYS:HB2 | 1.99 | 0.45 |
| 33:Lg:102:ALA:O | 33:Lg:106:VAL:HG13 | 2.16 | 0.45 |
| 45:S2:141:U:O4 | 65:ST:187:LYS:HD2 | 2.16 | 0.45 |
| 45:S2:888:U:H2' | 45:S2:889:U:C6 | 2.51 | 0.45 |
| 45:S2:998:A:H2' | 45:S2:999:U:C6 | 2.52 | 0.45 |
| 45:S2:1124:A:H2' | 45:S2:1125:A:C8 | 2.52 | 0.45 |
| 45:S2:1241:G:C8 | 50:SE:52:LYS:HD2 | 2.51 | 0.45 |
| 45:S2:1423:U:H4' | 45:S2:1423:U:OP1 | 2.16 | 0.45 |
| 47:SB:98:MET:HE1 | 47:SB:107:LYS:CG | 2.44 | 0.45 |
| 49:SD:32:LEU:HD23 | 49:SD:32:LEU:C | 2.41 | 0.45 |
| 49:SD:135:MET:HB3 | 49:SD:135:MET:HE3 | 1.68 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:SO:255:ALA:HB1 | 60:SO:289:ALA:HB3 | 1.99 | 0.45 |
| 62:SQ:171:ILE:HD13 | 62:SQ:196:GLU:HG3 | 1.97 | 0.45 |
| 1:LA:263:C:H2' | 1:LA:264:G:O4' | 2.17 | 0.45 |
| 1:LA:630:U:H2' | 1:LA:631:G:C8 | 2.51 | 0.45 |
| 1:LA:2129:G:O4' | 1:LA:2143:A:H4' | 2.16 | 0.45 |
| 13:LM:99:THR:O | 13:LM:154:THR:OG1 | 2.35 | 0.45 |
| 16:LP:36:ILE:HD11 | 16:LP:105:ARG:HB3 | 1.98 | 0.45 |
| 18:LR:88:VAL:O | 18:LR:92:GLN:HG2 | 2.16 | 0.45 |
| 26:LZ:117:ASN:OD1 | 26:LZ:119:THR:OG1 | 2.33 | 0.45 |
| 42:Lp:11:ARG:NH2 | 45:S2:1127:G:OP1 | 2.49 | 0.45 |
| 45:S2:59:C:H1' | 45:S2:452:A:C8 | 2.51 | 0.45 |
| 45:S2:161:U:OP2 | 65:ST:87:ARG:NH1 | 2.38 | 0.45 |
| 45:S2:368:U:N3 | 45:S2:369:A:N7 | 2.65 | 0.45 |
| 45:S2:828:U:O2' | 45:S2:829:A:OP1 | 2.32 | 0.45 |
| 45:S2:933:A:OP1 | 76:Se:70:LYS:NZ | 2.46 | 0.45 |
| 45:S2:1086:A:H2' | 45:S2:1087:A:C8 | 2.51 | 0.45 |
| 45:S2:1117:U:H2' | 45:S2:1118:G:C8 | 2.51 | 0.45 |
| 49:SD:130:THR:O | 49:SD:134:SER:HB3 | 2.16 | 0.45 |
| 50:SE:127:ARG:H | 50:SE:127:ARG:HD2 | 1.81 | 0.45 |
| 60:SO:122:ILE:CG2 | 60:SO:134:TRP:HB2 | 2.38 | 0.45 |
| 61:SP:38:PHE:CE1 | 61:SP:39:ASN:HB2 | 2.51 | 0.45 |
| 63:SR:139:ILE:HG13 | 63:SR:191:ALA:HB1 | 1.96 | 0.45 |
| 69:SX:6:THR:HG22 | 69:SX:8:GLN:H | 1.81 | 0.45 |
| 70:SY:64:ARG:O | 70:SY:64:ARG:HD3 | 2.16 | 0.45 |
| 1:LA:26:A:N3 | 1:LA:328:U:O2' | 2.47 | 0.45 |
| 1:LA:121:A:C2 | 10:LJ:129:PRO:HB3 | 2.50 | 0.45 |
| 1:LA:289:A:H2' | 1:LA:290:G:H8 | 1.81 | 0.45 |
| 1:LA:364:G:OP1 | 6:LF:60:THR:HG23 | 2.16 | 0.45 |
| 1:LA:439:C:O2 | 1:LA:493:G:N2 | 2.50 | 0.45 |
| 1:LA:795:U:H2' | 1:LA:796:U:C6 | 2.51 | 0.45 |
| 1:LA:1140:C:O2' | 1:LA:1152:A:N3 | 2.45 | 0.45 |
| 1:LA:1821:C:H5'' | 35:Li:66:SER:HB2 | 1.99 | 0.45 |
| 1:LA:2111:U:H5' | 1:LA:2112:A:H5' | 1.98 | 0.45 |
| 1:LA:3138:A:H2' | 1:LA:3139:G:O4' | 2.16 | 0.45 |
| 3:LC:94:C:H5'' | 38:Li:76:ASN:HD21 | 1.82 | 0.45 |
| 3:LC:121:U:O2 | 3:LC:132:G:N2 | 2.32 | 0.45 |
| 7:LG:236:LEU:HD23 | 7:LG:236:LEU:H | 1.81 | 0.45 |
| 10:LJ:71:VAL:CG2 | 10:LJ:75:ILE:HB | 2.47 | 0.45 |
| 11:LK:7:GLU:HB2 | 11:LK:54:LYS:HG3 | 1.99 | 0.45 |
| 14:LN:50:PRO:HA | 14:LN:138:VAL:O | 2.17 | 0.45 |
| 22:LV:126:VAL:HG23 | 22:LV:128:LEU:HD22 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:S2:330:G:H2' | 45:S2:331:A:C8 | 2.52 | 0.45 |
| 45:S2:333:A:H2' | 45:S2:334:G:C8 | 2.52 | 0.45 |
| 45:S2:1143:A:H4' | 45:S2:1144:U:OP1 | 2.15 | 0.45 |
| 45:S2:1220:C:H5' | 48:SC:51:SER:HB2 | 1.98 | 0.45 |
| 45:S2:1290:U:H2' | 45:S2:1291:G:N3 | 2.32 | 0.45 |
| 45:S2:1330:G:H3' | 45:S2:1331:A:H8 | 1.82 | 0.45 |
| 45:S2:1488:G:N2 | 45:S2:1512:G:H21 | 2.14 | 0.45 |
| 55:SJ:30:LYS:HD2 | 55:SJ:33:GLN:OE1 | 2.16 | 0.45 |
| 60:SO:132:LYS:HA | 60:SO:143:THR:HA | 1.99 | 0.45 |
| 61:SP:126:PRO:HG2 | 61:SP:152:PRO:HD2 | 1.99 | 0.45 |
| 71:SZ:92:LYS:HZ3 | 71:SZ:121:VAL:HG13 | 1.80 | 0.45 |
| 80:Tb:30:G:H2' | 80:Tb:31:G:H8 | 1.82 | 0.45 |
| 1:LA:169:U:O2' | 1:LA:170:G:O4' | 2.33 | 0.45 |
| 1:LA:177:U:N3 | 1:LA:241:G:C6 | 2.84 | 0.45 |
| 1:LA:1925:C:OP1 | 44:Lr:23:ARG:NH1 | 2.40 | 0.45 |
| 1:LA:2881:U:H2' | 1:LA:2882:U:C6 | 2.52 | 0.45 |
| 10:LJ:50:VAL:HG21 | 26:LZ:27:ARG:HD2 | 1.99 | 0.45 |
| 12:LL:177:ASP:OD1 | 12:LL:177:ASP:N | 2.49 | 0.45 |
| 14:LN:43:ALA:O | 14:LN:47:ALA:HA | 2.16 | 0.45 |
| 22:LV:116:ARG:HG2 | 22:LV:128:LEU:HD21 | 1.98 | 0.45 |
| 34:Lh:67:MET:HE1 | 34:Lh:90:PRO:HD3 | 1.99 | 0.45 |
| 42:Lp:1:MET:HB2 | 45:S2:1642:G:H5' | 1.99 | 0.45 |
| 45:S2:387:A:H4' | 45:S2:388:G:O5' | 2.17 | 0.45 |
| 45:S2:565:C:OP2 | 45:S2:577:G:O2' | 2.34 | 0.45 |
| 45:S2:707:A:OP2 | 45:S2:731:C:N4 | 2.45 | 0.45 |
| 45:S2:1531:G:H2' | 45:S2:1532:U:C6 | 2.52 | 0.45 |
| 46:SA:72:LEU:HD12 | 48:SC:65:TYR:HD1 | 1.82 | 0.45 |
| 48:SC:52:LYS:HE3 | 48:SC:54:TYR:CE2 | 2.51 | 0.45 |
| 51:SF:117:LEU:HA | 51:SF:117:LEU:HD23 | 1.61 | 0.45 |
| 51:SF:118:ILE:N | 51:SF:118:ILE:HD13 | 2.32 | 0.45 |
| 62:SQ:153:HIS:ND1 | 62:SQ:154:SER:N | 2.65 | 0.45 |
| 66:SU:166:LEU:O | 66:SU:170:GLN:HG3 | 2.16 | 0.45 |
| 68:SW:126:ARG:HG2 | 78:Sg:33:ARG:HD3 | 1.99 | 0.45 |
| 79:Ta:59:A:OP2 | 79:Ta:60:A:N6 | 2.47 | 0.45 |
| 1:LA:1152:A:O2' | 1:LA:1153:A:H5' | 2.17 | 0.45 |
| 1:LA:1747:G:OP1 | 39:Lm:44:LYS:NZ | 2.41 | 0.45 |
| 1:LA:2261:A:N1 | 45:S2:1758:U:O2' | 2.46 | 0.45 |
| 1:LA:2584:G:C6 | 26:LZ:24:LEU:HD13 | 2.52 | 0.45 |
| 1:LA:2837:A:N6 | 1:LA:2849:G:O2' | 2.43 | 0.45 |
| 1:LA:2932:A:O4' | 1:LA:3014:G:H5'' | 2.16 | 0.45 |
| 1:LA:3327:G:H2' | 1:LA:3328:U:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:LE:142:ALA:O | 5:LE:146:ARG:NE | 2.36 | 0.45 |
| 5:LE:158:VAL:HG13 | 5:LE:191:LYS:HD2 | 1.99 | 0.45 |
| 11:LK:47:LYS:HE2 | 11:LK:47:LYS:HB2 | 1.66 | 0.45 |
| 15:LO:112:LEU:HD21 | 17:LQ:197[A]:LEU:O | 2.17 | 0.45 |
| 19:LS:130:ARG:HE | 19:LS:130:ARG:HB2 | 1.49 | 0.45 |
| 26:LZ:108:LEU:N | 26:LZ:125:ARG:O | 2.44 | 0.45 |
| 45:S2:97:C:H1' | 45:S2:426:G:H5' | 1.99 | 0.45 |
| 45:S2:350:U:OP1 | 45:S2:351:C:O2' | 2.27 | 0.45 |
| 45:S2:689:G:H2' | 45:S2:690:G:C8 | 2.51 | 0.45 |
| 45:S2:905:A:O3' | 71:SZ:52:ARG:HB3 | 2.17 | 0.45 |
| 47:SB:98:MET:HE2 | 47:SB:105:GLY:O | 2.17 | 0.45 |
| 61:SP:144:ILE:HG23 | 61:SP:158:VAL:HG13 | 1.99 | 0.45 |
| 64:SS:180:LEU:HD21 | 64:SS:192:ILE:CG2 | 2.47 | 0.45 |
| 64:SS:180:LEU:HD21 | 64:SS:192:ILE:HG22 | 1.99 | 0.45 |
| 64:SS:192:ILE:N | 64:SS:192:ILE:HD12 | 2.31 | 0.45 |
| 1:LA:377:A:H1' | 1:LA:392:G:N2 | 2.31 | 0.45 |
| 1:LA:670:U:H2' | 1:LA:671:A:C8 | 2.51 | 0.45 |
| 1:LA:1228:G:H2' | 1:LA:1229:G:O4' | 2.17 | 0.45 |
| 1:LA:2523:A:H2 | 10:LJ:44:ARG:HH11 | 1.63 | 0.45 |
| 1:LA:2630:U:H4' | 1:LA:2696:A:H2 | 1.82 | 0.45 |
| 1:LA:2722:U:H2' | 1:LA:2723:U:C6 | 2.52 | 0.45 |
| 1:LA:3052:G:H2' | 1:LA:3053:U:H6 | 1.82 | 0.45 |
| 1:LA:3174:U:H5' | 34:Lh:10:LYS:CE | 2.47 | 0.45 |
| 1:LA:3314:G:OP2 | 5:LE:116:ARG:NH2 | 2.48 | 0.45 |
| 1:LA:3373:U:OP2 | 32:Lf:70:ARG:NH2 | 2.50 | 0.45 |
| 8:LH:145:LEU:HD23 | 8:LH:145:LEU:HA | 1.79 | 0.45 |
| 9:LI:98:LYS:HB3 | 9:LI:99:PRO:HD3 | 1.99 | 0.45 |
| 11:LK:151:VAL:O | 11:LK:155:SER:OG | 2.27 | 0.45 |
| 13:LM:54:VAL:CG1 | 13:LM:57:PHE:HB2 | 2.45 | 0.45 |
| 21:LU:71:LYS:HD3 | 21:LU:71:LYS:N | 2.31 | 0.45 |
| 35:Li:3:GLN:HE22 | 35:Li:29:ILE:HA | 1.81 | 0.45 |
| 35:Li:57:LEU:HB3 | 35:Li:61:GLN:HB2 | 1.99 | 0.45 |
| 37:Lk:59:ASP:OD1 | 37:Lk:60:LEU:N | 2.50 | 0.45 |
| 45:S2:1165:G:H2' | 45:S2:1166:A:C8 | 2.51 | 0.45 |
| 45:S2:1586:A:H2' | 45:S2:1587:A:O4' | 2.17 | 0.45 |
| 47:SB:128:ASN:HB3 | 47:SB:131:GLN:CB | 2.47 | 0.45 |
| 48:SC:71:GLU:HA | 48:SC:74:GLU:HG2 | 1.98 | 0.45 |
| 49:SD:68:GLU:OE2 | 49:SD:70:ASN:HB3 | 2.17 | 0.45 |
| 60:SO:150:TRP:NE1 | 60:SO:174:ASN:HD22 | 2.15 | 0.45 |
| 62:SQ:123:ALA:HB2 | 62:SQ:165:ARG:HG2 | 1.99 | 0.45 |
| 64:SS:246:LEU:HD12 | 64:SS:251:GLU:HG2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:Sc:79:ASN:HB3 | 74:Sc:81:LYS:HG3 | 1.99 | 0.45 |
| 75:Sd:84:LYS:HE3 | 75:Sd:85:PHE:CE1 | 2.52 | 0.45 |
| 79:Ta:37:G:C6 | 79:Ta:38:A:H8 | 2.35 | 0.45 |
| 1:LA:343:U:H1' | 6:LF:95:ARG:HG3 | 1.98 | 0.45 |
| 1:LA:575:C:H5'' | 9:LI:142:SER:OG | 2.17 | 0.45 |
| 1:LA:936:G:OP2 | 1:LA:937:C:N4 | 2.42 | 0.45 |
| 1:LA:1510:U:H5'' | 1:LA:1511:U:H5 | 1.82 | 0.45 |
| 1:LA:1565:A:H2' | 1:LA:1570:A:N1 | 2.32 | 0.45 |
| 1:LA:1611:A:H5'' | 39:Lm:51:LEU:HD22 | 1.97 | 0.45 |
| 1:LA:2862:G:H5' | 12:LL:109:ASP:HB3 | 1.98 | 0.45 |
| 1:LA:2897:G:O6 | 41:Lo:125:LYS:NZ | 2.50 | 0.45 |
| 11:LK:146:LEU:HD23 | 11:LK:146:LEU:HA | 1.77 | 0.45 |
| 16:LP:21:PHE:O | 16:LP:25:VAL:HG22 | 2.15 | 0.45 |
| 16:LP:192:LYS:O | 16:LP:196:THR:OG1 | 2.26 | 0.45 |
| 22:LV:149:GLN:NE2 | 22:LV:151:LEU:HD12 | 2.32 | 0.45 |
| 36:Lj:45:LYS:HE3 | 36:Lj:49:LYS:HD3 | 1.99 | 0.45 |
| 45:S2:372:G:H1' | 45:S2:613:G:O6 | 2.16 | 0.45 |
| 45:S2:555:A:H2' | 45:S2:555:A:N3 | 2.32 | 0.45 |
| 45:S2:1349:G:O2' | 45:S2:1350:U:O4' | 2.30 | 0.45 |
| 47:SB:136:ALA:HB2 | 47:SB:202:ALA:HB2 | 1.99 | 0.45 |
| 54:SI:38:LYS:HB2 | 54:SI:43:ASN:HD22 | 1.82 | 0.45 |
| 60:SO:93:ASP:HB2 | 60:SO:97:GLY:O | 2.16 | 0.45 |
| 68:SW:37:LYS:O | 68:SW:37:LYS:HG2 | 2.17 | 0.45 |
| 70:SY:104:ARG:NH1 | 70:SY:104:ARG:HB2 | 2.31 | 0.45 |
| 80:Tb:25:U:H2' | 80:Tb:26:C:C6 | 2.52 | 0.45 |
| 1:LA:1340:U:H2' | 1:LA:1341:C:C6 | 2.51 | 0.45 |
| 1:LA:1947:G:H5' | 20:LT:101:VAL:HG11 | 1.98 | 0.45 |
| 1:LA:2525:C:H2' | 1:LA:2526:G:H8 | 1.82 | 0.45 |
| 1:LA:2667:U:H2' | 1:LA:2668:G:H8 | 1.82 | 0.45 |
| 1:LA:3014:G:H2' | 1:LA:3015:A:H8 | 1.82 | 0.45 |
| 1:LA:3167:A:O2' | 1:LA:3168:U:OP1 | 2.27 | 0.45 |
| 1:LA:3382:G:H2' | 1:LA:3383:U:C6 | 2.52 | 0.45 |
| 2:LB:38:U:H2' | 2:LB:40:C:H5 | 1.82 | 0.45 |
| 3:LC:85:G:H4' | 3:LC:86:U:OP1 | 2.16 | 0.45 |
| 4:LD:82:VAL:HG13 | 4:LD:86:GLN:OE1 | 2.17 | 0.45 |
| 7:LG:214:ASP:OD1 | 7:LG:215:ASP:N | 2.49 | 0.45 |
| 13:LM:37:LEU:HD23 | 13:LM:37:LEU:HA | 1.80 | 0.45 |
| 13:LM:117:ASP:OD1 | 13:LM:118:PRO:HD2 | 2.17 | 0.45 |
| 16:LP:94:TYR:CE2 | 16:LP:96:ARG:HB2 | 2.52 | 0.45 |
| 18:LR:142:SER:O | 18:LR:142:SER:OG | 2.24 | 0.45 |
| 36:Lj:119:LYS:HD2 | 36:Lj:120:ALA:HB3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 37:Lk:47:ILE:O | 37:Lk:47:ILE:HG13 | 2.16 | 0.45 |
| 41:Lo:98:LYS:HG3 | 41:Lo:118:THR:HG21 | 1.98 | 0.45 |
| 45:S2:448:C:H2' | 45:S2:449:C:C6 | 2.52 | 0.45 |
| 45:S2:562:G:H2' | 45:S2:563:U:C6 | 2.51 | 0.45 |
| 45:S2:1098:U:H3' | 45:S2:1099:U:H5' | 1.99 | 0.45 |
| 45:S2:1691:A:H2' | 45:S2:1692:G:H8 | 1.81 | 0.45 |
| 45:S2:1775:U:H2' | 45:S2:1776:A:C8 | 2.51 | 0.45 |
| 58:SM:30:LEU:HA | 58:SM:39:CYS:HA | 1.99 | 0.45 |
| 61:SP:131:GLN:NE2 | 61:SP:135:GLU:OE2 | 2.45 | 0.45 |
| 62:SQ:103:MET:HE3 | 62:SQ:188:LEU:HD21 | 1.99 | 0.45 |
| 63:SR:81:MET:N | 63:SR:101:VAL:O | 2.44 | 0.45 |
| 63:SR:227:PRO:HA | 63:SR:230:TRP:CG | 2.52 | 0.45 |
| 64:SS:11:ARG:HH21 | 64:SS:25:GLY:HA3 | 1.80 | 0.45 |
| 65:ST:2:LYS:HE3 | 65:ST:2:LYS:HB3 | 1.71 | 0.45 |
| 1:LA:696:A:OP1 | 6:LF:272:VAL:HG21 | 2.18 | 0.44 |
| 1:LA:1127:U:H2' | 1:LA:1128:A:O4' | 2.16 | 0.44 |
| 1:LA:1193:G:H2' | 1:LA:1194:A:C8 | 2.52 | 0.44 |
| 1:LA:1554:U:H5' | 1:LA:1555:C:OP2 | 2.17 | 0.44 |
| 1:LA:2388:C:H2' | 1:LA:2389:A:C8 | 2.52 | 0.44 |
| 1:LA:2428:G:H2' | 1:LA:2429:A:C8 | 2.52 | 0.44 |
| 1:LA:2496:U:HO2' | 1:LA:2497:U:P | 2.39 | 0.44 |
| 1:LA:2552:U:C4 | 35:Li:95:ILE:HG12 | 2.52 | 0.44 |
| 1:LA:3386:U:H2' | 1:LA:3387:C:C6 | 2.52 | 0.44 |
| 10:LJ:149:LYS:H | 10:LJ:201:THR:HA | 1.82 | 0.44 |
| 15:LO:12:TRP:NE1 | 21:LU:151:PRO:HB2 | 2.32 | 0.44 |
| 17:LQ:50[A]:ASN:OD1 | 17:LQ:136[A]:THR:HG21 | 2.16 | 0.44 |
| 25:LY:50:ALA:HA | 25:LY:55:PHE:CG | 2.52 | 0.44 |
| 29:Lc:123:VAL:H | 29:Lc:143:GLY:HA3 | 1.81 | 0.44 |
| 35:Li:55:SER:O | 35:Li:62:TYR:OH | 2.32 | 0.44 |
| 45:S2:186:C:OP2 | 67:SV:142:LYS:NZ | 2.51 | 0.44 |
| 45:S2:386:G:OP2 | 67:SV:25:ARG:NH2 | 2.50 | 0.44 |
| 45:S2:481:A:H2' | 45:S2:482:U:C6 | 2.52 | 0.44 |
| 45:S2:872:G:H2' | 45:S2:873:U:O4' | 2.17 | 0.44 |
| 45:S2:990:C:H2' | 45:S2:991:G:O4' | 2.17 | 0.44 |
| 45:S2:1283:U:H5'' | 45:S2:1284:C:H2' | 1.99 | 0.44 |
| 47:SB:121:ILE:HG23 | 47:SB:129:PRO:HB3 | 1.99 | 0.44 |
| 48:SC:43:ILE:HG22 | 48:SC:47:GLN:OE1 | 2.18 | 0.44 |
| 50:SE:25:LEU:O | 50:SE:87:PRO:HB3 | 2.17 | 0.44 |
| 51:SF:129:PHE:HB2 | 55:SJ:79:TRP:CD1 | 2.52 | 0.44 |
| 62:SQ:33:LYS:HB3 | 62:SQ:33:LYS:HE3 | 1.76 | 0.44 |
| 65:ST:74:LYS:NZ | 65:ST:96:SER:HB2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:SW:110:GLN:NE2 | 68:SW:126:ARG:HB2 | 2.32 | 0.44 |
| 68:SW:113:VAL:HG13 | 68:SW:118:LEU:HB2 | 1.98 | 0.44 |
| 70:SY:6:SER:OG | 70:SY:7:ALA:N | 2.50 | 0.44 |
| 1:LA:114:A:H2' | 1:LA:115:A:O4' | 2.16 | 0.44 |
| 1:LA:1546:G:H2' | 1:LA:1547:C:C6 | 2.52 | 0.44 |
| 1:LA:1595:C:O2' | 1:LA:1695:A:N3 | 2.48 | 0.44 |
| 1:LA:2667:U:H2' | 1:LA:2668:G:C8 | 2.53 | 0.44 |
| 1:LA:2868:U:O2' | 1:LA:2872:U:OP1 | 2.35 | 0.44 |
| 1:LA:3040:U:H5' | 1:LA:3091:C:N4 | 2.31 | 0.44 |
| 5:LE:111:SER:O | 5:LE:115:LYS:HG2 | 2.18 | 0.44 |
| 10:LJ:78:PHE:C | 10:LJ:80:TYR:H | 2.24 | 0.44 |
| 21:LU:94:ILE:HD11 | 21:LU:102:ALA:HA | 2.00 | 0.44 |
| 21:LU:94:ILE:HD11 | 21:LU:102:ALA:HB1 | 1.98 | 0.44 |
| 29:Lc:22:ILE:HD12 | 29:Lc:22:ILE:N | 2.32 | 0.44 |
| 38:Ll:25:ARG:NH1 | 40:Ln:50:ASN:O | 2.50 | 0.44 |
| 45:S2:566:C:H2' | 45:S2:567:A:C8 | 2.53 | 0.44 |
| 45:S2:1046:G:H2' | 45:S2:1047:G:O4' | 2.17 | 0.44 |
| 45:S2:1145:U:H2' | 45:S2:1146:G:O4' | 2.17 | 0.44 |
| 45:S2:1501:C:H5 | 54:SI:102:ARG:NH1 | 2.15 | 0.44 |
| 50:SE:85:ILE:HD11 | 50:SE:116:LEU:HD13 | 1.99 | 0.44 |
| 51:SF:7:VAL:HG21 | 51:SF:91:ALA:HB1 | 1.99 | 0.44 |
| 51:SF:106:LYS:HE3 | 51:SF:117:LEU:HD21 | 1.99 | 0.44 |
| 52:SG:17:ILE:HD11 | 52:SG:54:THR:HG22 | 1.98 | 0.44 |
| 53:SH:66:LEU:O | 53:SH:70:VAL:HG23 | 2.17 | 0.44 |
| 62:SQ:26:ARG:O | 62:SQ:50:LYS:HG3 | 2.17 | 0.44 |
| 63:SR:41:LEU:HG | 63:SR:68:ILE:HD13 | 2.00 | 0.44 |
| 71:SZ:17:ALA:HA | 71:SZ:30:VAL:HG22 | 1.99 | 0.44 |
| 71:SZ:84:ARG:HG3 | 71:SZ:85:ALA:O | 2.16 | 0.44 |
| 1:LA:63:A:N3 | 1:LA:78:U:O2' | 2.43 | 0.44 |
| 1:LA:381:U:H2' | 1:LA:382:U:C6 | 2.52 | 0.44 |
| 1:LA:524:C:H2' | 1:LA:525:C:C6 | 2.50 | 0.44 |
| 1:LA:936:G:H5'' | 29:Lc:29:PRO:HA | 1.99 | 0.44 |
| 1:LA:1070:U:O2' | 1:LA:1071:G:H8 | 2.01 | 0.44 |
| 1:LA:1072:U:H2' | 1:LA:1073:U:C6 | 2.53 | 0.44 |
| 1:LA:1638:C:N4 | 35:Li:73:SER:HB2 | 2.32 | 0.44 |
| 1:LA:1900:A:O3' | 1:LA:2917:G:H5' | 2.17 | 0.44 |
| 1:LA:2231:A:H2' | 1:LA:2232:A:C8 | 2.51 | 0.44 |
| 1:LA:2565:C:H2' | 1:LA:2566:C:H6 | 1.79 | 0.44 |
| 1:LA:2666:A:N6 | 1:LA:2686:G:O2' | 2.50 | 0.44 |
| 4:LD:79:ASN:O | 4:LD:82:VAL:HG23 | 2.17 | 0.44 |
| 4:LD:168:VAL:HG13 | 44:Lr:79:VAL:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:LG:258:LYS:C | 7:LG:260:PHE:H | 2.25 | 0.44 |
| 11:LK:176:LEU:HD12 | 41:Lo:83:LYS:HG2 | 1.99 | 0.44 |
| 27:La:32:SER:HA | 27:La:49:PRO:HA | 1.99 | 0.44 |
| 45:S2:198:A:N3 | 45:S2:198:A:H2' | 2.32 | 0.44 |
| 45:S2:693:U:C2 | 45:S2:695:U:O4 | 2.70 | 0.44 |
| 45:S2:963:A:HO2' | 45:S2:964:U:P | 2.40 | 0.44 |
| 45:S2:1278:G:H2' | 45:S2:1279:C:O4' | 2.17 | 0.44 |
| 45:S2:1469:A:OP1 | 54:SI:91:TYR:OH | 2.36 | 0.44 |
| 49:SD:62:LEU:HD22 | 49:SD:63:VAL:O | 2.17 | 0.44 |
| 51:SF:73:GLY:N | 51:SF:76:SER:OG | 2.51 | 0.44 |
| 51:SF:140:LYS:HA | 51:SF:140:LYS:HD2 | 1.67 | 0.44 |
| 52:SG:86:PRO:HD3 | 61:SP:205:ARG:NH2 | 2.32 | 0.44 |
| 54:SI:73:VAL:HG21 | 54:SI:102:ARG:HG3 | 1.98 | 0.44 |
| 56:SK:91:PRO:HB3 | 56:SK:101:TYR:CE1 | 2.51 | 0.44 |
| 60:SO:149:ASP:HB2 | 60:SO:174:ASN:HB3 | 1.99 | 0.44 |
| 62:SQ:103:MET:CE | 62:SQ:188:LEU:HD21 | 2.47 | 0.44 |
| 65:ST:208:TYR:O | 65:ST:212:LEU:HG | 2.18 | 0.44 |
| 66:SU:47:ARG:HE | 66:SU:175:LYS:NZ | 2.16 | 0.44 |
| 66:SU:81:LEU:HD13 | 66:SU:81:LEU:HA | 1.82 | 0.44 |
| 69:SX:15:LYS:HE3 | 69:SX:15:LYS:HB3 | 1.72 | 0.44 |
| 1:LA:107:A:H1' | 1:LA:325:A:N3 | 2.31 | 0.44 |
| 1:LA:663:U:H2' | 1:LA:664:A:H8 | 1.77 | 0.44 |
| 1:LA:1121:U:C2 | 1:LA:1135:A:N6 | 2.84 | 0.44 |
| 1:LA:1169:A:H2' | 1:LA:1170:G:O4' | 2.18 | 0.44 |
| 1:LA:1645:G:H22 | 1:LA:1807:G:H1' | 1.83 | 0.44 |
| 4:LD:20:THR:HA | 4:LD:23:ARG:HG3 | 1.99 | 0.44 |
| 5:LE:113:GLU:HB2 | 5:LE:176:ALA:HB2 | 1.99 | 0.44 |
| 6:LF:181:VAL:HG11 | 6:LF:224:GLY:CA | 2.46 | 0.44 |
| 12:LL:139:ARG:HG2 | 12:LL:173:PHE:CZ | 2.52 | 0.44 |
| 14:LN:131:LYS:HG3 | 14:LN:133:PRO:HG3 | 2.00 | 0.44 |
| 24:LX:45:ARG:HD3 | 24:LX:46:LEU:N | 2.33 | 0.44 |
| 45:S2:94:U:O2' | 64:SS:8:HIS:ND1 | 2.45 | 0.44 |
| 45:S2:752:A:N6 | 45:S2:797:G:C6 | 2.80 | 0.44 |
| 45:S2:900:A:OP1 | 71:SZ:43:THR:OG1 | 2.24 | 0.44 |
| 45:S2:1047:G:C4 | 45:S2:1048:G:H1' | 2.52 | 0.44 |
| 45:S2:1064:G:O2' | 62:SQ:203:ASP:O | 2.35 | 0.44 |
| 45:S2:1488:G:H21 | 45:S2:1512:G:N2 | 2.15 | 0.44 |
| 45:S2:1770:U:H2' | 45:S2:1771:U:C6 | 2.52 | 0.44 |
| 46:SA:215:GLU:OE1 | 46:SA:215:GLU:N | 2.50 | 0.44 |
| 55:SJ:69:LYS:HD2 | 55:SJ:78:THR:HG23 | 2.00 | 0.44 |
| 57:SL:42:ARG:NH2 | 57:SL:59:SER:HA | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:SP:54:TRP:O | 61:SP:58:VAL:HG12 | 2.17 | 0.44 |
| 68:SW:55:ALA:O | 68:SW:59:LEU:HG | 2.17 | 0.44 |
| 72:Sa:1:MET:HE2 | 72:Sa:1:MET:HB2 | 1.82 | 0.44 |
| 78:Sg:14:VAL:HA | 78:Sg:17:GLN:NE2 | 2.31 | 0.44 |
| 1:LA:1156:G:O2' | 1:LA:1168:A:N3 | 2.45 | 0.44 |
| 1:LA:1363:C:H5'' | 19:LS:3:ILE:HD13 | 1.99 | 0.44 |
| 1:LA:1645:G:O2' | 1:LA:1646:A:O5' | 2.32 | 0.44 |
| 1:LA:1826:C:H2' | 1:LA:1827:A:H8 | 1.83 | 0.44 |
| 1:LA:1940:C:H2' | 1:LA:1941:U:C6 | 2.52 | 0.44 |
| 1:LA:2536:U:C5 | 62:SQ:97:LEU:HD13 | 2.52 | 0.44 |
| 1:LA:2834:U:H2' | 1:LA:2835:C:O2 | 2.17 | 0.44 |
| 1:LA:3065:U:H2' | 1:LA:3066:C:H6 | 1.82 | 0.44 |
| 1:LA:3149:A:H4' | 5:LE:128:LYS:O | 2.18 | 0.44 |
| 6:LF:23:PRO:HD2 | 6:LF:26:PHE:CE2 | 2.53 | 0.44 |
| 6:LF:90:PHE:O | 6:LF:98:ARG:NH2 | 2.50 | 0.44 |
| 7:LG:178:ASN:ND2 | 7:LG:179:ARG:HH11 | 2.15 | 0.44 |
| 12:LL:50:VAL:HG22 | 12:LL:167:LEU:HD23 | 1.99 | 0.44 |
| 14:LN:107:GLU:OE2 | 14:LN:107:GLU:N | 2.36 | 0.44 |
| 21:LU:43:TYR:OH | 21:LU:47:LYS:HE2 | 2.18 | 0.44 |
| 21:LU:104:GLU:O | 21:LU:108:GLN:HG2 | 2.18 | 0.44 |
| 27:La:56:VAL:HG22 | 27:La:104:LEU:HB3 | 2.00 | 0.44 |
| 29:Lc:99:ALA:HB1 | 29:Lc:123:VAL:HA | 2.00 | 0.44 |
| 42:Lp:1:MET:HG3 | 45:S2:1783:C:OP2 | 2.18 | 0.44 |
| 43:Lq:14:GLY:C | 43:Lq:16:THR:H | 2.23 | 0.44 |
| 45:S2:224:C:O2' | 45:S2:225:A:H5'' | 2.17 | 0.44 |
| 45:S2:1181:U:C2 | 45:S2:1458:G:C2 | 3.05 | 0.44 |
| 45:S2:1218:G:C4' | 45:S2:1220:C:H41 | 2.31 | 0.44 |
| 45:S2:1785:U:P | 71:SZ:133:ARG:HH22 | 2.40 | 0.44 |
| 46:SA:45:LYS:HD3 | 46:SA:83:THR:O | 2.18 | 0.44 |
| 46:SA:72:LEU:CD2 | 48:SC:20:VAL:HG21 | 2.48 | 0.44 |
| 64:SS:70:VAL:HG13 | 64:SS:92:LEU:CD1 | 2.47 | 0.44 |
| 66:SU:49:ILE:HG21 | 66:SU:172:VAL:HA | 1.99 | 0.44 |
| 70:SY:106:ARG:HB3 | 70:SY:106:ARG:CZ | 2.47 | 0.44 |
| 75:Sd:105:ARG:HG2 | 75:Sd:108:ARG:NH2 | 2.33 | 0.44 |
| 77:Sf:14:SER:O | 77:Sf:18:LYS:HG3 | 2.16 | 0.44 |
| 79:Ta:10:G:H5' | 79:Ta:46:G:C8 | 2.52 | 0.44 |
| 1:LA:291:C:OP1 | 16:LP:68:ARG:HB3 | 2.18 | 0.44 |
| 1:LA:374:A:N3 | 1:LA:376:G:H5'' | 2.33 | 0.44 |
| 1:LA:874:G:O2' | 1:LA:1890:A:OP1 | 2.36 | 0.44 |
| 1:LA:1045:A:H2' | 1:LA:1048:C:C5 | 2.53 | 0.44 |
| 1:LA:1113:U:OP1 | 29:Lc:23:GLY:N | 2.41 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 1:LA:1390:C:C2 | 33:Lg:103:LYS:HD3 | 2.53 | 0.44 |
| 1:LA:1472:G:H5' | 20:LT:23:TRP:CD1 | 2.53 | 0.44 |
| 1:LA:1491:G:N7 | 40:Ln:2:ALA:N | 2.66 | 0.44 |
| 1:LA:1502:A:H2' | 1:LA:1503:A:H8 | 1.82 | 0.44 |
| 1:LA:2661:G:H2' | 1:LA:2662:G:H8 | 1.83 | 0.44 |
| 1:LA:2767:U:H2' | 1:LA:2768:A:C8 | 2.52 | 0.44 |
| 1:LA:2897:G:OP2 | 1:LA:2898:C:H5'' | 2.17 | 0.44 |
| 3:LC:19:C:H2' | 3:LC:20:U:C6 | 2.53 | 0.44 |
| 6:LF:139:GLY:O | 6:LF:180:LYS:HE2 | 2.17 | 0.44 |
| 17:LQ:44[A]:SER:HB3 | 17:LQ:129[A]:LEU:HD21 | 2.00 | 0.44 |
| 45:S2:162:A:OP1 | 65:ST:83:CYS:HA | 2.17 | 0.44 |
| 45:S2:213:A:C6 | 45:S2:214:G:H1' | 2.53 | 0.44 |
| 45:S2:299:A:P | 64:SS:30:ARG:HH22 | 2.36 | 0.44 |
| 45:S2:1535:U:H3 | 47:SB:187:ILE:HD13 | 1.82 | 0.44 |
| 47:SB:25:LEU:HD22 | 51:SF:57:LEU:HD22 | 2.00 | 0.44 |
| 47:SB:162:VAL:CG1 | 57:SL:44:VAL:HG22 | 2.47 | 0.44 |
| 60:SO:72:THR:OG1 | 60:SO:73:LEU:N | 2.51 | 0.44 |
| 62:SQ:101:HIS:O | 62:SQ:217:LEU:HB2 | 2.17 | 0.44 |
| 62:SQ:225:VAL:O | 62:SQ:225:VAL:HG22 | 2.17 | 0.44 |
| 63:SR:63:VAL:HG12 | 63:SR:134:LEU:HD22 | 1.99 | 0.44 |
| 64:SS:89:VAL:HG13 | 64:SS:100:ARG:HD3 | 1.99 | 0.44 |
| 68:SW:125:ALA:O | 68:SW:128:LEU:N | 2.50 | 0.44 |
| 77:Sf:62:ILE:HG13 | 77:Sf:62:ILE:O | 2.17 | 0.44 |
| 1:LA:596:G:H2' | 1:LA:597:A:C8 | 2.52 | 0.44 |
| 1:LA:653:C:H2' | 1:LA:654:C:C6 | 2.53 | 0.44 |
| 1:LA:709:A:H2' | 1:LA:710:A:C8 | 2.52 | 0.44 |
| 1:LA:1361:G:H2' | 1:LA:1362:A:C8 | 2.53 | 0.44 |
| 1:LA:2444:A:O2' | 1:LA:2445:U:H3' | 2.18 | 0.44 |
| 1:LA:3012:U:H2' | 1:LA:3013:U:C6 | 2.52 | 0.44 |
| 1:LA:3109:C:H2' | 1:LA:3110:U:C6 | 2.52 | 0.44 |
| 3:LC:145:U:H2' | 3:LC:146:U:C6 | 2.53 | 0.44 |
| 7:LG:52:VAL:HA | 7:LG:147:ASP:HB3 | 1.99 | 0.44 |
| 9:LI:222:HIS:ND1 | 9:LI:224:ILE:HG12 | 2.32 | 0.44 |
| 15:LO:50:LYS:HG3 | 15:LO:85:TRP:CD1 | 2.52 | 0.44 |
| 16:LP:77:LYS:C | 16:LP:79:ALA:N | 2.75 | 0.44 |
| 19:LS:147:ARG:HB2 | 19:LS:150:VAL:HG13 | 2.00 | 0.44 |
| 20:LT:147:ALA:O | 20:LT:150:GLN:HG3 | 2.17 | 0.44 |
| 42:Lp:6:ARG:HH11 | 42:Lp:6:ARG:HG2 | 1.83 | 0.44 |
| 45:S2:267:U:O4 | 45:S2:268:C:N4 | 2.50 | 0.44 |
| 45:S2:1734:U:H2' | 45:S2:1735:U:C6 | 2.52 | 0.44 |
| 48:SC:38:LYS:HB2 | 48:SC:41:TYR:CD1 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|--------------------|--------------------------|-------------------|
| 55:SJ:26:LEU:HD12 | 55:SJ:26:LEU:O | 2.18 | 0.44 |
| 60:SO:133:VAL:HG12 | 60:SO:141:LEU:HB3 | 1.99 | 0.44 |
| 60:SO:179:LYS:CB | 60:SO:181:TRP:HE1 | 2.29 | 0.44 |
| 74:Sc:31:LYS:HB3 | 74:Sc:31:LYS:HE3 | 1.74 | 0.44 |
| 1:LA:1270:A:O2' | 1:LA:1271:C:OP1 | 2.28 | 0.44 |
| 6:LF:144:LYS:HD3 | 6:LF:144:LYS:HA | 1.62 | 0.44 |
| 7:LG:40:HIS:CE1 | 22:LV:69:LYS:HA | 2.52 | 0.44 |
| 7:LG:271:LYS:HE3 | 7:LG:271:LYS:HB3 | 1.85 | 0.44 |
| 15:LO:50:LYS:HE2 | 15:LO:82:SER:CB | 2.48 | 0.44 |
| 21:LU:79:VAL:HG11 | 21:LU:106:LEU:HD11 | 2.00 | 0.44 |
| 45:S2:1151:A:H2' | 45:S2:1152:A:H8 | 1.83 | 0.44 |
| 45:S2:1237:G:H2' | 45:S2:1237:G:N3 | 2.33 | 0.44 |
| 45:S2:1408:G:H3' | 45:S2:1409:G:H8 | 1.83 | 0.44 |
| 46:SA:209:ILE:HD12 | 46:SA:209:ILE:HA | 1.91 | 0.44 |
| 47:SB:45:LYS:HG2 | 47:SB:46:TRP:CE2 | 2.53 | 0.44 |
| 48:SC:59:PHE:CD1 | 48:SC:62:GLN:HA | 2.52 | 0.44 |
| 52:SG:6:THR:HG22 | 52:SG:8:THR:H | 1.82 | 0.44 |
| 62:SQ:143:THR:HA | 62:SQ:207:LEU:HA | 2.00 | 0.44 |
| 65:ST:27:PHE:CZ | 65:ST:111:LEU:HD11 | 2.52 | 0.44 |
| 1:LA:36:C:H4' | 1:LA:807:A:C2 | 2.53 | 0.44 |
| 1:LA:127:G:H2' | 1:LA:128:G:H8 | 1.82 | 0.44 |
| 1:LA:507:U:H2' | 1:LA:508:U:C6 | 2.52 | 0.44 |
| 1:LA:528:A:H2' | 1:LA:529:G:C8 | 2.53 | 0.44 |
| 1:LA:1479:G:O2' | 1:LA:1870:U:O4 | 2.33 | 0.44 |
| 1:LA:1832:G:O2' | 40:Ln:3:ALA:O | 2.35 | 0.44 |
| 1:LA:2812:A:H2' | 1:LA:2813:G:O4' | 2.17 | 0.44 |
| 2:LB:27:A:H2' | 2:LB:28:C:C6 | 2.53 | 0.44 |
| 5:LE:282:ILE:HG23 | 5:LE:322:ILE:HG23 | 2.00 | 0.44 |
| 6:LF:175:HIS:O | 6:LF:179:LEU:HG | 2.17 | 0.44 |
| 9:LI:120:THR:HB | 22:LV:132:PRO:HB2 | 1.99 | 0.44 |
| 17:LQ:127[A]:LEU:HD22 | 21:LU:156:VAL:HG13 | 1.99 | 0.44 |
| 19:LS:36:LEU:O | 19:LS:40:THR:HB | 2.18 | 0.44 |
| 22:LV:60:LYS:HB3 | 22:LV:76:ILE:HD12 | 2.00 | 0.44 |
| 45:S2:19:A:H2' | 45:S2:20:G:O4' | 2.17 | 0.44 |
| 45:S2:774:A:H61 | 45:S2:786:C:H42 | 1.66 | 0.44 |
| 45:S2:903:U:H2' | 45:S2:905:A:OP2 | 2.17 | 0.44 |
| 45:S2:1504:G:H2' | 45:S2:1505:A:C4 | 2.53 | 0.44 |
| 45:S2:1605:G:OP2 | 51:SF:127:LYS:HD3 | 2.18 | 0.44 |
| 49:SD:77:GLY:HA2 | 49:SD:80:ASN:ND2 | 2.32 | 0.44 |
| 57:SL:44:VAL:HG21 | 57:SL:48:VAL:HG11 | 2.00 | 0.44 |
| 60:SO:127:ARG:C | 60:SO:129:LYS:H | 2.26 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 68:SW:83:VAL:O | 68:SW:107:ARG:NE | 2.45 | 0.44 |
| 72:Sa:55:LEU:HD23 | 72:Sa:55:LEU:HA | 1.85 | 0.44 |
| 74:Sc:117:ILE:HD12 | 74:Sc:117:ILE:N | 2.32 | 0.44 |
| 1:LA:243:G:H2' | 1:LA:244:G:H8 | 1.82 | 0.43 |
| 1:LA:1516:G:OP1 | 40:Ln:41:ARG:NH1 | 2.33 | 0.43 |
| 1:LA:1750:G:H5' | 39:Lm:26:LYS:HE2 | 1.99 | 0.43 |
| 1:LA:2151:A:H2' | 1:LA:2152:U:C6 | 2.53 | 0.43 |
| 1:LA:2192:U:O2' | 1:LA:2312:A:OP2 | 2.21 | 0.43 |
| 1:LA:2242:A:H3' | 4:LD:244:GLY:HA2 | 1.99 | 0.43 |
| 1:LA:2422:U:H2' | 1:LA:2423:A:H8 | 1.83 | 0.43 |
| 1:LA:3145:G:H2' | 1:LA:3146:G:C8 | 2.53 | 0.43 |
| 6:LF:233:LEU:HD23 | 6:LF:233:LEU:HA | 1.66 | 0.43 |
| 12:LL:83:ASP:OD1 | 12:LL:83:ASP:N | 2.45 | 0.43 |
| 17:LQ:138[A]:LEU:HA | 17:LQ:138[A]:LEU:HD12 | 1.77 | 0.43 |
| 19:LS:133:LYS:HB2 | 19:LS:133:LYS:HE2 | 1.74 | 0.43 |
| 22:LV:50:LYS:O | 22:LV:92:ARG:HD2 | 2.17 | 0.43 |
| 43:Lq:6:LYS:HE2 | 43:Lq:94:GLY:HA2 | 2.00 | 0.43 |
| 45:S2:98:U:H2' | 45:S2:99:C:C6 | 2.53 | 0.43 |
| 45:S2:153:G:N2 | 45:S2:161:U:O2' | 2.35 | 0.43 |
| 45:S2:541:A:O2' | 45:S2:542:A:OP1 | 2.33 | 0.43 |
| 45:S2:604:A:H2' | 45:S2:605:A:O4' | 2.18 | 0.43 |
| 45:S2:732:G:H1 | 45:S2:737:A:H61 | 1.65 | 0.43 |
| 45:S2:1402:G:H5'' | 52:SG:3:ARG:CZ | 2.48 | 0.43 |
| 45:S2:1470:C:H5' | 45:S2:1540:G:N2 | 2.33 | 0.43 |
| 45:S2:1583:A:N6 | 47:SB:76:ARG:HA | 2.31 | 0.43 |
| 46:SA:202:LEU:HG | 46:SA:203:PRO:HD2 | 2.00 | 0.43 |
| 47:SB:117:THR:HG22 | 47:SB:191:ALA:O | 2.18 | 0.43 |
| 49:SD:32:LEU:CD1 | 49:SD:101:ALA:HA | 2.48 | 0.43 |
| 55:SJ:22:ILE:HD13 | 55:SJ:100:VAL:HG13 | 1.99 | 0.43 |
| 55:SJ:57:ARG:HG2 | 55:SJ:89:ARG:HD2 | 2.00 | 0.43 |
| 61:SP:3:LEU:HD12 | 72:Sa:80:LYS:HG3 | 1.99 | 0.43 |
| 63:SR:123:GLY:HA2 | 63:SR:126:ARG:HG2 | 1.98 | 0.43 |
| 64:SS:255:ARG:HD2 | 64:SS:255:ARG:C | 2.42 | 0.43 |
| 67:SV:104:ILE:O | 67:SV:164:ARG:HA | 2.17 | 0.43 |
| 71:SZ:25:ASP:N | 71:SZ:55:SER:HB3 | 2.33 | 0.43 |
| 73:Sb:18:GLU:HG3 | 73:Sb:69:LEU:HD22 | 2.00 | 0.43 |
| 75:Sd:5:VAL:HG13 | 75:Sd:32:ARG:NH2 | 2.33 | 0.43 |
| 75:Sd:18:LEU:HB2 | 75:Sd:20:ARG:NH1 | 2.32 | 0.43 |
| 80:Tb:71:G:H1' | 80:Tb:73:A:OP2 | 2.18 | 0.43 |
| 1:LA:355:A:H2' | 1:LA:356:C:O4' | 2.18 | 0.43 |
| 1:LA:428:A:H2' | 1:LA:429:U:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:791:G:H2' | 1:LA:792:C:H6 | 1.81 | 0.43 |
| 1:LA:870:U:H2' | 1:LA:871:U:C6 | 2.53 | 0.43 |
| 1:LA:2536:U:C6 | 62:SQ:229:MET:HB2 | 2.52 | 0.43 |
| 1:LA:2675:A:H4' | 1:LA:2676:G:O4' | 2.18 | 0.43 |
| 3:LC:121:U:H2' | 3:LC:122:U:C6 | 2.53 | 0.43 |
| 8:LH:36:PRO:HB3 | 8:LH:55:LEU:O | 2.18 | 0.43 |
| 13:LM:33:ALA:O | 13:LM:36:VAL:HG12 | 2.18 | 0.43 |
| 16:LP:77:LYS:C | 16:LP:79:ALA:H | 2.25 | 0.43 |
| 24:LX:59:MET:HE3 | 24:LX:73:VAL:CG1 | 2.48 | 0.43 |
| 27:La:63:LYS:HZ2 | 27:La:97:ILE:HD12 | 1.83 | 0.43 |
| 27:La:112:ASP:OD1 | 27:La:115:ARG:HB2 | 2.18 | 0.43 |
| 45:S2:95:G:OP1 | 64:SS:6:LYS:HD3 | 2.18 | 0.43 |
| 45:S2:912:U:OP2 | 62:SQ:8:ARG:NH2 | 2.50 | 0.43 |
| 45:S2:1117:U:H2' | 45:S2:1118:G:H8 | 1.83 | 0.43 |
| 45:S2:1545:A:H4' | 53:SH:127:HIS:HE1 | 1.82 | 0.43 |
| 50:SE:85:ILE:HG12 | 50:SE:107:ILE:HD12 | 2.00 | 0.43 |
| 51:SF:44:LEU:HD12 | 51:SF:78:VAL:HG21 | 1.99 | 0.43 |
| 55:SJ:68:ARG:HH12 | 55:SJ:77:LYS:HG3 | 1.83 | 0.43 |
| 60:SO:252:LEU:HD21 | 60:SO:263:PHE:HD2 | 1.83 | 0.43 |
| 64:SS:103:TYR:O | 64:SS:182:TYR:OH | 2.36 | 0.43 |
| 64:SS:248:ILE:HG13 | 68:SW:71:PHE:CE2 | 2.53 | 0.43 |
| 66:SU:113:PRO:HG2 | 66:SU:116:ARG:HD3 | 2.00 | 0.43 |
| 68:SW:44:ARG:O | 68:SW:48:GLN:HG2 | 2.17 | 0.43 |
| 68:SW:123:HIS:CD2 | 78:Sg:37:ARG:HE | 2.36 | 0.43 |
| 1:LA:299:G:C8 | 37:Lk:31:GLY:HA3 | 2.52 | 0.43 |
| 1:LA:428:A:H1' | 34:Lh:25:PRO:HG2 | 2.00 | 0.43 |
| 1:LA:808:G:H5'' | 16:LP:81:TYR:CE2 | 2.54 | 0.43 |
| 1:LA:1202:A:N6 | 1:LA:1299:G:H2' | 2.33 | 0.43 |
| 1:LA:2222:A:H2' | 1:LA:2223:A:C8 | 2.53 | 0.43 |
| 1:LA:2425:U:H2' | 1:LA:2426:U:C6 | 2.53 | 0.43 |
| 3:LC:10:A:H2' | 3:LC:11:C:C6 | 2.53 | 0.43 |
| 9:LI:229:PHE:CD1 | 9:LI:229:PHE:C | 2.96 | 0.43 |
| 15:LO:23:ILE:HG22 | 15:LO:31:LYS:O | 2.19 | 0.43 |
| 16:LP:140:LYS:HA | 16:LP:140:LYS:HD2 | 1.92 | 0.43 |
| 19:LS:150:VAL:HA | 19:LS:153:PHE:CD2 | 2.52 | 0.43 |
| 27:La:103:LYS:HA | 27:La:103:LYS:HD3 | 1.90 | 0.43 |
| 45:S2:603:U:H2' | 45:S2:604:A:C8 | 2.53 | 0.43 |
| 45:S2:1181:U:C2 | 45:S2:1458:G:N1 | 2.86 | 0.43 |
| 54:SI:38:LYS:O | 54:SI:39:THR:OG1 | 2.36 | 0.43 |
| 60:SO:22:SER:HB2 | 60:SO:71:CYS:SG | 2.59 | 0.43 |
| 65:ST:27:PHE:CD1 | 65:ST:36:VAL:HG21 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:SU:75:THR:HG23 | 66:SU:76:LYS:HE2 | 2.00 | 0.43 |
| 67:SV:26:LYS:HD2 | 67:SV:29:LEU:HD23 | 2.01 | 0.43 |
| 70:SY:34:ILE:O | 70:SY:38:VAL:HG22 | 2.17 | 0.43 |
| 1:LA:639:U:OP1 | 29:Lc:21:ARG:NH2 | 2.51 | 0.43 |
| 1:LA:1403:G:N2 | 1:LA:1406:A:OP2 | 2.40 | 0.43 |
| 1:LA:1494:U:C5 | 1:LA:1834:A:N1 | 2.86 | 0.43 |
| 1:LA:2990:A:N3 | 18:LR:69:ARG:NH2 | 2.67 | 0.43 |
| 10:LJ:158:ASP:HB3 | 10:LJ:159:PRO:HD3 | 2.01 | 0.43 |
| 12:LL:47:PRO:HB3 | 12:LL:171:TRP:CZ2 | 2.53 | 0.43 |
| 12:LL:100:ASN:OD1 | 12:LL:100:ASN:N | 2.51 | 0.43 |
| 13:LM:122:ILE:HD11 | 53:SH:110:ARG:HH12 | 1.83 | 0.43 |
| 27:La:79:ALA:CB | 27:La:98:ASN:HB3 | 2.48 | 0.43 |
| 40:Ln:25:GLN:OE1 | 40:Ln:28:ARG:NH1 | 2.49 | 0.43 |
| 45:S2:12:U:H2' | 45:S2:13:C:C6 | 2.53 | 0.43 |
| 45:S2:330:G:O2' | 45:S2:331:A:OP1 | 2.35 | 0.43 |
| 45:S2:406:U:H5'' | 65:ST:94:ARG:HB2 | 2.00 | 0.43 |
| 45:S2:1097:U:O3' | 63:SR:168:ARG:NH1 | 2.52 | 0.43 |
| 45:S2:1232:U:H2' | 45:S2:1233:G:O4' | 2.18 | 0.43 |
| 45:S2:1666:U:H5'' | 45:S2:1667:A:H8 | 1.83 | 0.43 |
| 49:SD:32:LEU:HD21 | 49:SD:102:GLY:CA | 2.46 | 0.43 |
| 51:SF:25:GLY:HA3 | 51:SF:64:ASP:CG | 2.42 | 0.43 |
| 51:SF:25:GLY:N | 51:SF:62:ASN:O | 2.48 | 0.43 |
| 51:SF:40:GLU:N | 51:SF:41:PRO:HD3 | 2.34 | 0.43 |
| 55:SJ:32:LYS:O | 55:SJ:36:ASN:ND2 | 2.51 | 0.43 |
| 55:SJ:102:ARG:O | 55:SJ:106:ILE:HG23 | 2.17 | 0.43 |
| 61:SP:67:ILE:CD1 | 61:SP:119:ARG:HB2 | 2.46 | 0.43 |
| 64:SS:194:THR:HG23 | 64:SS:194:THR:O | 2.18 | 0.43 |
| 65:ST:32:ILE:HD11 | 65:ST:63:MET:CE | 2.47 | 0.43 |
| 69:SX:75:VAL:HA | 69:SX:86:ILE:HA | 2.00 | 0.43 |
| 1:LA:412:G:H2' | 1:LA:413:U:C6 | 2.54 | 0.43 |
| 1:LA:517:G:OP1 | 9:LI:67:ARG:HD3 | 2.19 | 0.43 |
| 1:LA:648:A:H2' | 1:LA:649:C:C6 | 2.53 | 0.43 |
| 1:LA:1855:C:H2' | 1:LA:1856:C:C6 | 2.54 | 0.43 |
| 1:LA:2117:C:H2' | 1:LA:2118:A:O4' | 2.19 | 0.43 |
| 1:LA:2270:A:H2' | 1:LA:2271:G:O4' | 2.18 | 0.43 |
| 2:LB:75:G:N2 | 2:LB:104:A:C6 | 2.86 | 0.43 |
| 3:LC:62:C:H4' | 3:LC:63:G:O5' | 2.17 | 0.43 |
| 6:LF:98:ARG:HG2 | 6:LF:99:MET:O | 2.19 | 0.43 |
| 6:LF:150:LEU:HD23 | 6:LF:249:ILE:HG12 | 2.00 | 0.43 |
| 8:LH:40:LEU:HD11 | 8:LH:54:TYR:HB2 | 1.99 | 0.43 |
| 11:LK:103:ILE:HD11 | 11:LK:134:ILE:HG21 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:LT:167:ARG:NH1 | 20:LT:170:ARG:HH22 | 2.16 | 0.43 |
| 23:LW:35:LYS:NZ | 23:LW:39:ASP:HB3 | 2.33 | 0.43 |
| 27:La:119:ILE:HG23 | 27:La:124:GLY:HA3 | 2.00 | 0.43 |
| 33:Lg:74:PHE:CD1 | 33:Lg:85:LEU:HD11 | 2.54 | 0.43 |
| 45:S2:524:U:O2' | 45:S2:527:A:N6 | 2.51 | 0.43 |
| 45:S2:1011:G:H2' | 45:S2:1012:U:H5 | 1.84 | 0.43 |
| 45:S2:1586:A:C5 | 45:S2:1611:A:C8 | 3.06 | 0.43 |
| 48:SC:60:SER:HB2 | 48:SC:65:TYR:HE2 | 1.84 | 0.43 |
| 49:SD:42:ALA:HB3 | 49:SD:122:VAL:HG22 | 2.00 | 0.43 |
| 53:SH:126:ARG:HA | 53:SH:126:ARG:HD2 | 1.89 | 0.43 |
| 57:SL:7:VAL:HG13 | 57:SL:55:VAL:HG13 | 2.00 | 0.43 |
| 60:SO:307:ASP:OD1 | 60:SO:307:ASP:N | 2.38 | 0.43 |
| 62:SQ:90:GLU:HB3 | 62:SQ:97:LEU:HD12 | 2.00 | 0.43 |
| 62:SQ:131:ASP:OD1 | 62:SQ:131:ASP:N | 2.48 | 0.43 |
| 66:SU:77:LEU:HD23 | 66:SU:92:PHE:HE2 | 1.83 | 0.43 |
| 69:SX:59:PRO:HB3 | 69:SX:66:ILE:HD11 | 2.00 | 0.43 |
| 1:LA:291:C:OP2 | 16:LP:128:LYS:NZ | 2.52 | 0.43 |
| 1:LA:722:U:O2' | 30:Ld:29:TYR:OH | 2.12 | 0.43 |
| 1:LA:1116:G:OP1 | 30:Ld:4:SER:HB2 | 2.18 | 0.43 |
| 1:LA:1621:U:H2' | 1:LA:1622:G:C8 | 2.53 | 0.43 |
| 1:LA:2596:U:H2' | 1:LA:2597:G:C8 | 2.53 | 0.43 |
| 1:LA:3037:U:H2' | 1:LA:3038:C:O4' | 2.19 | 0.43 |
| 1:LA:3112:A:N1 | 1:LA:3121:A:C8 | 2.87 | 0.43 |
| 1:LA:3253:G:H2' | 1:LA:3254:U:C6 | 2.53 | 0.43 |
| 4:LD:211:HIS:CD2 | 4:LD:219:ILE:HG23 | 2.53 | 0.43 |
| 7:LG:208:MET:HE3 | 7:LG:226:TYR:CD2 | 2.53 | 0.43 |
| 7:LG:258:LYS:O | 7:LG:265:TYR:OH | 2.29 | 0.43 |
| 11:LK:90:MET:HE3 | 11:LK:144:ILE:CG2 | 2.48 | 0.43 |
| 21:LU:23:LYS:HA | 21:LU:23:LYS:HD2 | 1.57 | 0.43 |
| 22:LV:92:ARG:HB3 | 22:LV:94:GLU:OE1 | 2.19 | 0.43 |
| 28:Lb:93:LYS:HE3 | 28:Lb:93:LYS:HB3 | 1.89 | 0.43 |
| 40:Ln:25:GLN:NE2 | 40:Ln:28:ARG:NH1 | 2.67 | 0.43 |
| 45:S2:567:A:H5' | 78:Sg:10:ARG:O | 2.19 | 0.43 |
| 45:S2:688:G:H2' | 45:S2:689:G:C8 | 2.54 | 0.43 |
| 45:S2:1584:G:N7 | 51:SF:14:LYS:HE3 | 2.33 | 0.43 |
| 45:S2:1719:A:H5'' | 45:S2:1720:G:OP2 | 2.19 | 0.43 |
| 47:SB:174:LEU:HD23 | 47:SB:177:ILE:HD11 | 2.01 | 0.43 |
| 62:SQ:99:ASN:OD1 | 62:SQ:100:PHE:N | 2.47 | 0.43 |
| 63:SR:82:ASN:O | 63:SR:83:ILE:HD13 | 2.18 | 0.43 |
| 64:SS:104:ASP:HB3 | 64:SS:110:ALA:HB2 | 2.00 | 0.43 |
| 64:SS:105:VAL:HG23 | 64:SS:245:LYS:H | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 65:ST:27:PHE:HZ | 65:ST:111:LEU:HD21 | 1.84 | 0.43 |
| 65:ST:195:VAL:O | 65:ST:199:GLN:HG2 | 2.19 | 0.43 |
| 79:Ta:38:A:H3' | 79:Ta:38:A:N3 | 2.34 | 0.43 |
| 1:LA:71:A:P | 29:Lc:67:HIS:HE2 | 2.41 | 0.43 |
| 1:LA:199:A:C4 | 1:LA:201:A:C8 | 3.07 | 0.43 |
| 1:LA:309:U:H6 | 1:LA:310:U:H5 | 1.67 | 0.43 |
| 1:LA:1876:U:H5'' | 1:LA:1877:G:H5' | 2.00 | 0.43 |
| 1:LA:2702:A:OP2 | 7:LG:23:ARG:NE | 2.39 | 0.43 |
| 2:LB:47:C:H2' | 2:LB:48:U:C6 | 2.54 | 0.43 |
| 5:LE:226:PHE:CE1 | 5:LE:268:GLY:HA2 | 2.53 | 0.43 |
| 7:LG:177:GLU:HB2 | 7:LG:190:ILE:HD12 | 2.01 | 0.43 |
| 17:LQ:50[A]:ASN:OD1 | 17:LQ:136[A]:THR:CG2 | 2.67 | 0.43 |
| 21:LU:167:ARG:HG3 | 21:LU:168:PRO:HD2 | 2.01 | 0.43 |
| 36:Lj:86:ARG:O | 36:Lj:90:ARG:HG2 | 2.19 | 0.43 |
| 45:S2:736:C:H2' | 45:S2:737:A:H8 | 1.83 | 0.43 |
| 45:S2:1198:G:OP1 | 45:S2:1199:G:O2' | 2.26 | 0.43 |
| 47:SB:54:LYS:HE2 | 47:SB:54:LYS:HB3 | 1.91 | 0.43 |
| 47:SB:148:ARG:HH21 | 57:SL:22:ARG:NH2 | 2.16 | 0.43 |
| 47:SB:188:LYS:HB3 | 56:SK:63:SER:OG | 2.19 | 0.43 |
| 52:SG:85:VAL:HG21 | 61:SP:198:MET:HG3 | 1.99 | 0.43 |
| 57:SL:53:ILE:HG22 | 57:SL:54:LEU:H | 1.83 | 0.43 |
| 62:SQ:163:ALA:O | 62:SQ:167:VAL:HG13 | 2.18 | 0.43 |
| 63:SR:59:HIS:CG | 63:SR:239:PRO:HD3 | 2.53 | 0.43 |
| 65:ST:78:THR:HG22 | 65:ST:79:LYS:H | 1.84 | 0.43 |
| 68:SW:109:LEU:O | 68:SW:112:GLN:HB2 | 2.19 | 0.43 |
| 71:SZ:31:THR:HA | 71:SZ:38:THR:HA | 2.00 | 0.43 |
| 73:Sb:122:SER:OG | 73:Sb:123:GLY:N | 2.47 | 0.43 |
| 76:Se:66:LYS:HB3 | 76:Se:66:LYS:HE3 | 1.82 | 0.43 |
| 1:LA:209:A:H4' | 1:LA:211:A:N7 | 2.33 | 0.43 |
| 1:LA:523:U:H5' | 1:LA:524:C:H5 | 1.84 | 0.43 |
| 1:LA:1323:U:OP1 | 21:LU:2:ALA:N | 2.51 | 0.43 |
| 1:LA:2655:A:OP2 | 43:Lq:97:LYS:HG3 | 2.19 | 0.43 |
| 1:LA:2857:U:O5' | 1:LA:2857:U:H6 | 2.01 | 0.43 |
| 1:LA:3171:A:O2' | 17:LQ:101[A]:ARG:NH1 | 2.52 | 0.43 |
| 2:LB:45:A:H2' | 2:LB:46:A:H8 | 1.84 | 0.43 |
| 3:LC:67:U:H2' | 3:LC:68:G:C8 | 2.53 | 0.43 |
| 3:LC:149:A:H2' | 3:LC:150:G:C8 | 2.54 | 0.43 |
| 15:LO:102:LYS:HA | 15:LO:102:LYS:HD2 | 1.67 | 0.43 |
| 23:LW:77:LYS:HG3 | 23:LW:95:PHE:CD1 | 2.54 | 0.43 |
| 34:Lh:67:MET:CE | 34:Lh:89:LEU:HD23 | 2.48 | 0.43 |
| 35:Li:41:ARG:HA | 35:Li:56:THR:HG22 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:Lj:31:LEU:HA | 36:Lj:31:LEU:HD23 | 1.84 | 0.43 |
| 45:S2:810:G:C5 | 66:SU:111:LYS:HD3 | 2.54 | 0.43 |
| 46:SA:25:PHE:O | 46:SA:29:LEU:HB2 | 2.19 | 0.43 |
| 54:SI:21:PHE:HD2 | 54:SI:22:LEU:HD12 | 1.83 | 0.43 |
| 57:SL:30:VAL:O | 57:SL:39:THR:HA | 2.19 | 0.43 |
| 61:SP:78:SER:OG | 61:SP:128:SER:OG | 2.32 | 0.43 |
| 62:SQ:24:PHE:CE2 | 71:SZ:70:LYS:CE | 2.98 | 0.43 |
| 65:ST:48:TYR:CE2 | 65:ST:121:LEU:HD11 | 2.53 | 0.43 |
| 75:Sd:44:LEU:HA | 75:Sd:44:LEU:HD23 | 1.75 | 0.43 |
| 1:LA:673:G:O6 | 19:LS:56:LYS:NZ | 2.52 | 0.43 |
| 1:LA:826:A:H5'' | 35:Li:14:ASN:O | 2.19 | 0.43 |
| 1:LA:991:A:O2' | 1:LA:992:G:H5' | 2.18 | 0.43 |
| 1:LA:1034:G:N2 | 1:LA:1035:A:N7 | 2.67 | 0.43 |
| 1:LA:1615:U:H2' | 1:LA:1616:G:C8 | 2.54 | 0.43 |
| 1:LA:1843:C:O2 | 38:Ll:9:GLY:HA2 | 2.19 | 0.43 |
| 1:LA:2745:A:O2' | 7:LG:175:HIS:HA | 2.19 | 0.43 |
| 1:LA:3002:G:P | 5:LE:26:ARG:HH22 | 2.42 | 0.43 |
| 5:LE:298:PHE:HB3 | 5:LE:357:LYS:O | 2.19 | 0.43 |
| 11:LK:10:ILE:CG2 | 11:LK:53:ILE:HB | 2.48 | 0.43 |
| 11:LK:20:ILE:HB | 15:LO:7:VAL:HG23 | 2.00 | 0.43 |
| 12:LL:145:LYS:O | 12:LL:149:VAL:HG13 | 2.18 | 0.43 |
| 23:LW:50:LEU:HD12 | 23:LW:50:LEU:O | 2.18 | 0.43 |
| 33:Lg:79:VAL:HG13 | 33:Lg:111:ARG:HG2 | 2.01 | 0.43 |
| 39:Lm:8:ILE:HD12 | 39:Lm:65:LEU:HD21 | 2.00 | 0.43 |
| 45:S2:471:A:O2' | 68:SW:8:TYR:HB2 | 2.19 | 0.43 |
| 45:S2:611:U:H5'' | 74:Sc:5:LYS:HD3 | 2.01 | 0.43 |
| 45:S2:896:U:H2' | 45:S2:897:C:C2 | 2.54 | 0.43 |
| 46:SA:75:LYS:HZ1 | 48:SC:20:VAL:C | 2.27 | 0.43 |
| 47:SB:189:THR:O | 47:SB:192:GLU:HG2 | 2.18 | 0.43 |
| 48:SC:2:LEU:HD23 | 48:SC:2:LEU:H | 1.83 | 0.43 |
| 50:SE:28:MET:HG3 | 50:SE:29:SER:N | 2.33 | 0.43 |
| 50:SE:83:MET:O | 50:SE:116:LEU:N | 2.52 | 0.43 |
| 55:SJ:63:LEU:HB3 | 58:SM:34:TYR:CZ | 2.54 | 0.43 |
| 64:SS:152:PRO:HD2 | 65:ST:215:ARG:NH1 | 2.34 | 0.43 |
| 68:SW:74:ASN:HB3 | 68:SW:78:ARG:HH21 | 1.84 | 0.43 |
| 69:SX:79:LYS:HD3 | 69:SX:79:LYS:HA | 1.88 | 0.43 |
| 75:Sd:112:LYS:HB3 | 75:Sd:112:LYS:HE3 | 1.68 | 0.43 |
| 1:LA:230:U:H2' | 1:LA:231:G:O4' | 2.18 | 0.43 |
| 1:LA:1071:G:H2' | 1:LA:1072:U:C6 | 2.54 | 0.43 |
| 1:LA:1413:G:C6 | 1:LA:1414:U:C4 | 3.07 | 0.43 |
| 1:LA:1594:U:C2 | 1:LA:1595:C:C5 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:LA:1743:G:H2' | 1:LA:1744:C:H6 | 1.84 | 0.43 |
| 1:LA:1908:A:H2' | 1:LA:1909:A:C8 | 2.53 | 0.43 |
| 1:LA:2156:G:N7 | 4:LD:152:SER:OG | 2.47 | 0.43 |
| 1:LA:3068:G:H2' | 1:LA:3068:G:N3 | 2.34 | 0.43 |
| 1:LA:3380:U:H4' | 1:LA:3381:U:OP2 | 2.14 | 0.43 |
| 4:LD:126:LEU:HD13 | 4:LD:150:LEU:HD21 | 2.01 | 0.43 |
| 14:LN:3:ILE:HG21 | 29:Lc:45:MET:CE | 2.43 | 0.43 |
| 21:LU:27:MET:HE3 | 21:LU:27:MET:HB2 | 1.88 | 0.43 |
| 26:LZ:57:LEU:HD12 | 26:LZ:57:LEU:HA | 1.79 | 0.43 |
| 28:Lb:16:GLY:O | 35:Li:74:ARG:HG3 | 2.19 | 0.43 |
| 32:Lf:13:THR:OG1 | 32:Lf:72:ARG:NH1 | 2.43 | 0.43 |
| 37:Lk:38:LYS:HB2 | 37:Lk:38:LYS:HE2 | 1.53 | 0.43 |
| 45:S2:747:C:H2' | 45:S2:748:U:C6 | 2.54 | 0.43 |
| 45:S2:886:U:H2' | 45:S2:887:A:H8 | 1.84 | 0.43 |
| 45:S2:952:A:O2' | 70:SY:114:ARG:HG3 | 2.18 | 0.43 |
| 45:S2:1107:G:O2' | 45:S2:1108:G:H5' | 2.18 | 0.43 |
| 45:S2:1232:U:H3' | 45:S2:1233:G:H8 | 1.84 | 0.43 |
| 45:S2:1502:G:N2 | 45:S2:1505:A:OP2 | 2.52 | 0.43 |
| 45:S2:1505:A:O2' | 45:S2:1551:U:O4' | 2.29 | 0.43 |
| 45:S2:1609:U:H2' | 45:S2:1610:G:O4' | 2.18 | 0.43 |
| 54:SI:40:SER:HB3 | 54:SI:43:ASN:ND2 | 2.31 | 0.43 |
| 60:SO:23:LEU:HD22 | 60:SO:291:SER:HB2 | 2.00 | 0.43 |
| 63:SR:73:LEU:O | 63:SR:76:LEU:HD22 | 2.19 | 0.43 |
| 64:SS:15:PRO:HG2 | 64:SS:18:TRP:CE2 | 2.53 | 0.43 |
| 66:SU:114:ARG:HA | 66:SU:114:ARG:HD2 | 1.94 | 0.43 |
| 66:SU:170:GLN:NE2 | 66:SU:182:VAL:HA | 2.33 | 0.43 |
| 76:Se:91:ASP:OD1 | 76:Se:91:ASP:C | 2.61 | 0.43 |
| 1:LA:138:U:H2' | 1:LA:139:G:H5'' | 2.01 | 0.42 |
| 1:LA:552:U:H3' | 1:LA:553:A:C8 | 2.54 | 0.42 |
| 1:LA:1009:G:H5'' | 12:LL:40:LYS:HZ2 | 1.83 | 0.42 |
| 1:LA:1062:G:C6 | 22:LV:109:VAL:HG22 | 2.54 | 0.42 |
| 1:LA:1679:G:H2' | 1:LA:1680:U:C6 | 2.54 | 0.42 |
| 1:LA:2110:G:H5'' | 25:LY:48:ARG:NH2 | 2.34 | 0.42 |
| 1:LA:2153:U:H2' | 1:LA:2154:G:C8 | 2.54 | 0.42 |
| 1:LA:2244:C:O2' | 4:LD:220:GLY:O | 2.36 | 0.42 |
| 1:LA:2529:G:N3 | 1:LA:2529:G:H2' | 2.33 | 0.42 |
| 1:LA:3168:U:O5' | 1:LA:3168:U:H6 | 2.02 | 0.42 |
| 2:LB:46:A:OP1 | 7:LG:158:ARG:HG3 | 2.19 | 0.42 |
| 3:LC:75:G:H2' | 3:LC:76:C:C6 | 2.53 | 0.42 |
| 4:LD:65:ASP:HB3 | 4:LD:68:LYS:O | 2.19 | 0.42 |
| 4:LD:103:PRO:O | 4:LD:107:VAL:HG13 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:LD:109:GLU:HG2 | 4:LD:138:GLY:HA2 | 2.01 | 0.42 |
| 9:LI:104:GLN:HG2 | 19:LS:6:THR:HG22 | 2.00 | 0.42 |
| 45:S2:916:U:O2 | 45:S2:916:U:H2' | 2.19 | 0.42 |
| 45:S2:959:U:H5' | 70:SY:15:ALA:O | 2.19 | 0.42 |
| 45:S2:1160:A:H2' | 45:S2:1161:C:H6 | 1.82 | 0.42 |
| 47:SB:26:ALA:HB3 | 51:SF:26:LYS:HZ3 | 1.84 | 0.42 |
| 47:SB:117:THR:HG21 | 47:SB:194:LEU:HD22 | 2.01 | 0.42 |
| 47:SB:140:THR:HG21 | 47:SB:175:LEU:HD21 | 2.01 | 0.42 |
| 51:SF:97:VAL:HG12 | 51:SF:98:ASP:H | 1.83 | 0.42 |
| 54:SI:110:LYS:HA | 54:SI:110:LYS:HD2 | 1.72 | 0.42 |
| 62:SQ:133:TYR:CD2 | 62:SQ:217:LEU:HD11 | 2.51 | 0.42 |
| 64:SS:133:LYS:HA | 64:SS:133:LYS:HD2 | 1.86 | 0.42 |
| 66:SU:49:ILE:HD12 | 66:SU:172:VAL:HB | 2.01 | 0.42 |
| 66:SU:94:ALA:HB3 | 66:SU:96:ARG:NH1 | 2.34 | 0.42 |
| 77:Sf:70:LYS:H | 77:Sf:70:LYS:HD3 | 1.84 | 0.42 |
| 1:LA:352:A:H61 | 1:LA:365:A:H5'' | 1.84 | 0.42 |
| 1:LA:375:A:H1' | 27:La:87:LYS:HE3 | 2.01 | 0.42 |
| 1:LA:1230:A:H2 | 1:LA:1259:A:N3 | 2.16 | 0.42 |
| 1:LA:1728:A:C6 | 31:Le:49:PRO:HD3 | 2.54 | 0.42 |
| 1:LA:2673:A:H2' | 1:LA:2674:C:C6 | 2.55 | 0.42 |
| 1:LA:2676:G:H2' | 1:LA:2676:G:N3 | 2.33 | 0.42 |
| 1:LA:3213:U:C5 | 15:LO:121:MET:HE3 | 2.54 | 0.42 |
| 6:LF:150:LEU:HD21 | 6:LF:172:VAL:CG1 | 2.49 | 0.42 |
| 7:LG:55:PHE:CZ | 7:LG:158:ARG:HB2 | 2.54 | 0.42 |
| 8:LH:136:GLU:OE1 | 8:LH:136:GLU:HA | 2.18 | 0.42 |
| 13:LM:133:ARG:HG3 | 13:LM:152:HIS:NE2 | 2.33 | 0.42 |
| 13:LM:155:THR:OG1 | 13:LM:156:LYS:N | 2.52 | 0.42 |
| 13:LM:158:ASP:OD1 | 13:LM:159:THR:N | 2.52 | 0.42 |
| 15:LO:72:LEU:HD21 | 15:LO:81:VAL:HG22 | 2.01 | 0.42 |
| 16:LP:83:LYS:HB2 | 16:LP:85:THR:HG22 | 2.01 | 0.42 |
| 19:LS:90:ASP:OD2 | 19:LS:92:ARG:NH2 | 2.45 | 0.42 |
| 25:LY:23:ARG:HB3 | 25:LY:25:ASP:OD1 | 2.19 | 0.42 |
| 45:S2:115:G:O2' | 45:S2:116:U:H5'' | 2.20 | 0.42 |
| 45:S2:345:U:H1' | 45:S2:346:G:C8 | 2.53 | 0.42 |
| 45:S2:768:C:C2 | 68:SW:143:ILE:HG21 | 2.54 | 0.42 |
| 45:S2:1440:C:H2' | 45:S2:1441:C:H6 | 1.83 | 0.42 |
| 45:S2:1483:A:C5' | 51:SF:71:GLY:HA2 | 2.45 | 0.42 |
| 45:S2:1561:U:H2' | 45:S2:1562:G:C8 | 2.54 | 0.42 |
| 45:S2:1597:A:OP2 | 58:SM:19:ARG:NE | 2.50 | 0.42 |
| 45:S2:1638:G:H2' | 45:S2:1639:C:O4' | 2.18 | 0.42 |
| 46:SA:11:LEU:HD11 | 55:SJ:86:ILE:HD11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:SA:140:GLY:HA3 | 46:SA:182:LEU:HD23 | 2.01 | 0.42 |
| 47:SB:162:VAL:HG13 | 57:SL:54:LEU:HD21 | 2.01 | 0.42 |
| 47:SB:163:SER:O | 47:SB:167:ARG:HB2 | 2.18 | 0.42 |
| 52:SG:35:CYS:HA | 52:SG:38:ILE:CG2 | 2.41 | 0.42 |
| 55:SJ:57:ARG:HE | 55:SJ:89:ARG:NH1 | 2.17 | 0.42 |
| 56:SK:91:PRO:HB3 | 56:SK:101:TYR:HE1 | 1.83 | 0.42 |
| 60:SO:288:HIS:O | 60:SO:306:THR:HG23 | 2.19 | 0.42 |
| 62:SQ:134:VAL:HG12 | 62:SQ:218:LEU:HD12 | 2.01 | 0.42 |
| 62:SQ:194:ASN:O | 62:SQ:198:GLU:HG3 | 2.19 | 0.42 |
| 63:SR:240:LEU:O | 63:SR:244:SER:OG | 2.26 | 0.42 |
| 64:SS:70:VAL:HG13 | 64:SS:92:LEU:HD11 | 2.00 | 0.42 |
| 68:SW:31:ALA:HB2 | 68:SW:42:ILE:HD11 | 2.01 | 0.42 |
| 72:Sa:3:ASN:OD1 | 72:Sa:7:GLN:HB2 | 2.19 | 0.42 |
| 1:LA:253:A:H2' | 1:LA:253:A:N3 | 2.34 | 0.42 |
| 1:LA:639:U:OP1 | 29:Lc:21:ARG:NH1 | 2.49 | 0.42 |
| 1:LA:692:A:H3' | 1:LA:693:C:H6 | 1.84 | 0.42 |
| 1:LA:846:A:H2' | 1:LA:847:A:C8 | 2.55 | 0.42 |
| 1:LA:1122:U:H2' | 1:LA:1123:U:O4' | 2.19 | 0.42 |
| 1:LA:1181:A:H2 | 1:LA:1323:U:O4 | 2.03 | 0.42 |
| 1:LA:1595:C:H2' | 1:LA:1596:C:H6 | 1.84 | 0.42 |
| 1:LA:2196:C:N4 | 1:LA:2240:U:H2' | 2.34 | 0.42 |
| 2:LB:68:C:OP1 | 7:LG:14:SER:OG | 2.20 | 0.42 |
| 3:LC:37:A:OP2 | 36:Lj:86:ARG:HD2 | 2.18 | 0.42 |
| 3:LC:154:C:H2' | 3:LC:155:A:H8 | 1.84 | 0.42 |
| 5:LE:148:LEU:O | 5:LE:152:LYS:HG3 | 2.19 | 0.42 |
| 5:LE:283:TYR:N | 5:LE:323:MET:O | 2.46 | 0.42 |
| 6:LF:5:GLN:HB3 | 6:LF:19:ALA:HB1 | 2.00 | 0.42 |
| 8:LH:75:PRO:HG2 | 8:LH:77:ARG:HG3 | 2.01 | 0.42 |
| 10:LJ:238:LEU:HA | 10:LJ:238:LEU:HD13 | 1.81 | 0.42 |
| 14:LN:7:LEU:O | 29:Lc:49:HIS:NE2 | 2.43 | 0.42 |
| 20:LT:24:LEU:HD12 | 20:LT:50:ILE:HG23 | 2.01 | 0.42 |
| 25:LY:60:LYS:HE2 | 25:LY:60:LYS:HB2 | 1.59 | 0.42 |
| 43:Lq:13:LYS:H | 43:Lq:13:LYS:HG2 | 1.66 | 0.42 |
| 45:S2:521:A:N6 | 45:S2:528:U:OP1 | 2.52 | 0.42 |
| 45:S2:534:A:H2' | 45:S2:535:A:O4' | 2.19 | 0.42 |
| 45:S2:605:A:OP2 | 45:S2:606:A:O2' | 2.34 | 0.42 |
| 45:S2:864:U:O4 | 73:Sb:60:LYS:NZ | 2.52 | 0.42 |
| 45:S2:959:U:OP2 | 77:Sf:20:LYS:NZ | 2.51 | 0.42 |
| 45:S2:1183:A:O2' | 45:S2:1210:C:H4' | 2.19 | 0.42 |
| 45:S2:1280:C:H2' | 45:S2:1281:G:H8 | 1.83 | 0.42 |
| 45:S2:1478:G:O2' | 54:SI:56:LYS:HG2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:SA:106:LYS:HE2 | 46:SA:174:HIS:C | 2.44 | 0.42 |
| 59:SN:117:LEU:C | 59:SN:118:ARG:HD3 | 2.44 | 0.42 |
| 61:SP:23:HIS:CE1 | 61:SP:24:LEU:HG | 2.54 | 0.42 |
| 62:SQ:35:PRO:HD3 | 62:SQ:98:THR:HG23 | 2.01 | 0.42 |
| 63:SR:118:ALA:HB3 | 63:SR:124:ALA:HB2 | 2.00 | 0.42 |
| 68:SW:73:GLY:O | 68:SW:77:ILE:HD12 | 2.19 | 0.42 |
| 68:SW:179:ARG:HA | 68:SW:179:ARG:HD3 | 1.75 | 0.42 |
| 72:Sa:68:SER:O | 72:Sa:72:LEU:HG | 2.19 | 0.42 |
| 75:Sd:10:ARG:HB2 | 75:Sd:24:VAL:HG13 | 2.01 | 0.42 |
| 75:Sd:53:ASP:HB2 | 75:Sd:79:VAL:HG22 | 2.01 | 0.42 |
| 79:Ta:52:C:H2' | 79:Ta:53:G:O4' | 2.19 | 0.42 |
| 1:LA:86:G:O2' | 1:LA:98:G:O6 | 2.29 | 0.42 |
| 1:LA:590:G:H1' | 8:LH:19:LYS:HG3 | 2.01 | 0.42 |
| 1:LA:691:A:H4' | 6:LF:46:LYS:HB2 | 2.01 | 0.42 |
| 1:LA:845:A:H2' | 1:LA:846:A:O4' | 2.19 | 0.42 |
| 1:LA:1339:G:H2' | 1:LA:1340:U:C6 | 2.54 | 0.42 |
| 1:LA:1872:U:OP1 | 20:LT:21:LYS:NZ | 2.45 | 0.42 |
| 1:LA:1925:C:H5' | 44:Lr:8:VAL:HG13 | 2.01 | 0.42 |
| 1:LA:1939:G:OP1 | 20:LT:75:HIS:ND1 | 2.51 | 0.42 |
| 4:LD:117:GLU:OE1 | 4:LD:163:ARG:NH2 | 2.50 | 0.42 |
| 9:LI:156:ILE:HD13 | 9:LI:161:VAL:HG22 | 2.01 | 0.42 |
| 13:LM:157:GLU:O | 13:LM:161:SER:OG | 2.35 | 0.42 |
| 14:LN:126:PHE:HD2 | 36:Lj:115:LYS:HG2 | 1.84 | 0.42 |
| 16:LP:158:HIS:HB3 | 16:LP:161:ALA:HB3 | 2.01 | 0.42 |
| 18:LR:119:VAL:HA | 18:LR:145:HIS:O | 2.19 | 0.42 |
| 19:LS:17:THR:HA | 19:LS:53:PHE:CD2 | 2.54 | 0.42 |
| 22:LV:75:ILE:HD11 | 22:LV:88:ARG:NH2 | 2.34 | 0.42 |
| 22:LV:107:GLU:HA | 22:LV:107:GLU:OE1 | 2.17 | 0.42 |
| 24:LX:35:TYR:HE1 | 24:LX:37:ILE:HG22 | 1.84 | 0.42 |
| 24:LX:54:LEU:HD12 | 24:LX:54:LEU:HA | 1.89 | 0.42 |
| 33:Lg:55:ILE:HD12 | 33:Lg:55:ILE:HA | 1.82 | 0.42 |
| 36:Lj:41:LEU:HD12 | 36:Lj:41:LEU:HA | 1.85 | 0.42 |
| 45:S2:55:A:H2' | 45:S2:403:G:H1 | 1.85 | 0.42 |
| 45:S2:566:C:O2' | 45:S2:567:A:P | 2.77 | 0.42 |
| 45:S2:1252:C:H2' | 45:S2:1253:U:O4' | 2.18 | 0.42 |
| 46:SA:107:PHE:N | 46:SA:107:PHE:CD1 | 2.84 | 0.42 |
| 46:SA:113:LEU:HD11 | 46:SA:117:ARG:HB3 | 2.00 | 0.42 |
| 47:SB:144:GLU:OE1 | 47:SB:222:LYS:HG2 | 2.19 | 0.42 |
| 60:SO:221:MET:HA | 60:SO:221:MET:HE3 | 2.01 | 0.42 |
| 60:SO:252:LEU:CG | 60:SO:263:PHE:HB3 | 2.46 | 0.42 |
| 61:SP:89:PHE:CD2 | 61:SP:174:TRP:HE3 | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:SQ:24:PHE:HE2 | 71:SZ:70:LYS:NZ | 2.16 | 0.42 |
| 62:SQ:33:LYS:O | 62:SQ:98:THR:HG22 | 2.19 | 0.42 |
| 65:ST:199:GLN:HA | 65:ST:202:ARG:HG2 | 2.01 | 0.42 |
| 67:SV:191:PHE:O | 67:SV:195:ARG:HG2 | 2.18 | 0.42 |
| 72:Sa:71:ARG:HG3 | 72:Sa:83:TRP:CZ2 | 2.54 | 0.42 |
| 77:Sf:26:GLN:O | 77:Sf:26:GLN:HG2 | 2.19 | 0.42 |
| 77:Sf:74:SER:O | 77:Sf:77:THR:OG1 | 2.38 | 0.42 |
| 1:LA:253:A:O3' | 1:LA:254:A:H8 | 2.02 | 0.42 |
| 1:LA:429:U:O2' | 34:Lh:88:ASN:O | 2.30 | 0.42 |
| 1:LA:1589:G:OP1 | 35:Li:15:THR:HG21 | 2.19 | 0.42 |
| 1:LA:1791:C:O2 | 1:LA:1793:G:O2' | 2.35 | 0.42 |
| 1:LA:2136:U:C6 | 1:LA:2140:U:C4 | 3.08 | 0.42 |
| 1:LA:2614:G:H2' | 1:LA:2615:C:C6 | 2.55 | 0.42 |
| 1:LA:3126:A:H2' | 1:LA:3127:G:O4' | 2.18 | 0.42 |
| 1:LA:3268:U:H4' | 1:LA:3269:U:O5' | 2.18 | 0.42 |
| 8:LH:92:SER:O | 8:LH:148:GLU:HG2 | 2.19 | 0.42 |
| 10:LJ:227:ASP:CG | 10:LJ:231:LYS:HZ1 | 2.27 | 0.42 |
| 21:LU:66:GLU:OE2 | 21:LU:99:ARG:N | 2.47 | 0.42 |
| 29:Lc:82:ILE:O | 29:Lc:87:ARG:NH2 | 2.48 | 0.42 |
| 35:Li:84:CYS:O | 35:Li:88:ARG:HG3 | 2.19 | 0.42 |
| 45:S2:127:G:H1' | 45:S2:178:U:N3 | 2.34 | 0.42 |
| 45:S2:976:G:N1 | 45:S2:1023:A:O2' | 2.45 | 0.42 |
| 45:S2:1583:A:H1' | 45:S2:1585:U:H5 | 1.83 | 0.42 |
| 47:SB:29:ILE:HG22 | 47:SB:34:GLN:HG3 | 2.01 | 0.42 |
| 60:SO:297:ASP:OD1 | 60:SO:299:GLN:HG3 | 2.20 | 0.42 |
| 62:SQ:32:ILE:HA | 62:SQ:96:LEU:CD1 | 2.48 | 0.42 |
| 65:ST:65:GLN:HA | 65:ST:100:ALA:HB2 | 1.99 | 0.42 |
| 66:SU:48:GLU:OE1 | 66:SU:58:LEU:HD22 | 2.19 | 0.42 |
| 1:LA:1173:G:H2' | 1:LA:1174:C:C6 | 2.54 | 0.42 |
| 1:LA:1496:C:H2' | 1:LA:1497:A:H8 | 1.81 | 0.42 |
| 1:LA:1921:A:H2' | 1:LA:1922:C:O4' | 2.19 | 0.42 |
| 1:LA:2388:C:H2' | 1:LA:2389:A:H8 | 1.84 | 0.42 |
| 1:LA:2514:A:H5'' | 16:LP:28:TRP:CD1 | 2.55 | 0.42 |
| 1:LA:2563:G:OP2 | 28:Lb:55:LYS:HD3 | 2.20 | 0.42 |
| 1:LA:3088:C:H2' | 1:LA:3089:U:O4' | 2.20 | 0.42 |
| 6:LF:170:LYS:HA | 6:LF:175:HIS:HB2 | 2.01 | 0.42 |
| 7:LG:40:HIS:HB3 | 7:LG:43:LYS:HG3 | 2.02 | 0.42 |
| 10:LJ:100:GLU:OE2 | 10:LJ:108:ARG:NH2 | 2.47 | 0.42 |
| 11:LK:123:ILE:O | 11:LK:123:ILE:HG13 | 2.20 | 0.42 |
| 12:LL:47:PRO:HD2 | 12:LL:141:LYS:HA | 2.01 | 0.42 |
| 12:LL:78:THR:HG23 | 12:LL:79:VAL:HG13 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:Li:19:LYS:HD3 | 35:Li:19:LYS:HA | 1.65 | 0.42 |
| 45:S2:623:A:O2' | 45:S2:624:G:OP1 | 2.25 | 0.42 |
| 45:S2:1233:G:H21 | 59:SN:145:HIS:CE1 | 2.37 | 0.42 |
| 45:S2:1280:C:H2' | 45:S2:1281:G:C8 | 2.54 | 0.42 |
| 45:S2:1593:A:H2' | 45:S2:1594:G:C8 | 2.54 | 0.42 |
| 45:S2:1649:G:H2' | 45:S2:1650:U:H6 | 1.84 | 0.42 |
| 46:SA:22:ASN:OD1 | 46:SA:34:TYR:OH | 2.35 | 0.42 |
| 60:SO:36:ALA:HB2 | 60:SO:42:LEU:HG | 2.01 | 0.42 |
| 61:SP:105:GLY:O | 61:SP:109:ASN:HB3 | 2.20 | 0.42 |
| 66:SU:79:ARG:HD3 | 66:SU:79:ARG:C | 2.44 | 0.42 |
| 67:SV:110:ARG:O | 67:SV:114:GLU:HG2 | 2.18 | 0.42 |
| 68:SW:110:GLN:HG3 | 68:SW:144:PRO:HB3 | 2.02 | 0.42 |
| 72:Sa:60:ARG:NH1 | 72:Sa:60:ARG:HG2 | 2.35 | 0.42 |
| 74:Sc:63:GLN:HA | 74:Sc:64:PRO:HA | 1.90 | 0.42 |
| 75:Sd:51:GLU:HG2 | 75:Sd:79:VAL:HG23 | 2.02 | 0.42 |
| 1:LA:226:C:H2' | 1:LA:227:G:O4' | 2.19 | 0.42 |
| 1:LA:406:G:N2 | 3:LC:16:G:N3 | 2.68 | 0.42 |
| 1:LA:674:C:O2' | 1:LA:678:U:OP1 | 2.30 | 0.42 |
| 1:LA:1138:G:O6 | 30:Ld:10:HIS:NE2 | 2.50 | 0.42 |
| 1:LA:1511:U:O3' | 20:LT:5:ARG:NH2 | 2.53 | 0.42 |
| 1:LA:1648:U:C4 | 1:LA:1806:G:N2 | 2.87 | 0.42 |
| 1:LA:1947:G:H4' | 20:LT:101:VAL:HG21 | 2.00 | 0.42 |
| 1:LA:3269:U:C5 | 8:LH:46:ARG:HD2 | 2.55 | 0.42 |
| 7:LG:60:ILE:HB | 7:LG:80:SER:HB2 | 2.01 | 0.42 |
| 8:LH:92:SER:HB3 | 8:LH:148:GLU:OE2 | 2.19 | 0.42 |
| 16:LP:77:LYS:O | 16:LP:79:ALA:N | 2.53 | 0.42 |
| 22:LV:39:ILE:HG22 | 22:LV:99:SER:HB3 | 2.01 | 0.42 |
| 27:La:58:VAL:HA | 27:La:104:LEU:HD23 | 2.02 | 0.42 |
| 31:Le:57:GLU:OE2 | 31:Le:69:TYR:OH | 2.30 | 0.42 |
| 39:Lm:9:LYS:O | 39:Lm:13:GLU:HG2 | 2.20 | 0.42 |
| 40:Ln:13:MET:CE | 40:Ln:49:MET:HE1 | 2.50 | 0.42 |
| 45:S2:116:U:H2' | 45:S2:117:U:H6 | 1.85 | 0.42 |
| 45:S2:1024:U:OP2 | 45:S2:1027:A:N6 | 2.46 | 0.42 |
| 45:S2:1071:U:C5 | 77:Sf:19:HIS:HD2 | 2.38 | 0.42 |
| 45:S2:1544:U:H2' | 45:S2:1545:A:C8 | 2.55 | 0.42 |
| 46:SA:75:LYS:HD2 | 48:SC:22:VAL:HG13 | 2.00 | 0.42 |
| 46:SA:120:TYR:O | 46:SA:124:ARG:HD3 | 2.19 | 0.42 |
| 48:SC:10:LYS:O | 48:SC:13:GLN:HG2 | 2.19 | 0.42 |
| 54:SI:37:VAL:HG23 | 54:SI:39:THR:H | 1.85 | 0.42 |
| 61:SP:10:THR:OG1 | 61:SP:13:ASP:OD2 | 2.37 | 0.42 |
| 61:SP:56:LYS:HE3 | 61:SP:158:VAL:HG23 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 61:SP:191:ARG:HA | 61:SP:191:ARG:HD2 | 1.74 | 0.42 |
| 73:Sb:93:LEU:HD12 | 73:Sb:93:LEU:O | 2.19 | 0.42 |
| 75:Sd:40:LEU:HB3 | 75:Sd:57:VAL:HG21 | 2.01 | 0.42 |
| 79:Ta:65:G:O2' | 79:Ta:66:C:OP1 | 2.36 | 0.42 |
| 1:LA:302:U:H5'' | 16:LP:179:LYS:HE3 | 2.00 | 0.42 |
| 1:LA:307:A:O2' | 1:LA:2222:A:H1' | 2.20 | 0.42 |
| 1:LA:1156:G:H2' | 1:LA:1157:A:O4' | 2.20 | 0.42 |
| 1:LA:1863:A:H2' | 1:LA:1864:A:C8 | 2.54 | 0.42 |
| 1:LA:2420:U:O2' | 43:Lq:52:GLY:HA3 | 2.20 | 0.42 |
| 1:LA:2560:A:O2' | 1:LA:2561:A:H5'' | 2.20 | 0.42 |
| 1:LA:2745:A:H2' | 1:LA:2746:A:O4' | 2.20 | 0.42 |
| 1:LA:3088:C:OP1 | 5:LE:222:LYS:HE2 | 2.19 | 0.42 |
| 1:LA:3378:C:H2' | 1:LA:3379:U:C5 | 2.54 | 0.42 |
| 3:LC:139:U:H2' | 3:LC:140:G:H8 | 1.85 | 0.42 |
| 4:LD:149:ARG:HE | 4:LD:155:LYS:NZ | 2.18 | 0.42 |
| 10:LJ:29:SER:C | 10:LJ:31:PRO:HD3 | 2.45 | 0.42 |
| 13:LM:141:ARG:NH2 | 13:LM:144:CYS:O | 2.53 | 0.42 |
| 18:LR:108:ASP:OD1 | 18:LR:110:THR:OG1 | 2.24 | 0.42 |
| 26:LZ:75:LYS:HG2 | 26:LZ:81:ILE:HB | 2.01 | 0.42 |
| 45:S2:11:A:H2' | 45:S2:12:U:H5' | 2.00 | 0.42 |
| 45:S2:52:U:C2 | 45:S2:53:G:N7 | 2.88 | 0.42 |
| 45:S2:398:G:OP1 | 67:SV:49:ARG:HA | 2.20 | 0.42 |
| 45:S2:448:C:H2' | 45:S2:449:C:H6 | 1.85 | 0.42 |
| 45:S2:591:A:H2' | 45:S2:592:A:C8 | 2.54 | 0.42 |
| 45:S2:876:G:H1' | 45:S2:944:A:O4' | 2.20 | 0.42 |
| 45:S2:1408:G:OP2 | 51:SF:114:ARG:NH1 | 2.46 | 0.42 |
| 54:SI:30:VAL:HG22 | 54:SI:31:PRO:HD2 | 2.01 | 0.42 |
| 62:SQ:195:LYS:HE2 | 62:SQ:195:LYS:N | 2.35 | 0.42 |
| 64:SS:44:LEU:HD11 | 64:SS:90:ILE:HD13 | 2.00 | 0.42 |
| 67:SV:84:HIS:NE2 | 67:SV:97:THR:OG1 | 2.53 | 0.42 |
| 69:SX:75:VAL:HG12 | 69:SX:86:ILE:HG22 | 2.02 | 0.42 |
| 74:Sc:102:VAL:HB | 74:Sc:124:VAL:HG13 | 2.01 | 0.42 |
| 75:Sd:15:ASN:OD1 | 75:Sd:15:ASN:N | 2.53 | 0.42 |
| 1:LA:492:U:H5'' | 1:LA:493:G:C5 | 2.55 | 0.42 |
| 1:LA:800:A:N6 | 14:LN:19:GLN:OE1 | 2.53 | 0.42 |
| 1:LA:883:A:N7 | 1:LA:2138:A:C4 | 2.88 | 0.42 |
| 1:LA:1168:A:H4' | 9:LI:219:LYS:HE2 | 2.01 | 0.42 |
| 1:LA:2687:U:H5' | 1:LA:2689:G:O6 | 2.20 | 0.42 |
| 1:LA:2688:A:N3 | 1:LA:2688:A:H2' | 2.35 | 0.42 |
| 1:LA:3038:C:OP1 | 5:LE:62:ARG:NH1 | 2.47 | 0.42 |
| 1:LA:3189:C:OP1 | 17:LQ:172[A]:ARG:NH1 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LV:144:GLU:O | 22:LV:144:GLU:HG2 | 2.19 | 0.42 |
| 36:Lj:14:LYS:NZ | 36:Lj:14:LYS:HB2 | 2.34 | 0.42 |
| 39:Lm:3:ARG:HH21 | 39:Lm:50:SER:HG | 1.58 | 0.42 |
| 45:S2:305:C:H5' | 69:SX:71:LEU:HD21 | 2.02 | 0.42 |
| 45:S2:446:A:H2' | 45:S2:446:A:N3 | 2.34 | 0.42 |
| 45:S2:762:A:P | 68:SW:79:ARG:HH12 | 2.43 | 0.42 |
| 45:S2:1179:G:H2' | 45:S2:1180:C:C5 | 2.55 | 0.42 |
| 45:S2:1198:G:H5' | 45:S2:1199:G:H4' | 2.02 | 0.42 |
| 45:S2:1276:U:H2' | 45:S2:1277:G:H8 | 1.84 | 0.42 |
| 50:SE:73:PRO:HG3 | 50:SE:91:GLY:O | 2.18 | 0.42 |
| 51:SF:5:PRO:HB2 | 51:SF:96:TYR:CZ | 2.54 | 0.42 |
| 52:SG:5:ARG:HD3 | 52:SG:5:ARG:N | 2.35 | 0.42 |
| 55:SJ:88:LYS:O | 55:SJ:89:ARG:HD3 | 2.20 | 0.42 |
| 55:SJ:95:ALA:HB1 | 55:SJ:99:ILE:HD11 | 2.02 | 0.42 |
| 60:SO:88:THR:HG21 | 60:SO:102:ARG:HH22 | 1.84 | 0.42 |
| 64:SS:104:ASP:OD1 | 64:SS:104:ASP:N | 2.52 | 0.42 |
| 68:SW:11:THR:O | 68:SW:44:ARG:HA | 2.20 | 0.42 |
| 79:Ta:43:G:H2' | 79:Ta:43:G:N3 | 2.35 | 0.42 |
| 1:LA:35:A:OP1 | 16:LP:83:LYS:HG2 | 2.20 | 0.42 |
| 1:LA:209:A:N3 | 6:LF:221:ASN:ND2 | 2.63 | 0.42 |
| 1:LA:287:G:OP1 | 16:LP:179:LYS:HD3 | 2.20 | 0.42 |
| 1:LA:414:U:C2 | 1:LA:415:G:C8 | 3.07 | 0.42 |
| 1:LA:595:C:OP1 | 9:LI:33:ARG:NE | 2.47 | 0.42 |
| 1:LA:1259:A:H4' | 1:LA:1278:C:N3 | 2.35 | 0.42 |
| 1:LA:1674:G:H2' | 1:LA:1675:A:H8 | 1.85 | 0.42 |
| 1:LA:2195:C:O2' | 1:LA:2269:A:N3 | 2.48 | 0.42 |
| 1:LA:2880:C:H2' | 1:LA:2881:U:H6 | 1.81 | 0.42 |
| 4:LD:53:GLY:O | 4:LD:192:LYS:HE3 | 2.19 | 0.42 |
| 6:LF:3:ARG:H | 6:LF:3:ARG:HG2 | 1.63 | 0.42 |
| 12:LL:176:LEU:HD11 | 12:LL:199:PHE:CZ | 2.54 | 0.42 |
| 19:LS:151:ARG:O | 19:LS:162:ALA:HB3 | 2.20 | 0.42 |
| 38:Ll:43:LYS:HB2 | 38:Ll:43:LYS:HE3 | 1.67 | 0.42 |
| 38:Ll:68:LYS:HG3 | 38:Ll:69:HIS:CE1 | 2.55 | 0.42 |
| 38:Ll:75:LYS:HD2 | 38:Ll:75:LYS:C | 2.45 | 0.42 |
| 45:S2:129:U:H5' | 45:S2:203:U:OP2 | 2.20 | 0.42 |
| 45:S2:954:G:H2' | 45:S2:955:A:H8 | 1.85 | 0.42 |
| 45:S2:1010:C:H2' | 45:S2:1011:G:O4' | 2.19 | 0.42 |
| 45:S2:1336:A:H2' | 45:S2:1337:A:C8 | 2.55 | 0.42 |
| 45:S2:1580:C:H4' | 51:SF:137:ARG:HB2 | 2.02 | 0.42 |
| 47:SB:195:ALA:O | 47:SB:199:ILE:HG23 | 2.20 | 0.42 |
| 49:SD:70:ASN:O | 49:SD:74:LEU:HD23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 50:SE:51:SER:HB2 | 50:SE:54:ALA:HB2 | 2.00 | 0.42 |
| 51:SF:58:ASP:OD1 | 51:SF:58:ASP:N | 2.50 | 0.42 |
| 53:SH:41:ARG:HH21 | 54:SI:38:LYS:HE2 | 1.85 | 0.42 |
| 60:SO:67:ILE:HB | 60:SO:85:TRP:CG | 2.55 | 0.42 |
| 62:SQ:23:PRO:HA | 62:SQ:26:ARG:CZ | 2.50 | 0.42 |
| 65:ST:136:LYS:HG3 | 65:ST:136:LYS:O | 2.19 | 0.42 |
| 67:SV:67:TRP:HD1 | 67:SV:185:GLU:OE2 | 2.03 | 0.42 |
| 68:SW:13:SER:HB3 | 68:SW:47:PHE:HD1 | 1.85 | 0.42 |
| 68:SW:65:LYS:HE2 | 68:SW:65:LYS:HB2 | 1.77 | 0.42 |
| 68:SW:124:HIS:O | 68:SW:127:VAL:HG12 | 2.19 | 0.42 |
| 70:SY:16:ILE:O | 73:Sb:57:ARG:NH2 | 2.53 | 0.42 |
| 80:Tb:49:C:C2 | 80:Tb:60:A:H1' | 2.54 | 0.42 |
| 1:LA:19:U:H2' | 1:LA:20:A:H8 | 1.85 | 0.41 |
| 1:LA:276:U:H2' | 1:LA:277:G:C8 | 2.55 | 0.41 |
| 1:LA:690:A:N1 | 3:LC:28:C:O2' | 2.48 | 0.41 |
| 1:LA:695:C:OP2 | 6:LF:119:ARG:NH2 | 2.48 | 0.41 |
| 1:LA:1189:A:H2' | 1:LA:1189:A:N3 | 2.35 | 0.41 |
| 1:LA:1340:U:H2' | 1:LA:1341:C:H6 | 1.85 | 0.41 |
| 1:LA:1576:G:H2' | 1:LA:1577:C:C6 | 2.54 | 0.41 |
| 1:LA:2853:U:OP2 | 12:LL:3:ARG:NH1 | 2.52 | 0.41 |
| 1:LA:2946:G:OP2 | 1:LA:2946:G:H4' | 2.20 | 0.41 |
| 1:LA:3138:A:OP1 | 5:LE:274:SER:HB3 | 2.20 | 0.41 |
| 3:LC:65:A:H2' | 3:LC:66:A:H8 | 1.85 | 0.41 |
| 6:LF:317:PRO:C | 6:LF:319:LYS:N | 2.78 | 0.41 |
| 12:LL:89:VAL:HG13 | 12:LL:136:PHE:HE1 | 1.85 | 0.41 |
| 17:LQ:47[A]:PHE:HA | 17:LQ:136[A]:THR:CG2 | 2.49 | 0.41 |
| 21:LU:24:LEU:O | 21:LU:24:LEU:HD23 | 2.20 | 0.41 |
| 24:LX:24:ASN:ND2 | 24:LX:97:ASP:OD2 | 2.51 | 0.41 |
| 25:LY:45:ASN:O | 25:LY:49:ILE:HG12 | 2.20 | 0.41 |
| 25:LY:46:PRO:O | 25:LY:52:THR:OG1 | 2.35 | 0.41 |
| 31:Le:42:ILE:O | 31:Le:42:ILE:HG13 | 2.20 | 0.41 |
| 41:Lo:82:LEU:HD12 | 41:Lo:82:LEU:HA | 1.84 | 0.41 |
| 45:S2:183:U:H2' | 45:S2:184:C:H6 | 1.85 | 0.41 |
| 45:S2:402:C:N4 | 45:S2:423:G:OP2 | 2.53 | 0.41 |
| 45:S2:959:U:O2 | 45:S2:959:U:H2' | 2.20 | 0.41 |
| 45:S2:1022:C:O2' | 45:S2:1125:A:N1 | 2.45 | 0.41 |
| 46:SA:40:ARG:HD2 | 46:SA:40:ARG:C | 2.45 | 0.41 |
| 49:SD:26:ASP:HA | 49:SD:29:LYS:HE2 | 2.02 | 0.41 |
| 64:SS:106:LYS:NZ | 64:SS:251:GLU:OE2 | 2.46 | 0.41 |
| 66:SU:123:ASP:OD1 | 66:SU:124:LYS:N | 2.52 | 0.41 |
| 67:SV:81:VAL:HG22 | 67:SV:94:ASN:HA | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:128:G:H2' | 1:LA:129:U:C6 | 2.55 | 0.41 |
| 1:LA:181:U:C4' | 38:LI:75:LYS:HD3 | 2.48 | 0.41 |
| 1:LA:491:C:OP1 | 8:LH:112:THR:OG1 | 2.36 | 0.41 |
| 1:LA:506:U:O2' | 1:LA:1165:G:H4' | 2.20 | 0.41 |
| 1:LA:713:G:N1 | 29:Lc:72:VAL:HG11 | 2.35 | 0.41 |
| 1:LA:723:U:H2' | 1:LA:724:G:O4' | 2.20 | 0.41 |
| 1:LA:1096:G:H4' | 22:LV:129:LYS:HG2 | 2.02 | 0.41 |
| 1:LA:1563:U:N3 | 1:LA:1564:G:N7 | 2.68 | 0.41 |
| 1:LA:1666:A:H2' | 1:LA:1667:G:H8 | 1.85 | 0.41 |
| 1:LA:1686:U:H1' | 23:LW:75:TYR:CD2 | 2.54 | 0.41 |
| 1:LA:2536:U:H5'' | 62:SQ:229:MET:CG | 2.48 | 0.41 |
| 1:LA:3131:C:H2' | 1:LA:3132:C:C6 | 2.55 | 0.41 |
| 1:LA:3157:G:H2' | 1:LA:3157:G:N3 | 2.34 | 0.41 |
| 1:LA:3202:U:H2' | 1:LA:3203:C:C6 | 2.56 | 0.41 |
| 6:LF:170:LYS:HB2 | 6:LF:170:LYS:HE2 | 1.72 | 0.41 |
| 6:LF:327:LEU:HD21 | 9:LI:165:ASP:N | 2.34 | 0.41 |
| 7:LG:78:ALA:HB3 | 7:LG:105:ILE:HB | 2.02 | 0.41 |
| 10:LJ:47:SER:HA | 10:LJ:50:VAL:HG23 | 2.02 | 0.41 |
| 12:LL:150:GLU:OE2 | 12:LL:153:ARG:NH1 | 2.53 | 0.41 |
| 15:LO:102:LYS:HG3 | 15:LO:106:ARG:NH2 | 2.35 | 0.41 |
| 16:LP:94:TYR:CZ | 16:LP:96:ARG:HB2 | 2.56 | 0.41 |
| 19:LS:23:ASN:HB3 | 19:LS:26:LEU:HB3 | 2.02 | 0.41 |
| 20:LT:155:LEU:HD23 | 20:LT:155:LEU:HA | 1.84 | 0.41 |
| 45:S2:62:A:O2' | 45:S2:268:C:O2 | 2.37 | 0.41 |
| 45:S2:92:A:OP2 | 45:S2:398:G:N1 | 2.41 | 0.41 |
| 45:S2:371:G:O4' | 73:Sb:88:LYS:HE2 | 2.20 | 0.41 |
| 45:S2:562:G:H2' | 45:S2:563:U:H6 | 1.86 | 0.41 |
| 45:S2:881:A:H2' | 45:S2:882:U:O4' | 2.20 | 0.41 |
| 45:S2:1551:U:P | 50:SE:43:ARG:HH12 | 2.43 | 0.41 |
| 46:SA:40:ARG:HG2 | 55:SJ:110:PRO:HB3 | 2.03 | 0.41 |
| 46:SA:172:THR:O | 46:SA:173:ARG:HD3 | 2.20 | 0.41 |
| 47:SB:61:TYR:CE1 | 47:SB:165:LEU:HD13 | 2.55 | 0.41 |
| 52:SG:74:GLN:O | 52:SG:78:ARG:HG2 | 2.20 | 0.41 |
| 60:SO:81:LEU:HD11 | 60:SO:115:ILE:HG23 | 2.00 | 0.41 |
| 62:SQ:138:PHE:HD1 | 62:SQ:214:LYS:O | 2.03 | 0.41 |
| 63:SR:52:THR:OG1 | 63:SR:54:GLU:OE1 | 2.30 | 0.41 |
| 64:SS:244:ILE:HD12 | 64:SS:244:ILE:C | 2.46 | 0.41 |
| 66:SU:23:ALA:HA | 66:SU:26:GLU:CD | 2.45 | 0.41 |
| 67:SV:65:PHE:CE2 | 67:SV:104:ILE:HG21 | 2.56 | 0.41 |
| 68:SW:60:LEU:HD11 | 68:SW:97:LEU:HD21 | 2.01 | 0.41 |
| 68:SW:109:LEU:HB2 | 68:SW:146:PHE:HB3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 73:Sb:5:SER:HB3 | 73:Sb:8:ALA:HB3 | 2.02 | 0.41 |
| 79:Ta:14:A:H62 | 79:Ta:23:G:N2 | 2.09 | 0.41 |
| 1:LA:87:U:H2' | 1:LA:88:A:H8 | 1.85 | 0.41 |
| 1:LA:700:G:H2' | 1:LA:701:C:C6 | 2.55 | 0.41 |
| 1:LA:809:A:OP1 | 16:LP:81:TYR:HB2 | 2.21 | 0.41 |
| 1:LA:833:U:H2' | 1:LA:834:G:O4' | 2.20 | 0.41 |
| 1:LA:2277:C:P | 42:Lp:23:ARG:HH21 | 2.43 | 0.41 |
| 1:LA:2761:A:H2' | 1:LA:2762:U:H6 | 1.84 | 0.41 |
| 1:LA:3048:A:C5 | 5:LE:75:ALA:HB2 | 2.56 | 0.41 |
| 1:LA:3242:A:H4' | 5:LE:95:THR:HG22 | 2.01 | 0.41 |
| 1:LA:3321:A:H2' | 1:LA:3322:A:H8 | 1.83 | 0.41 |
| 1:LA:3370:G:H2' | 1:LA:3371:A:C8 | 2.55 | 0.41 |
| 2:LB:3:U:H2' | 2:LB:4:U:C6 | 2.56 | 0.41 |
| 5:LE:24:SER:O | 5:LE:220:VAL:HG21 | 2.20 | 0.41 |
| 5:LE:48:GLY:O | 5:LE:335:ILE:HD12 | 2.19 | 0.41 |
| 5:LE:66:LYS:HE3 | 24:LX:11:PHE:CD2 | 2.55 | 0.41 |
| 6:LF:22:LEU:HA | 6:LF:23:PRO:HD3 | 1.83 | 0.41 |
| 6:LF:53:SER:OG | 6:LF:56:ALA:HB2 | 2.20 | 0.41 |
| 6:LF:159:ILE:HG12 | 6:LF:164:GLU:HG3 | 2.01 | 0.41 |
| 7:LG:120:LYS:HE2 | 7:LG:120:LYS:HB2 | 1.90 | 0.41 |
| 7:LG:282:ARG:O | 7:LG:286:VAL:HG23 | 2.20 | 0.41 |
| 14:LN:21:ARG:HB3 | 16:LP:196:THR:HA | 2.02 | 0.41 |
| 20:LT:110:ARG:HE | 20:LT:110:ARG:HB3 | 1.53 | 0.41 |
| 23:LW:46:ALA:HB3 | 23:LW:49:ASN:OD1 | 2.20 | 0.41 |
| 39:Lm:7:ASP:CG | 39:Lm:9:LYS:HZ3 | 2.29 | 0.41 |
| 42:Lp:14:LYS:HB2 | 42:Lp:14:LYS:HE3 | 1.76 | 0.41 |
| 45:S2:547:U:O2' | 45:S2:596:C:O2 | 2.32 | 0.41 |
| 45:S2:856:A:H1' | 66:SU:64:VAL:HG13 | 2.03 | 0.41 |
| 45:S2:1208:A:H1' | 45:S2:1270:G:P | 2.61 | 0.41 |
| 45:S2:1217:A:H4' | 45:S2:1219:A:H5'' | 2.02 | 0.41 |
| 45:S2:1264:G:N2 | 45:S2:1265:G:H1' | 2.35 | 0.41 |
| 45:S2:1533:C:OP2 | 56:SK:77:ARG:NH2 | 2.53 | 0.41 |
| 51:SF:82:ARG:HA | 51:SF:85:ILE:HG12 | 2.01 | 0.41 |
| 60:SO:25:THR:HG22 | 60:SO:32:LEU:O | 2.20 | 0.41 |
| 66:SU:39:ARG:N | 66:SU:40:PRO:HD2 | 2.36 | 0.41 |
| 68:SW:139:GLN:NE2 | 75:Sd:64:PHE:HB3 | 2.35 | 0.41 |
| 1:LA:75:G:H5' | 14:LN:58:VAL:HB | 2.01 | 0.41 |
| 1:LA:716:C:OP1 | 1:LA:750:A:O2' | 2.38 | 0.41 |
| 1:LA:1106:C:O2' | 1:LA:1107:U:H6 | 2.03 | 0.41 |
| 1:LA:1395:C:H2' | 1:LA:1396:C:C6 | 2.55 | 0.41 |
| 1:LA:1506:G:H1' | 18:LR:139:TYR:CE2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:LA:1743:G:H2' | 1:LA:1744:C:C6 | 2.55 | 0.41 |
| 1:LA:1941:U:H2' | 1:LA:1942:C:O4' | 2.20 | 0.41 |
| 1:LA:2396:A:H8 | 1:LA:2940:A:N1 | 2.19 | 0.41 |
| 4:LD:180:LEU:HG | 44:Lr:26:VAL:HG21 | 2.02 | 0.41 |
| 7:LG:63:GLN:HB2 | 7:LG:65:ILE:HD11 | 2.02 | 0.41 |
| 9:LI:232:ARG:O | 9:LI:233:GLU:C | 2.63 | 0.41 |
| 11:LK:18:VAL:H | 15:LO:5:SER:HB2 | 1.85 | 0.41 |
| 13:LM:13:LYS:N | 13:LM:132:ASN:O | 2.40 | 0.41 |
| 23:LW:80:THR:HG21 | 23:LW:95:PHE:HD2 | 1.85 | 0.41 |
| 24:LX:11:PHE:CE1 | 24:LX:88:ARG:HD2 | 2.56 | 0.41 |
| 32:Lf:37:LYS:HG3 | 32:Lf:51:LEU:HD11 | 2.01 | 0.41 |
| 37:Lk:5:THR:OG1 | 37:Lk:7:ILE:HG12 | 2.21 | 0.41 |
| 45:S2:164:A:N3 | 65:ST:13:GLN:NE2 | 2.68 | 0.41 |
| 45:S2:371:G:O5' | 73:Sb:88:LYS:HE2 | 2.20 | 0.41 |
| 45:S2:992:A:H2 | 45:S2:1012:U:O4 | 2.03 | 0.41 |
| 49:SD:32:LEU:HD13 | 49:SD:101:ALA:HA | 2.02 | 0.41 |
| 49:SD:45:LEU:O | 49:SD:49:THR:HG22 | 2.19 | 0.41 |
| 49:SD:131:ASP:HA | 49:SD:134:SER:OG | 2.20 | 0.41 |
| 52:SG:18:GLU:OE2 | 52:SG:19:ARG:HB3 | 2.20 | 0.41 |
| 52:SG:30:THR:O | 52:SG:34:LEU:HD23 | 2.21 | 0.41 |
| 54:SI:21:PHE:O | 54:SI:25:GLN:HG2 | 2.21 | 0.41 |
| 57:SL:10:ALA:O | 57:SL:54:LEU:HB2 | 2.21 | 0.41 |
| 61:SP:110:TYR:HA | 61:SP:115:PHE:CD1 | 2.56 | 0.41 |
| 62:SQ:229:MET:HG2 | 62:SQ:229:MET:H | 1.59 | 0.41 |
| 66:SU:9:LEU:HD21 | 66:SU:12:ALA:O | 2.20 | 0.41 |
| 67:SV:65:PHE:CD2 | 67:SV:104:ILE:HG21 | 2.55 | 0.41 |
| 68:SW:45:ILE:HA | 68:SW:48:GLN:HE21 | 1.85 | 0.41 |
| 75:Sd:111:LYS:HE2 | 75:Sd:115:ASP:OD2 | 2.21 | 0.41 |
| 79:Ta:59:A:H4' | 79:Ta:60:A:C8 | 2.55 | 0.41 |
| 1:LA:946:G:H2' | 1:LA:947:C:H6 | 1.86 | 0.41 |
| 1:LA:1034:G:N2 | 1:LA:1035:A:H62 | 2.18 | 0.41 |
| 1:LA:1238:C:H5'' | 1:LA:1239:A:OP1 | 2.21 | 0.41 |
| 1:LA:2661:G:H2' | 1:LA:2662:G:C8 | 2.56 | 0.41 |
| 1:LA:3208:A:H8 | 1:LA:3208:A:OP1 | 2.04 | 0.41 |
| 1:LA:3228:G:O6 | 1:LA:3257:U:O2 | 2.39 | 0.41 |
| 3:LC:64:U:C2 | 3:LC:65:A:C8 | 3.08 | 0.41 |
| 10:LJ:73:PRO:HD3 | 10:LJ:233:TRP:CE2 | 2.55 | 0.41 |
| 12:LL:150:GLU:O | 12:LL:154:ARG:HG2 | 2.20 | 0.41 |
| 12:LL:175:ASN:OD1 | 12:LL:175:ASN:N | 2.51 | 0.41 |
| 19:LS:175:ALA:C | 29:Lc:51:GLY:HA2 | 2.45 | 0.41 |
| 20:LT:28:GLU:O | 20:LT:32:ILE:HG13 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:LU:94:ILE:HD11 | 21:LU:102:ALA:CA | 2.51 | 0.41 |
| 28:Lb:62:VAL:O | 28:Lb:66:THR:OG1 | 2.34 | 0.41 |
| 44:Lr:8:VAL:O | 44:Lr:11:THR:OG1 | 2.37 | 0.41 |
| 44:Lr:84:ARG:O | 44:Lr:88:GLU:HG2 | 2.20 | 0.41 |
| 45:S2:205:U:N3 | 45:S2:206:A:N7 | 2.69 | 0.41 |
| 45:S2:339:C:H2' | 45:S2:340:U:C6 | 2.55 | 0.41 |
| 45:S2:641:G:N2 | 66:SU:177:THR:O | 2.53 | 0.41 |
| 45:S2:958:U:O2' | 45:S2:960:U:OP2 | 2.38 | 0.41 |
| 45:S2:1517:U:H5'' | 45:S2:1518:C:H5 | 1.84 | 0.41 |
| 47:SB:148:ARG:HH21 | 57:SL:22:ARG:HH21 | 1.68 | 0.41 |
| 49:SD:103:LEU:HD12 | 49:SD:103:LEU:HA | 1.92 | 0.41 |
| 50:SE:90:ILE:HD11 | 50:SE:112:LEU:HD21 | 2.02 | 0.41 |
| 56:SK:46:LYS:O | 56:SK:50:ILE:HG23 | 2.21 | 0.41 |
| 60:SO:305:TYR:HB2 | 60:SO:309:VAL:HG23 | 2.02 | 0.41 |
| 61:SP:36:TYR:CD2 | 61:SP:161:PRO:HB3 | 2.55 | 0.41 |
| 62:SQ:195:LYS:NZ | 62:SQ:198:GLU:OE2 | 2.54 | 0.41 |
| 64:SS:20:LEU:HD23 | 64:SS:20:LEU:HA | 1.89 | 0.41 |
| 66:SU:96:ARG:NH1 | 66:SU:128:ASP:OD2 | 2.54 | 0.41 |
| 66:SU:139:ARG:HG2 | 66:SU:139:ARG:HH11 | 1.85 | 0.41 |
| 68:SW:27:GLU:HG2 | 68:SW:42:ILE:HG21 | 2.02 | 0.41 |
| 68:SW:180:LYS:HB2 | 68:SW:180:LYS:HE2 | 1.90 | 0.41 |
| 70:SY:3:ARG:HB3 | 70:SY:6:SER:HB3 | 2.01 | 0.41 |
| 75:Sd:26:ASP:OD1 | 75:Sd:26:ASP:N | 2.54 | 0.41 |
| 1:LA:63:A:H5'' | 16:LP:174:ILE:HG21 | 2.02 | 0.41 |
| 1:LA:252:U:O2' | 1:LA:253:A:OP1 | 2.31 | 0.41 |
| 1:LA:294:U:H4' | 37:Lk:77:LEU:HD23 | 2.02 | 0.41 |
| 1:LA:412:G:OP1 | 18:LR:62:ARG:NH1 | 2.53 | 0.41 |
| 1:LA:911:G:H2' | 1:LA:913:A:C5 | 2.56 | 0.41 |
| 1:LA:1481:A:N3 | 1:LA:1481:A:H2' | 2.36 | 0.41 |
| 1:LA:1906:C:H3' | 1:LA:1907:A:C8 | 2.55 | 0.41 |
| 1:LA:3112:A:H2' | 1:LA:3113:A:O4' | 2.20 | 0.41 |
| 3:LC:9:A:H2' | 3:LC:10:A:H8 | 1.86 | 0.41 |
| 3:LC:151:C:C5 | 26:LZ:24:LEU:HD21 | 2.56 | 0.41 |
| 4:LD:104:LEU:CD1 | 4:LD:158:ILE:HD11 | 2.47 | 0.41 |
| 5:LE:367:LYS:HD2 | 25:LY:33:ASN:HB2 | 2.02 | 0.41 |
| 9:LI:86:VAL:O | 9:LI:114:GLY:HA2 | 2.21 | 0.41 |
| 9:LI:163:LEU:HD13 | 9:LI:169:ILE:HD11 | 2.02 | 0.41 |
| 15:LO:56:GLN:HE21 | 15:LO:58:ILE:HD12 | 1.85 | 0.41 |
| 19:LS:147:ARG:O | 19:LS:150:VAL:HG22 | 2.20 | 0.41 |
| 29:Lc:7:LYS:HD3 | 29:Lc:7:LYS:HA | 1.91 | 0.41 |
| 45:S2:477:A:H62 | 45:S2:539:G:N2 | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 45:S2:566:C:N4 | 45:S2:576:G:O2' | 2.51 | 0.41 |
| 45:S2:962:C:H2' | 45:S2:963:A:O4' | 2.21 | 0.41 |
| 45:S2:1584:G:C5 | 51:SF:14:LYS:HE3 | 2.56 | 0.41 |
| 45:S2:1731:A:H2' | 45:S2:1731:A:N3 | 2.35 | 0.41 |
| 46:SA:67:ASN:HA | 46:SA:70:THR:HG22 | 2.02 | 0.41 |
| 47:SB:93:LEU:HD22 | 47:SB:172:ILE:HG23 | 2.02 | 0.41 |
| 49:SD:130:THR:CG2 | 49:SD:133:LEU:HD22 | 2.51 | 0.41 |
| 56:SK:53:GLU:O | 56:SK:57:TYR:CD2 | 2.74 | 0.41 |
| 56:SK:70:LYS:HE3 | 56:SK:70:LYS:HB3 | 1.94 | 0.41 |
| 59:SN:141:CYS:HB3 | 59:SN:144:CYS:HB2 | 2.02 | 0.41 |
| 60:SO:15:GLY:HA3 | 60:SO:45:TRP:CH2 | 2.53 | 0.41 |
| 60:SO:19:TRP:HB2 | 60:SO:38:ARG:HD2 | 2.03 | 0.41 |
| 60:SO:156:VAL:HG23 | 60:SO:169:ILE:HG22 | 2.03 | 0.41 |
| 61:SP:13:ASP:HA | 61:SP:16:LEU:HD12 | 2.02 | 0.41 |
| 63:SR:59:HIS:CD2 | 63:SR:239:PRO:HD3 | 2.55 | 0.41 |
| 71:SZ:92:LYS:HE3 | 71:SZ:92:LYS:HB2 | 1.86 | 0.41 |
| 74:Sc:37:ALA:HA | 74:Sc:41:SER:HB3 | 2.03 | 0.41 |
| 1:LA:82:C:H4' | 16:LP:204:LYS:HE2 | 2.02 | 0.41 |
| 1:LA:112:U:OP1 | 36:Lj:107:LYS:HE3 | 2.21 | 0.41 |
| 1:LA:121:A:O2' | 10:LJ:105:LYS:HE2 | 2.20 | 0.41 |
| 1:LA:163:C:H2' | 1:LA:164:A:H5' | 2.03 | 0.41 |
| 1:LA:431:U:H2' | 1:LA:432:G:H8 | 1.86 | 0.41 |
| 1:LA:615:G:H2' | 1:LA:616:G:H8 | 1.84 | 0.41 |
| 1:LA:691:A:C2 | 1:LA:692:A:H1' | 2.56 | 0.41 |
| 1:LA:762:G:H2' | 1:LA:763:U:O4' | 2.20 | 0.41 |
| 1:LA:848:C:H2' | 1:LA:849:U:C6 | 2.55 | 0.41 |
| 1:LA:1059:U:H2' | 1:LA:1060:A:C8 | 2.55 | 0.41 |
| 1:LA:1380:A:H2' | 1:LA:1381:G:C8 | 2.55 | 0.41 |
| 1:LA:1546:G:OP1 | 16:LP:108:ARG:NH2 | 2.53 | 0.41 |
| 1:LA:2536:U:P | 62:SQ:227:ALA:H | 2.44 | 0.41 |
| 2:LB:101:G:N7 | 21:LU:52:LYS:NZ | 2.62 | 0.41 |
| 5:LE:165:GLN:OE1 | 5:LE:167:ARG:NH1 | 2.41 | 0.41 |
| 5:LE:287:LYS:HB2 | 5:LE:287:LYS:HE2 | 1.93 | 0.41 |
| 6:LF:159:ILE:CG1 | 6:LF:164:GLU:HG3 | 2.51 | 0.41 |
| 15:LO:50:LYS:NZ | 15:LO:82:SER:O | 2.39 | 0.41 |
| 16:LP:24:ARG:O | 16:LP:27:VAL:HG12 | 2.21 | 0.41 |
| 17:LQ:12[A]:LYS:HA | 17:LQ:40[A]:GLU:HB3 | 2.03 | 0.41 |
| 18:LR:53:ASP:HB3 | 18:LR:55:GLN:HG2 | 2.03 | 0.41 |
| 19:LS:138:LEU:HD22 | 19:LS:140:LEU:HD21 | 2.02 | 0.41 |
| 43:Lq:32:LYS:HE2 | 43:Lq:32:LYS:HB3 | 1.83 | 0.41 |
| 45:S2:55:A:H3' | 45:S2:403:G:H22 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 45:S2:617:U:H2' | 45:S2:618:U:C6 | 2.56 | 0.41 |
| 45:S2:788:A:C5 | 64:SS:19:LEU:HD22 | 2.55 | 0.41 |
| 45:S2:802:G:H2' | 45:S2:803:A:N9 | 2.35 | 0.41 |
| 45:S2:803:A:H2 | 45:S2:804:A:H62 | 1.69 | 0.41 |
| 45:S2:919:A:N7 | 45:S2:920:U:N3 | 2.69 | 0.41 |
| 45:S2:1552:U:O2 | 45:S2:1556:A:C6 | 2.73 | 0.41 |
| 47:SB:57:SER:HB2 | 57:SL:55:VAL:HG23 | 2.02 | 0.41 |
| 60:SO:23:LEU:HD21 | 60:SO:292:LEU:C | 2.45 | 0.41 |
| 60:SO:250:TYR:HE1 | 60:SO:265:LEU:HD23 | 1.86 | 0.41 |
| 61:SP:77:SER:HB2 | 61:SP:86:VAL:HG11 | 2.02 | 0.41 |
| 71:SZ:13:VAL:HG23 | 71:SZ:77:THR:H | 1.85 | 0.41 |
| 75:Sd:29:HIS:ND1 | 75:Sd:32:ARG:HB2 | 2.35 | 0.41 |
| 77:Sf:55:THR:HA | 77:Sf:63:LEU:HD12 | 2.03 | 0.41 |
| 77:Sf:70:LYS:HD3 | 77:Sf:70:LYS:N | 2.36 | 0.41 |
| 1:LA:22:G:H1' | 3:LC:104:A:N3 | 2.34 | 0.41 |
| 1:LA:1154:C:H1' | 1:LA:1197:C:O2 | 2.19 | 0.41 |
| 1:LA:1173:G:N2 | 17:LQ:87[A]:MET:HE2 | 2.35 | 0.41 |
| 1:LA:1183:A:H2' | 1:LA:1184:C:C6 | 2.55 | 0.41 |
| 1:LA:1497:A:H2' | 1:LA:1498:C:H6 | 1.86 | 0.41 |
| 1:LA:1583:U:H2' | 1:LA:1584:C:C6 | 2.55 | 0.41 |
| 1:LA:1947:G:H2' | 1:LA:1948:G:C8 | 2.54 | 0.41 |
| 1:LA:2669:G:H2' | 1:LA:2670:A:H8 | 1.85 | 0.41 |
| 1:LA:2896:A:H5' | 41:Lo:125:LYS:HB2 | 2.02 | 0.41 |
| 5:LE:37:ARG:HH12 | 5:LE:191:LYS:NZ | 2.18 | 0.41 |
| 9:LI:221:LYS:HB2 | 9:LI:227:GLY:HA3 | 2.02 | 0.41 |
| 13:LM:60:ARG:O | 13:LM:63:GLU:HB2 | 2.19 | 0.41 |
| 18:LR:37:ASN:OD1 | 18:LR:117:ILE:HG22 | 2.21 | 0.41 |
| 18:LR:116:HIS:HB3 | 18:LR:149:VAL:HB | 2.02 | 0.41 |
| 24:LX:81:GLN:O | 24:LX:98:ASN:HB3 | 2.21 | 0.41 |
| 26:LZ:68:THR:HG23 | 36:Lj:36:LEU:HD13 | 2.02 | 0.41 |
| 33:Lg:113:LYS:HE3 | 33:Lg:113:LYS:HB3 | 1.83 | 0.41 |
| 35:Li:51:LEU:HB3 | 35:Li:54:ILE:HD13 | 2.02 | 0.41 |
| 36:Lj:20:GLN:HA | 36:Lj:23:ASP:OD2 | 2.21 | 0.41 |
| 45:S2:312:A:H4' | 45:S2:313:U:H5' | 2.03 | 0.41 |
| 45:S2:1125:A:C5 | 45:S2:1126:G:H1' | 2.56 | 0.41 |
| 45:S2:1253:U:O2' | 45:S2:1254:U:OP1 | 2.31 | 0.41 |
| 45:S2:1364:G:H2' | 45:S2:1365:C:H6 | 1.84 | 0.41 |
| 45:S2:1505:A:N1 | 45:S2:1549:C:O2' | 2.48 | 0.41 |
| 45:S2:1524:A:H4' | 54:SI:93:HIS:CG | 2.56 | 0.41 |
| 45:S2:1767:G:H4' | 45:S2:1768:G:C4 | 2.56 | 0.41 |
| 46:SA:158:ILE:CD1 | 46:SA:163:PRO:HB2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 49:SD:108:ARG:O | 49:SD:110:GLY:N | 2.54 | 0.41 |
| 54:SI:21:PHE:CD2 | 54:SI:22:LEU:HD12 | 2.56 | 0.41 |
| 59:SN:118:ARG:HB2 | 59:SN:134:ASN:HD22 | 1.85 | 0.41 |
| 64:SS:198:LYS:HB2 | 64:SS:208:VAL:HG12 | 2.02 | 0.41 |
| 1:LA:24:G:H2' | 1:LA:25:U:O4' | 2.20 | 0.41 |
| 1:LA:71:A:OP1 | 29:Lc:67:HIS:NE2 | 2.54 | 0.41 |
| 1:LA:492:U:H3' | 1:LA:493:G:C8 | 2.55 | 0.41 |
| 1:LA:760:A:H2' | 1:LA:761:U:H6 | 1.85 | 0.41 |
| 1:LA:834:G:O2' | 1:LA:856:G:N2 | 2.32 | 0.41 |
| 1:LA:854:U:H5'' | 20:LT:95:TRP:CG | 2.55 | 0.41 |
| 1:LA:1039:A:H61 | 7:LG:9:SER:HB2 | 1.85 | 0.41 |
| 1:LA:1076:U:O3' | 7:LG:43:LYS:HD3 | 2.20 | 0.41 |
| 1:LA:1161:U:H4' | 33:Lg:57:TYR:CE1 | 2.56 | 0.41 |
| 1:LA:1243:A:O2' | 1:LA:1244:A:H5' | 2.21 | 0.41 |
| 1:LA:1590:G:H5'' | 35:Li:37:LYS:NZ | 2.35 | 0.41 |
| 1:LA:1810:G:H2' | 1:LA:1811:G:C8 | 2.56 | 0.41 |
| 1:LA:2177:A:H5'' | 4:LD:132:ASN:OD1 | 2.21 | 0.41 |
| 1:LA:2421:C:O5' | 43:Lq:52:GLY:HA2 | 2.20 | 0.41 |
| 1:LA:2587:U:H2' | 1:LA:2588:G:C8 | 2.56 | 0.41 |
| 1:LA:2766:U:H2' | 1:LA:2767:U:H6 | 1.85 | 0.41 |
| 1:LA:2823:G:H2' | 1:LA:2824:C:H6 | 1.86 | 0.41 |
| 1:LA:3117:C:H2' | 1:LA:3118:U:O4' | 2.21 | 0.41 |
| 1:LA:3205:C:N3 | 15:LO:13:ARG:NH2 | 2.62 | 0.41 |
| 1:LA:3262:G:C2 | 1:LA:3263:G:C8 | 3.09 | 0.41 |
| 1:LA:3307:C:O2' | 18:LR:69:ARG:O | 2.38 | 0.41 |
| 1:LA:3327:G:N2 | 5:LE:309:GLY:O | 2.51 | 0.41 |
| 5:LE:103:THR:HG21 | 5:LE:147:GLU:OE1 | 2.20 | 0.41 |
| 6:LF:105:THR:O | 14:LN:26:PHE:HZ | 2.03 | 0.41 |
| 7:LG:84:PRO:HD3 | 7:LG:88:ILE:O | 2.21 | 0.41 |
| 7:LG:88:ILE:HD13 | 7:LG:240:TYR:CE1 | 2.56 | 0.41 |
| 7:LG:262:LYS:HE2 | 7:LG:262:LYS:HB3 | 1.78 | 0.41 |
| 8:LH:40:LEU:HD13 | 8:LH:84:VAL:HG21 | 2.03 | 0.41 |
| 9:LI:138:TYR:CE2 | 9:LI:233:GLU:HB3 | 2.56 | 0.41 |
| 9:LI:141:TYR:HD1 | 9:LI:189:ILE:CD1 | 2.30 | 0.41 |
| 10:LJ:94:PHE:CB | 10:LJ:189:LEU:HD21 | 2.51 | 0.41 |
| 11:LK:3:TYR:HA | 21:LU:142:GLN:OE1 | 2.21 | 0.41 |
| 13:LM:60:ARG:HB2 | 13:LM:63:GLU:CD | 2.45 | 0.41 |
| 16:LP:99:ARG:HG3 | 16:LP:130:PHE:CD1 | 2.56 | 0.41 |
| 16:LP:180:PHE:O | 16:LP:184:LYS:HG3 | 2.21 | 0.41 |
| 17:LQ:128[A]:ARG:HD2 | 17:LQ:128[A]:ARG:HA | 1.70 | 0.41 |
| 20:LT:183:ALA:O | 20:LT:187:GLU:HB3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:LZ:50:ALA:O | 36:Lj:66:VAL:HG21 | 2.21 | 0.41 |
| 27:La:60:ARG:HD3 | 27:La:60:ARG:HA | 1.83 | 0.41 |
| 28:Lb:54:THR:H | 28:Lb:57:HIS:CD2 | 2.39 | 0.41 |
| 34:Lh:16:TYR:OH | 34:Lh:91:ALA:HB2 | 2.21 | 0.41 |
| 35:Li:102:LYS:HB2 | 35:Li:102:LYS:HE3 | 1.69 | 0.41 |
| 36:Lj:118:ILE:HG21 | 36:Lj:118:ILE:HD13 | 1.51 | 0.41 |
| 37:Lk:86:LYS:O | 37:Lk:90:MET:HG2 | 2.21 | 0.41 |
| 45:S2:31:C:O3' | 74:Sc:139:LYS:HE2 | 2.21 | 0.41 |
| 45:S2:158:U:O2 | 45:S2:420:A:O2' | 2.37 | 0.41 |
| 45:S2:271:A:C6 | 45:S2:285:G:N2 | 2.89 | 0.41 |
| 45:S2:383:G:H2' | 45:S2:384:G:H5'' | 2.02 | 0.41 |
| 45:S2:389:G:H2' | 45:S2:390:G:N3 | 2.36 | 0.41 |
| 45:S2:577:G:H2' | 79:Ta:36:G:H1' | 2.02 | 0.41 |
| 45:S2:610:G:H21 | 74:Sc:19:ARG:HH22 | 1.68 | 0.41 |
| 45:S2:889:U:H2' | 45:S2:890:C:O4' | 2.21 | 0.41 |
| 45:S2:1167:G:N2 | 51:SF:139:GLN:HE22 | 2.18 | 0.41 |
| 45:S2:1170:G:C2 | 45:S2:1171:A:C8 | 3.09 | 0.41 |
| 45:S2:1256:A:H4' | 45:S2:1257:U:O5' | 2.20 | 0.41 |
| 45:S2:1408:G:H5'' | 45:S2:1409:G:N7 | 2.36 | 0.41 |
| 45:S2:1552:U:N3 | 45:S2:1556:A:C5 | 2.88 | 0.41 |
| 45:S2:1573:A:N6 | 47:SB:181:GLU:HA | 2.35 | 0.41 |
| 45:S2:1676:U:OP1 | 67:SV:44:HIS:ND1 | 2.54 | 0.41 |
| 45:S2:1682:U:H2' | 45:S2:1683:C:C6 | 2.56 | 0.41 |
| 45:S2:1760:G:H1' | 45:S2:1781:A:C2 | 2.56 | 0.41 |
| 47:SB:76:ARG:HD3 | 47:SB:76:ARG:N | 2.35 | 0.41 |
| 48:SC:3:MET:HE1 | 48:SC:41:TYR:CD2 | 2.56 | 0.41 |
| 49:SD:33:ARG:HD3 | 49:SD:33:ARG:HA | 1.90 | 0.41 |
| 49:SD:130:THR:HG22 | 49:SD:133:LEU:HD22 | 2.02 | 0.41 |
| 53:SH:60:GLU:OE1 | 53:SH:60:GLU:N | 2.53 | 0.41 |
| 54:SI:135:ILE:HD13 | 54:SI:135:ILE:HA | 1.87 | 0.41 |
| 56:SK:65:LEU:HD22 | 56:SK:80:LEU:HG | 2.03 | 0.41 |
| 58:SM:30:LEU:HA | 58:SM:30:LEU:HD12 | 1.88 | 0.41 |
| 60:SO:51:ASP:OD1 | 60:SO:51:ASP:N | 2.49 | 0.41 |
| 61:SP:98:ILE:HG21 | 61:SP:102:PHE:HD1 | 1.86 | 0.41 |
| 63:SR:82:ASN:OD1 | 63:SR:82:ASN:C | 2.63 | 0.41 |
| 65:ST:38:GLY:HA2 | 65:ST:41:VAL:HG12 | 2.03 | 0.41 |
| 65:ST:58:LYS:O | 65:ST:59:GLN:HB2 | 2.21 | 0.41 |
| 66:SU:9:LEU:HD21 | 66:SU:13:PRO:HA | 2.02 | 0.41 |
| 66:SU:44:LYS:HG3 | 66:SU:63:PRO:CG | 2.51 | 0.41 |
| 68:SW:93:LEU:HD12 | 68:SW:96:VAL:HG21 | 2.02 | 0.41 |
| 70:SY:96:VAL:CG1 | 70:SY:100:LYS:HE3 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:SZ:49:LYS:HE2 | 71:SZ:49:LYS:HB2 | 1.90 | 0.41 |
| 73:Sb:57:ARG:H | 73:Sb:57:ARG:HG2 | 1.63 | 0.41 |
| 1:LA:513:G:N3 | 6:LF:341:SER:OG | 2.50 | 0.41 |
| 1:LA:650:G:O2' | 1:LA:1434:A:OP1 | 2.39 | 0.41 |
| 1:LA:659:A:N1 | 1:LA:940:G:O2' | 2.42 | 0.41 |
| 1:LA:761:U:O4 | 1:LA:768:G:C2 | 2.74 | 0.41 |
| 1:LA:971:A:H2' | 1:LA:972:A:C8 | 2.55 | 0.41 |
| 1:LA:1739:U:H4' | 1:LA:1740:A:H5' | 2.03 | 0.41 |
| 1:LA:1827:A:H2' | 1:LA:1828:G:C8 | 2.56 | 0.41 |
| 1:LA:1882:A:H2' | 1:LA:1883:A:C8 | 2.56 | 0.41 |
| 1:LA:2192:U:H5'' | 1:LA:2193:G:O5' | 2.21 | 0.41 |
| 1:LA:2828:U:C2 | 1:LA:2829:G:C8 | 3.09 | 0.41 |
| 1:LA:3349:C:HO2' | 1:LA:3350:U:P | 2.42 | 0.41 |
| 3:LC:121:U:H2' | 3:LC:122:U:H6 | 1.86 | 0.41 |
| 5:LE:377:HIS:C | 5:LE:377:HIS:ND1 | 2.78 | 0.41 |
| 6:LF:104:LYS:HD2 | 6:LF:106:TRP:CH2 | 2.56 | 0.41 |
| 7:LG:127:GLY:O | 7:LG:195:LEU:HD23 | 2.20 | 0.41 |
| 12:LL:46:PHE:HB2 | 12:LL:139:ARG:HD2 | 2.03 | 0.41 |
| 14:LN:137:GLN:O | 14:LN:137:GLN:HG3 | 2.21 | 0.41 |
| 31:Le:25:LEU:CD2 | 31:Le:81:VAL:HG11 | 2.48 | 0.41 |
| 33:Lg:111:ARG:HH21 | 33:Lg:115:LEU:HD21 | 1.86 | 0.41 |
| 34:Lh:20:LYS:HE3 | 34:Lh:20:LYS:HB2 | 1.67 | 0.41 |
| 35:Li:67:LYS:HA | 35:Li:70:LYS:HE3 | 2.02 | 0.41 |
| 37:Lk:9:ILE:HD12 | 37:Lk:10:GLY:H | 1.85 | 0.41 |
| 39:Lm:7:ASP:CG | 39:Lm:9:LYS:NZ | 2.79 | 0.41 |
| 44:Lr:14:TYR:CE2 | 44:Lr:26:VAL:HG11 | 2.56 | 0.41 |
| 45:S2:37:U:H2' | 45:S2:38:C:C6 | 2.56 | 0.41 |
| 45:S2:327:U:O2' | 69:SX:10:GLU:HG2 | 2.20 | 0.41 |
| 45:S2:476:U:OP1 | 78:Sg:33:ARG:NH2 | 2.53 | 0.41 |
| 45:S2:1085:G:H2' | 45:S2:1087:A:OP2 | 2.21 | 0.41 |
| 45:S2:1389:C:O2 | 45:S2:1390:U:H4' | 2.21 | 0.41 |
| 45:S2:1504:G:H2' | 45:S2:1505:A:N3 | 2.36 | 0.41 |
| 45:S2:1729:C:H1' | 67:SV:2:GLY:HA3 | 2.03 | 0.41 |
| 47:SB:162:VAL:HG12 | 57:SL:44:VAL:HG22 | 2.03 | 0.41 |
| 60:SO:7:LEU:HD12 | 60:SO:313:TRP:HB3 | 2.02 | 0.41 |
| 62:SQ:194:ASN:ND2 | 62:SQ:211:HIS:HA | 2.36 | 0.41 |
| 64:SS:181:VAL:HG22 | 64:SS:193:GLY:HA3 | 2.02 | 0.41 |
| 64:SS:198:LYS:CB | 64:SS:208:VAL:HG12 | 2.51 | 0.41 |
| 68:SW:125:ALA:O | 68:SW:126:ARG:C | 2.64 | 0.41 |
| 74:Sc:131:SER:OG | 74:Sc:133:LEU:HD23 | 2.20 | 0.41 |
| 77:Sf:21:LEU:HA | 77:Sf:26:GLN:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:Sf:79:PHE:CD1 | 77:Sf:79:PHE:C | 2.99 | 0.41 |
| 80:Tb:23:G:H2' | 80:Tb:24:C:C5 | 2.55 | 0.41 |
| 1:LA:8:C:H2' | 1:LA:9:U:C6 | 2.56 | 0.40 |
| 1:LA:27:C:H42 | 1:LA:57:A:N6 | 2.20 | 0.40 |
| 1:LA:47:C:H5'' | 14:LN:16:LYS:HG2 | 2.03 | 0.40 |
| 1:LA:123:A:H5' | 1:LA:124:U:OP2 | 2.21 | 0.40 |
| 1:LA:345:G:O2' | 3:LC:25:G:N3 | 2.52 | 0.40 |
| 1:LA:1383:U:O5' | 6:LF:202:ARG:HD3 | 2.20 | 0.40 |
| 1:LA:1500:U:O2' | 1:LA:1501:C:O5' | 2.35 | 0.40 |
| 1:LA:2282:G:H1' | 1:LA:2284:C:N4 | 2.36 | 0.40 |
| 1:LA:2562:G:C4 | 1:LA:2563:G:C8 | 3.09 | 0.40 |
| 1:LA:3066:C:H3' | 20:LT:62:ARG:HH22 | 1.87 | 0.40 |
| 1:LA:3312:U:OP1 | 5:LE:117:ARG:NH2 | 2.52 | 0.40 |
| 4:LD:46:LYS:HA | 4:LD:46:LYS:HD2 | 1.71 | 0.40 |
| 5:LE:256:HIS:HA | 5:LE:257:PRO:C | 2.46 | 0.40 |
| 18:LR:94:LEU:HB3 | 18:LR:148:LEU:HD21 | 2.02 | 0.40 |
| 22:LV:84:TYR:HE1 | 30:Ld:21:ILE:HG22 | 1.85 | 0.40 |
| 23:LW:100:THR:O | 23:LW:102:GLU:HG2 | 2.21 | 0.40 |
| 29:Lc:114:GLY:O | 29:Lc:137:LYS:NZ | 2.52 | 0.40 |
| 35:Li:58:ARG:HA | 35:Li:58:ARG:HD2 | 1.74 | 0.40 |
| 41:Lo:111:ARG:HG3 | 41:Lo:112:LYS:HD2 | 2.03 | 0.40 |
| 45:S2:97:C:H2' | 45:S2:98:U:H6 | 1.85 | 0.40 |
| 45:S2:1273:G:H4' | 45:S2:1274:C:H5'' | 2.03 | 0.40 |
| 45:S2:1565:C:OP2 | 53:SH:41:ARG:HG3 | 2.21 | 0.40 |
| 45:S2:1678:A:H8 | 45:S2:1678:A:OP2 | 2.04 | 0.40 |
| 53:SH:29:VAL:HG13 | 53:SH:30:TYR:CD2 | 2.56 | 0.40 |
| 65:ST:147:LEU:HD23 | 65:ST:147:LEU:H | 1.85 | 0.40 |
| 68:SW:89:ASP:OD1 | 68:SW:89:ASP:N | 2.51 | 0.40 |
| 72:Sa:4:ASP:N | 72:Sa:4:ASP:OD1 | 2.53 | 0.40 |
| 75:Sd:18:LEU:HD23 | 75:Sd:18:LEU:HA | 1.79 | 0.40 |
| 76:Se:52:ASP:O | 76:Se:55:GLU:HG3 | 2.21 | 0.40 |
| 1:LA:764:C:H41 | 14:LN:176:GLU:CD | 2.29 | 0.40 |
| 1:LA:967:G:H21 | 30:Ld:15:LYS:NZ | 2.19 | 0.40 |
| 1:LA:2390:G:H2' | 1:LA:2391:C:O4' | 2.21 | 0.40 |
| 1:LA:3168:U:OP2 | 34:Lh:56:SER:OG | 2.32 | 0.40 |
| 3:LC:18:U:H2' | 3:LC:19:C:C6 | 2.56 | 0.40 |
| 6:LF:27:SER:O | 6:LF:279:HIS:NE2 | 2.49 | 0.40 |
| 14:LN:165:SER:C | 14:LN:167:PHE:H | 2.28 | 0.40 |
| 16:LP:98:LEU:HD12 | 16:LP:128:LYS:HD2 | 2.03 | 0.40 |
| 21:LU:94:ILE:HD11 | 21:LU:102:ALA:CB | 2.51 | 0.40 |
| 22:LV:6:GLY:H | 22:LV:9:SER:HB2 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:LX:125:LEU:HB3 | 24:LX:126:TRP:CD1 | 2.57 | 0.40 |
| 45:S2:607:G:H21 | 45:S2:614:C:H5'' | 1.87 | 0.40 |
| 45:S2:636:A:H5'' | 73:Sb:31:SER:HB2 | 2.04 | 0.40 |
| 45:S2:640:U:N3 | 66:SU:118:LEU:HD21 | 2.35 | 0.40 |
| 45:S2:767:U:H2' | 68:SW:143:ILE:HD13 | 2.04 | 0.40 |
| 45:S2:1291:G:C8 | 45:S2:1292:G:C8 | 3.10 | 0.40 |
| 45:S2:1691:A:C8 | 45:S2:1692:G:N7 | 2.89 | 0.40 |
| 60:SO:169:ILE:CD1 | 60:SO:181:TRP:CE3 | 2.98 | 0.40 |
| 62:SQ:138:PHE:O | 62:SQ:213:ARG:N | 2.54 | 0.40 |
| 62:SQ:160:HIS:O | 62:SQ:164:ILE:HG12 | 2.20 | 0.40 |
| 64:SS:136:VAL:HG11 | 64:SS:148:ARG:HE | 1.85 | 0.40 |
| 68:SW:136:VAL:HA | 68:SW:156:ILE:HD13 | 2.03 | 0.40 |
| 76:Se:7:SER:HB2 | 76:Se:10:ARG:O | 2.22 | 0.40 |
| 76:Se:82:ARG:HH11 | 76:Se:82:ARG:HG2 | 1.86 | 0.40 |
| 1:LA:181:U:C5 | 1:LA:182:U:H1' | 2.56 | 0.40 |
| 1:LA:354:U:C5 | 1:LA:365:A:N7 | 2.89 | 0.40 |
| 1:LA:630:U:H2' | 1:LA:631:G:H8 | 1.87 | 0.40 |
| 1:LA:972:A:H2' | 1:LA:973:G:O4' | 2.21 | 0.40 |
| 1:LA:2383:A:N1 | 17:LQ:96[A]:LYS:HE2 | 2.37 | 0.40 |
| 1:LA:2429:A:H2' | 1:LA:2430:C:C6 | 2.57 | 0.40 |
| 1:LA:2939:A:OP2 | 5:LE:2:SER:N | 2.54 | 0.40 |
| 1:LA:2980:U:OP2 | 5:LE:244:ARG:NH1 | 2.49 | 0.40 |
| 1:LA:2986:A:O2' | 5:LE:259:HIS:HB3 | 2.21 | 0.40 |
| 1:LA:3332:G:N2 | 1:LA:3368:G:O2' | 2.53 | 0.40 |
| 2:LB:28:C:OP1 | 13:LM:137:ARG:NE | 2.44 | 0.40 |
| 11:LK:50:ASN:O | 11:LK:50:ASN:ND2 | 2.48 | 0.40 |
| 12:LL:150:GLU:OE2 | 12:LL:150:GLU:HA | 2.22 | 0.40 |
| 13:LM:93:ASP:N | 13:LM:93:ASP:OD1 | 2.54 | 0.40 |
| 14:LN:106:GLN:HB3 | 37:Lk:18:THR:OG1 | 2.22 | 0.40 |
| 16:LP:47:LYS:HD2 | 16:LP:47:LYS:HA | 1.81 | 0.40 |
| 22:LV:44:ALA:HB2 | 22:LV:53:PRO:HG2 | 2.02 | 0.40 |
| 37:Lk:21:THR:HG23 | 37:Lk:21:THR:O | 2.22 | 0.40 |
| 44:Lr:89:MET:HE2 | 44:Lr:89:MET:HB3 | 1.78 | 0.40 |
| 45:S2:393:C:H2' | 45:S2:394:C:H6 | 1.86 | 0.40 |
| 45:S2:590:C:OP2 | 78:Sg:35:TYR:OH | 2.39 | 0.40 |
| 45:S2:1173:C:H2' | 45:S2:1174:C:H6 | 1.87 | 0.40 |
| 45:S2:1631:A:H8 | 45:S2:1631:A:OP1 | 2.04 | 0.40 |
| 45:S2:1741:U:O2 | 45:S2:1741:U:H2' | 2.20 | 0.40 |
| 47:SB:162:VAL:HG13 | 57:SL:54:LEU:CD1 | 2.46 | 0.40 |
| 48:SC:20:VAL:HG12 | 48:SC:67:THR:HA | 2.03 | 0.40 |
| 51:SF:128:LYS:HE2 | 51:SF:128:LYS:HB2 | 1.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------------|--------------------------|-------------------|
| 53:SH:110:ARG:CZ | 53:SH:110:ARG:HB3 | 2.51 | 0.40 |
| 56:SK:50:ILE:HG13 | 56:SK:51:LEU:N | 2.35 | 0.40 |
| 61:SP:127:ARG:NH1 | 61:SP:150:ASP:O | 2.51 | 0.40 |
| 62:SQ:210:ILE:N | 62:SQ:210:ILE:CD1 | 2.84 | 0.40 |
| 66:SU:123:ASP:O | 66:SU:127:GLU:OE2 | 2.39 | 0.40 |
| 69:SX:46:LYS:H | 69:SX:46:LYS:HG2 | 1.67 | 0.40 |
| 1:LA:619:U:H4' | 18:LR:167:ARG:NE | 2.37 | 0.40 |
| 1:LA:686:U:H5 | 14:LN:36:ARG:CZ | 2.35 | 0.40 |
| 1:LA:920:A:C6 | 38:Ll:8:PHE:HE2 | 2.39 | 0.40 |
| 1:LA:970:G:H2' | 1:LA:971:A:C8 | 2.56 | 0.40 |
| 1:LA:1126:G:N2 | 1:LA:1128:A:H3' | 2.36 | 0.40 |
| 1:LA:1285:A:H4' | 1:LA:1286:A:H5' | 2.03 | 0.40 |
| 1:LA:1596:C:H2' | 1:LA:1597:G:H8 | 1.85 | 0.40 |
| 1:LA:1919:U:O2' | 1:LA:1931:A:N7 | 2.45 | 0.40 |
| 1:LA:2200:G:H2' | 1:LA:2201:C:H6 | 1.86 | 0.40 |
| 1:LA:2800:A:O2' | 1:LA:2801:A:H3' | 2.22 | 0.40 |
| 1:LA:2889:A:O2' | 1:LA:2932:A:N3 | 2.51 | 0.40 |
| 1:LA:2986:A:OP1 | 17:LQ:68[A]:ARG:NH2 | 2.48 | 0.40 |
| 1:LA:3372:U:H5'' | 32:Lf:69:TYR:CD2 | 2.56 | 0.40 |
| 6:LF:11:LEU:HD23 | 6:LF:11:LEU:HA | 1.69 | 0.40 |
| 9:LI:96:PRO:O | 9:LI:100:ARG:HB2 | 2.21 | 0.40 |
| 10:LJ:78:PHE:C | 10:LJ:80:TYR:N | 2.79 | 0.40 |
| 10:LJ:151:VAL:HG11 | 10:LJ:170:CYS:SG | 2.62 | 0.40 |
| 11:LK:128:VAL:HA | 11:LK:157:ASN:OD1 | 2.22 | 0.40 |
| 11:LK:173:ARG:HE | 11:LK:173:ARG:HB2 | 1.80 | 0.40 |
| 14:LN:46:ILE:HD11 | 14:LN:51:LEU:HA | 2.04 | 0.40 |
| 14:LN:119:TYR:CZ | 14:LN:123:ILE:HG21 | 2.56 | 0.40 |
| 17:LQ:37[A]:ARG:CG | 17:LQ:108[A]:ILE:HD11 | 2.51 | 0.40 |
| 18:LR:67:ILE:HD11 | 18:LR:80:LYS:HB3 | 2.03 | 0.40 |
| 19:LS:19:PRO:HD3 | 19:LS:53:PHE:HD1 | 1.85 | 0.40 |
| 20:LT:74:ARG:HB2 | 20:LT:75:HIS:CD2 | 2.56 | 0.40 |
| 29:Lc:135:GLU:O | 29:Lc:139:ARG:HG2 | 2.21 | 0.40 |
| 41:Lo:78:ILE:H | 41:Lo:83:LYS:HZ2 | 1.68 | 0.40 |
| 45:S2:57:G:OP1 | 75:Sd:112:LYS:NZ | 2.31 | 0.40 |
| 45:S2:473:A:OP1 | 68:SW:44:ARG:HD3 | 2.21 | 0.40 |
| 45:S2:1141:G:O6 | 45:S2:1142:A:N6 | 2.54 | 0.40 |
| 45:S2:1639:C:H2' | 45:S2:1640:C:O4' | 2.21 | 0.40 |
| 45:S2:1705:C:H6 | 45:S2:1705:C:H2' | 1.71 | 0.40 |
| 46:SA:32:GLU:HA | 46:SA:54:ARG:HD3 | 2.04 | 0.40 |
| 48:SC:44:LYS:HA | 48:SC:44:LYS:HD2 | 1.76 | 0.40 |
| 50:SE:74:ALA:HA | 50:SE:75:PRO:HD3 | 1.93 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:SE:110:GLU:HB2 | 53:SH:119:ILE:CD1 | 2.52 | 0.40 |
| 62:SQ:187:LYS:C | 62:SQ:190:PRO:HD2 | 2.47 | 0.40 |
| 65:ST:208:TYR:CZ | 65:ST:212:LEU:HD21 | 2.57 | 0.40 |
| 71:SZ:72:LYS:NZ | 71:SZ:77:THR:CA | 2.81 | 0.40 |
| 1:LA:107:A:H2' | 1:LA:108:A:O4' | 2.22 | 0.40 |
| 1:LA:213:A:O4' | 27:La:2:ALA:HA | 2.22 | 0.40 |
| 1:LA:1339:G:H2' | 1:LA:1340:U:H6 | 1.85 | 0.40 |
| 1:LA:1385:A:H5'' | 6:LF:141:ARG:NH2 | 2.36 | 0.40 |
| 1:LA:1592:A:O5' | 35:Li:60:ARG:HD3 | 2.20 | 0.40 |
| 1:LA:2145:C:H5'' | 4:LD:203:ALA:HB1 | 2.02 | 0.40 |
| 1:LA:2147:U:H2' | 1:LA:2148:A:C8 | 2.56 | 0.40 |
| 1:LA:2415:U:H2' | 1:LA:2416:U:C6 | 2.56 | 0.40 |
| 1:LA:2512:U:H4' | 10:LJ:238:LEU:CD1 | 2.51 | 0.40 |
| 1:LA:3049:U:H4' | 25:LY:17:ARG:HD3 | 2.02 | 0.40 |
| 1:LA:3170:U:C4 | 34:Lh:54:ARG:HD3 | 2.57 | 0.40 |
| 4:LD:104:LEU:HD22 | 4:LD:136:ILE:HD11 | 2.03 | 0.40 |
| 4:LD:155:LYS:HA | 4:LD:155:LYS:HD3 | 1.76 | 0.40 |
| 10:LJ:152:LEU:HG | 10:LJ:180:VAL:HG11 | 2.04 | 0.40 |
| 18:LR:51:VAL:HA | 18:LR:56:ARG:O | 2.21 | 0.40 |
| 20:LT:21:LYS:HD3 | 20:LT:21:LYS:HA | 1.87 | 0.40 |
| 26:LZ:127:THR:HG22 | 26:LZ:128:ALA:H | 1.87 | 0.40 |
| 45:S2:91:G:H2' | 45:S2:92:A:O4' | 2.21 | 0.40 |
| 45:S2:1215:C:H2' | 45:S2:1216:C:H6 | 1.87 | 0.40 |
| 45:S2:1478:G:OP1 | 54:SI:39:THR:OG1 | 2.28 | 0.40 |
| 45:S2:1527:C:O2 | 51:SF:74:HIS:NE2 | 2.47 | 0.40 |
| 45:S2:1553:G:N1 | 45:S2:1556:A:OP2 | 2.54 | 0.40 |
| 47:SB:105:GLY:C | 47:SB:106:LYS:HG2 | 2.47 | 0.40 |
| 47:SB:177:ILE:HD12 | 47:SB:178:GLY:H | 1.87 | 0.40 |
| 53:SH:30:TYR:HA | 53:SH:33:THR:HG23 | 2.04 | 0.40 |
| 60:SO:132:LYS:HG3 | 60:SO:133:VAL:N | 2.36 | 0.40 |
| 61:SP:30:GLN:NE2 | 61:SP:149:LEU:HB3 | 2.36 | 0.40 |
| 61:SP:74:VAL:O | 61:SP:121:VAL:HA | 2.21 | 0.40 |
| 62:SQ:105:PHE:CE1 | 62:SQ:109:LYS:CG | 2.96 | 0.40 |
| 66:SU:27:LEU:HD22 | 66:SU:27:LEU:HA | 1.91 | 0.40 |
| 74:Sc:127:VAL:O | 74:Sc:130:VAL:HG12 | 2.22 | 0.40 |
| 75:Sd:31:ASN:C | 75:Sd:32:ARG:HG2 | 2.46 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 4 | LD | 249/251 (99%) | 236 (95%) | 13 (5%) | 0 | 100 | 100 |
| 5 | LE | 384/386 (100%) | 356 (93%) | 28 (7%) | 0 | 100 | 100 |
| 6 | LF | 359/361 (99%) | 333 (93%) | 26 (7%) | 0 | 100 | 100 |
| 7 | LG | 292/294 (99%) | 275 (94%) | 17 (6%) | 0 | 100 | 100 |
| 8 | LH | 163/175 (93%) | 154 (94%) | 9 (6%) | 0 | 100 | 100 |
| 9 | LI | 220/222 (99%) | 210 (96%) | 10 (4%) | 0 | 100 | 100 |
| 10 | LJ | 231/233 (99%) | 217 (94%) | 14 (6%) | 0 | 100 | 100 |
| 11 | LK | 189/191 (99%) | 176 (93%) | 13 (7%) | 0 | 100 | 100 |
| 12 | LL | 216/218 (99%) | 208 (96%) | 8 (4%) | 0 | 100 | 100 |
| 13 | LM | 167/169 (99%) | 158 (95%) | 9 (5%) | 0 | 100 | 100 |
| 14 | LN | 191/193 (99%) | 174 (91%) | 17 (9%) | 0 | 100 | 100 |
| 15 | LO | 134/136 (98%) | 128 (96%) | 6 (4%) | 0 | 100 | 100 |
| 16 | LP | 201/203 (99%) | 188 (94%) | 11 (6%) | 2 (1%) | 13 | 29 |
| 17 | LQ | 195/197 (99%) | 193 (99%) | 2 (1%) | 0 | 100 | 100 |
| 18 | LR | 181/183 (99%) | 172 (95%) | 9 (5%) | 0 | 100 | 100 |
| 19 | LS | 183/185 (99%) | 174 (95%) | 9 (5%) | 0 | 100 | 100 |
| 20 | LT | 186/188 (99%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 21 | LU | 169/171 (99%) | 162 (96%) | 7 (4%) | 0 | 100 | 100 |
| 22 | LV | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 23 | LW | 98/100 (98%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 24 | LX | 134/136 (98%) | 131 (98%) | 3 (2%) | 0 | 100 | 100 |
| 25 | LY | 63/65 (97%) | 61 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | LZ | 119/121 (98%) | 117 (98%) | 2 (2%) | 0 | 100 | 100 |
| 27 | La | 123/125 (98%) | 118 (96%) | 5 (4%) | 0 | 100 | 100 |
| 28 | Lb | 133/135 (98%) | 122 (92%) | 11 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 29 | Lc | 146/148 (99%) | 136 (93%) | 10 (7%) | 0 | 100 | 100 |
| 30 | Ld | 56/58 (97%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 31 | Le | 94/96 (98%) | 94 (100%) | 0 | 0 | 100 | 100 |
| 32 | Lf | 107/109 (98%) | 103 (96%) | 4 (4%) | 0 | 100 | 100 |
| 33 | Lg | 125/127 (98%) | 119 (95%) | 6 (5%) | 0 | 100 | 100 |
| 34 | Lh | 104/106 (98%) | 99 (95%) | 5 (5%) | 0 | 100 | 100 |
| 35 | Li | 110/112 (98%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 36 | Lj | 117/119 (98%) | 110 (94%) | 7 (6%) | 0 | 100 | 100 |
| 37 | Lk | 97/99 (98%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 38 | Ll | 79/81 (98%) | 77 (98%) | 2 (2%) | 0 | 100 | 100 |
| 39 | Lm | 75/77 (97%) | 73 (97%) | 2 (3%) | 0 | 100 | 100 |
| 40 | Ln | 48/50 (96%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 41 | Lo | 50/52 (96%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 42 | Lp | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 43 | Lq | 101/103 (98%) | 95 (94%) | 6 (6%) | 0 | 100 | 100 |
| 44 | Lr | 89/91 (98%) | 84 (94%) | 5 (6%) | 0 | 100 | 100 |
| 46 | SA | 220/223 (99%) | 211 (96%) | 9 (4%) | 0 | 100 | 100 |
| 47 | SB | 204/206 (99%) | 191 (94%) | 12 (6%) | 1 (0%) | 25 | 47 |
| 48 | SC | 90/92 (98%) | 81 (90%) | 9 (10%) | 0 | 100 | 100 |
| 49 | SD | 119/124 (96%) | 90 (76%) | 29 (24%) | 0 | 100 | 100 |
| 50 | SE | 115/117 (98%) | 112 (97%) | 3 (3%) | 0 | 100 | 100 |
| 51 | SF | 139/141 (99%) | 129 (93%) | 10 (7%) | 0 | 100 | 100 |
| 52 | SG | 117/125 (94%) | 117 (100%) | 0 | 0 | 100 | 100 |
| 53 | SH | 143/145 (99%) | 137 (96%) | 6 (4%) | 0 | 100 | 100 |
| 54 | SI | 141/143 (99%) | 131 (93%) | 10 (7%) | 0 | 100 | 100 |
| 55 | SJ | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 56 | SK | 80/82 (98%) | 72 (90%) | 8 (10%) | 0 | 100 | 100 |
| 57 | SL | 61/63 (97%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 58 | SM | 51/53 (96%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 59 | SN | 71/73 (97%) | 56 (79%) | 15 (21%) | 0 | 100 | 100 |
| 60 | SO | 310/312 (99%) | 283 (91%) | 27 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 61 | SP | 204/206 (99%) | 185 (91%) | 19 (9%) | 0 | 100 | 100 |
| 62 | SQ | 222/232 (96%) | 201 (90%) | 21 (10%) | 0 | 100 | 100 |
| 63 | SR | 214/217 (99%) | 202 (94%) | 12 (6%) | 0 | 100 | 100 |
| 64 | SS | 256/260 (98%) | 229 (90%) | 27 (10%) | 0 | 100 | 100 |
| 65 | ST | 226/228 (99%) | 213 (94%) | 11 (5%) | 2 (1%) | 14 | 31 |
| 66 | SU | 182/185 (98%) | 169 (93%) | 13 (7%) | 0 | 100 | 100 |
| 67 | SV | 183/199 (92%) | 176 (96%) | 7 (4%) | 0 | 100 | 100 |
| 68 | SW | 182/185 (98%) | 172 (94%) | 10 (6%) | 0 | 100 | 100 |
| 69 | SX | 140/146 (96%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 70 | SY | 148/150 (99%) | 136 (92%) | 12 (8%) | 0 | 100 | 100 |
| 71 | SZ | 125/128 (98%) | 114 (91%) | 11 (9%) | 0 | 100 | 100 |
| 72 | Sa | 85/87 (98%) | 77 (91%) | 8 (9%) | 0 | 100 | 100 |
| 73 | Sb | 127/129 (98%) | 115 (91%) | 12 (9%) | 0 | 100 | 100 |
| 74 | Sc | 142/144 (99%) | 126 (89%) | 16 (11%) | 0 | 100 | 100 |
| 75 | Sd | 132/134 (98%) | 129 (98%) | 3 (2%) | 0 | 100 | 100 |
| 76 | Se | 95/97 (98%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 77 | Sf | 79/81 (98%) | 75 (95%) | 4 (5%) | 0 | 100 | 100 |
| 78 | Sg | 55/57 (96%) | 47 (86%) | 8 (14%) | 0 | 100 | 100 |
| All | All | 10914/11115 (98%) | 10242 (94%) | 667 (6%) | 5 (0%) | 100 | 100 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65 | ST | 177 | ARG |
| 65 | ST | 175 | ILE |
| 47 | SB | 162 | VAL |
| 16 | LP | 78 | GLY |
| 16 | LP | 76 | PRO |

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4 | LD | 190/193 (98%) | 187 (98%) | 3 (2%) | 58 | 79 |
| 5 | LE | 318/322 (99%) | 300 (94%) | 18 (6%) | 17 | 37 |
| 6 | LF | 288/288 (100%) | 275 (96%) | 13 (4%) | 23 | 47 |
| 7 | LG | 241/243 (99%) | 227 (94%) | 14 (6%) | 17 | 36 |
| 8 | LH | 139/154 (90%) | 135 (97%) | 4 (3%) | 37 | 64 |
| 9 | LI | 186/186 (100%) | 178 (96%) | 8 (4%) | 25 | 49 |
| 10 | LJ | 187/191 (98%) | 173 (92%) | 14 (8%) | 11 | 24 |
| 11 | LK | 168/171 (98%) | 160 (95%) | 8 (5%) | 21 | 44 |
| 12 | LL | 185/185 (100%) | 177 (96%) | 8 (4%) | 25 | 49 |
| 13 | LM | 145/147 (99%) | 139 (96%) | 6 (4%) | 26 | 51 |
| 14 | LN | 154/154 (100%) | 146 (95%) | 8 (5%) | 19 | 41 |
| 15 | LO | 107/107 (100%) | 97 (91%) | 10 (9%) | 7 | 15 |
| 16 | LP | 175/175 (100%) | 170 (97%) | 5 (3%) | 37 | 64 |
| 17 | LQ | 160/160 (100%) | 154 (96%) | 6 (4%) | 28 | 54 |
| 18 | LR | 138/145 (95%) | 134 (97%) | 4 (3%) | 37 | 64 |
| 19 | LS | 150/150 (100%) | 145 (97%) | 5 (3%) | 33 | 59 |
| 20 | LT | 152/153 (99%) | 146 (96%) | 6 (4%) | 27 | 53 |
| 21 | LU | 155/155 (100%) | 145 (94%) | 10 (6%) | 14 | 31 |
| 22 | LV | 135/136 (99%) | 129 (96%) | 6 (4%) | 24 | 48 |
| 23 | LW | 87/87 (100%) | 81 (93%) | 6 (7%) | 13 | 28 |
| 24 | LX | 104/104 (100%) | 97 (93%) | 7 (7%) | 13 | 29 |
| 25 | LY | 54/57 (95%) | 51 (94%) | 3 (6%) | 17 | 38 |
| 26 | LZ | 104/105 (99%) | 97 (93%) | 7 (7%) | 13 | 29 |
| 27 | La | 108/108 (100%) | 105 (97%) | 3 (3%) | 38 | 65 |
| 28 | Lb | 112/115 (97%) | 106 (95%) | 6 (5%) | 18 | 39 |
| 29 | Lc | 117/118 (99%) | 114 (97%) | 3 (3%) | 41 | 67 |
| 30 | Ld | 46/46 (100%) | 45 (98%) | 1 (2%) | 47 | 72 |
| 31 | Le | 81/81 (100%) | 77 (95%) | 4 (5%) | 21 | 43 |
| 32 | Lf | 92/96 (96%) | 88 (96%) | 4 (4%) | 25 | 49 |
| 33 | Lg | 108/109 (99%) | 105 (97%) | 3 (3%) | 38 | 65 |
| 34 | Lh | 90/90 (100%) | 89 (99%) | 1 (1%) | 70 | 86 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 35 | Li | 95/95 (100%) | 90 (95%) | 5 (5%) | 19 | 40 |
| 36 | Lj | 104/104 (100%) | 104 (100%) | 0 | 100 | 100 |
| 37 | Lk | 80/81 (99%) | 77 (96%) | 3 (4%) | 28 | 54 |
| 38 | Ll | 67/67 (100%) | 64 (96%) | 3 (4%) | 23 | 47 |
| 39 | Lm | 68/68 (100%) | 64 (94%) | 4 (6%) | 16 | 35 |
| 40 | Ln | 45/45 (100%) | 42 (93%) | 3 (7%) | 13 | 29 |
| 41 | Lo | 45/47 (96%) | 44 (98%) | 1 (2%) | 47 | 72 |
| 42 | Lp | 22/23 (96%) | 21 (96%) | 1 (4%) | 23 | 47 |
| 43 | Lq | 87/88 (99%) | 84 (97%) | 3 (3%) | 32 | 58 |
| 44 | Lr | 71/71 (100%) | 70 (99%) | 1 (1%) | 62 | 82 |
| 46 | SA | 182/182 (100%) | 170 (93%) | 12 (7%) | 14 | 30 |
| 47 | SB | 172/173 (99%) | 169 (98%) | 3 (2%) | 56 | 78 |
| 48 | SC | 77/85 (91%) | 73 (95%) | 4 (5%) | 19 | 41 |
| 49 | SD | 88/100 (88%) | 82 (93%) | 6 (7%) | 13 | 28 |
| 50 | SE | 95/98 (97%) | 91 (96%) | 4 (4%) | 25 | 50 |
| 51 | SF | 117/117 (100%) | 109 (93%) | 8 (7%) | 13 | 28 |
| 52 | SG | 101/113 (89%) | 96 (95%) | 5 (5%) | 20 | 43 |
| 53 | SH | 127/128 (99%) | 123 (97%) | 4 (3%) | 35 | 62 |
| 54 | SI | 115/115 (100%) | 111 (96%) | 4 (4%) | 31 | 57 |
| 55 | SJ | 93/94 (99%) | 89 (96%) | 4 (4%) | 25 | 49 |
| 56 | SK | 67/73 (92%) | 67 (100%) | 0 | 100 | 100 |
| 57 | SL | 55/56 (98%) | 51 (93%) | 4 (7%) | 11 | 25 |
| 58 | SM | 47/47 (100%) | 46 (98%) | 1 (2%) | 48 | 73 |
| 59 | SN | 56/64 (88%) | 55 (98%) | 1 (2%) | 54 | 77 |
| 60 | SO | 250/257 (97%) | 243 (97%) | 7 (3%) | 38 | 65 |
| 61 | SP | 170/173 (98%) | 163 (96%) | 7 (4%) | 26 | 51 |
| 62 | SQ | 200/205 (98%) | 190 (95%) | 10 (5%) | 20 | 43 |
| 63 | SR | 175/176 (99%) | 166 (95%) | 9 (5%) | 20 | 42 |
| 64 | SS | 220/221 (100%) | 206 (94%) | 14 (6%) | 14 | 32 |
| 65 | ST | 189/195 (97%) | 176 (93%) | 13 (7%) | 13 | 28 |
| 66 | SU | 163/165 (99%) | 158 (97%) | 5 (3%) | 35 | 62 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 67 | SV | 148/160 (92%) | 145 (98%) | 3 (2%) | 50 | 74 |
| 68 | SW | 156/158 (99%) | 145 (93%) | 11 (7%) | 12 | 26 |
| 69 | SX | 126/129 (98%) | 122 (97%) | 4 (3%) | 34 | 60 |
| 70 | SY | 127/127 (100%) | 119 (94%) | 8 (6%) | 15 | 32 |
| 71 | SZ | 90/97 (93%) | 87 (97%) | 3 (3%) | 33 | 59 |
| 72 | Sa | 71/74 (96%) | 66 (93%) | 5 (7%) | 12 | 27 |
| 73 | Sb | 110/110 (100%) | 109 (99%) | 1 (1%) | 75 | 90 |
| 74 | Sc | 119/119 (100%) | 116 (98%) | 3 (2%) | 42 | 68 |
| 75 | Sd | 102/112 (91%) | 94 (92%) | 8 (8%) | 10 | 22 |
| 76 | Se | 82/83 (99%) | 81 (99%) | 1 (1%) | 67 | 85 |
| 77 | Sf | 70/70 (100%) | 64 (91%) | 6 (9%) | 8 | 18 |
| 78 | Sg | 48/49 (98%) | 47 (98%) | 1 (2%) | 48 | 73 |
| All | All | 9168/9345 (98%) | 8761 (96%) | 407 (4%) | 26 | 48 |

All (407) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | LD | 96 | LEU |
| 4 | LD | 113 | VAL |
| 4 | LD | 130 | SER |
| 5 | LE | 25 | ILE |
| 5 | LE | 44 | THR |
| 5 | LE | 56 | ILE |
| 5 | LE | 102 | LEU |
| 5 | LE | 104 | THR |
| 5 | LE | 112 | ASP |
| 5 | LE | 114 | VAL |
| 5 | LE | 125 | SER |
| 5 | LE | 140 | ASP |
| 5 | LE | 148 | LEU |
| 5 | LE | 158 | VAL |
| 5 | LE | 189 | SER |
| 5 | LE | 208 | VAL |
| 5 | LE | 296 | THR |
| 5 | LE | 324 | VAL |
| 5 | LE | 344 | THR |
| 5 | LE | 346 | THR |
| 5 | LE | 369 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | LF | 11 | LEU |
| 6 | LF | 116 | ASN |
| 6 | LF | 159 | ILE |
| 6 | LF | 169 | LEU |
| 6 | LF | 170 | LYS |
| 6 | LF | 172 | VAL |
| 6 | LF | 182 | LEU |
| 6 | LF | 219 | LEU |
| 6 | LF | 230 | VAL |
| 6 | LF | 265 | GLU |
| 6 | LF | 280 | ILE |
| 6 | LF | 333 | VAL |
| 6 | LF | 349 | THR |
| 7 | LG | 46 | THR |
| 7 | LG | 56 | THR |
| 7 | LG | 80 | SER |
| 7 | LG | 109 | THR |
| 7 | LG | 125 | VAL |
| 7 | LG | 144 | VAL |
| 7 | LG | 163 | LEU |
| 7 | LG | 173 | VAL |
| 7 | LG | 187 | THR |
| 7 | LG | 197 | SER |
| 7 | LG | 199 | ILE |
| 7 | LG | 208 | MET |
| 7 | LG | 242 | SER |
| 7 | LG | 262 | LYS |
| 8 | LH | 91 | VAL |
| 8 | LH | 96 | VAL |
| 8 | LH | 98 | VAL |
| 8 | LH | 141 | VAL |
| 9 | LI | 57 | THR |
| 9 | LI | 83 | LEU |
| 9 | LI | 123 | THR |
| 9 | LI | 124 | LEU |
| 9 | LI | 142 | SER |
| 9 | LI | 161 | VAL |
| 9 | LI | 189 | ILE |
| 9 | LI | 232 | ARG |
| 10 | LJ | 71 | VAL |
| 10 | LJ | 74 | THR |
| 10 | LJ | 90 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | LJ | 95 | ASN |
| 10 | LJ | 101 | THR |
| 10 | LJ | 104 | GLU |
| 10 | LJ | 132 | VAL |
| 10 | LJ | 158 | ASP |
| 10 | LJ | 175 | VAL |
| 10 | LJ | 192 | GLN |
| 10 | LJ | 197 | VAL |
| 10 | LJ | 203 | VAL |
| 10 | LJ | 214 | LEU |
| 10 | LJ | 229 | VAL |
| 11 | LK | 18 | VAL |
| 11 | LK | 78 | MET |
| 11 | LK | 82 | VAL |
| 11 | LK | 114 | VAL |
| 11 | LK | 126 | VAL |
| 11 | LK | 133 | THR |
| 11 | LK | 140 | VAL |
| 11 | LK | 157 | ASN |
| 12 | LL | 21 | ARG |
| 12 | LL | 26 | VAL |
| 12 | LL | 80 | SER |
| 12 | LL | 87 | LEU |
| 12 | LL | 123 | HIS |
| 12 | LL | 129 | VAL |
| 12 | LL | 167 | LEU |
| 12 | LL | 176 | LEU |
| 13 | LM | 18 | VAL |
| 13 | LM | 44 | THR |
| 13 | LM | 95 | ASN |
| 13 | LM | 129 | VAL |
| 13 | LM | 155 | THR |
| 13 | LM | 161 | SER |
| 14 | LN | 4 | SER |
| 14 | LN | 24 | VAL |
| 14 | LN | 41 | THR |
| 14 | LN | 63 | VAL |
| 14 | LN | 69 | VAL |
| 14 | LN | 103 | ASN |
| 14 | LN | 138 | VAL |
| 14 | LN | 155 | GLU |
| 15 | LO | 7 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 15 | LO | 15 | VAL |
| 15 | LO | 36 | VAL |
| 15 | LO | 56 | GLN |
| 15 | LO | 90 | VAL |
| 15 | LO | 105 | GLN |
| 15 | LO | 107 | GLU |
| 15 | LO | 120 | VAL |
| 15 | LO | 131 | VAL |
| 15 | LO | 133 | LYS |
| 16 | LP | 19 | LEU |
| 16 | LP | 32 | GLN |
| 16 | LP | 54 | LYS |
| 16 | LP | 60 | VAL |
| 16 | LP | 101 | THR |
| 17 | LQ | 3[A] | VAL |
| 17 | LQ | 136[A] | THR |
| 17 | LQ | 142[A] | SER |
| 17 | LQ | 150[A] | GLU |
| 17 | LQ | 175[A] | THR |
| 17 | LQ | 197[A] | LEU |
| 18 | LR | 16 | SER |
| 18 | LR | 87 | SER |
| 18 | LR | 119 | VAL |
| 18 | LR | 146 | ILE |
| 19 | LS | 9 | GLN |
| 19 | LS | 17 | THR |
| 19 | LS | 24 | VAL |
| 19 | LS | 100 | THR |
| 19 | LS | 129 | VAL |
| 20 | LT | 14 | VAL |
| 20 | LT | 29 | THR |
| 20 | LT | 55 | VAL |
| 20 | LT | 72 | GLU |
| 20 | LT | 119 | LEU |
| 20 | LT | 166 | ASN |
| 21 | LU | 19 | VAL |
| 21 | LU | 32 | SER |
| 21 | LU | 50 | LYS |
| 21 | LU | 55 | SER |
| 21 | LU | 59 | VAL |
| 21 | LU | 79 | VAL |
| 21 | LU | 82 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | LU | 120 | SER |
| 21 | LU | 159 | SER |
| 21 | LU | 162 | THR |
| 22 | LV | 16 | GLN |
| 22 | LV | 25 | VAL |
| 22 | LV | 33 | VAL |
| 22 | LV | 61 | THR |
| 22 | LV | 138 | SER |
| 22 | LV | 149 | GLN |
| 23 | LW | 39 | ASP |
| 23 | LW | 56 | VAL |
| 23 | LW | 66 | VAL |
| 23 | LW | 68 | THR |
| 23 | LW | 87 | ASN |
| 23 | LW | 100 | THR |
| 24 | LX | 57 | MET |
| 24 | LX | 74 | MET |
| 24 | LX | 98 | ASN |
| 24 | LX | 110 | LYS |
| 24 | LX | 112 | SER |
| 24 | LX | 125 | LEU |
| 24 | LX | 137 | VAL |
| 25 | LY | 19 | THR |
| 25 | LY | 26 | SER |
| 25 | LY | 33 | ASN |
| 26 | LZ | 57 | LEU |
| 26 | LZ | 62 | VAL |
| 26 | LZ | 75 | LYS |
| 26 | LZ | 107 | VAL |
| 26 | LZ | 119 | THR |
| 26 | LZ | 129 | ASP |
| 26 | LZ | 142 | ILE |
| 27 | La | 63 | LYS |
| 27 | La | 105 | VAL |
| 27 | La | 119 | ILE |
| 28 | Lb | 55 | LYS |
| 28 | Lb | 57 | HIS |
| 28 | Lb | 66 | THR |
| 28 | Lb | 95 | VAL |
| 28 | Lb | 100 | THR |
| 28 | Lb | 113 | VAL |
| 29 | Lc | 16 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | Lc | 102 | ILE |
| 29 | Lc | 112 | ILE |
| 30 | Ld | 13 | THR |
| 31 | Le | 17 | VAL |
| 31 | Le | 36 | GLN |
| 31 | Le | 40 | LYS |
| 31 | Le | 90 | VAL |
| 32 | Lf | 64 | VAL |
| 32 | Lf | 96 | VAL |
| 32 | Lf | 106 | THR |
| 32 | Lf | 109 | VAL |
| 33 | Lg | 55 | ILE |
| 33 | Lg | 78 | ASN |
| 33 | Lg | 84 | THR |
| 34 | Lh | 37 | THR |
| 35 | Li | 38 | LEU |
| 35 | Li | 66 | SER |
| 35 | Li | 68 | THR |
| 35 | Li | 84 | CYS |
| 35 | Li | 101 | VAL |
| 37 | Lk | 17 | VAL |
| 37 | Lk | 37 | THR |
| 37 | Lk | 57 | LEU |
| 38 | Ll | 36 | SER |
| 38 | Ll | 57 | HIS |
| 38 | Ll | 79 | GLN |
| 39 | Lm | 10 | GLN |
| 39 | Lm | 54 | LEU |
| 39 | Lm | 65 | LEU |
| 39 | Lm | 72 | THR |
| 40 | Ln | 9 | ILE |
| 40 | Ln | 19 | GLN |
| 40 | Ln | 27 | ILE |
| 41 | Lo | 82 | LEU |
| 42 | Lp | 18 | ARG |
| 43 | Lq | 7 | THR |
| 43 | Lq | 10 | THR |
| 43 | Lq | 26 | THR |
| 44 | Lr | 81 | SER |
| 46 | SA | 32 | GLU |
| 46 | SA | 77 | PHE |
| 46 | SA | 85 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | SA | 96 | LEU |
| 46 | SA | 97 | SER |
| 46 | SA | 122 | VAL |
| 46 | SA | 170 | THR |
| 46 | SA | 175 | VAL |
| 46 | SA | 181 | VAL |
| 46 | SA | 190 | ARG |
| 46 | SA | 194 | LYS |
| 46 | SA | 206 | VAL |
| 47 | SB | 64 | VAL |
| 47 | SB | 93 | LEU |
| 47 | SB | 133 | VAL |
| 48 | SC | 40 | LEU |
| 48 | SC | 57 | THR |
| 48 | SC | 59 | PHE |
| 48 | SC | 63 | TYR |
| 49 | SD | 56 | GLU |
| 49 | SD | 84 | ASN |
| 49 | SD | 88 | LEU |
| 49 | SD | 99 | GLU |
| 49 | SD | 116 | VAL |
| 49 | SD | 120 | VAL |
| 50 | SE | 82 | ASN |
| 50 | SE | 86 | VAL |
| 50 | SE | 93 | VAL |
| 50 | SE | 116 | LEU |
| 51 | SF | 4 | VAL |
| 51 | SF | 19 | VAL |
| 51 | SF | 29 | ILE |
| 51 | SF | 52 | LEU |
| 51 | SF | 54 | LEU |
| 51 | SF | 59 | LYS |
| 51 | SF | 90 | VAL |
| 51 | SF | 117 | LEU |
| 52 | SG | 17 | ILE |
| 52 | SG | 61 | ILE |
| 52 | SG | 85 | VAL |
| 52 | SG | 88 | VAL |
| 52 | SG | 113 | LEU |
| 53 | SH | 29 | VAL |
| 53 | SH | 45 | LEU |
| 53 | SH | 91 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | SH | 94 | ASP |
| 54 | SI | 37 | VAL |
| 54 | SI | 43 | ASN |
| 54 | SI | 71 | VAL |
| 54 | SI | 129 | GLN |
| 55 | SJ | 52 | LYS |
| 55 | SJ | 62 | VAL |
| 55 | SJ | 81 | THR |
| 55 | SJ | 103 | ILE |
| 57 | SL | 9 | LEU |
| 57 | SL | 18 | ARG |
| 57 | SL | 40 | ILE |
| 57 | SL | 43 | ASN |
| 58 | SM | 28 | THR |
| 59 | SN | 87 | THR |
| 60 | SO | 17 | ASN |
| 60 | SO | 25 | THR |
| 60 | SO | 82 | SER |
| 60 | SO | 114 | ASP |
| 60 | SO | 122 | ILE |
| 60 | SO | 195 | HIS |
| 60 | SO | 240 | VAL |
| 61 | SP | 8 | ASP |
| 61 | SP | 32 | HIS |
| 61 | SP | 50 | VAL |
| 61 | SP | 56 | LYS |
| 61 | SP | 58 | VAL |
| 61 | SP | 180 | GLU |
| 61 | SP | 183 | ARG |
| 62 | SQ | 32 | ILE |
| 62 | SQ | 48 | VAL |
| 62 | SQ | 61 | LEU |
| 62 | SQ | 65 | VAL |
| 62 | SQ | 91 | VAL |
| 62 | SQ | 97 | LEU |
| 62 | SQ | 106 | THR |
| 62 | SQ | 124 | ASN |
| 62 | SQ | 137 | ILE |
| 62 | SQ | 215 | VAL |
| 63 | SR | 39 | THR |
| 63 | SR | 73 | LEU |
| 63 | SR | 80 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63 | SR | 102 | VAL |
| 63 | SR | 184 | VAL |
| 63 | SR | 196 | VAL |
| 63 | SR | 232 | GLU |
| 63 | SR | 235 | LEU |
| 63 | SR | 238 | SER |
| 64 | SS | 17 | HIS |
| 64 | SS | 45 | ILE |
| 64 | SS | 81 | THR |
| 64 | SS | 89 | VAL |
| 64 | SS | 95 | THR |
| 64 | SS | 126 | VAL |
| 64 | SS | 140 | VAL |
| 64 | SS | 141 | THR |
| 64 | SS | 170 | THR |
| 64 | SS | 210 | ILE |
| 64 | SS | 219 | VAL |
| 64 | SS | 225 | VAL |
| 64 | SS | 227 | VAL |
| 64 | SS | 228 | ILE |
| 65 | ST | 15 | THR |
| 65 | ST | 18 | ILE |
| 65 | ST | 67 | VAL |
| 65 | ST | 71 | THR |
| 65 | ST | 74 | LYS |
| 65 | ST | 75 | LEU |
| 65 | ST | 106 | LEU |
| 65 | ST | 109 | LEU |
| 65 | ST | 112 | VAL |
| 65 | ST | 121 | LEU |
| 65 | ST | 171 | LYS |
| 65 | ST | 185 | GLN |
| 65 | ST | 216 | LEU |
| 66 | SU | 20 | VAL |
| 66 | SU | 38 | LEU |
| 66 | SU | 74 | GLN |
| 66 | SU | 127 | GLU |
| 66 | SU | 182 | VAL |
| 67 | SV | 14 | THR |
| 67 | SV | 58 | LEU |
| 67 | SV | 169 | ILE |
| 68 | SW | 14 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68 | SW | 21 | SER |
| 68 | SW | 50 | SER |
| 68 | SW | 70 | LEU |
| 68 | SW | 80 | LEU |
| 68 | SW | 89 | ASP |
| 68 | SW | 121 | SER |
| 68 | SW | 122 | VAL |
| 68 | SW | 127 | VAL |
| 68 | SW | 161 | THR |
| 68 | SW | 163 | PRO |
| 69 | SX | 74 | THR |
| 69 | SX | 99 | ARG |
| 69 | SX | 107 | VAL |
| 69 | SX | 131 | ILE |
| 70 | SY | 14 | SER |
| 70 | SY | 52 | VAL |
| 70 | SY | 62 | GLN |
| 70 | SY | 66 | ILE |
| 70 | SY | 75 | LEU |
| 70 | SY | 77 | SER |
| 70 | SY | 87 | ASP |
| 70 | SY | 143 | SER |
| 71 | SZ | 26 | THR |
| 71 | SZ | 29 | HIS |
| 71 | SZ | 86 | THR |
| 72 | Sa | 2 | GLU |
| 72 | Sa | 13 | VAL |
| 72 | Sa | 51 | VAL |
| 72 | Sa | 65 | SER |
| 72 | Sa | 84 | SER |
| 73 | Sb | 11 | LEU |
| 74 | Sc | 53 | VAL |
| 74 | Sc | 112 | LYS |
| 74 | Sc | 131 | SER |
| 75 | Sd | 5 | VAL |
| 75 | Sd | 23 | PHE |
| 75 | Sd | 24 | VAL |
| 75 | Sd | 25 | VAL |
| 75 | Sd | 36 | SER |
| 75 | Sd | 62 | THR |
| 75 | Sd | 107 | GLN |
| 75 | Sd | 121 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 76 | Se | 68 | TYR |
| 77 | Sf | 3 | LEU |
| 77 | Sf | 33 | LEU |
| 77 | Sf | 45 | THR |
| 77 | Sf | 54 | VAL |
| 77 | Sf | 61 | THR |
| 77 | Sf | 77 | THR |
| 78 | Sg | 8 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 4 | LD | 83 | HIS |
| 4 | LD | 97 | ASN |
| 4 | LD | 205 | ASN |
| 5 | LE | 109 | HIS |
| 5 | LE | 139 | GLN |
| 5 | LE | 182 | GLN |
| 5 | LE | 224 | HIS |
| 6 | LF | 5 | GLN |
| 6 | LF | 9 | HIS |
| 6 | LF | 213 | ASN |
| 6 | LF | 296 | GLN |
| 6 | LF | 316 | ASN |
| 7 | LG | 57 | ASN |
| 8 | LH | 138 | GLN |
| 9 | LI | 25 | GLN |
| 9 | LI | 64 | GLN |
| 9 | LI | 80 | GLN |
| 9 | LI | 146 | GLN |
| 9 | LI | 194 | HIS |
| 11 | LK | 125 | ASN |
| 11 | LK | 157 | ASN |
| 12 | LL | 73 | ASN |
| 13 | LM | 43 | GLN |
| 14 | LN | 103 | ASN |
| 14 | LN | 160 | GLN |
| 14 | LN | 162 | ASN |
| 15 | LO | 59 | ASN |
| 15 | LO | 105 | GLN |
| 16 | LP | 15 | GLN |
| 17 | LQ | 31[A] | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | LR | 10 | ASN |
| 18 | LR | 172 | GLN |
| 18 | LR | 179 | GLN |
| 19 | LS | 45 | ASN |
| 20 | LT | 27 | ASN |
| 20 | LT | 92 | GLN |
| 20 | LT | 166 | ASN |
| 22 | LV | 5 | HIS |
| 22 | LV | 16 | GLN |
| 22 | LV | 122 | GLN |
| 22 | LV | 131 | GLN |
| 23 | LW | 88 | GLN |
| 26 | LZ | 117 | ASN |
| 28 | Lb | 36 | HIS |
| 28 | Lb | 122 | HIS |
| 29 | Lc | 62 | HIS |
| 30 | Ld | 6 | ASN |
| 31 | Le | 11 | ASN |
| 31 | Le | 71 | GLN |
| 32 | Lf | 17 | HIS |
| 33 | Lg | 13 | HIS |
| 33 | Lg | 49 | ASN |
| 34 | Lh | 5 | HIS |
| 34 | Lh | 17 | GLN |
| 34 | Lh | 26 | ASN |
| 34 | Lh | 42 | GLN |
| 35 | Li | 3 | GLN |
| 36 | Lj | 62 | GLN |
| 38 | Ll | 69 | HIS |
| 38 | Ll | 76 | ASN |
| 39 | Lm | 57 | ASN |
| 40 | Ln | 19 | GLN |
| 43 | Lq | 3 | ASN |
| 46 | SA | 74 | GLN |
| 46 | SA | 92 | GLN |
| 46 | SA | 111 | ASN |
| 46 | SA | 159 | HIS |
| 47 | SB | 66 | GLN |
| 47 | SB | 158 | GLN |
| 48 | SC | 81 | ASN |
| 49 | SD | 96 | GLN |
| 49 | SD | 143 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | SE | 98 | ASN |
| 50 | SE | 104 | GLN |
| 51 | SF | 8 | GLN |
| 52 | SG | 74 | GLN |
| 52 | SG | 101 | ASN |
| 54 | SI | 43 | ASN |
| 55 | SJ | 40 | ASN |
| 57 | SL | 27 | GLN |
| 58 | SM | 10 | HIS |
| 60 | SO | 174 | ASN |
| 60 | SO | 195 | HIS |
| 60 | SO | 198 | ASN |
| 61 | SP | 21 | ASN |
| 61 | SP | 23 | HIS |
| 61 | SP | 140 | ASN |
| 62 | SQ | 146 | GLN |
| 63 | SR | 87 | GLN |
| 63 | SR | 189 | GLN |
| 63 | SR | 220 | ASN |
| 64 | SS | 197 | HIS |
| 64 | SS | 209 | HIS |
| 64 | SS | 224 | ASN |
| 65 | ST | 4 | ASN |
| 65 | ST | 119 | GLN |
| 66 | SU | 19 | GLN |
| 66 | SU | 174 | ASN |
| 67 | SV | 32 | GLN |
| 67 | SV | 64 | ASN |
| 67 | SV | 159 | GLN |
| 68 | SW | 38 | ASN |
| 68 | SW | 48 | GLN |
| 68 | SW | 74 | ASN |
| 68 | SW | 124 | HIS |
| 69 | SX | 81 | HIS |
| 69 | SX | 127 | GLN |
| 70 | SY | 78 | ASN |
| 71 | SZ | 12 | GLN |
| 71 | SZ | 24 | ASN |
| 71 | SZ | 65 | GLN |
| 73 | Sb | 64 | GLN |
| 73 | Sb | 70 | ASN |
| 74 | Sc | 10 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 77 | Sf | 49 | HIS |
| 78 | Sg | 17 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | LA | 3180/3393 (93%) | 852 (26%) | 35 (1%) |
| 2 | LB | 120/121 (99%) | 24 (20%) | 1 (0%) |
| 3 | LC | 157/158 (99%) | 43 (27%) | 2 (1%) |
| 45 | S2 | 1768/1799 (98%) | 720 (40%) | 26 (1%) |
| 79 | Ta | 76/77 (98%) | 48 (63%) | 0 |
| 80 | Tb | 76/77 (98%) | 38 (50%) | 0 |
| 81 | mR | 0/25 | - | - |
| All | All | 5377/5650 (95%) | 1725 (32%) | 64 (1%) |

All (1725) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | LA | 6 | A |
| 1 | LA | 22 | G |
| 1 | LA | 26 | A |
| 1 | LA | 34 | A |
| 1 | LA | 40 | A |
| 1 | LA | 43 | A |
| 1 | LA | 49 | A |
| 1 | LA | 59 | G |
| 1 | LA | 60 | A |
| 1 | LA | 65 | A |
| 1 | LA | 66 | A |
| 1 | LA | 80 | G |
| 1 | LA | 81 | C |
| 1 | LA | 89 | A |
| 1 | LA | 92 | G |
| 1 | LA | 99 | A |
| 1 | LA | 108 | A |
| 1 | LA | 109 | A |
| 1 | LA | 110 | G |
| 1 | LA | 111 | C |
| 1 | LA | 116 | A |
| 1 | LA | 122 | A |
| 1 | LA | 130 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | LA | 135 | C |
| 1 | LA | 136 | G |
| 1 | LA | 139 | G |
| 1 | LA | 146 | U |
| 1 | LA | 148 | G |
| 1 | LA | 155 | G |
| 1 | LA | 156 | G |
| 1 | LA | 157 | A |
| 1 | LA | 159 | A |
| 1 | LA | 160 | G |
| 1 | LA | 161 | G |
| 1 | LA | 162 | G |
| 1 | LA | 163 | C |
| 1 | LA | 164 | A |
| 1 | LA | 165 | A |
| 1 | LA | 166 | C |
| 1 | LA | 167 | U |
| 1 | LA | 168 | U |
| 1 | LA | 169 | U |
| 1 | LA | 170 | G |
| 1 | LA | 175 | C |
| 1 | LA | 176 | G |
| 1 | LA | 177 | U |
| 1 | LA | 178 | U |
| 1 | LA | 182 | U |
| 1 | LA | 189 | G |
| 1 | LA | 190 | U |
| 1 | LA | 191 | U |
| 1 | LA | 192 | C |
| 1 | LA | 199 | A |
| 1 | LA | 200 | C |
| 1 | LA | 202 | G |
| 1 | LA | 206 | G |
| 1 | LA | 210 | U |
| 1 | LA | 211 | A |
| 1 | LA | 218 | G |
| 1 | LA | 219 | A |
| 1 | LA | 235 | A |
| 1 | LA | 236 | G |
| 1 | LA | 240 | U |
| 1 | LA | 243 | G |
| 1 | LA | 246 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | LA | 247 | C |
| 1 | LA | 249 | U |
| 1 | LA | 251 | G |
| 1 | LA | 252 | U |
| 1 | LA | 253 | A |
| 1 | LA | 254 | A |
| 1 | LA | 255 | A |
| 1 | LA | 258 | G |
| 1 | LA | 259 | C |
| 1 | LA | 260 | C |
| 1 | LA | 261 | U |
| 1 | LA | 263 | C |
| 1 | LA | 269 | G |
| 1 | LA | 270 | U |
| 1 | LA | 286 | U |
| 1 | LA | 295 | A |
| 1 | LA | 297 | G |
| 1 | LA | 298 | U |
| 1 | LA | 305 | U |
| 1 | LA | 308 | A |
| 1 | LA | 309 | U |
| 1 | LA | 310 | U |
| 1 | LA | 311 | C |
| 1 | LA | 312 | C |
| 1 | LA | 315 | C |
| 1 | LA | 323 | A |
| 1 | LA | 329 | U |
| 1 | LA | 337 | G |
| 1 | LA | 341 | G |
| 1 | LA | 350 | C |
| 1 | LA | 351 | A |
| 1 | LA | 357 | A |
| 1 | LA | 370 | U |
| 1 | LA | 376 | G |
| 1 | LA | 381 | U |
| 1 | LA | 384 | A |
| 1 | LA | 387 | A |
| 1 | LA | 397 | A |
| 1 | LA | 398 | A |
| 1 | LA | 399 | A |
| 1 | LA | 402 | A |
| 1 | LA | 403 | C |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | LA | 404 | G |
| 1 | LA | 406 | G |
| 1 | LA | 407 | A |
| 1 | LA | 416 | A |
| 1 | LA | 418 | A |
| 1 | LA | 421 | G |
| 1 | LA | 422 | A |
| 1 | LA | 433 | A |
| 1 | LA | 438 | A |
| 1 | LA | 443 | G |
| 1 | LA | 444 | U |
| 1 | LA | 448 | U |
| 1 | LA | 449 | U |
| 1 | LA | 486 | U |
| 1 | LA | 488 | U |
| 1 | LA | 490 | A |
| 1 | LA | 494 | G |
| 1 | LA | 509 | G |
| 1 | LA | 512 | G |
| 1 | LA | 513 | G |
| 1 | LA | 520 | A |
| 1 | LA | 521 | A |
| 1 | LA | 522 | A |
| 1 | LA | 523 | U |
| 1 | LA | 524 | C |
| 1 | LA | 530 | G |
| 1 | LA | 534 | G |
| 1 | LA | 538 | C |
| 1 | LA | 539 | U |
| 1 | LA | 540 | U |
| 1 | LA | 543 | C |
| 1 | LA | 546 | G |
| 1 | LA | 547 | G |
| 1 | LA | 548 | U |
| 1 | LA | 551 | G |
| 1 | LA | 556 | A |
| 1 | LA | 558 | A |
| 1 | LA | 559 | G |
| 1 | LA | 560 | C |
| 1 | LA | 561 | C |
| 1 | LA | 566 | G |
| 1 | LA | 567 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | LA | 568 | A |
| 1 | LA | 569 | A |
| 1 | LA | 571 | A |
| 1 | LA | 577 | A |
| 1 | LA | 578 | G |
| 1 | LA | 579 | C |
| 1 | LA | 591 | A |
| 1 | LA | 592 | C |
| 1 | LA | 593 | U |
| 1 | LA | 599 | G |
| 1 | LA | 600 | U |
| 1 | LA | 602 | A |
| 1 | LA | 603 | G |
| 1 | LA | 608 | G |
| 1 | LA | 610 | A |
| 1 | LA | 619 | U |
| 1 | LA | 620 | A |
| 1 | LA | 621 | A |
| 1 | LA | 634 | G |
| 1 | LA | 636 | C |
| 1 | LA | 648 | A |
| 1 | LA | 652 | A |
| 1 | LA | 660 | G |
| 1 | LA | 666 | C |
| 1 | LA | 676 | A |
| 1 | LA | 689 | A |
| 1 | LA | 690 | A |
| 1 | LA | 692 | A |
| 1 | LA | 698 | A |
| 1 | LA | 704 | A |
| 1 | LA | 710 | A |
| 1 | LA | 711 | G |
| 1 | LA | 715 | A |
| 1 | LA | 716 | C |
| 1 | LA | 717 | G |
| 1 | LA | 726 | G |
| 1 | LA | 731 | C |
| 1 | LA | 732 | G |
| 1 | LA | 733 | C |
| 1 | LA | 735 | A |
| 1 | LA | 757 | C |
| 1 | LA | 759 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | LA | 760 | A |
| 1 | LA | 764 | C |
| 1 | LA | 765 | U |
| 1 | LA | 766 | U |
| 1 | LA | 773 | G |
| 1 | LA | 775 | U |
| 1 | LA | 776 | U |
| 1 | LA | 778 | G |
| 1 | LA | 780 | G |
| 1 | LA | 784 | G |
| 1 | LA | 805 | A |
| 1 | LA | 807 | A |
| 1 | LA | 816 | A |
| 1 | LA | 829 | A |
| 1 | LA | 848 | C |
| 1 | LA | 859 | G |
| 1 | LA | 860 | C |
| 1 | LA | 873 | U |
| 1 | LA | 878 | U |
| 1 | LA | 879 | G |
| 1 | LA | 888 | U |
| 1 | LA | 889 | C |
| 1 | LA | 895 | A |
| 1 | LA | 896 | U |
| 1 | LA | 906 | G |
| 1 | LA | 907 | G |
| 1 | LA | 913 | A |
| 1 | LA | 915 | G |
| 1 | LA | 916 | A |
| 1 | LA | 920 | A |
| 1 | LA | 922 | C |
| 1 | LA | 923 | G |
| 1 | LA | 924 | A |
| 1 | LA | 926 | C |
| 1 | LA | 936 | G |
| 1 | LA | 943 | C |
| 1 | LA | 958 | C |
| 1 | LA | 959 | U |
| 1 | LA | 961 | A |
| 1 | LA | 973 | G |
| 1 | LA | 980 | U |
| 1 | LA | 981 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 993 | G |
| 1 | LA | 994 | U |
| 1 | LA | 1005 | A |
| 1 | LA | 1014 | U |
| 1 | LA | 1015 | C |
| 1 | LA | 1016 | C |
| 1 | LA | 1017 | G |
| 1 | LA | 1020 | G |
| 1 | LA | 1022 | C |
| 1 | LA | 1023 | G |
| 1 | LA | 1025 | A |
| 1 | LA | 1027 | U |
| 1 | LA | 1028 | G |
| 1 | LA | 1029 | A |
| 1 | LA | 1039 | A |
| 1 | LA | 1040 | U |
| 1 | LA | 1041 | U |
| 1 | LA | 1042 | C |
| 1 | LA | 1046 | A |
| 1 | LA | 1048 | C |
| 1 | LA | 1049 | U |
| 1 | LA | 1062 | G |
| 1 | LA | 1063 | A |
| 1 | LA | 1065 | G |
| 1 | LA | 1067 | C |
| 1 | LA | 1068 | C |
| 1 | LA | 1069 | U |
| 1 | LA | 1070 | U |
| 1 | LA | 1071 | G |
| 1 | LA | 1078 | A |
| 1 | LA | 1080 | U |
| 1 | LA | 1092 | A |
| 1 | LA | 1093 | U |
| 1 | LA | 1096 | G |
| 1 | LA | 1097 | A |
| 1 | LA | 1102 | A |
| 1 | LA | 1103 | G |
| 1 | LA | 1104 | A |
| 1 | LA | 1105 | G |
| 1 | LA | 1106 | C |
| 1 | LA | 1107 | U |
| 1 | LA | 1116 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 1121 | U |
| 1 | LA | 1130 | G |
| 1 | LA | 1135 | A |
| 1 | LA | 1136 | C |
| 1 | LA | 1137 | U |
| 1 | LA | 1142 | A |
| 1 | LA | 1143 | U |
| 1 | LA | 1153 | A |
| 1 | LA | 1158 | A |
| 1 | LA | 1160 | G |
| 1 | LA | 1164 | A |
| 1 | LA | 1178 | A |
| 1 | LA | 1179 | A |
| 1 | LA | 1180 | U |
| 1 | LA | 1189 | A |
| 1 | LA | 1191 | C |
| 1 | LA | 1192 | A |
| 1 | LA | 1195 | C |
| 1 | LA | 1197 | C |
| 1 | LA | 1200 | C |
| 1 | LA | 1201 | A |
| 1 | LA | 1207 | U |
| 1 | LA | 1213 | U |
| 1 | LA | 1217 | U |
| 1 | LA | 1218 | C |
| 1 | LA | 1220 | A |
| 1 | LA | 1224 | A |
| 1 | LA | 1227 | C |
| 1 | LA | 1233 | G |
| 1 | LA | 1235 | G |
| 1 | LA | 1237 | C |
| 1 | LA | 1238 | C |
| 1 | LA | 1239 | A |
| 1 | LA | 1240 | U |
| 1 | LA | 1241 | G |
| 1 | LA | 1244 | A |
| 1 | LA | 1245 | G |
| 1 | LA | 1246 | U |
| 1 | LA | 1248 | G |
| 1 | LA | 1250 | A |
| 1 | LA | 1251 | A |
| 1 | LA | 1253 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 1254 | C |
| 1 | LA | 1259 | A |
| 1 | LA | 1260 | G |
| 1 | LA | 1261 | G |
| 1 | LA | 1262 | A |
| 1 | LA | 1263 | G |
| 1 | LA | 1267 | G |
| 1 | LA | 1268 | U |
| 1 | LA | 1271 | C |
| 1 | LA | 1274 | C |
| 1 | LA | 1277 | A |
| 1 | LA | 1278 | C |
| 1 | LA | 1283 | C |
| 1 | LA | 1284 | G |
| 1 | LA | 1285 | A |
| 1 | LA | 1306 | G |
| 1 | LA | 1307 | A |
| 1 | LA | 1308 | U |
| 1 | LA | 1312 | G |
| 1 | LA | 1324 | U |
| 1 | LA | 1329 | A |
| 1 | LA | 1330 | U |
| 1 | LA | 1335 | U |
| 1 | LA | 1343 | G |
| 1 | LA | 1347 | U |
| 1 | LA | 1349 | A |
| 1 | LA | 1351 | A |
| 1 | LA | 1352 | U |
| 1 | LA | 1353 | G |
| 1 | LA | 1354 | A |
| 1 | LA | 1355 | U |
| 1 | LA | 1356 | G |
| 1 | LA | 1360 | U |
| 1 | LA | 1373 | G |
| 1 | LA | 1374 | G |
| 1 | LA | 1382 | G |
| 1 | LA | 1385 | A |
| 1 | LA | 1390 | C |
| 1 | LA | 1394 | G |
| 1 | LA | 1398 | A |
| 1 | LA | 1399 | G |
| 1 | LA | 1415 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 1416 | G |
| 1 | LA | 1417 | A |
| 1 | LA | 1418 | A |
| 1 | LA | 1433 | G |
| 1 | LA | 1436 | C |
| 1 | LA | 1445 | A |
| 1 | LA | 1449 | G |
| 1 | LA | 1451 | A |
| 1 | LA | 1467 | A |
| 1 | LA | 1468 | C |
| 1 | LA | 1476 | A |
| 1 | LA | 1480 | A |
| 1 | LA | 1481 | A |
| 1 | LA | 1482 | G |
| 1 | LA | 1483 | U |
| 1 | LA | 1486 | G |
| 1 | LA | 1493 | U |
| 1 | LA | 1499 | G |
| 1 | LA | 1501 | C |
| 1 | LA | 1502 | A |
| 1 | LA | 1507 | C |
| 1 | LA | 1510 | U |
| 1 | LA | 1523 | A |
| 1 | LA | 1535 | G |
| 1 | LA | 1538 | A |
| 1 | LA | 1555 | C |
| 1 | LA | 1556 | A |
| 1 | LA | 1557 | A |
| 1 | LA | 1558 | A |
| 1 | LA | 1559 | G |
| 1 | LA | 1560 | G |
| 1 | LA | 1561 | C |
| 1 | LA | 1562 | C |
| 1 | LA | 1566 | U |
| 1 | LA | 1567 | U |
| 1 | LA | 1569 | U |
| 1 | LA | 1574 | A |
| 1 | LA | 1575 | G |
| 1 | LA | 1576 | G |
| 1 | LA | 1578 | C |
| 1 | LA | 1579 | A |
| 1 | LA | 1580 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 1581 | C |
| 1 | LA | 1582 | A |
| 1 | LA | 1586 | A |
| 1 | LA | 1588 | A |
| 1 | LA | 1589 | G |
| 1 | LA | 1592 | A |
| 1 | LA | 1604 | A |
| 1 | LA | 1617 | G |
| 1 | LA | 1618 | A |
| 1 | LA | 1620 | A |
| 1 | LA | 1621 | U |
| 1 | LA | 1624 | A |
| 1 | LA | 1625 | U |
| 1 | LA | 1627 | C |
| 1 | LA | 1628 | U |
| 1 | LA | 1638 | C |
| 1 | LA | 1641 | A |
| 1 | LA | 1642 | A |
| 1 | LA | 1646 | A |
| 1 | LA | 1656 | C |
| 1 | LA | 1679 | G |
| 1 | LA | 1682 | A |
| 1 | LA | 1683 | U |
| 1 | LA | 1685 | U |
| 1 | LA | 1687 | U |
| 1 | LA | 1693 | U |
| 1 | LA | 1695 | A |
| 1 | LA | 1705 | C |
| 1 | LA | 1709 | C |
| 1 | LA | 1712 | G |
| 1 | LA | 1713 | A |
| 1 | LA | 1714 | A |
| 1 | LA | 1720 | U |
| 1 | LA | 1723 | U |
| 1 | LA | 1724 | C |
| 1 | LA | 1729 | G |
| 1 | LA | 1735 | G |
| 1 | LA | 1740 | A |
| 1 | LA | 1741 | U |
| 1 | LA | 1749 | A |
| 1 | LA | 1750 | G |
| 1 | LA | 1758 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 1760 | C |
| 1 | LA | 1764 | U |
| 1 | LA | 1768 | G |
| 1 | LA | 1769 | G |
| 1 | LA | 1772 | C |
| 1 | LA | 1774 | G |
| 1 | LA | 1779 | G |
| 1 | LA | 1787 | C |
| 1 | LA | 1795 | G |
| 1 | LA | 1796 | A |
| 1 | LA | 1797 | A |
| 1 | LA | 1805 | A |
| 1 | LA | 1806 | G |
| 1 | LA | 1807 | G |
| 1 | LA | 1809 | A |
| 1 | LA | 1812 | A |
| 1 | LA | 1813 | A |
| 1 | LA | 1814 | U |
| 1 | LA | 1815 | A |
| 1 | LA | 1820 | U |
| 1 | LA | 1822 | A |
| 1 | LA | 1825 | C |
| 1 | LA | 1838 | A |
| 1 | LA | 1839 | U |
| 1 | LA | 1841 | A |
| 1 | LA | 1845 | C |
| 1 | LA | 1848 | C |
| 1 | LA | 1849 | A |
| 1 | LA | 1857 | A |
| 1 | LA | 1865 | C |
| 1 | LA | 1866 | A |
| 1 | LA | 1867 | G |
| 1 | LA | 1868 | C |
| 1 | LA | 1877 | G |
| 1 | LA | 1879 | U |
| 1 | LA | 1885 | A |
| 1 | LA | 1892 | A |
| 1 | LA | 1905 | G |
| 1 | LA | 1906 | C |
| 1 | LA | 1925 | C |
| 1 | LA | 1947 | G |
| 1 | LA | 1950 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 1952 | G |
| 1 | LA | 1953 | G |
| 1 | LA | 1954 | U |
| 1 | LA | 2093 | C |
| 1 | LA | 2096 | U |
| 1 | LA | 2097 | C |
| 1 | LA | 2098 | A |
| 1 | LA | 2100 | C |
| 1 | LA | 2106 | A |
| 1 | LA | 2110 | G |
| 1 | LA | 2111 | U |
| 1 | LA | 2112 | A |
| 1 | LA | 2120 | G |
| 1 | LA | 2121 | G |
| 1 | LA | 2130 | A |
| 1 | LA | 2139 | U |
| 1 | LA | 2141 | A |
| 1 | LA | 2143 | A |
| 1 | LA | 2145 | C |
| 1 | LA | 2157 | A |
| 1 | LA | 2165 | A |
| 1 | LA | 2168 | G |
| 1 | LA | 2169 | U |
| 1 | LA | 2180 | C |
| 1 | LA | 2187 | A |
| 1 | LA | 2188 | U |
| 1 | LA | 2191 | C |
| 1 | LA | 2193 | G |
| 1 | LA | 2196 | C |
| 1 | LA | 2204 | U |
| 1 | LA | 2206 | A |
| 1 | LA | 2208 | U |
| 1 | LA | 2209 | G |
| 1 | LA | 2216 | U |
| 1 | LA | 2217 | G |
| 1 | LA | 2218 | A |
| 1 | LA | 2219 | A |
| 1 | LA | 2220 | G |
| 1 | LA | 2221 | A |
| 1 | LA | 2222 | A |
| 1 | LA | 2223 | A |
| 1 | LA | 2227 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 2229 | C |
| 1 | LA | 2231 | A |
| 1 | LA | 2233 | G |
| 1 | LA | 2235 | G |
| 1 | LA | 2243 | A |
| 1 | LA | 2254 | A |
| 1 | LA | 2255 | A |
| 1 | LA | 2256 | C |
| 1 | LA | 2257 | U |
| 1 | LA | 2258 | A |
| 1 | LA | 2259 | U |
| 1 | LA | 2260 | G |
| 1 | LA | 2271 | G |
| 1 | LA | 2272 | G |
| 1 | LA | 2275 | G |
| 1 | LA | 2280 | A |
| 1 | LA | 2283 | C |
| 1 | LA | 2284 | C |
| 1 | LA | 2294 | A |
| 1 | LA | 2304 | G |
| 1 | LA | 2306 | G |
| 1 | LA | 2307 | C |
| 1 | LA | 2309 | U |
| 1 | LA | 2312 | A |
| 1 | LA | 2313 | U |
| 1 | LA | 2314 | G |
| 1 | LA | 2333 | U |
| 1 | LA | 2334 | G |
| 1 | LA | 2335 | U |
| 1 | LA | 2372 | A |
| 1 | LA | 2373 | C |
| 1 | LA | 2374 | G |
| 1 | LA | 2384 | G |
| 1 | LA | 2387 | U |
| 1 | LA | 2392 | G |
| 1 | LA | 2393 | G |
| 1 | LA | 2396 | A |
| 1 | LA | 2401 | A |
| 1 | LA | 2402 | G |
| 1 | LA | 2403 | A |
| 1 | LA | 2410 | U |
| 1 | LA | 2424 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 2433 | U |
| 1 | LA | 2434 | G |
| 1 | LA | 2438 | A |
| 1 | LA | 2439 | G |
| 1 | LA | 2441 | G |
| 1 | LA | 2442 | A |
| 1 | LA | 2443 | C |
| 1 | LA | 2444 | A |
| 1 | LA | 2445 | U |
| 1 | LA | 2446 | A |
| 1 | LA | 2447 | G |
| 1 | LA | 2448 | A |
| 1 | LA | 2450 | G |
| 1 | LA | 2492 | U |
| 1 | LA | 2493 | A |
| 1 | LA | 2495 | C |
| 1 | LA | 2497 | U |
| 1 | LA | 2499 | A |
| 1 | LA | 2500 | U |
| 1 | LA | 2501 | A |
| 1 | LA | 2502 | G |
| 1 | LA | 2503 | U |
| 1 | LA | 2509 | U |
| 1 | LA | 2513 | U |
| 1 | LA | 2523 | A |
| 1 | LA | 2530 | C |
| 1 | LA | 2531 | U |
| 1 | LA | 2535 | A |
| 1 | LA | 2536 | U |
| 1 | LA | 2537 | U |
| 1 | LA | 2538 | C |
| 1 | LA | 2539 | A |
| 1 | LA | 2540 | U |
| 1 | LA | 2541 | U |
| 1 | LA | 2544 | C |
| 1 | LA | 2545 | C |
| 1 | LA | 2547 | C |
| 1 | LA | 2548 | G |
| 1 | LA | 2553 | A |
| 1 | LA | 2554 | G |
| 1 | LA | 2557 | U |
| 1 | LA | 2558 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 2560 | A |
| 1 | LA | 2564 | U |
| 1 | LA | 2568 | A |
| 1 | LA | 2569 | U |
| 1 | LA | 2570 | U |
| 1 | LA | 2571 | C |
| 1 | LA | 2572 | G |
| 1 | LA | 2573 | G |
| 1 | LA | 2579 | A |
| 1 | LA | 2584 | G |
| 1 | LA | 2585 | G |
| 1 | LA | 2592 | A |
| 1 | LA | 2605 | G |
| 1 | LA | 2606 | G |
| 1 | LA | 2609 | G |
| 1 | LA | 2611 | U |
| 1 | LA | 2613 | G |
| 1 | LA | 2628 | U |
| 1 | LA | 2636 | A |
| 1 | LA | 2650 | G |
| 1 | LA | 2651 | U |
| 1 | LA | 2655 | A |
| 1 | LA | 2656 | A |
| 1 | LA | 2657 | G |
| 1 | LA | 2671 | G |
| 1 | LA | 2673 | A |
| 1 | LA | 2675 | A |
| 1 | LA | 2676 | G |
| 1 | LA | 2677 | A |
| 1 | LA | 2679 | A |
| 1 | LA | 2680 | U |
| 1 | LA | 2681 | C |
| 1 | LA | 2687 | U |
| 1 | LA | 2688 | A |
| 1 | LA | 2690 | A |
| 1 | LA | 2695 | A |
| 1 | LA | 2703 | A |
| 1 | LA | 2711 | U |
| 1 | LA | 2713 | G |
| 1 | LA | 2718 | U |
| 1 | LA | 2719 | G |
| 1 | LA | 2726 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 2727 | G |
| 1 | LA | 2728 | U |
| 1 | LA | 2752 | G |
| 1 | LA | 2754 | C |
| 1 | LA | 2761 | A |
| 1 | LA | 2771 | C |
| 1 | LA | 2776 | G |
| 1 | LA | 2777 | G |
| 1 | LA | 2779 | A |
| 1 | LA | 2780 | U |
| 1 | LA | 2782 | U |
| 1 | LA | 2795 | G |
| 1 | LA | 2796 | C |
| 1 | LA | 2798 | A |
| 1 | LA | 2799 | G |
| 1 | LA | 2800 | A |
| 1 | LA | 2801 | A |
| 1 | LA | 2804 | G |
| 1 | LA | 2809 | C |
| 1 | LA | 2813 | G |
| 1 | LA | 2816 | A |
| 1 | LA | 2841 | U |
| 1 | LA | 2844 | A |
| 1 | LA | 2848 | C |
| 1 | LA | 2852 | A |
| 1 | LA | 2855 | G |
| 1 | LA | 2856 | C |
| 1 | LA | 2857 | U |
| 1 | LA | 2858 | U |
| 1 | LA | 2859 | U |
| 1 | LA | 2866 | C |
| 1 | LA | 2870 | G |
| 1 | LA | 2871 | A |
| 1 | LA | 2875 | C |
| 1 | LA | 2886 | A |
| 1 | LA | 2887 | U |
| 1 | LA | 2888 | C |
| 1 | LA | 2895 | A |
| 1 | LA | 2897 | G |
| 1 | LA | 2901 | A |
| 1 | LA | 2910 | A |
| 1 | LA | 2915 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 2917 | G |
| 1 | LA | 2922 | U |
| 1 | LA | 2924 | C |
| 1 | LA | 2925 | A |
| 1 | LA | 2926 | C |
| 1 | LA | 2929 | A |
| 1 | LA | 2932 | A |
| 1 | LA | 2934 | U |
| 1 | LA | 2935 | A |
| 1 | LA | 2941 | C |
| 1 | LA | 2944 | G |
| 1 | LA | 2946 | G |
| 1 | LA | 2954 | U |
| 1 | LA | 2970 | A |
| 1 | LA | 2977 | U |
| 1 | LA | 2982 | C |
| 1 | LA | 2989 | G |
| 1 | LA | 2991 | U |
| 1 | LA | 2995 | U |
| 1 | LA | 2996 | G |
| 1 | LA | 3010 | A |
| 1 | LA | 3011 | A |
| 1 | LA | 3014 | G |
| 1 | LA | 3016 | A |
| 1 | LA | 3017 | C |
| 1 | LA | 3019 | U |
| 1 | LA | 3020 | A |
| 1 | LA | 3021 | G |
| 1 | LA | 3026 | A |
| 1 | LA | 3027 | G |
| 1 | LA | 3031 | A |
| 1 | LA | 3033 | C |
| 1 | LA | 3035 | G |
| 1 | LA | 3040 | U |
| 1 | LA | 3047 | A |
| 1 | LA | 3048 | A |
| 1 | LA | 3054 | U |
| 1 | LA | 3057 | U |
| 1 | LA | 3068 | G |
| 1 | LA | 3069 | A |
| 1 | LA | 3070 | U |
| 1 | LA | 3071 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 3073 | G |
| 1 | LA | 3077 | U |
| 1 | LA | 3085 | A |
| 1 | LA | 3091 | C |
| 1 | LA | 3092 | C |
| 1 | LA | 3108 | G |
| 1 | LA | 3112 | A |
| 1 | LA | 3114 | C |
| 1 | LA | 3121 | A |
| 1 | LA | 3128 | A |
| 1 | LA | 3129 | A |
| 1 | LA | 3130 | U |
| 1 | LA | 3136 | C |
| 1 | LA | 3137 | U |
| 1 | LA | 3140 | A |
| 1 | LA | 3141 | A |
| 1 | LA | 3142 | C |
| 1 | LA | 3151 | U |
| 1 | LA | 3152 | U |
| 1 | LA | 3154 | U |
| 1 | LA | 3155 | U |
| 1 | LA | 3156 | U |
| 1 | LA | 3157 | G |
| 1 | LA | 3158 | C |
| 1 | LA | 3160 | C |
| 1 | LA | 3161 | C |
| 1 | LA | 3164 | A |
| 1 | LA | 3165 | C |
| 1 | LA | 3167 | A |
| 1 | LA | 3168 | U |
| 1 | LA | 3169 | A |
| 1 | LA | 3170 | U |
| 1 | LA | 3171 | A |
| 1 | LA | 3172 | G |
| 1 | LA | 3173 | A |
| 1 | LA | 3174 | U |
| 1 | LA | 3178 | U |
| 1 | LA | 3179 | A |
| 1 | LA | 3180 | C |
| 1 | LA | 3181 | G |
| 1 | LA | 3186 | A |
| 1 | LA | 3194 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 3197 | U |
| 1 | LA | 3198 | G |
| 1 | LA | 3206 | U |
| 1 | LA | 3208 | A |
| 1 | LA | 3209 | A |
| 1 | LA | 3213 | U |
| 1 | LA | 3215 | G |
| 1 | LA | 3216 | C |
| 1 | LA | 3217 | A |
| 1 | LA | 3218 | G |
| 1 | LA | 3225 | A |
| 1 | LA | 3226 | A |
| 1 | LA | 3228 | G |
| 1 | LA | 3234 | C |
| 1 | LA | 3238 | G |
| 1 | LA | 3242 | A |
| 1 | LA | 3245 | G |
| 1 | LA | 3246 | G |
| 1 | LA | 3247 | C |
| 1 | LA | 3248 | C |
| 1 | LA | 3250 | U |
| 1 | LA | 3256 | C |
| 1 | LA | 3258 | U |
| 1 | LA | 3259 | G |
| 1 | LA | 3267 | A |
| 1 | LA | 3268 | U |
| 1 | LA | 3269 | U |
| 1 | LA | 3272 | A |
| 1 | LA | 3275 | G |
| 1 | LA | 3278 | A |
| 1 | LA | 3280 | U |
| 1 | LA | 3284 | C |
| 1 | LA | 3285 | G |
| 1 | LA | 3288 | G |
| 1 | LA | 3291 | A |
| 1 | LA | 3293 | A |
| 1 | LA | 3294 | A |
| 1 | LA | 3295 | A |
| 1 | LA | 3296 | U |
| 1 | LA | 3302 | G |
| 1 | LA | 3303 | U |
| 1 | LA | 3304 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 3306 | A |
| 1 | LA | 3315 | A |
| 1 | LA | 3316 | U |
| 1 | LA | 3318 | U |
| 1 | LA | 3319 | A |
| 1 | LA | 3325 | G |
| 1 | LA | 3335 | A |
| 1 | LA | 3340 | U |
| 1 | LA | 3344 | G |
| 1 | LA | 3346 | A |
| 1 | LA | 3347 | G |
| 1 | LA | 3350 | U |
| 1 | LA | 3352 | G |
| 1 | LA | 3353 | U |
| 1 | LA | 3354 | U |
| 1 | LA | 3355 | G |
| 1 | LA | 3356 | U |
| 1 | LA | 3358 | A |
| 1 | LA | 3359 | C |
| 1 | LA | 3368 | G |
| 1 | LA | 3377 | C |
| 1 | LA | 3378 | C |
| 1 | LA | 3379 | U |
| 1 | LA | 3380 | U |
| 1 | LA | 3381 | U |
| 1 | LA | 3382 | G |
| 1 | LA | 3385 | G |
| 1 | LA | 3389 | G |
| 1 | LA | 3390 | A |
| 1 | LA | 3391 | U |
| 1 | LA | 3394 | G |
| 2 | LB | 7 | G |
| 2 | LB | 16 | U |
| 2 | LB | 17 | A |
| 2 | LB | 33 | U |
| 2 | LB | 37 | G |
| 2 | LB | 42 | A |
| 2 | LB | 43 | U |
| 2 | LB | 44 | C |
| 2 | LB | 51 | A |
| 2 | LB | 52 | G |
| 2 | LB | 53 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | LB | 54 | U |
| 2 | LB | 55 | A |
| 2 | LB | 65 | G |
| 2 | LB | 73 | C |
| 2 | LB | 74 | C |
| 2 | LB | 76 | A |
| 2 | LB | 102 | A |
| 2 | LB | 105 | C |
| 2 | LB | 106 | U |
| 2 | LB | 112 | G |
| 2 | LB | 113 | C |
| 2 | LB | 117 | A |
| 2 | LB | 121 | U |
| 3 | LC | 6 | U |
| 3 | LC | 14 | C |
| 3 | LC | 15 | G |
| 3 | LC | 16 | G |
| 3 | LC | 17 | A |
| 3 | LC | 22 | U |
| 3 | LC | 23 | U |
| 3 | LC | 26 | U |
| 3 | LC | 27 | U |
| 3 | LC | 34 | U |
| 3 | LC | 35 | C |
| 3 | LC | 49 | G |
| 3 | LC | 52 | A |
| 3 | LC | 53 | A |
| 3 | LC | 54 | A |
| 3 | LC | 55 | U |
| 3 | LC | 59 | A |
| 3 | LC | 62 | C |
| 3 | LC | 63 | G |
| 3 | LC | 81 | U |
| 3 | LC | 82 | U |
| 3 | LC | 84 | C |
| 3 | LC | 86 | U |
| 3 | LC | 87 | G |
| 3 | LC | 88 | A |
| 3 | LC | 90 | U |
| 3 | LC | 95 | G |
| 3 | LC | 97 | A |
| 3 | LC | 100 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | LC | 102 | U |
| 3 | LC | 104 | A |
| 3 | LC | 106 | C |
| 3 | LC | 107 | G |
| 3 | LC | 111 | A |
| 3 | LC | 113 | U |
| 3 | LC | 117 | C |
| 3 | LC | 125 | U |
| 3 | LC | 126 | A |
| 3 | LC | 127 | U |
| 3 | LC | 151 | C |
| 3 | LC | 153 | U |
| 3 | LC | 155 | A |
| 3 | LC | 158 | U |
| 45 | S2 | 3 | U |
| 45 | S2 | 4 | C |
| 45 | S2 | 9 | U |
| 45 | S2 | 10 | G |
| 45 | S2 | 13 | C |
| 45 | S2 | 14 | C |
| 45 | S2 | 15 | U |
| 45 | S2 | 16 | G |
| 45 | S2 | 17 | C |
| 45 | S2 | 22 | A |
| 45 | S2 | 25 | C |
| 45 | S2 | 26 | A |
| 45 | S2 | 34 | G |
| 45 | S2 | 40 | A |
| 45 | S2 | 42 | G |
| 45 | S2 | 45 | U |
| 45 | S2 | 47 | A |
| 45 | S2 | 56 | U |
| 45 | S2 | 57 | G |
| 45 | S2 | 61 | A |
| 45 | S2 | 63 | G |
| 45 | S2 | 65 | A |
| 45 | S2 | 66 | U |
| 45 | S2 | 68 | A |
| 45 | S2 | 69 | G |
| 45 | S2 | 73 | U |
| 45 | S2 | 74 | U |
| 45 | S2 | 75 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 76 | A |
| 45 | S2 | 77 | U |
| 45 | S2 | 80 | A |
| 45 | S2 | 81 | G |
| 45 | S2 | 84 | A |
| 45 | S2 | 85 | A |
| 45 | S2 | 86 | A |
| 45 | S2 | 88 | U |
| 45 | S2 | 89 | G |
| 45 | S2 | 99 | C |
| 45 | S2 | 100 | A |
| 45 | S2 | 104 | A |
| 45 | S2 | 106 | U |
| 45 | S2 | 114 | C |
| 45 | S2 | 115 | G |
| 45 | S2 | 116 | U |
| 45 | S2 | 121 | U |
| 45 | S2 | 125 | U |
| 45 | S2 | 131 | C |
| 45 | S2 | 132 | U |
| 45 | S2 | 133 | U |
| 45 | S2 | 134 | U |
| 45 | S2 | 135 | A |
| 45 | S2 | 136 | C |
| 45 | S2 | 138 | A |
| 45 | S2 | 140 | A |
| 45 | S2 | 141 | U |
| 45 | S2 | 146 | U |
| 45 | S2 | 147 | A |
| 45 | S2 | 148 | A |
| 45 | S2 | 149 | C |
| 45 | S2 | 150 | U |
| 45 | S2 | 154 | G |
| 45 | S2 | 155 | U |
| 45 | S2 | 156 | A |
| 45 | S2 | 161 | U |
| 45 | S2 | 168 | A |
| 45 | S2 | 171 | A |
| 45 | S2 | 173 | A |
| 45 | S2 | 176 | C |
| 45 | S2 | 178 | U |
| 45 | S2 | 180 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 183 | U |
| 45 | S2 | 185 | U |
| 45 | S2 | 191 | C |
| 45 | S2 | 192 | U |
| 45 | S2 | 194 | U |
| 45 | S2 | 195 | G |
| 45 | S2 | 199 | G |
| 45 | S2 | 200 | A |
| 45 | S2 | 201 | G |
| 45 | S2 | 202 | A |
| 45 | S2 | 204 | G |
| 45 | S2 | 208 | U |
| 45 | S2 | 209 | U |
| 45 | S2 | 211 | U |
| 45 | S2 | 212 | U |
| 45 | S2 | 214 | G |
| 45 | S2 | 215 | A |
| 45 | S2 | 216 | U |
| 45 | S2 | 217 | A |
| 45 | S2 | 218 | A |
| 45 | S2 | 219 | A |
| 45 | S2 | 220 | A |
| 45 | S2 | 221 | A |
| 45 | S2 | 222 | A |
| 45 | S2 | 225 | A |
| 45 | S2 | 227 | U |
| 45 | S2 | 230 | C |
| 45 | S2 | 231 | U |
| 45 | S2 | 233 | C |
| 45 | S2 | 234 | G |
| 45 | S2 | 235 | G |
| 45 | S2 | 236 | A |
| 45 | S2 | 239 | C |
| 45 | S2 | 240 | U |
| 45 | S2 | 241 | U |
| 45 | S2 | 242 | U |
| 45 | S2 | 248 | U |
| 45 | S2 | 249 | U |
| 45 | S2 | 253 | A |
| 45 | S2 | 255 | U |
| 45 | S2 | 256 | A |
| 45 | S2 | 258 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 260 | U |
| 45 | S2 | 261 | U |
| 45 | S2 | 262 | U |
| 45 | S2 | 265 | A |
| 45 | S2 | 266 | A |
| 45 | S2 | 267 | U |
| 45 | S2 | 271 | A |
| 45 | S2 | 272 | U |
| 45 | S2 | 273 | G |
| 45 | S2 | 276 | C |
| 45 | S2 | 277 | U |
| 45 | S2 | 280 | U |
| 45 | S2 | 281 | G |
| 45 | S2 | 283 | U |
| 45 | S2 | 288 | A |
| 45 | S2 | 291 | G |
| 45 | S2 | 293 | U |
| 45 | S2 | 295 | A |
| 45 | S2 | 296 | U |
| 45 | S2 | 297 | U |
| 45 | S2 | 299 | A |
| 45 | S2 | 304 | U |
| 45 | S2 | 313 | U |
| 45 | S2 | 314 | C |
| 45 | S2 | 316 | A |
| 45 | S2 | 319 | U |
| 45 | S2 | 320 | U |
| 45 | S2 | 322 | G |
| 45 | S2 | 323 | A |
| 45 | S2 | 324 | U |
| 45 | S2 | 325 | G |
| 45 | S2 | 331 | A |
| 45 | S2 | 333 | A |
| 45 | S2 | 334 | G |
| 45 | S2 | 337 | G |
| 45 | S2 | 338 | C |
| 45 | S2 | 339 | C |
| 45 | S2 | 341 | A |
| 45 | S2 | 345 | U |
| 45 | S2 | 346 | G |
| 45 | S2 | 352 | A |
| 45 | S2 | 359 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 360 | A |
| 45 | S2 | 361 | C |
| 45 | S2 | 365 | G |
| 45 | S2 | 366 | A |
| 45 | S2 | 368 | U |
| 45 | S2 | 370 | A |
| 45 | S2 | 371 | G |
| 45 | S2 | 373 | G |
| 45 | S2 | 374 | U |
| 45 | S2 | 380 | U |
| 45 | S2 | 384 | G |
| 45 | S2 | 388 | G |
| 45 | S2 | 389 | G |
| 45 | S2 | 400 | A |
| 45 | S2 | 401 | A |
| 45 | S2 | 402 | C |
| 45 | S2 | 404 | G |
| 45 | S2 | 408 | C |
| 45 | S2 | 410 | A |
| 45 | S2 | 412 | A |
| 45 | S2 | 413 | U |
| 45 | S2 | 414 | C |
| 45 | S2 | 416 | A |
| 45 | S2 | 417 | A |
| 45 | S2 | 418 | G |
| 45 | S2 | 420 | A |
| 45 | S2 | 424 | C |
| 45 | S2 | 425 | A |
| 45 | S2 | 439 | U |
| 45 | S2 | 440 | U |
| 45 | S2 | 441 | A |
| 45 | S2 | 444 | C |
| 45 | S2 | 445 | A |
| 45 | S2 | 447 | U |
| 45 | S2 | 451 | A |
| 45 | S2 | 452 | A |
| 45 | S2 | 453 | U |
| 45 | S2 | 454 | U |
| 45 | S2 | 455 | C |
| 45 | S2 | 473 | A |
| 45 | S2 | 475 | A |
| 45 | S2 | 477 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 479 | C |
| 45 | S2 | 481 | A |
| 45 | S2 | 485 | A |
| 45 | S2 | 486 | G |
| 45 | S2 | 487 | G |
| 45 | S2 | 489 | C |
| 45 | S2 | 492 | A |
| 45 | S2 | 494 | U |
| 45 | S2 | 495 | C |
| 45 | S2 | 496 | G |
| 45 | S2 | 498 | G |
| 45 | S2 | 500 | C |
| 45 | S2 | 501 | U |
| 45 | S2 | 502 | U |
| 45 | S2 | 506 | A |
| 45 | S2 | 511 | A |
| 45 | S2 | 512 | A |
| 45 | S2 | 518 | A |
| 45 | S2 | 519 | C |
| 45 | S2 | 520 | A |
| 45 | S2 | 522 | U |
| 45 | S2 | 523 | G |
| 45 | S2 | 524 | U |
| 45 | S2 | 525 | A |
| 45 | S2 | 527 | A |
| 45 | S2 | 529 | A |
| 45 | S2 | 534 | A |
| 45 | S2 | 537 | G |
| 45 | S2 | 538 | A |
| 45 | S2 | 539 | G |
| 45 | S2 | 541 | A |
| 45 | S2 | 542 | A |
| 45 | S2 | 543 | C |
| 45 | S2 | 545 | A |
| 45 | S2 | 549 | G |
| 45 | S2 | 550 | A |
| 45 | S2 | 551 | G |
| 45 | S2 | 555 | A |
| 45 | S2 | 556 | A |
| 45 | S2 | 558 | U |
| 45 | S2 | 559 | C |
| 45 | S2 | 562 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 565 | C |
| 45 | S2 | 566 | C |
| 45 | S2 | 567 | A |
| 45 | S2 | 568 | G |
| 45 | S2 | 578 | U |
| 45 | S2 | 579 | A |
| 45 | S2 | 580 | A |
| 45 | S2 | 581 | U |
| 45 | S2 | 585 | A |
| 45 | S2 | 586 | G |
| 45 | S2 | 587 | C |
| 45 | S2 | 588 | U |
| 45 | S2 | 589 | C |
| 45 | S2 | 590 | C |
| 45 | S2 | 591 | A |
| 45 | S2 | 594 | A |
| 45 | S2 | 606 | A |
| 45 | S2 | 610 | G |
| 45 | S2 | 611 | U |
| 45 | S2 | 619 | A |
| 45 | S2 | 620 | A |
| 45 | S2 | 623 | A |
| 45 | S2 | 624 | G |
| 45 | S2 | 635 | A |
| 45 | S2 | 639 | U |
| 45 | S2 | 640 | U |
| 45 | S2 | 643 | G |
| 45 | S2 | 649 | U |
| 45 | S2 | 650 | U |
| 45 | S2 | 652 | G |
| 45 | S2 | 653 | C |
| 45 | S2 | 654 | C |
| 45 | S2 | 655 | G |
| 45 | S2 | 656 | G |
| 45 | S2 | 657 | U |
| 45 | S2 | 658 | C |
| 45 | S2 | 677 | G |
| 45 | S2 | 679 | U |
| 45 | S2 | 680 | U |
| 45 | S2 | 682 | C |
| 45 | S2 | 683 | C |
| 45 | S2 | 687 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 688 | G |
| 45 | S2 | 689 | G |
| 45 | S2 | 694 | U |
| 45 | S2 | 695 | U |
| 45 | S2 | 696 | C |
| 45 | S2 | 697 | C |
| 45 | S2 | 698 | U |
| 45 | S2 | 699 | U |
| 45 | S2 | 700 | C |
| 45 | S2 | 704 | C |
| 45 | S2 | 705 | U |
| 45 | S2 | 706 | A |
| 45 | S2 | 709 | C |
| 45 | S2 | 711 | U |
| 45 | S2 | 712 | G |
| 45 | S2 | 713 | A |
| 45 | S2 | 714 | G |
| 45 | S2 | 727 | U |
| 45 | S2 | 729 | G |
| 45 | S2 | 730 | G |
| 45 | S2 | 732 | G |
| 45 | S2 | 733 | A |
| 45 | S2 | 735 | C |
| 45 | S2 | 738 | G |
| 45 | S2 | 740 | A |
| 45 | S2 | 741 | C |
| 45 | S2 | 742 | U |
| 45 | S2 | 743 | U |
| 45 | S2 | 744 | U |
| 45 | S2 | 749 | U |
| 45 | S2 | 750 | U |
| 45 | S2 | 751 | G |
| 45 | S2 | 752 | A |
| 45 | S2 | 753 | A |
| 45 | S2 | 754 | A |
| 45 | S2 | 755 | A |
| 45 | S2 | 756 | A |
| 45 | S2 | 758 | U |
| 45 | S2 | 759 | U |
| 45 | S2 | 760 | A |
| 45 | S2 | 761 | G |
| 45 | S2 | 762 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | S2 | 763 | G |
| 45 | S2 | 765 | G |
| 45 | S2 | 767 | U |
| 45 | S2 | 768 | C |
| 45 | S2 | 771 | A |
| 45 | S2 | 772 | G |
| 45 | S2 | 773 | C |
| 45 | S2 | 774 | A |
| 45 | S2 | 775 | G |
| 45 | S2 | 780 | A |
| 45 | S2 | 782 | U |
| 45 | S2 | 783 | G |
| 45 | S2 | 789 | A |
| 45 | S2 | 790 | U |
| 45 | S2 | 792 | U |
| 45 | S2 | 798 | C |
| 45 | S2 | 806 | A |
| 45 | S2 | 809 | A |
| 45 | S2 | 812 | A |
| 45 | S2 | 813 | U |
| 45 | S2 | 814 | A |
| 45 | S2 | 816 | G |
| 45 | S2 | 818 | C |
| 45 | S2 | 820 | U |
| 45 | S2 | 821 | U |
| 45 | S2 | 822 | U |
| 45 | S2 | 823 | G |
| 45 | S2 | 824 | G |
| 45 | S2 | 825 | U |
| 45 | S2 | 827 | C |
| 45 | S2 | 828 | U |
| 45 | S2 | 829 | A |
| 45 | S2 | 830 | U |
| 45 | S2 | 832 | U |
| 45 | S2 | 836 | U |
| 45 | S2 | 837 | G |
| 45 | S2 | 840 | U |
| 45 | S2 | 841 | U |
| 45 | S2 | 843 | U |
| 45 | S2 | 845 | G |
| 45 | S2 | 846 | G |
| 45 | S2 | 847 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 848 | C |
| 45 | S2 | 849 | C |
| 45 | S2 | 850 | A |
| 45 | S2 | 852 | C |
| 45 | S2 | 855 | A |
| 45 | S2 | 857 | U |
| 45 | S2 | 863 | A |
| 45 | S2 | 864 | U |
| 45 | S2 | 865 | A |
| 45 | S2 | 893 | U |
| 45 | S2 | 896 | U |
| 45 | S2 | 902 | G |
| 45 | S2 | 905 | A |
| 45 | S2 | 906 | A |
| 45 | S2 | 908 | U |
| 45 | S2 | 909 | U |
| 45 | S2 | 913 | G |
| 45 | S2 | 914 | G |
| 45 | S2 | 916 | U |
| 45 | S2 | 919 | A |
| 45 | S2 | 921 | U |
| 45 | S2 | 930 | A |
| 45 | S2 | 931 | C |
| 45 | S2 | 933 | A |
| 45 | S2 | 934 | C |
| 45 | S2 | 935 | U |
| 45 | S2 | 942 | G |
| 45 | S2 | 946 | U |
| 45 | S2 | 951 | A |
| 45 | S2 | 960 | U |
| 45 | S2 | 964 | U |
| 45 | S2 | 966 | A |
| 45 | S2 | 973 | A |
| 45 | S2 | 984 | G |
| 45 | S2 | 988 | A |
| 45 | S2 | 992 | A |
| 45 | S2 | 993 | A |
| 45 | S2 | 1004 | U |
| 45 | S2 | 1005 | A |
| 45 | S2 | 1012 | U |
| 45 | S2 | 1017 | U |
| 45 | S2 | 1021 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1024 | U |
| 45 | S2 | 1026 | A |
| 45 | S2 | 1028 | C |
| 45 | S2 | 1030 | A |
| 45 | S2 | 1038 | U |
| 45 | S2 | 1039 | A |
| 45 | S2 | 1047 | G |
| 45 | S2 | 1048 | G |
| 45 | S2 | 1049 | U |
| 45 | S2 | 1050 | G |
| 45 | S2 | 1052 | U |
| 45 | S2 | 1053 | G |
| 45 | S2 | 1054 | U |
| 45 | S2 | 1055 | U |
| 45 | S2 | 1056 | U |
| 45 | S2 | 1057 | U |
| 45 | S2 | 1058 | U |
| 45 | S2 | 1059 | U |
| 45 | S2 | 1060 | U |
| 45 | S2 | 1061 | A |
| 45 | S2 | 1062 | A |
| 45 | S2 | 1063 | U |
| 45 | S2 | 1064 | G |
| 45 | S2 | 1068 | C |
| 45 | S2 | 1069 | A |
| 45 | S2 | 1070 | C |
| 45 | S2 | 1071 | U |
| 45 | S2 | 1072 | C |
| 45 | S2 | 1076 | A |
| 45 | S2 | 1079 | U |
| 45 | S2 | 1082 | C |
| 45 | S2 | 1091 | A |
| 45 | S2 | 1092 | A |
| 45 | S2 | 1096 | C |
| 45 | S2 | 1098 | U |
| 45 | S2 | 1099 | U |
| 45 | S2 | 1100 | G |
| 45 | S2 | 1109 | G |
| 45 | S2 | 1111 | G |
| 45 | S2 | 1137 | A |
| 45 | S2 | 1138 | A |
| 45 | S2 | 1142 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1143 | A |
| 45 | S2 | 1144 | U |
| 45 | S2 | 1145 | U |
| 45 | S2 | 1150 | G |
| 45 | S2 | 1157 | A |
| 45 | S2 | 1158 | C |
| 45 | S2 | 1160 | A |
| 45 | S2 | 1162 | C |
| 45 | S2 | 1163 | A |
| 45 | S2 | 1170 | G |
| 45 | S2 | 1174 | C |
| 45 | S2 | 1179 | G |
| 45 | S2 | 1182 | U |
| 45 | S2 | 1186 | U |
| 45 | S2 | 1192 | C |
| 45 | S2 | 1194 | A |
| 45 | S2 | 1195 | C |
| 45 | S2 | 1196 | A |
| 45 | S2 | 1199 | G |
| 45 | S2 | 1200 | G |
| 45 | S2 | 1202 | A |
| 45 | S2 | 1203 | A |
| 45 | S2 | 1204 | A |
| 45 | S2 | 1208 | A |
| 45 | S2 | 1209 | C |
| 45 | S2 | 1213 | G |
| 45 | S2 | 1217 | A |
| 45 | S2 | 1219 | A |
| 45 | S2 | 1223 | A |
| 45 | S2 | 1227 | A |
| 45 | S2 | 1232 | U |
| 45 | S2 | 1237 | G |
| 45 | S2 | 1238 | A |
| 45 | S2 | 1239 | U |
| 45 | S2 | 1243 | G |
| 45 | S2 | 1244 | A |
| 45 | S2 | 1245 | G |
| 45 | S2 | 1246 | C |
| 45 | S2 | 1247 | U |
| 45 | S2 | 1248 | C |
| 45 | S2 | 1249 | U |
| 45 | S2 | 1250 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1254 | U |
| 45 | S2 | 1255 | G |
| 45 | S2 | 1257 | U |
| 45 | S2 | 1258 | U |
| 45 | S2 | 1259 | U |
| 45 | S2 | 1260 | U |
| 45 | S2 | 1261 | G |
| 45 | S2 | 1263 | G |
| 45 | S2 | 1275 | A |
| 45 | S2 | 1281 | G |
| 45 | S2 | 1285 | U |
| 45 | S2 | 1287 | A |
| 45 | S2 | 1291 | G |
| 45 | S2 | 1295 | G |
| 45 | S2 | 1301 | U |
| 45 | S2 | 1302 | U |
| 45 | S2 | 1307 | U |
| 45 | S2 | 1308 | G |
| 45 | S2 | 1310 | U |
| 45 | S2 | 1314 | U |
| 45 | S2 | 1315 | U |
| 45 | S2 | 1316 | G |
| 45 | S2 | 1321 | A |
| 45 | S2 | 1322 | A |
| 45 | S2 | 1325 | A |
| 45 | S2 | 1337 | A |
| 45 | S2 | 1338 | C |
| 45 | S2 | 1339 | C |
| 45 | S2 | 1340 | U |
| 45 | S2 | 1344 | A |
| 45 | S2 | 1345 | A |
| 45 | S2 | 1346 | A |
| 45 | S2 | 1348 | A |
| 45 | S2 | 1349 | G |
| 45 | S2 | 1350 | U |
| 45 | S2 | 1351 | G |
| 45 | S2 | 1353 | U |
| 45 | S2 | 1354 | G |
| 45 | S2 | 1359 | C |
| 45 | S2 | 1360 | A |
| 45 | S2 | 1362 | U |
| 45 | S2 | 1363 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1367 | G |
| 45 | S2 | 1368 | G |
| 45 | S2 | 1371 | A |
| 45 | S2 | 1372 | U |
| 45 | S2 | 1377 | U |
| 45 | S2 | 1379 | C |
| 45 | S2 | 1383 | G |
| 45 | S2 | 1384 | A |
| 45 | S2 | 1385 | G |
| 45 | S2 | 1390 | U |
| 45 | S2 | 1391 | A |
| 45 | S2 | 1392 | U |
| 45 | S2 | 1398 | U |
| 45 | S2 | 1399 | C |
| 45 | S2 | 1401 | A |
| 45 | S2 | 1402 | G |
| 45 | S2 | 1406 | A |
| 45 | S2 | 1409 | G |
| 45 | S2 | 1412 | G |
| 45 | S2 | 1413 | U |
| 45 | S2 | 1414 | U |
| 45 | S2 | 1422 | A |
| 45 | S2 | 1423 | U |
| 45 | S2 | 1424 | A |
| 45 | S2 | 1426 | C |
| 45 | S2 | 1427 | A |
| 45 | S2 | 1428 | G |
| 45 | S2 | 1431 | C |
| 45 | S2 | 1432 | U |
| 45 | S2 | 1433 | G |
| 45 | S2 | 1434 | U |
| 45 | S2 | 1436 | A |
| 45 | S2 | 1439 | C |
| 45 | S2 | 1444 | A |
| 45 | S2 | 1445 | G |
| 45 | S2 | 1448 | G |
| 45 | S2 | 1449 | U |
| 45 | S2 | 1451 | C |
| 45 | S2 | 1452 | U |
| 45 | S2 | 1453 | G |
| 45 | S2 | 1456 | C |
| 45 | S2 | 1457 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1458 | G |
| 45 | S2 | 1459 | C |
| 45 | S2 | 1460 | A |
| 45 | S2 | 1461 | C |
| 45 | S2 | 1465 | C |
| 45 | S2 | 1466 | G |
| 45 | S2 | 1469 | A |
| 45 | S2 | 1471 | A |
| 45 | S2 | 1472 | C |
| 45 | S2 | 1473 | U |
| 45 | S2 | 1474 | G |
| 45 | S2 | 1478 | G |
| 45 | S2 | 1481 | C |
| 45 | S2 | 1482 | C |
| 45 | S2 | 1483 | A |
| 45 | S2 | 1485 | C |
| 45 | S2 | 1486 | G |
| 45 | S2 | 1487 | A |
| 45 | S2 | 1489 | U |
| 45 | S2 | 1491 | U |
| 45 | S2 | 1492 | A |
| 45 | S2 | 1494 | C |
| 45 | S2 | 1496 | U |
| 45 | S2 | 1497 | U |
| 45 | S2 | 1500 | C |
| 45 | S2 | 1501 | C |
| 45 | S2 | 1502 | G |
| 45 | S2 | 1503 | A |
| 45 | S2 | 1504 | G |
| 45 | S2 | 1505 | A |
| 45 | S2 | 1506 | G |
| 45 | S2 | 1507 | G |
| 45 | S2 | 1508 | U |
| 45 | S2 | 1509 | C |
| 45 | S2 | 1510 | U |
| 45 | S2 | 1512 | G |
| 45 | S2 | 1514 | U |
| 45 | S2 | 1516 | A |
| 45 | S2 | 1517 | U |
| 45 | S2 | 1518 | C |
| 45 | S2 | 1521 | G |
| 45 | S2 | 1522 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1523 | G |
| 45 | S2 | 1527 | C |
| 45 | S2 | 1530 | C |
| 45 | S2 | 1535 | U |
| 45 | S2 | 1536 | G |
| 45 | S2 | 1537 | C |
| 45 | S2 | 1539 | G |
| 45 | S2 | 1541 | G |
| 45 | S2 | 1542 | G |
| 45 | S2 | 1543 | A |
| 45 | S2 | 1548 | G |
| 45 | S2 | 1549 | C |
| 45 | S2 | 1550 | A |
| 45 | S2 | 1555 | A |
| 45 | S2 | 1556 | A |
| 45 | S2 | 1557 | U |
| 45 | S2 | 1558 | U |
| 45 | S2 | 1559 | A |
| 45 | S2 | 1560 | U |
| 45 | S2 | 1561 | U |
| 45 | S2 | 1565 | C |
| 45 | S2 | 1567 | U |
| 45 | S2 | 1569 | A |
| 45 | S2 | 1572 | G |
| 45 | S2 | 1573 | A |
| 45 | S2 | 1574 | G |
| 45 | S2 | 1580 | C |
| 45 | S2 | 1582 | U |
| 45 | S2 | 1583 | A |
| 45 | S2 | 1584 | G |
| 45 | S2 | 1586 | A |
| 45 | S2 | 1593 | A |
| 45 | S2 | 1597 | A |
| 45 | S2 | 1598 | U |
| 45 | S2 | 1601 | G |
| 45 | S2 | 1609 | U |
| 45 | S2 | 1611 | A |
| 45 | S2 | 1612 | U |
| 45 | S2 | 1613 | U |
| 45 | S2 | 1614 | A |
| 45 | S2 | 1615 | C |
| 45 | S2 | 1618 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1622 | G |
| 45 | S2 | 1634 | C |
| 45 | S2 | 1647 | U |
| 45 | S2 | 1657 | U |
| 45 | S2 | 1658 | G |
| 45 | S2 | 1662 | G |
| 45 | S2 | 1667 | A |
| 45 | S2 | 1672 | G |
| 45 | S2 | 1677 | C |
| 45 | S2 | 1678 | A |
| 45 | S2 | 1684 | U |
| 45 | S2 | 1685 | G |
| 45 | S2 | 1687 | U |
| 45 | S2 | 1688 | U |
| 45 | S2 | 1689 | A |
| 45 | S2 | 1690 | G |
| 45 | S2 | 1691 | A |
| 45 | S2 | 1694 | A |
| 45 | S2 | 1695 | G |
| 45 | S2 | 1696 | G |
| 45 | S2 | 1697 | G |
| 45 | S2 | 1698 | G |
| 45 | S2 | 1699 | G |
| 45 | S2 | 1700 | C |
| 45 | S2 | 1702 | A |
| 45 | S2 | 1703 | C |
| 45 | S2 | 1704 | U |
| 45 | S2 | 1706 | C |
| 45 | S2 | 1707 | A |
| 45 | S2 | 1708 | U |
| 45 | S2 | 1710 | U |
| 45 | S2 | 1711 | C |
| 45 | S2 | 1713 | G |
| 45 | S2 | 1717 | G |
| 45 | S2 | 1719 | A |
| 45 | S2 | 1720 | G |
| 45 | S2 | 1721 | A |
| 45 | S2 | 1722 | A |
| 45 | S2 | 1723 | U |
| 45 | S2 | 1727 | G |
| 45 | S2 | 1731 | A |
| 45 | S2 | 1733 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1737 | G |
| 45 | S2 | 1738 | U |
| 45 | S2 | 1741 | U |
| 45 | S2 | 1742 | U |
| 45 | S2 | 1755 | A |
| 45 | S2 | 1760 | G |
| 45 | S2 | 1762 | A |
| 45 | S2 | 1766 | A |
| 45 | S2 | 1767 | G |
| 45 | S2 | 1769 | U |
| 45 | S2 | 1780 | G |
| 45 | S2 | 1782 | A |
| 45 | S2 | 1783 | C |
| 45 | S2 | 1792 | G |
| 45 | S2 | 1793 | G |
| 45 | S2 | 1794 | A |
| 45 | S2 | 1795 | U |
| 45 | S2 | 1796 | C |
| 45 | S2 | 1797 | A |
| 45 | S2 | 1799 | U |
| 79 | Ta | 3 | C |
| 79 | Ta | 4 | G |
| 79 | Ta | 5 | G |
| 79 | Ta | 7 | G |
| 79 | Ta | 8 | U |
| 79 | Ta | 9 | G |
| 79 | Ta | 11 | A |
| 79 | Ta | 13 | C |
| 79 | Ta | 14 | A |
| 79 | Ta | 15 | G |
| 79 | Ta | 18 | C |
| 79 | Ta | 19 | G |
| 79 | Ta | 20 | G |
| 79 | Ta | 22 | A |
| 79 | Ta | 24 | C |
| 79 | Ta | 26 | C |
| 79 | Ta | 27 | G |
| 79 | Ta | 29 | C |
| 79 | Ta | 30 | G |
| 79 | Ta | 31 | G |
| 79 | Ta | 32 | G |
| 79 | Ta | 34 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79 | Ta | 35 | A |
| 79 | Ta | 36 | G |
| 79 | Ta | 37 | G |
| 79 | Ta | 40 | C |
| 79 | Ta | 43 | G |
| 79 | Ta | 44 | A |
| 79 | Ta | 47 | G |
| 79 | Ta | 48 | U |
| 79 | Ta | 49 | C |
| 79 | Ta | 51 | U |
| 79 | Ta | 52 | C |
| 79 | Ta | 55 | U |
| 79 | Ta | 56 | U |
| 79 | Ta | 57 | C |
| 79 | Ta | 60 | A |
| 79 | Ta | 62 | C |
| 79 | Ta | 63 | C |
| 79 | Ta | 65 | G |
| 79 | Ta | 66 | C |
| 79 | Ta | 67 | C |
| 79 | Ta | 70 | C |
| 79 | Ta | 71 | G |
| 79 | Ta | 72 | C |
| 79 | Ta | 74 | A |
| 79 | Ta | 75 | C |
| 79 | Ta | 76 | C |
| 80 | Tb | 3 | C |
| 80 | Tb | 6 | G |
| 80 | Tb | 8 | U |
| 80 | Tb | 10 | G |
| 80 | Tb | 11 | A |
| 80 | Tb | 12 | G |
| 80 | Tb | 18 | C |
| 80 | Tb | 20 | G |
| 80 | Tb | 21 | U |
| 80 | Tb | 23 | G |
| 80 | Tb | 24 | C |
| 80 | Tb | 28 | U |
| 80 | Tb | 30 | G |
| 80 | Tb | 32 | G |
| 80 | Tb | 33 | C |
| 80 | Tb | 34 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 80 | Tb | 37 | C |
| 80 | Tb | 38 | A |
| 80 | Tb | 39 | A |
| 80 | Tb | 41 | C |
| 80 | Tb | 43 | G |
| 80 | Tb | 46 | G |
| 80 | Tb | 47 | G |
| 80 | Tb | 48 | U |
| 80 | Tb | 49 | C |
| 80 | Tb | 50 | G |
| 80 | Tb | 51 | U |
| 80 | Tb | 52 | C |
| 80 | Tb | 56 | U |
| 80 | Tb | 57 | C |
| 80 | Tb | 60 | A |
| 80 | Tb | 68 | C |
| 80 | Tb | 70 | C |
| 80 | Tb | 71 | G |
| 80 | Tb | 72 | C |
| 80 | Tb | 73 | A |
| 80 | Tb | 75 | C |
| 80 | Tb | 77 | A |

All (64) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 245 | U |
| 1 | LA | 252 | U |
| 1 | LA | 253 | A |
| 1 | LA | 258 | G |
| 1 | LA | 260 | C |
| 1 | LA | 915 | G |
| 1 | LA | 1106 | C |
| 1 | LA | 1196 | A |
| 1 | LA | 1234 | U |
| 1 | LA | 1237 | C |
| 1 | LA | 1270 | A |
| 1 | LA | 1306 | G |
| 1 | LA | 1342 | A |
| 1 | LA | 1415 | C |
| 1 | LA | 1500 | U |
| 1 | LA | 1682 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | LA | 2095 | A |
| 1 | LA | 2219 | A |
| 1 | LA | 2253 | U |
| 1 | LA | 2259 | U |
| 1 | LA | 2279 | A |
| 1 | LA | 2283 | C |
| 1 | LA | 2443 | C |
| 1 | LA | 2444 | A |
| 1 | LA | 2446 | A |
| 1 | LA | 2447 | G |
| 1 | LA | 2496 | U |
| 1 | LA | 2779 | A |
| 1 | LA | 3070 | U |
| 1 | LA | 3120 | U |
| 1 | LA | 3167 | A |
| 1 | LA | 3227 | C |
| 1 | LA | 3268 | U |
| 1 | LA | 3349 | C |
| 1 | LA | 3380 | U |
| 2 | LB | 116 | C |
| 3 | LC | 14 | C |
| 3 | LC | 85 | G |
| 45 | S2 | 139 | C |
| 45 | S2 | 330 | G |
| 45 | S2 | 387 | A |
| 45 | S2 | 400 | A |
| 45 | S2 | 474 | A |
| 45 | S2 | 511 | A |
| 45 | S2 | 541 | A |
| 45 | S2 | 549 | G |
| 45 | S2 | 550 | A |
| 45 | S2 | 566 | C |
| 45 | S2 | 609 | U |
| 45 | S2 | 639 | U |
| 45 | S2 | 705 | U |
| 45 | S2 | 740 | A |
| 45 | S2 | 828 | U |
| 45 | S2 | 963 | A |
| 45 | S2 | 1143 | A |
| 45 | S2 | 1191 | U |
| 45 | S2 | 1226 | A |
| 45 | S2 | 1253 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | S2 | 1256 | A |
| 45 | S2 | 1274 | C |
| 45 | S2 | 1337 | A |
| 45 | S2 | 1382 | A |
| 45 | S2 | 1450 | U |
| 45 | S2 | 1471 | A |

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

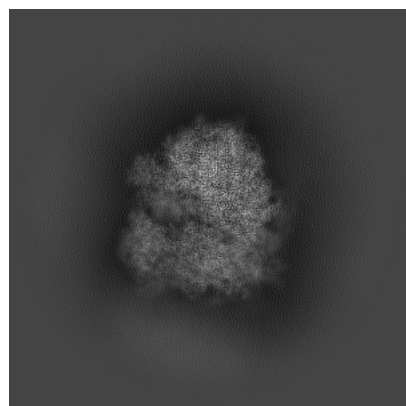
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60097. These allow visual inspection of the internal detail of the map and identification of artifacts.

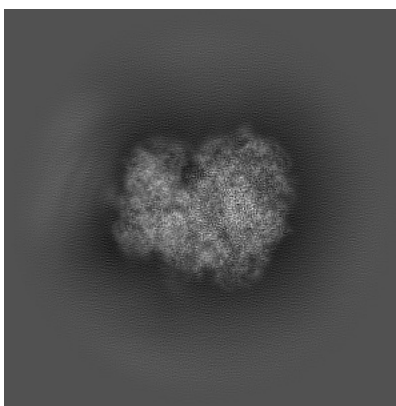
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

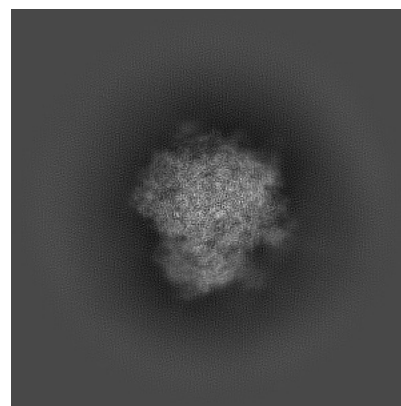
6.1.1 Primary map



X

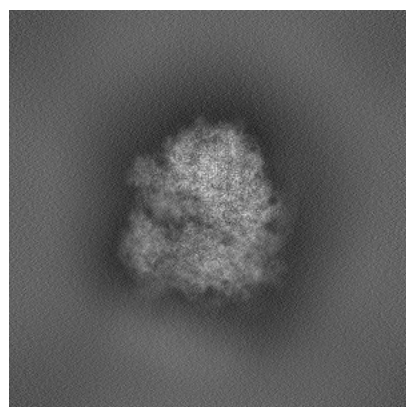


Y

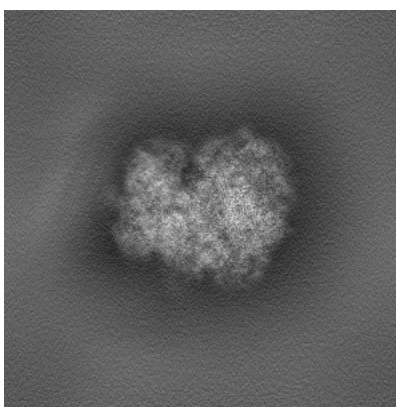


Z

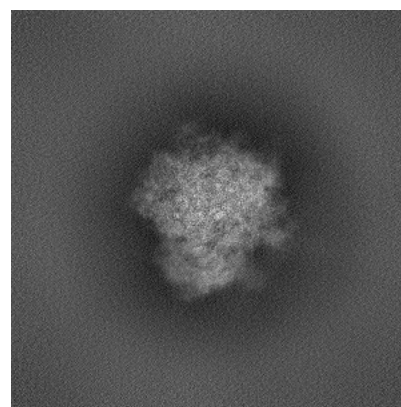
6.1.2 Raw map



X



Y

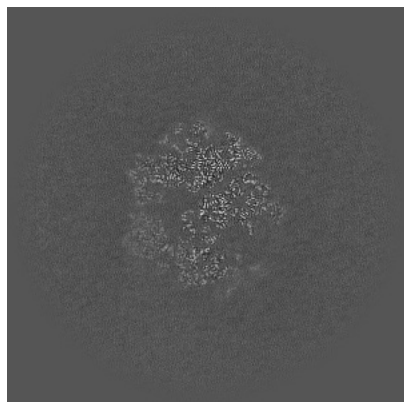


Z

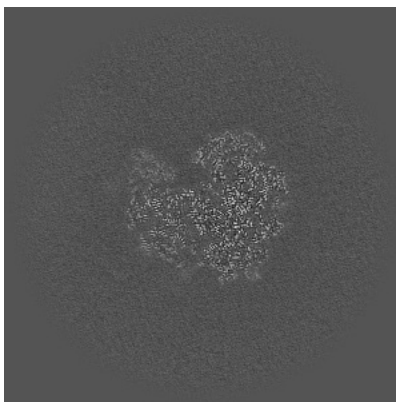
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

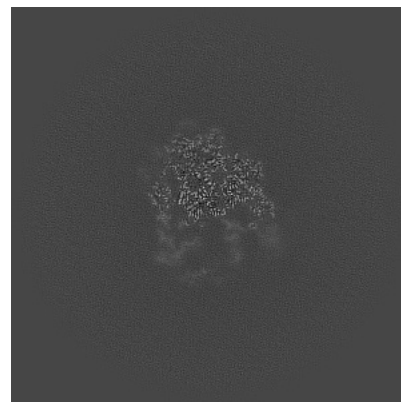
6.2.1 Primary map



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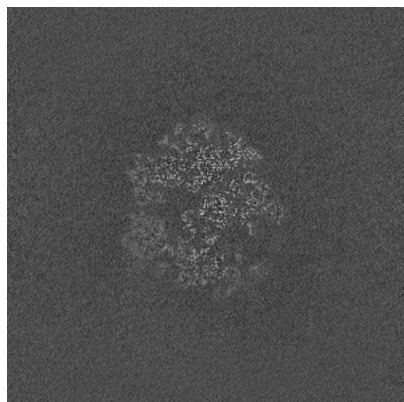


Y Index: 300

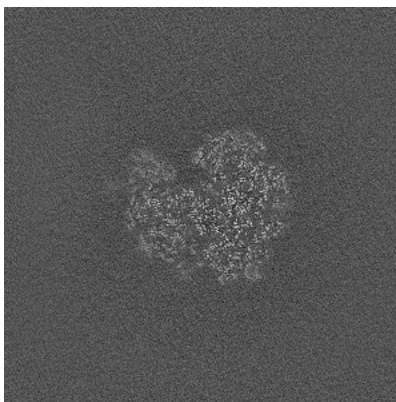


Z Index: 300

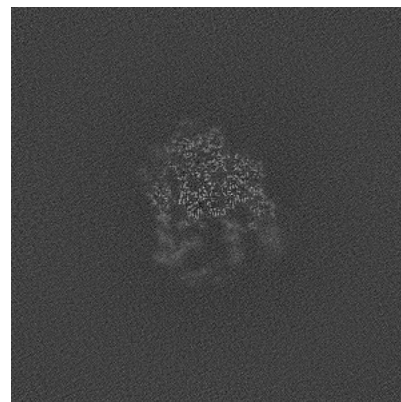
6.2.2 Raw map



X Index: 300



Y Index: 300

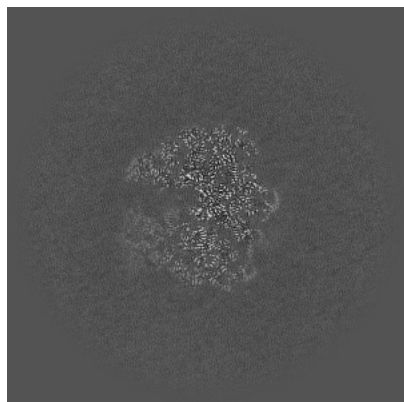


Z Index: 300

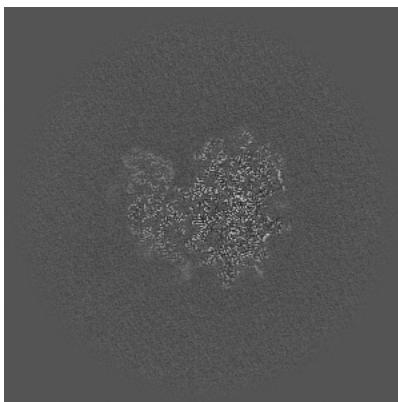
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

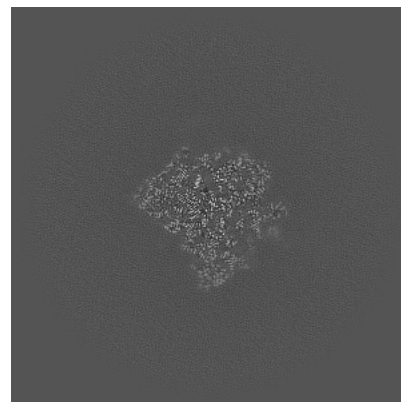
6.3.1 Primary map



X Index: 283

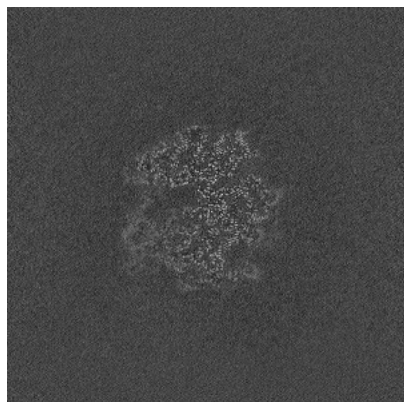


Y Index: 307

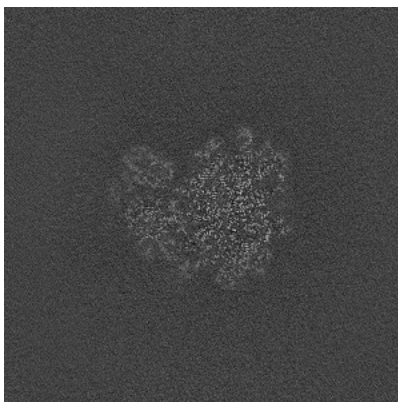


Z Index: 345

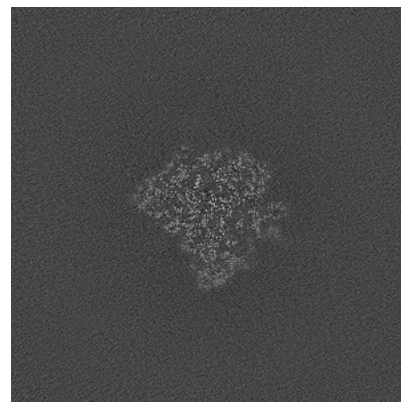
6.3.2 Raw map



X Index: 288



Y Index: 310

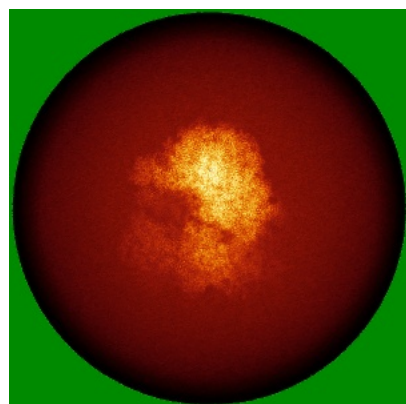


Z Index: 345

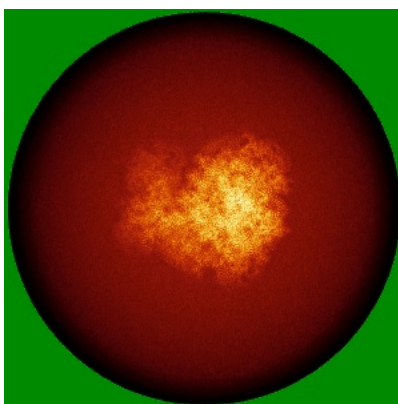
The images above show the largest variance slices of the map in three orthogonal directions.

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

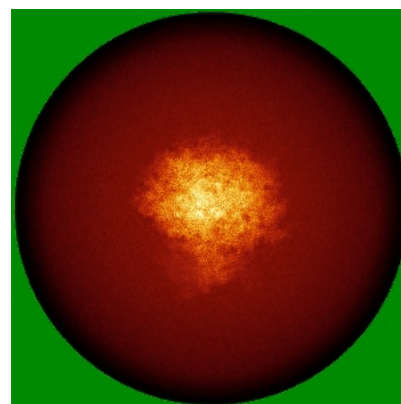
6.4.1 Primary map



X

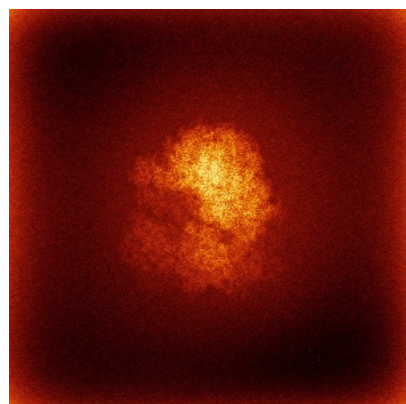


Y

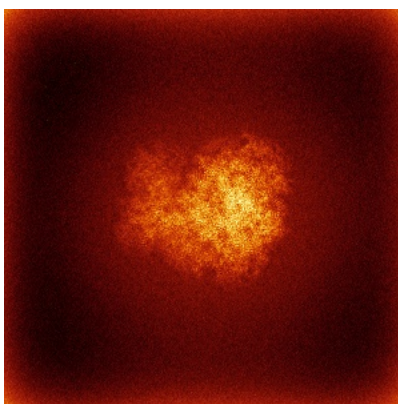


Z

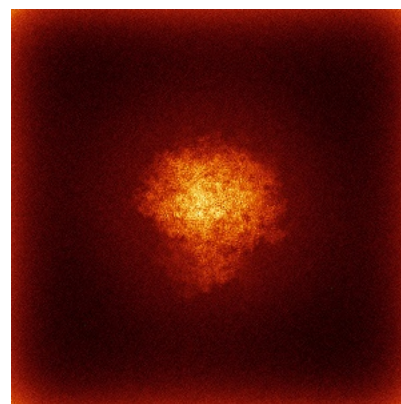
6.4.2 Raw map



X



Y

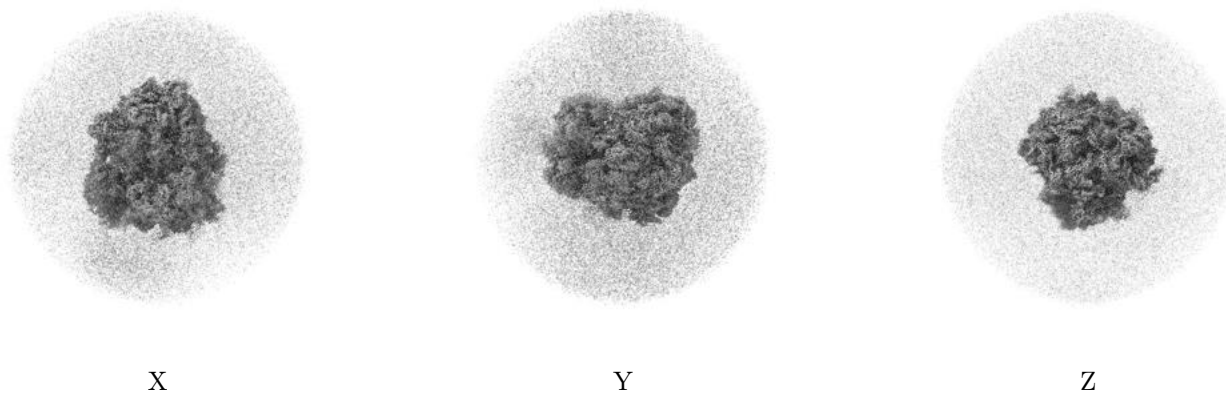


Z

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.

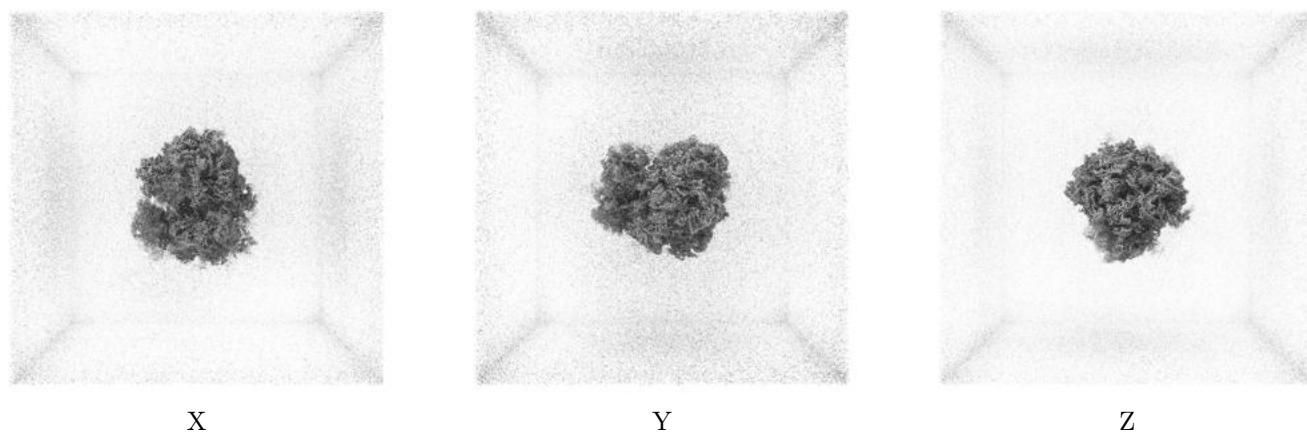
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. 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.

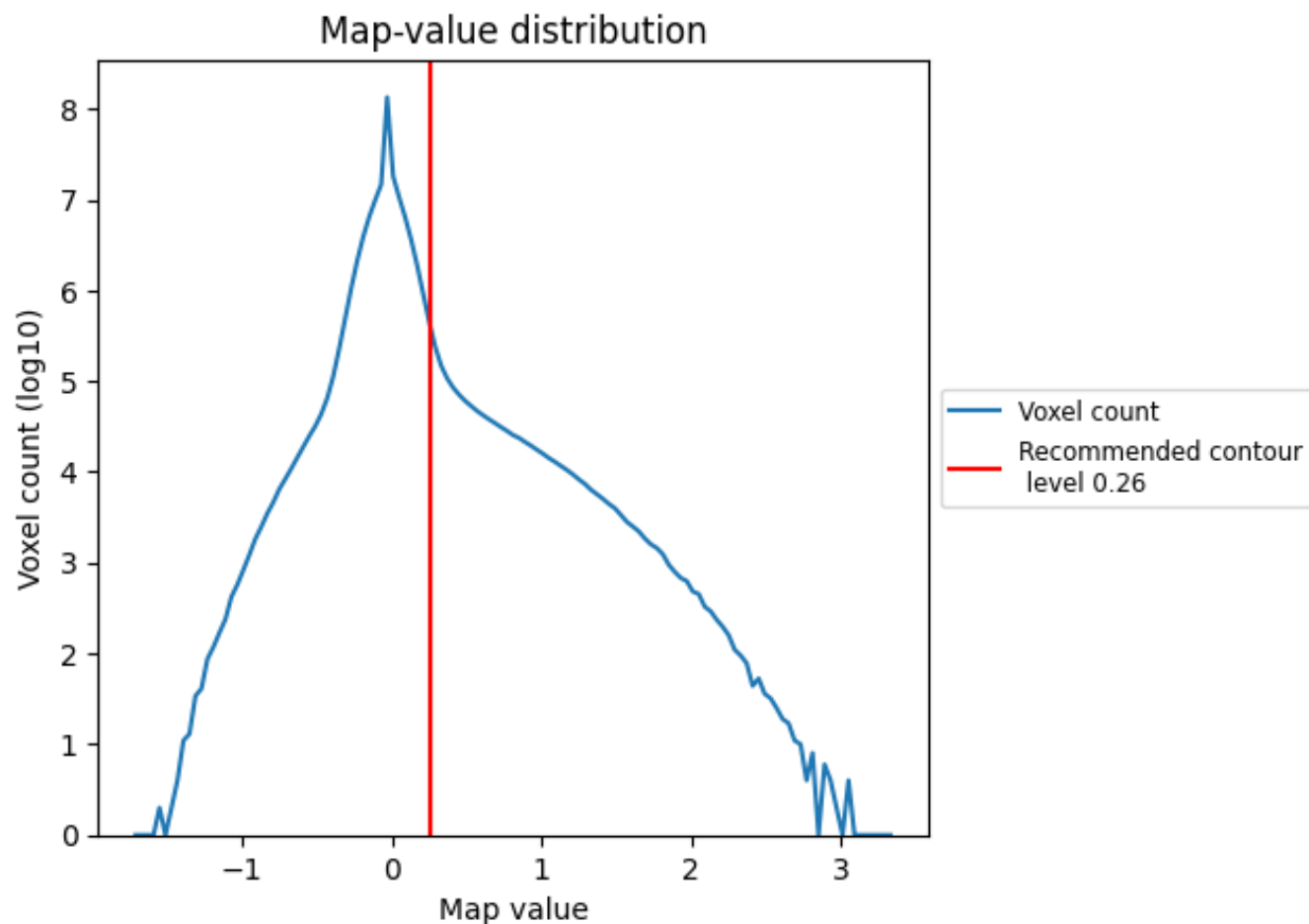
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

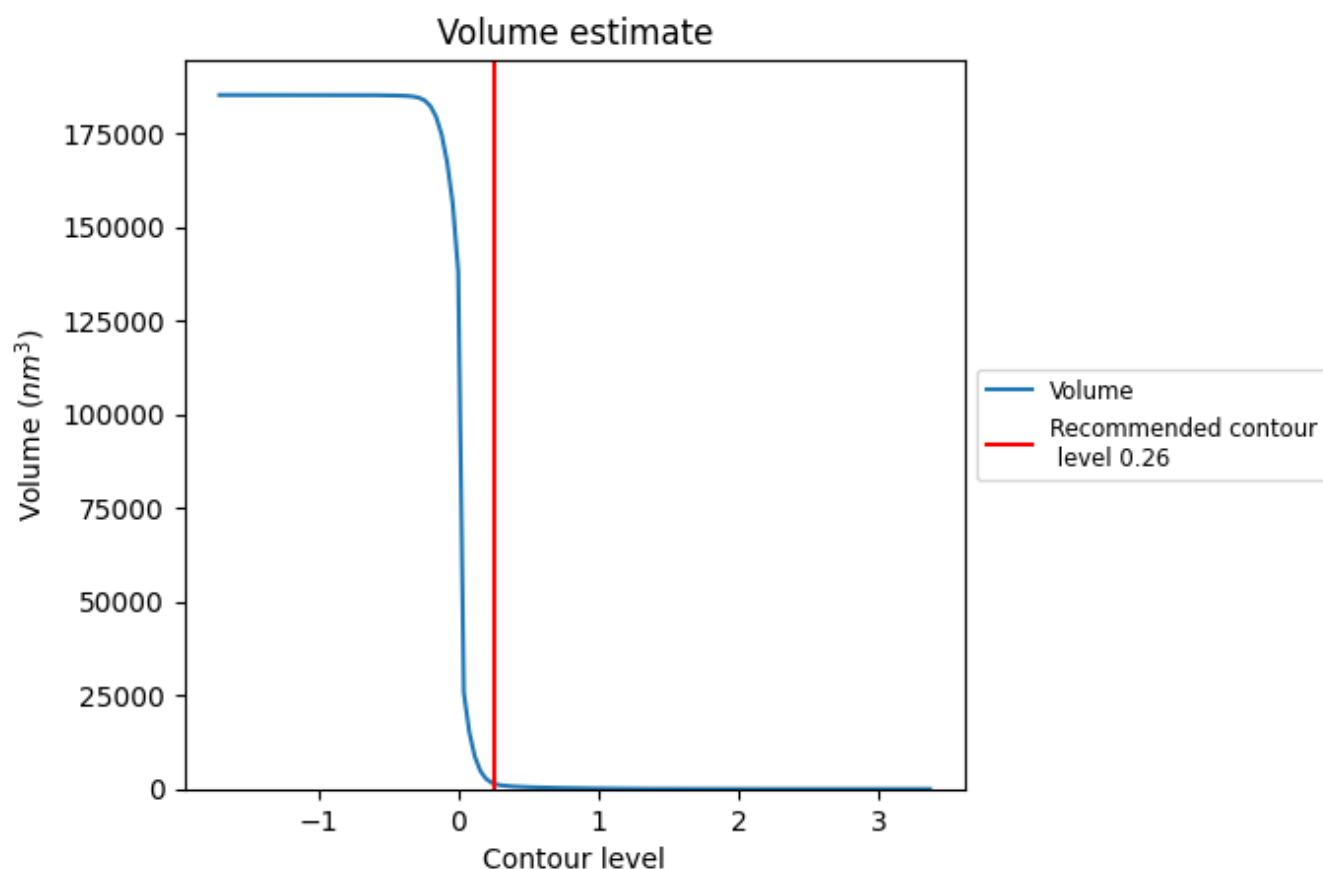
This section contains the results of statistical analysis of the map.

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.

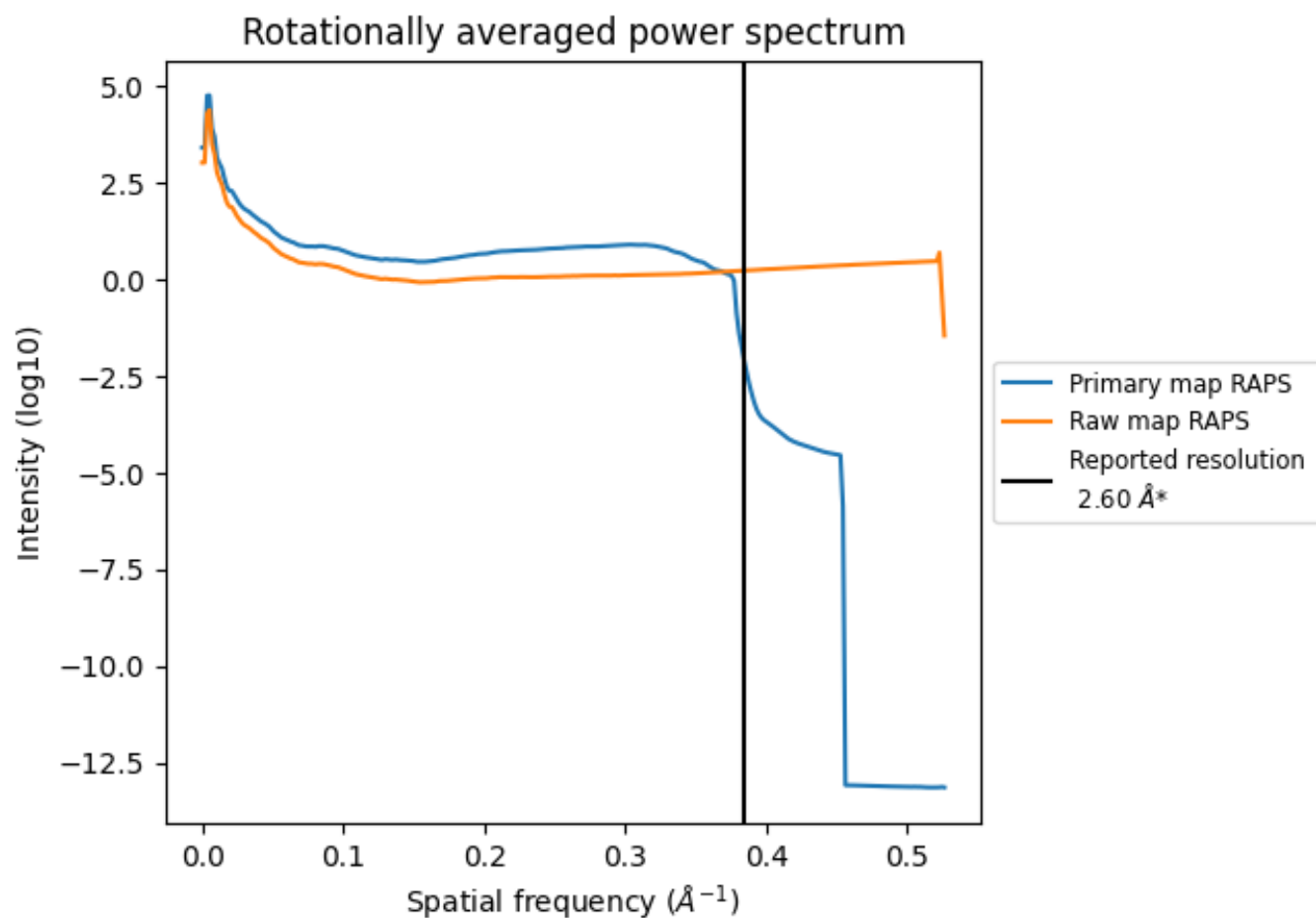
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1368 nm^3 ; this corresponds to an approximate mass of 1236 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 ⓘ

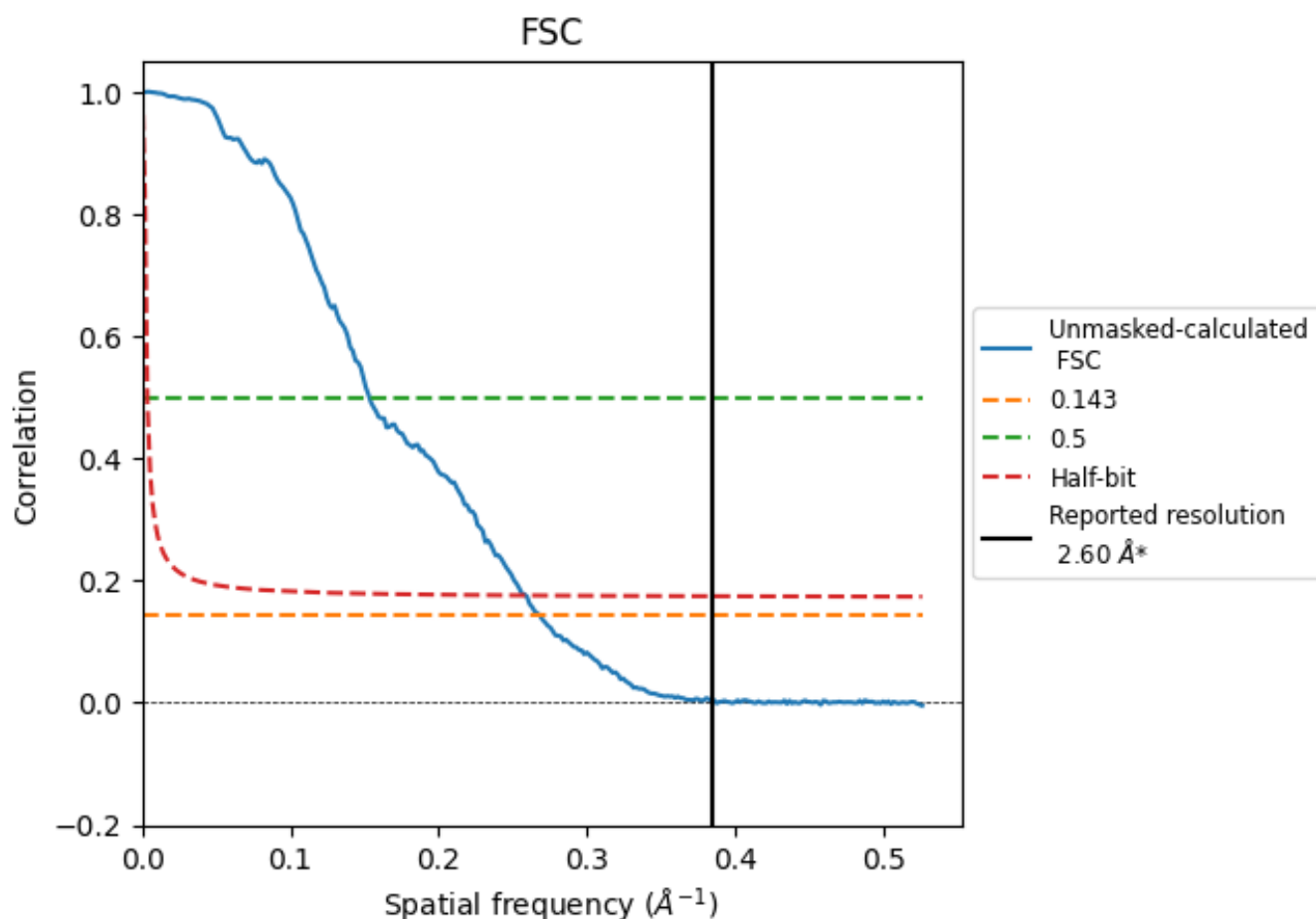


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

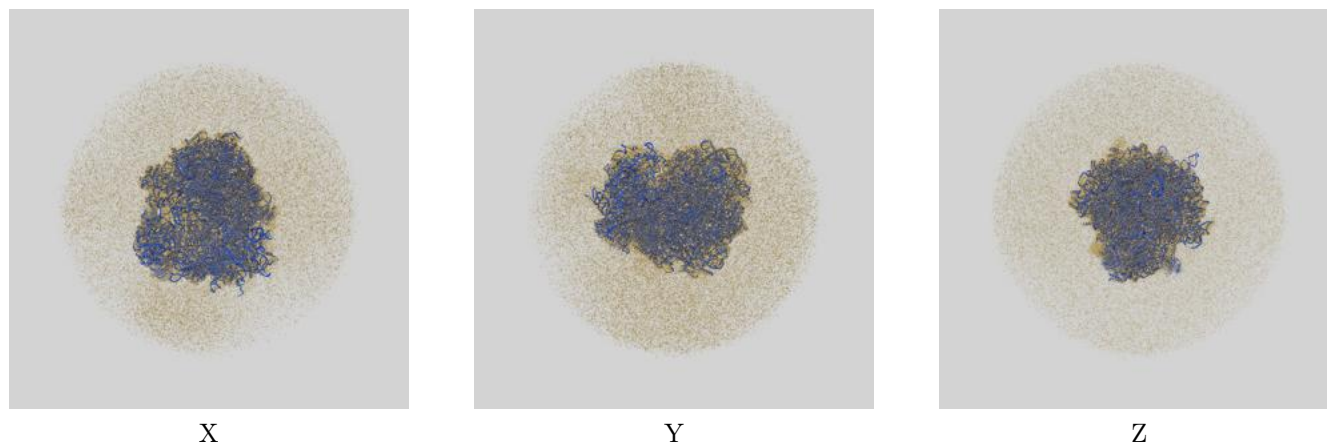
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.60 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.73 | 6.52 | 3.87 |

*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 3.73 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

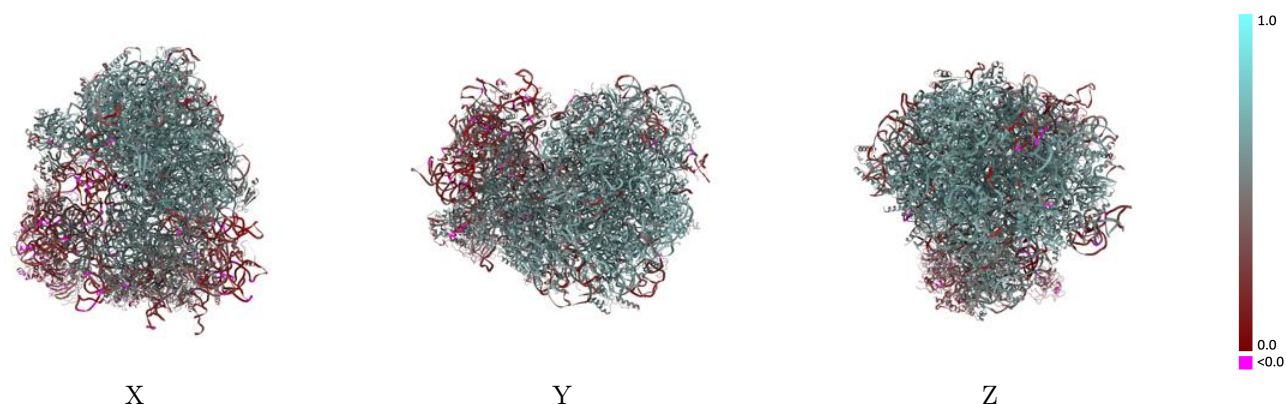
This section contains information regarding the fit between EMDB map EMD-60097 and PDB model 8ZHB. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



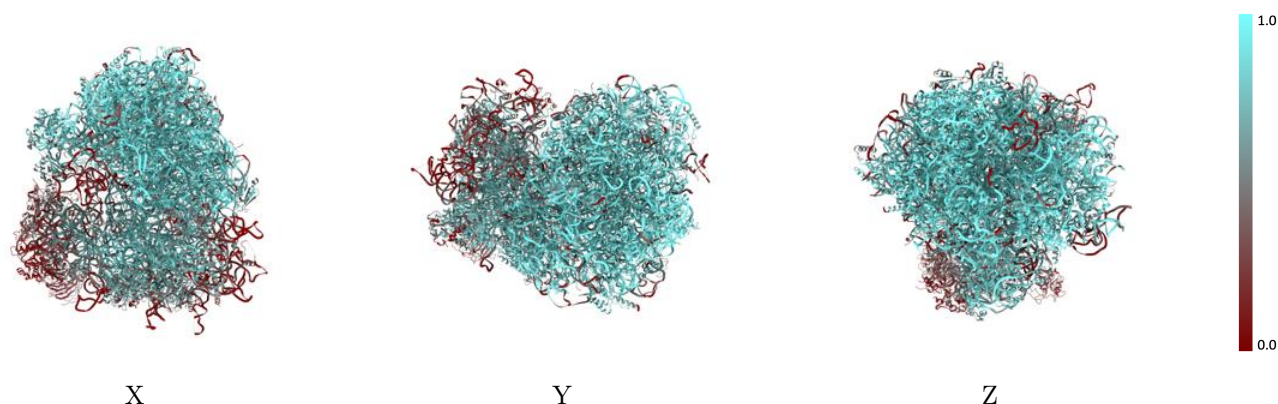
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



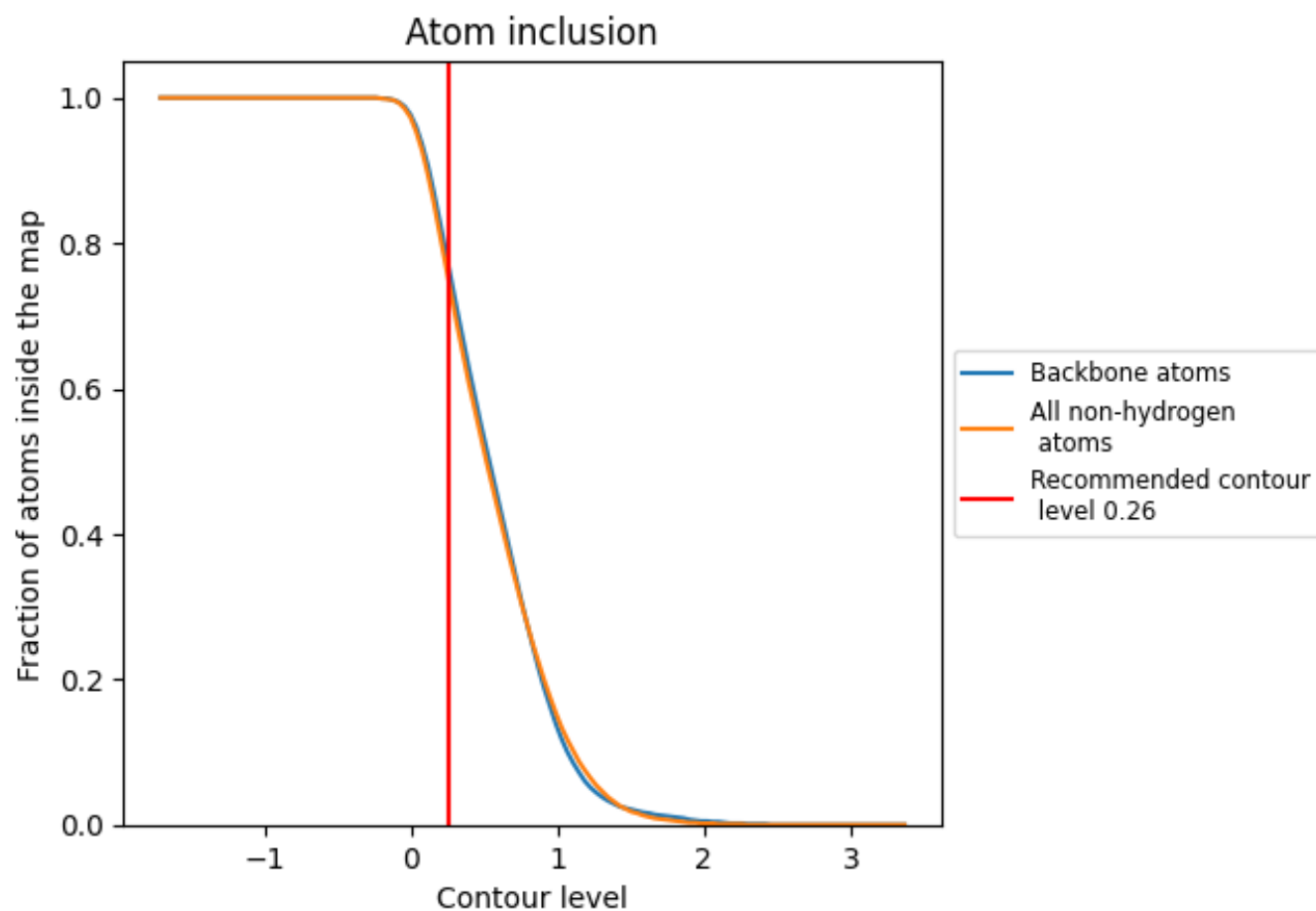
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.26) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7450 |  0.5010 |
| LA |  0.8730 |  0.5600 |
| LB |  0.9030 |  0.5570 |
| LC |  0.9190 |  0.5920 |
| LD |  0.9350 |  0.6380 |
| LE |  0.9030 |  0.6050 |
| LF |  0.9080 |  0.6130 |
| LG |  0.7830 |  0.5400 |
| LH |  0.7970 |  0.5500 |
| LI |  0.9200 |  0.6200 |
| LJ |  0.8190 |  0.5620 |
| LK |  0.8410 |  0.5750 |
| LL |  0.8160 |  0.5790 |
| LM |  0.6630 |  0.4660 |
| LN |  0.8780 |  0.5980 |
| LO |  0.8590 |  0.5750 |
| LP |  0.9450 |  0.6320 |
| LQ |  0.8980 |  0.6050 |
| LR |  0.8900 |  0.6050 |
| LS |  0.9380 |  0.6320 |
| LT |  0.7870 |  0.5450 |
| LU |  0.9030 |  0.6120 |
| LV |  0.9010 |  0.6070 |
| LW |  0.6960 |  0.4940 |
| LX |  0.8890 |  0.6150 |
| LY |  0.9020 |  0.6160 |
| LZ |  0.8570 |  0.6010 |
| La |  0.9100 |  0.6170 |
| Lb |  0.8590 |  0.5870 |
| Lc |  0.9360 |  0.6300 |
| Ld |  0.8520 |  0.5850 |
| Le |  0.8650 |  0.5920 |
| Lf |  0.8320 |  0.5780 |
| Lg |  0.8780 |  0.6090 |
| Lh |  0.9390 |  0.6330 |













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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Li |  0.8850 |  0.6070 |
| Lj |  0.8820 |  0.5940 |
| Lk |  0.8370 |  0.5580 |
| Ll |  0.9660 |  0.6460 |
| Lm |  0.6490 |  0.4910 |
| Ln |  0.9130 |  0.6240 |
| Lo |  0.8810 |  0.6060 |
| Lp |  0.8460 |  0.6160 |
| Lq |  0.8960 |  0.6160 |
| Lr |  0.8710 |  0.6280 |
| S2 |  0.6190 |  0.3850 |
| SA |  0.3760 |  0.3680 |
| SB |  0.2820 |  0.3250 |
| SC |  0.2740 |  0.2810 |
| SD |  0.0380 |  0.1800 |
| SE |  0.3460 |  0.3000 |
| SF |  0.3070 |  0.3280 |
| SG |  0.4600 |  0.3990 |
| SH |  0.3370 |  0.3190 |
| SI |  0.2980 |  0.3150 |
| SJ |  0.3020 |  0.3170 |
| SK |  0.1230 |  0.2190 |
| SL |  0.3340 |  0.3290 |
| SM |  0.4440 |  0.3690 |
| SN |  0.0660 |  0.1860 |
| SO |  0.1650 |  0.2310 |
| SP |  0.6650 |  0.4900 |
| SQ |  0.7030 |  0.5060 |
| SR |  0.7710 |  0.5580 |
| SS |  0.5860 |  0.4520 |
| ST |  0.3940 |  0.3540 |
| SU |  0.5800 |  0.4630 |
| SV |  0.5810 |  0.4360 |
| SW |  0.5180 |  0.3950 |
| SX |  0.7170 |  0.5210 |
| SY |  0.8050 |  0.5670 |
| SZ |  0.7800 |  0.5420 |
| Sa |  0.7370 |  0.5330 |
| Sb |  0.8940 |  0.6110 |
| Sc |  0.7000 |  0.4990 |
| Sd |  0.4770 |  0.3820 |
| Se |  0.8350 |  0.5660 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Sf |  0.7260 |  0.4980 |
| Sg |  0.4440 |  0.3480 |
| Ta |  0.2480 |  0.1590 |
| Tb |  0.3430 |  0.2300 |
| mR |  0.5870 |  0.3670 |