# Full wwPDB EM Validation Report

Mar 9, 2026 – 01:13 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 8BTD / pdb_00008btd |
| EMDB ID | : | EMD-16228 |
| Title | : | Giardia Ribosome in PRE-T Hybrid State (D1) |
| Authors | : | Majumdar, S.; Emmerich, A.G.; Sanyal, S. |
| Deposited on | : | 2022-11-28 |
| Resolution | : | 4.90 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

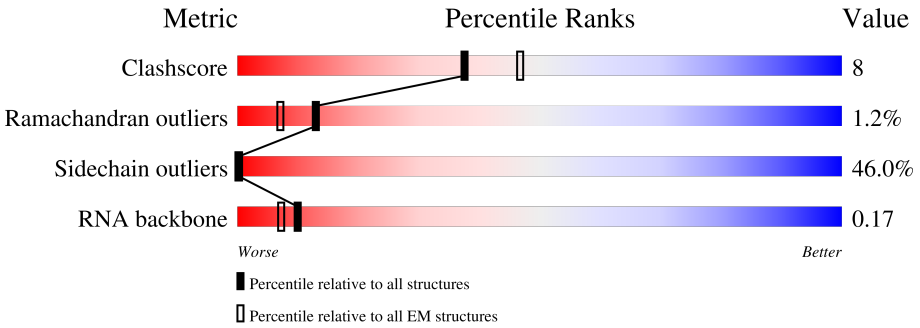
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025)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

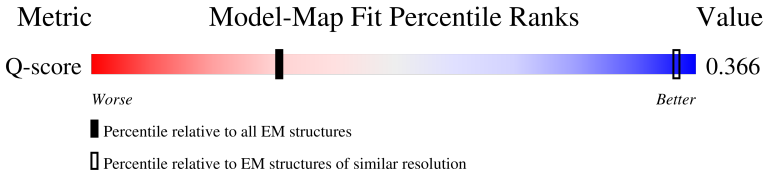
# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.90 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 1274 ( 4.40 - 5.40 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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 | 251 | 32% 52% 38% 8% |
| 2 | LB | 379 | 21% 54% 35% 10% |
| 3 | LC | 316 | 25% 53% 34% 12% |

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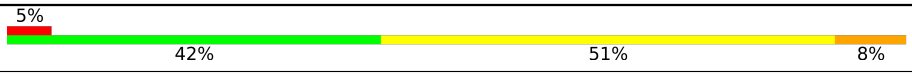
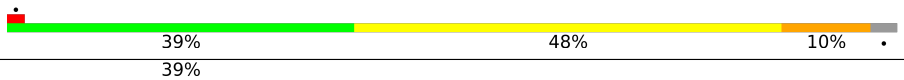
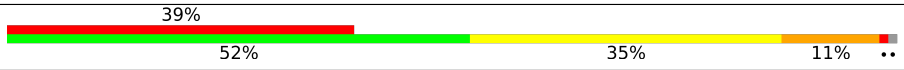
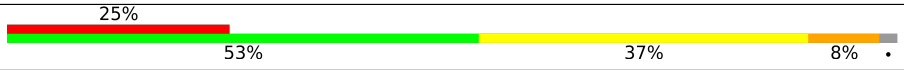
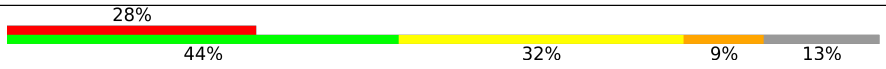
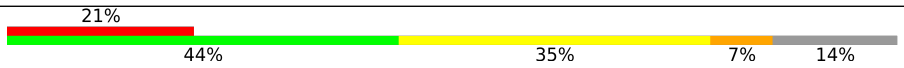
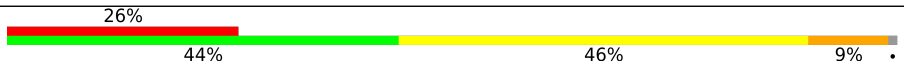
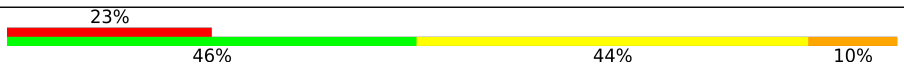
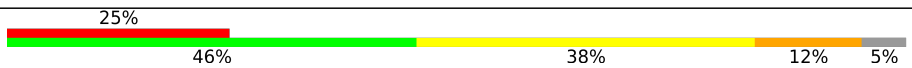
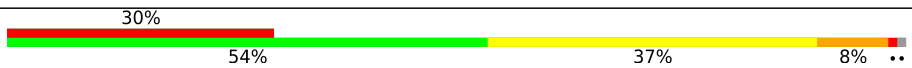
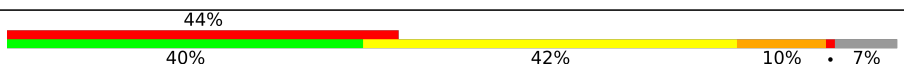
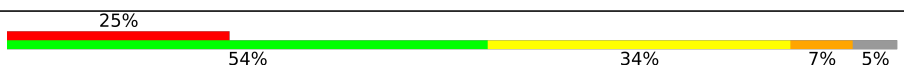
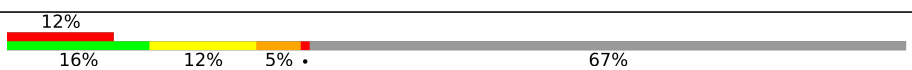
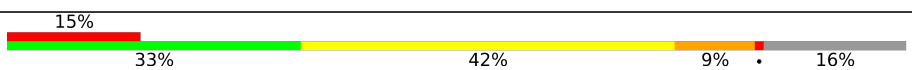
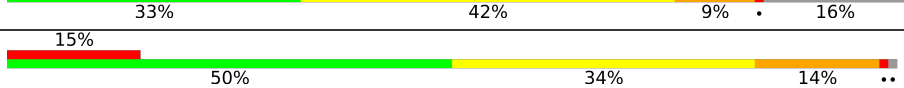
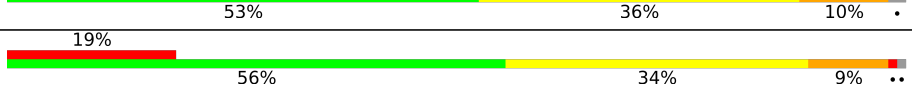
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | LD | 142 |   |
| 5 | LE | 121 |   |
| 6 | LF | 297 |   |
| 7 | LG | 51 |   |
| 8 | LH | 235 | |
| 9 | LI | 225 |   |
| 10 | LJ | 185 | |
| 11 | LK | 210 | |
| 12 | LL | 173 | |
| 13 | LM | 234 |   |
| 14 | LN | 131 |   |
| 15 | LO | 204 |   |
| 16 | LP | 197 | |
| 17 | LQ | 164 |   |
| 18 | LR | 179 |   |
| 19 | LS | 196 | |
| 20 | LT | 173 | |
| 21 | LU | 159 | |
| 22 | LV | 124 |   |
| 23 | LW | 142 |   |
| 24 | LX | 189 |   |
| 25 | LY | 141 |   |
| 26 | LZ | 135 |   |
| 27 | La | 135 | |
| 28 | Lb | 149 |   |

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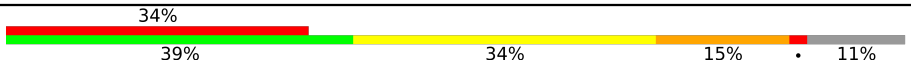
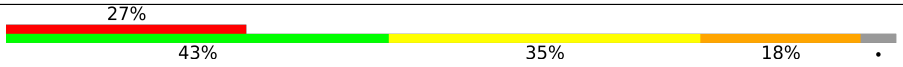
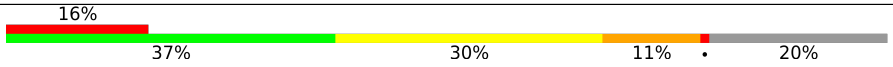
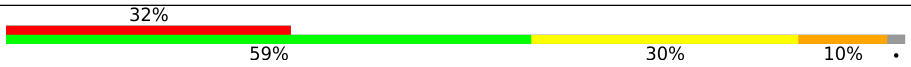
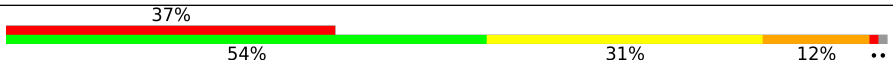
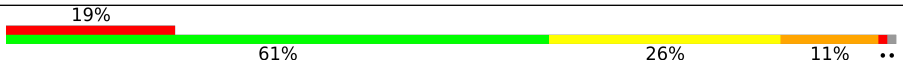
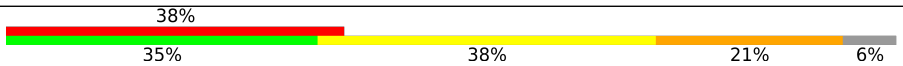
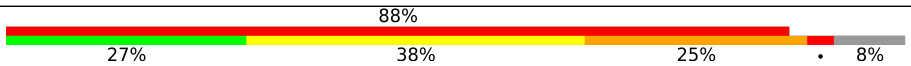
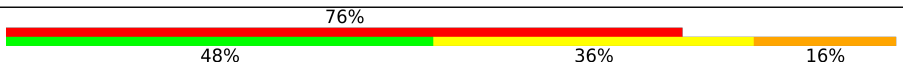
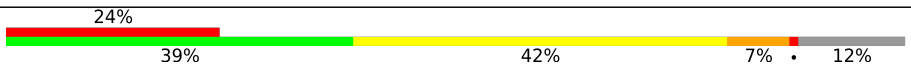
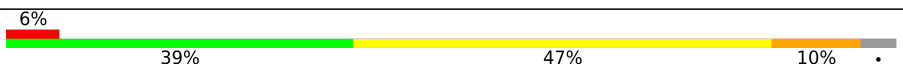
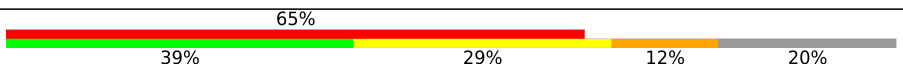
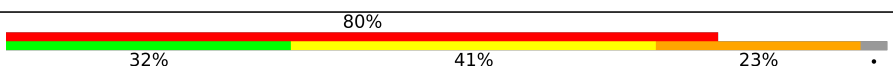
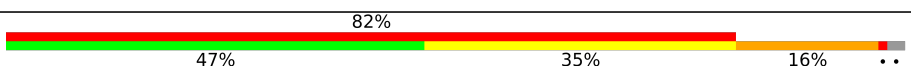
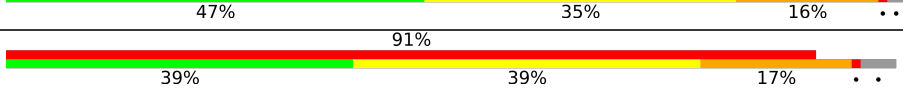
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | Lc | 62 |   |
| 30 | Ld | 109 | |
| 31 | Le | 106 | |
| 32 | Lf | 136 |   |
| 33 | Lg | 123 |   |
| 34 | Lh | 120 | |
| 35 | Li | 124 |   |
| 36 | Lj | 90 |   |
| 37 | Lk | 89 |   |
| 38 | Ll | 77 |   |
| 39 | Ln | 217 |   |
| 40 | Lo | 25 |   |
| 41 | Lp | 106 |   |
| 42 | Lq | 94 | |
| 43 | Ls | 127 | |
| 44 | Lt | 2697 |   |
| 45 | SA | 245 |   |
| 46 | SB | 242 | |
| 47 | SC | 217 | |
| 48 | SD | 248 | |
| 49 | SE | 268 |   |
| 50 | SF | 190 |   |
| 51 | SG | 248 |   |
| 52 | SH | 190 | |
| 53 | SI | 174 | |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | SJ | 130 | 67% 37% 47% 15% |
| 55 | SK | 189 | 77% 39% 38% 15% 7% |
| 56 | SL | 134 | 65% 41% 29% 10% 20% |
| 57 | SM | 154 | 87% 44% 39% 16% |
| 58 | SO | 144 | 69% 44% 40% 12% |
| 59 | SP | 154 | 70% 52% 34% 11% |
| 60 | SQ | 145 | 48% 50% 30% 7% 12% |
| 61 | SR | 145 | 67% 30% 37% 12% 20% |
| 62 | ST | 158 | 80% 34% 46% 15% |
| 63 | SU | 137 | 70% 39% 34% 15% 12% |
| 64 | SV | 154 | 69% 42% 36% 14% 5% |
| 65 | SW | 139 | 81% 42% 41% 14% |
| 66 | SX | 126 | 71% 37% 37% 6% 20% |
| 67 | SY | 89 | 84% 44% 38% 15% |
| 68 | Sb | 132 | 78% 31% 44% 14% 9% |
| 69 | Sc | 88 | 70% 28% 36% 20% 15% |
| 70 | Sd | 109 | 60% 42% 39% 17% |
| 71 | Se | 81 | 78% 38% 46% 14% |
| 72 | Sg | 64 | 81% 20% 58% 19% |
| 73 | Sh | 51 | 69% 37% 39% 22% |
| 74 | Sj | 69 | 84% 42% 35% 19% |
| 75 | St | 1454 | 32% 32% 53% 15% |
| 76 | u | 75 | 48% 36% 48% 16% |
| 77 | v | 75 | 95% 11% 71% 19% |
| 78 | y | 11 | 64% 27% 45% 18% 9% |

# 2 Entry composition

There are 78 unique types of molecules in this entry. The entry contains 178901 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | LA | 250 | 1886 | 1163 | 389 | 322 | 12 | 0 | 0 |

- Molecule 2 is a protein called Ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | LB | 378 | 2987 | 1886 | 566 | 514 | 21 | 0 | 0 |

- Molecule 3 is a protein called Ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | LC | 315 | 2454 | 1543 | 476 | 426 | 9 | 0 | 0 |

- Molecule 4 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | LD | 142 | 3038 | 1350 | 563 | 983 | 142 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | LE | 117 | 2502 | 1116 | 457 | 812 | 117 | 0 | 0 |

- Molecule 6 is a protein called Ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | LF | 293 | 2355 | 1490 | 439 | 418 | 8 | 0 | 0 |

- Molecule 7 is a protein called Ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 7 | LG | 50 | Total | C | N | O | 0 | 0 |
| | | | 439 | 281 | 94 | 64 | | |

- Molecule 8 is a protein called Ribosomal protein L7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | LH | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1742 | 1106 | 317 | 314 | 5 | | |

- Molecule 9 is a protein called Ribosomal protein L7a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | LI | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1554 | 989 | 284 | 276 | 5 | | |

- Molecule 10 is a protein called Ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | LJ | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1452 | 917 | 264 | 261 | 10 | | |

- Molecule 11 is a protein called Ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | LK | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1671 | 1046 | 330 | 286 | 9 | | |

- Molecule 12 is a protein called Ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | LL | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1349 | 850 | 250 | 244 | 5 | | |

- Molecule 13 is a protein called Ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | LM | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1605 | 999 | 325 | 274 | 7 | | |

- Molecule 14 is a protein called Ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | LN | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1024 | 649 | 186 | 183 | 6 | | |

- Molecule 15 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | LO | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1708 | 1080 | 357 | 265 | 6 | | |

- Molecule 16 is a protein called Ribosomal protein L13a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | LP | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1578 | 994 | 306 | 266 | 12 | | |

- Molecule 17 is a protein called Ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | LQ | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 793 | 242 | 215 | 4 | | |

- Molecule 18 is a protein called Ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | LR | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1402 | 871 | 279 | 243 | 9 | | |

- Molecule 19 is a protein called Ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | LS | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1592 | 983 | 334 | 270 | 5 | | |

- Molecule 20 is a protein called Ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | LT | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1423 | 899 | 272 | 243 | 9 | | |

- Molecule 21 is a protein called Ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | LU | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1264 | 789 | 260 | 208 | 7 | | |

- Molecule 22 is a protein called Ribosomal protein L22e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | LV | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 935 | 589 | 157 | 187 | 2 | | |

- Molecule 23 is a protein called Ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | LW | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1029 | 648 | 196 | 180 | 5 | | |

- Molecule 24 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | LX | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 340 | 109 | 82 | 7 | | |

- Molecule 25 is a protein called Ribosomal protein L23A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | LY | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 962 | 619 | 174 | 166 | 3 | | |

- Molecule 26 is a protein called Ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | LZ | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1076 | 665 | 219 | 184 | 8 | | |

- Molecule 27 is a protein called Ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | La | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1051 | 660 | 198 | 186 | 7 | | |

- Molecule 28 is a protein called Ribosomal protein L27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | Lb | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1201 | 759 | 240 | 199 | 3 | | |

- Molecule 29 is a protein called Ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | Lc | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 456 | 275 | 103 | 76 | 2 | | |

- Molecule 30 is a protein called Ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | Ld | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 731 | 461 | 127 | 139 | 4 | | |

- Molecule 31 is a protein called Ribosomal protein L31B.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 31 | Le | 100 | Total | C | N | O | 0 | 0 |
| | | | 818 | 518 | 158 | 142 | | |

- Molecule 32 is a protein called Ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | Lf | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1077 | 683 | 215 | 173 | 6 | | |

- Molecule 33 is a protein called Ribosomal protein L35a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | Lg | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 778 | 498 | 147 | 130 | 3 | | |

- Molecule 34 is a protein called Ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Lh | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 914 | 563 | 189 | 158 | 4 | | |

- Molecule 35 is a protein called Ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | Li | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 983 | 623 | 192 | 163 | 5 | | |

- Molecule 36 is a protein called Ribosomal protein L36-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | Lj | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 731 | 462 | 146 | 119 | 4 | | |

- Molecule 37 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | Lk | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 711 | 435 | 152 | 117 | 7 | | |

- Molecule 38 is a protein called Ribosomal protein L38e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | Ll | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 558 | 353 | 99 | 102 | 4 | | |

- Molecule 39 is a protein called Ribosomal protein L10a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | Ln | 200 | Total | C | N | O | S | 0 | 0 |
| | | | 1592 | 1025 | 278 | 284 | 5 | | |

- Molecule 40 is a protein called Ribosomal protein L41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | Lo | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 227 | 140 | 57 | 27 | 3 | | |

- Molecule 41 is a protein called Ribosomal protein L44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | Lp | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 767 | 478 | 159 | 125 | 5 | | |

- Molecule 42 is a protein called Ribosomal protein L37a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | Lq | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 708 | 437 | 144 | 120 | 7 | | |

- Molecule 43 is a protein called Ubiquitin/Ribosomal protein L40e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | Ls | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 388 | 234 | 83 | 64 | 7 | | |

- Molecule 44 is a RNA chain called Large Subunit rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | Lt | 2593 | Total | C | N | O | P | 0 | 0 |
| | | | 55643 | 24727 | 10311 | 18012 | 2593 | | |

- Molecule 45 is a protein called Ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | SA | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1578 | 1018 | 276 | 276 | 8 | | |

- Molecule 46 is a protein called Ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | SB | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1059 | 302 | 301 | 5 | | |

- Molecule 47 is a protein called Ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | SC | 210 | Total | C | N | O | S | 0 | 0 |
| | | | 1665 | 1050 | 306 | 293 | 16 | | |

- Molecule 48 is a protein called Ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | SD | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1868 | 1180 | 349 | 326 | 13 | | |

- Molecule 49 is a protein called Ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | SE | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2085 | 1333 | 384 | 356 | 12 | | |

- Molecule 50 is a protein called Ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | SF | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1442 | 896 | 275 | 262 | 9 | | |

- Molecule 51 is a protein called Ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | SG | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1889 | 1188 | 360 | 331 | 10 | | |

- Molecule 52 is a protein called Ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | SH | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1481 | 948 | 258 | 268 | 7 | | |

- Molecule 53 is a protein called Ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | SI | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1357 | 850 | 260 | 244 | 3 | | |

- Molecule 54 is a protein called Ribosomal protein S15A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | SJ | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1031 | 659 | 192 | 177 | 3 | | |

- Molecule 55 is a protein called Ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | SK | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1423 | 889 | 281 | 247 | 6 | | |

- Molecule 56 is a protein called Ribosomal protein S10B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | SL | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 568 | 147 | 158 | 3 | | |

- Molecule 57 is a protein called Ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | SM | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1265 | 802 | 248 | 209 | 6 | | |

- Molecule 58 is a protein called Ribosomal protein S23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | SO | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1089 | 688 | 216 | 182 | 3 | | |

- Molecule 59 is a protein called Ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | SP | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 762 | 225 | 202 | 4 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| SP | 6 | ALA | SER | conflict | UNP A8BE02 |
| SP | 7 | PRO | LYS | conflict | UNP A8BE02 |
| SP | 38 | TYR | CYS | conflict | UNP A8BE02 |
| SP | 49 | GLN | ARG | conflict | UNP A8BE02 |

- Molecule 60 is a protein called Ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | SQ | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 926 | 569 | 190 | 164 | 3 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| SQ | 110 | GLY | GLN | conflict | UNP E2RU83 |
| SQ | 112 | SER | GLY | conflict | UNP E2RU83 |
| SQ | 113 | ALA | SER | conflict | UNP E2RU83 |
| SQ | 115 | GLY | ALA | conflict | UNP E2RU83 |

- Molecule 61 is a protein called Ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | SR | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 943 | 601 | 184 | 150 | 8 | | |

- Molecule 62 is a protein called Ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | ST | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1180 | 736 | 229 | 212 | 3 | | |

- Molecule 63 is a protein called Ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | SU | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 965 | 598 | 184 | 178 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| SU | 104 | THR | ALA | conflict | UNP A8BRG5 |

- Molecule 64 is a protein called Ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | SV | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 715 | 238 | 203 | 6 | | |

- Molecule 65 is a protein called Ribosomal protein S19e.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | SW | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1080 | 686 | 204 | 187 | 3 | | |

- Molecule 66 is a protein called Ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | SX | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 802 | 511 | 146 | 140 | 5 | | |

- Molecule 67 is a protein called Ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | SY | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 651 | 403 | 120 | 122 | 6 | | |

- Molecule 68 is a protein called Ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | Sb | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 952 | 604 | 179 | 163 | 6 | | |

- Molecule 69 is a protein called Ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | Sc | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 597 | 377 | 107 | 107 | 6 | | |

- Molecule 70 is a protein called Ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | Sd | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 544 | 184 | 149 | 7 | | |

- Molecule 71 is a protein called Ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | Se | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 629 | 397 | 110 | 116 | 6 | | |

- Molecule 72 is a protein called Ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | Sg | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 505 | 311 | 100 | 92 | 2 | | |

- Molecule 73 is a protein called Ribosomal protein S29A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 73 | Sh | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 417 | 264 | 80 | 67 | 6 | | |

- Molecule 74 is a protein called Ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 74 | Sj | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 543 | 341 | 114 | 87 | 1 | | |

- Molecule 75 is a RNA chain called Small Subunit rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 75 | St | 1454 | Total | C | N | O | P | 0 | 0 |
| | | | 31176 | 13861 | 5772 | 10090 | 1453 | | |

- Molecule 76 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 76 | u | 75 | Total | C | N | O | P | 0 | 0 |
| | | | 1604 | 717 | 298 | 515 | 74 | | |

- Molecule 77 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 77 | v | 75 | Total | C | N | O | P | 0 | 0 |
| | | | 1602 | 716 | 296 | 516 | 74 | | |

- Molecule 78 is a RNA chain called mRNA.

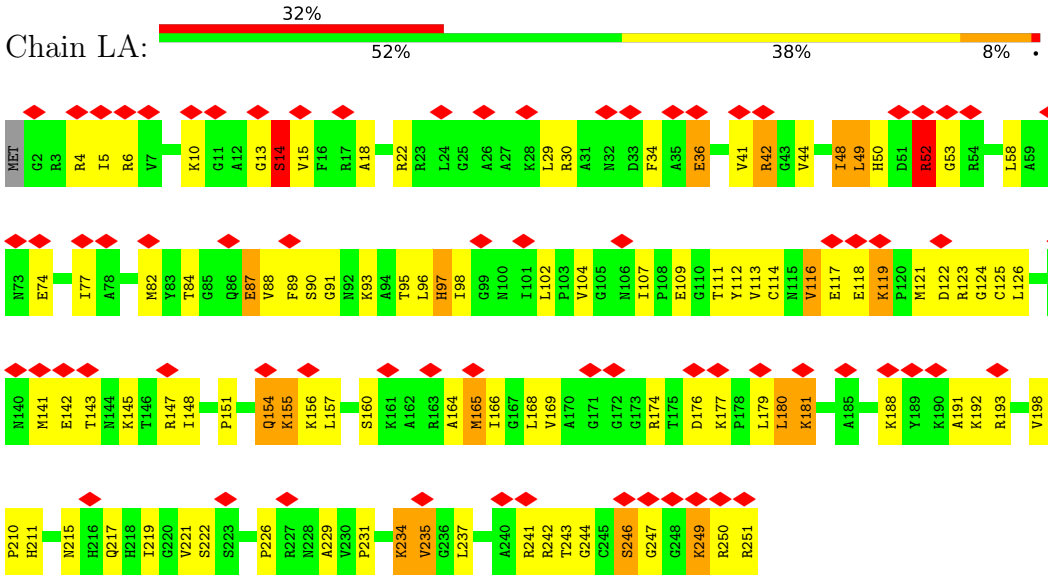
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | y | 10 | Total | C | N | O | P | 0 | 0 |
| | | | 221 | 99 | 47 | 65 | 10 | | |

# 3 Residue-property plots (i)

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

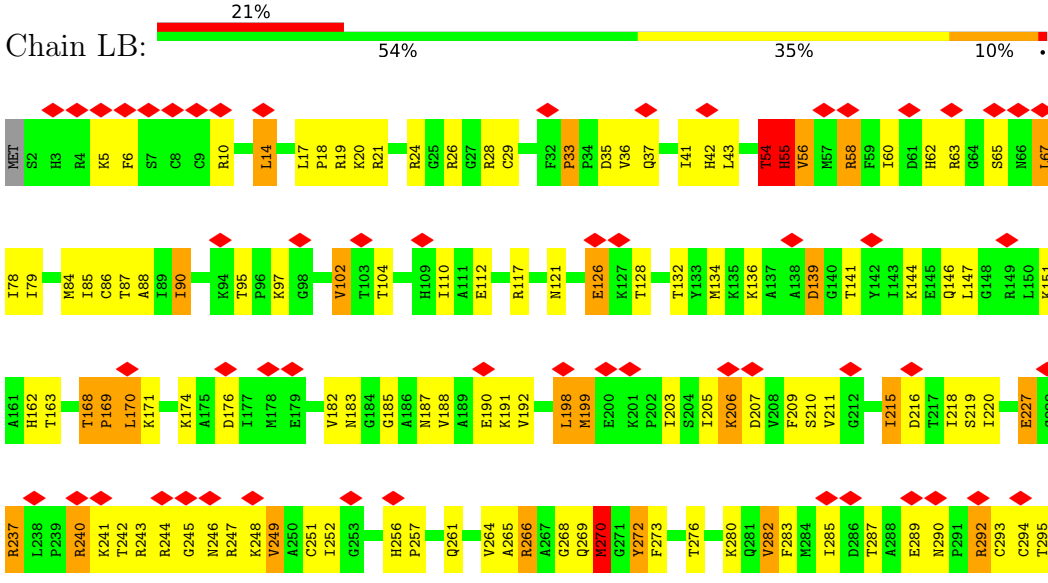
• Molecule 1: Ribosomal protein L2

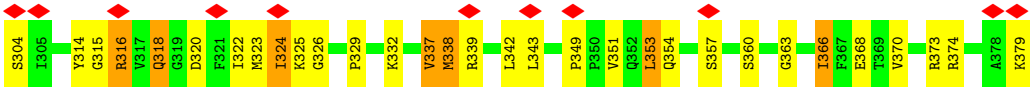
Chain LA:




• Molecule 2: Ribosomal protein L3

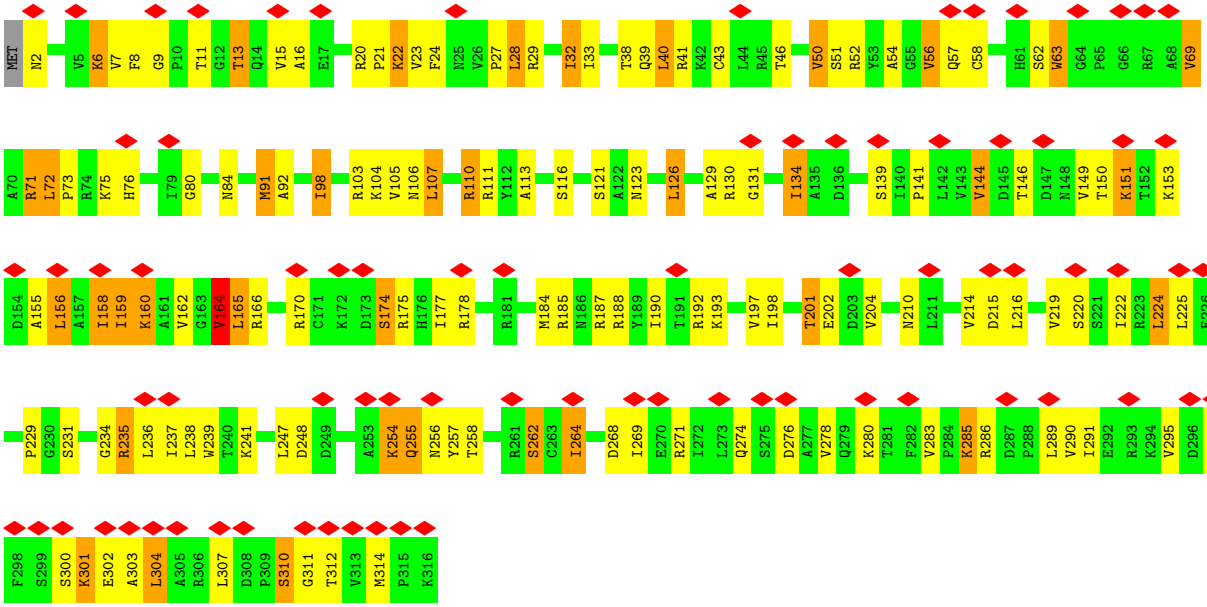
Chain LB:





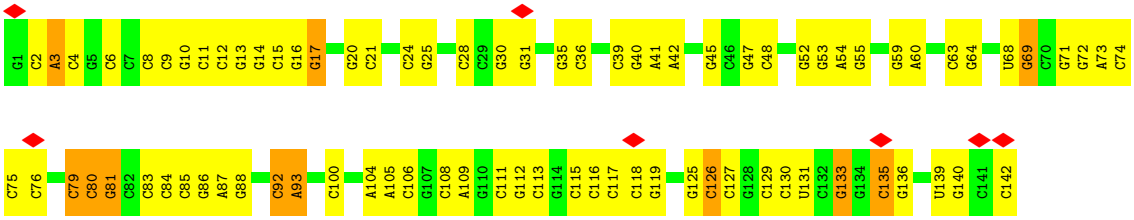

• Molecule 3: Ribosomal protein L4

Chain LC:



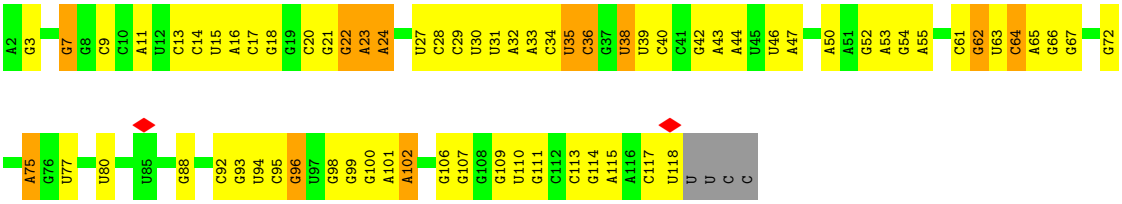

• Molecule 4: 5.8S rRNA

Chain LD:



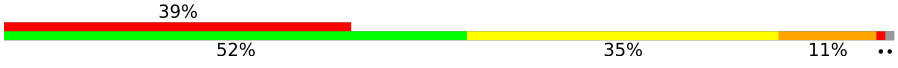

• Molecule 5: 5S rRNA

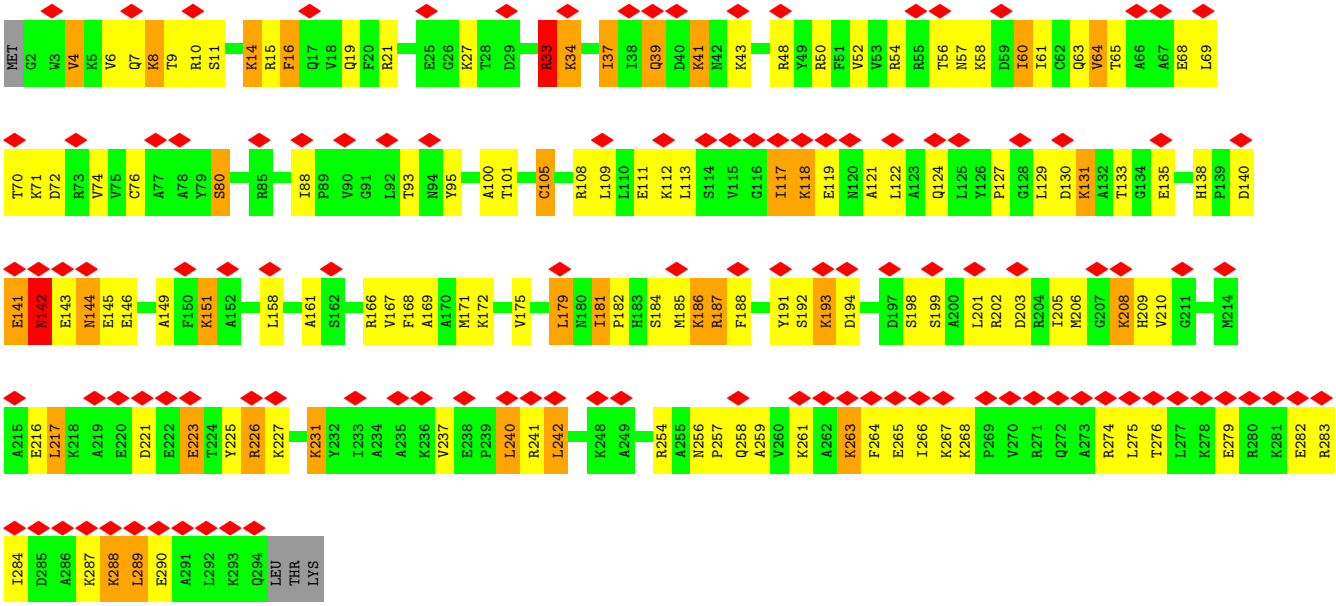
Chain LE:



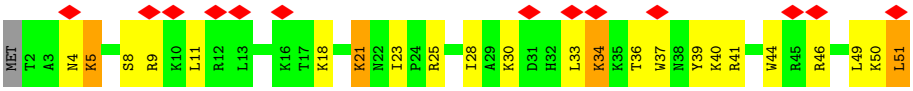

• Molecule 6: Ribosomal protein L5

Chain LF:



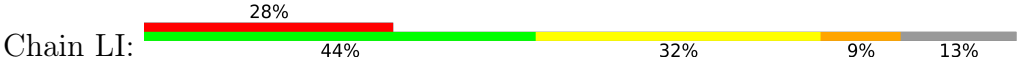


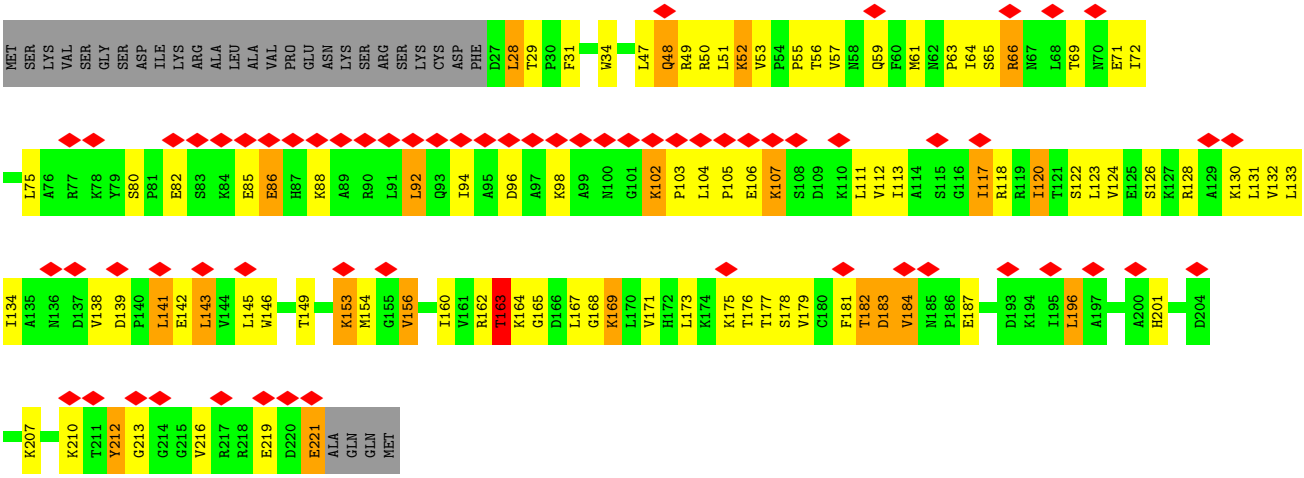

• Molecule 7: Ribosomal protein L39




• Molecule 8: Ribosomal protein L7

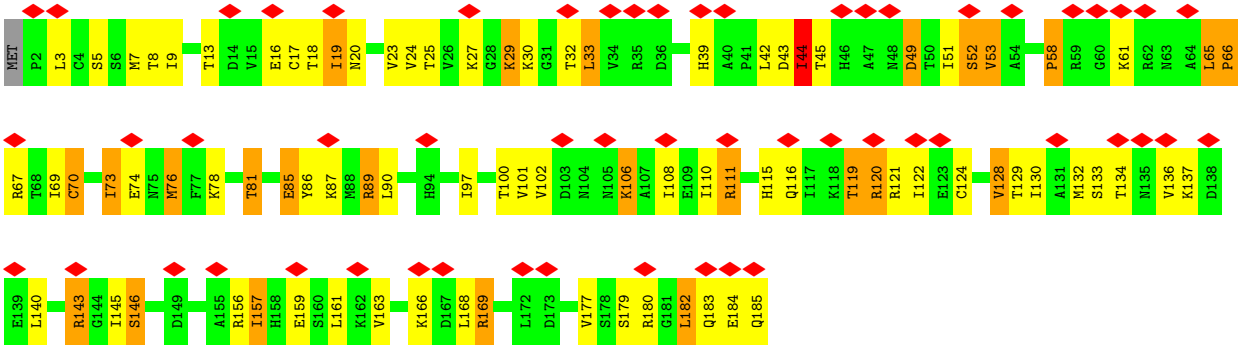
• Molecule 9: Ribosomal protein L7a






• Molecule 10: Ribosomal protein L6

Chain LJ:

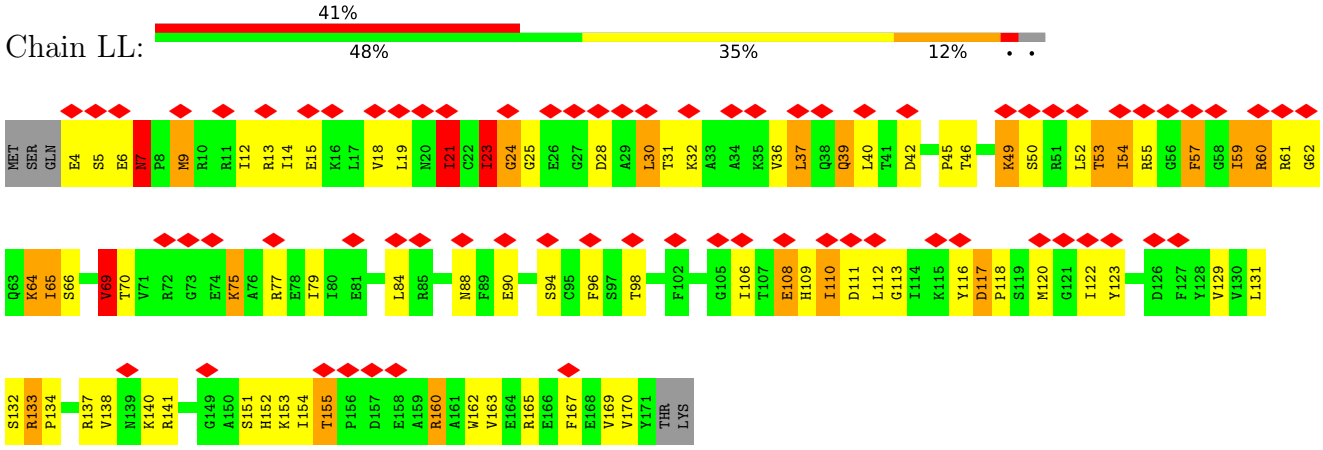



• Molecule 11: Ribosomal protein L10

Chain LK:

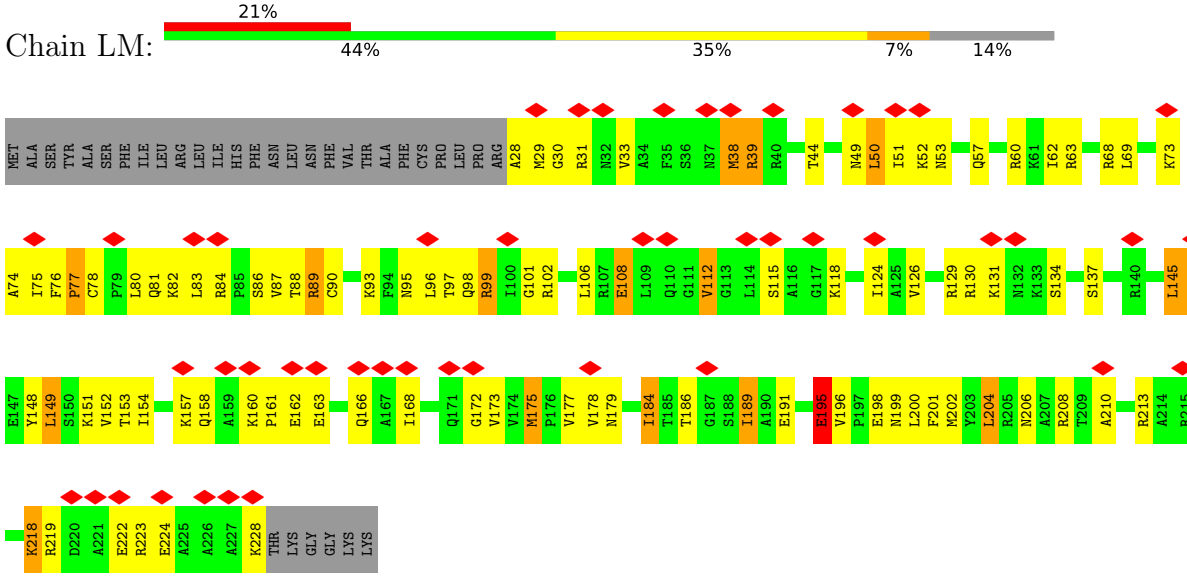
• Molecule 12: Ribosomal protein L11

Chain LL:



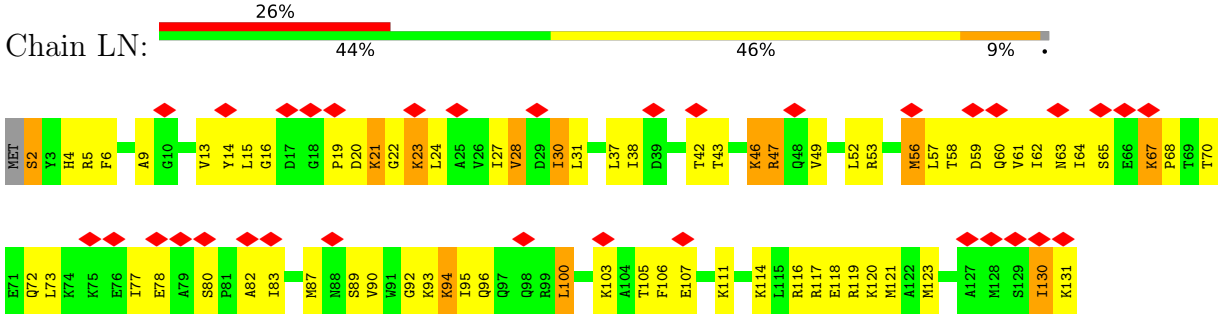

• Molecule 13: Ribosomal protein L13

Chain LM:



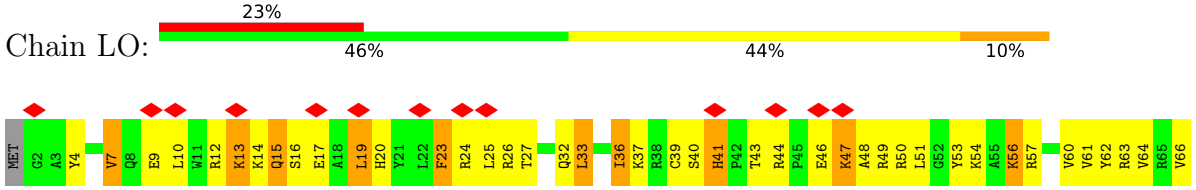

• Molecule 14: Ribosomal protein L14

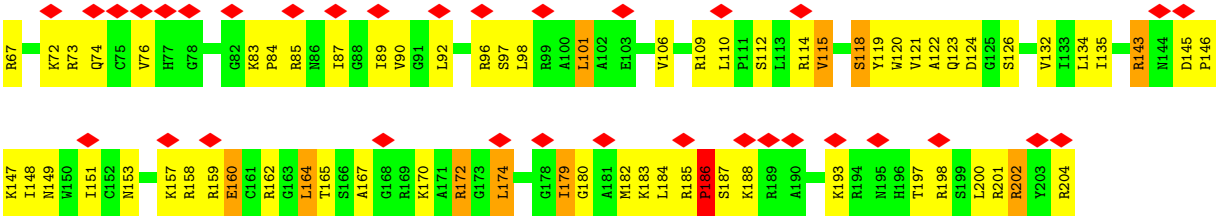
Chain LN:



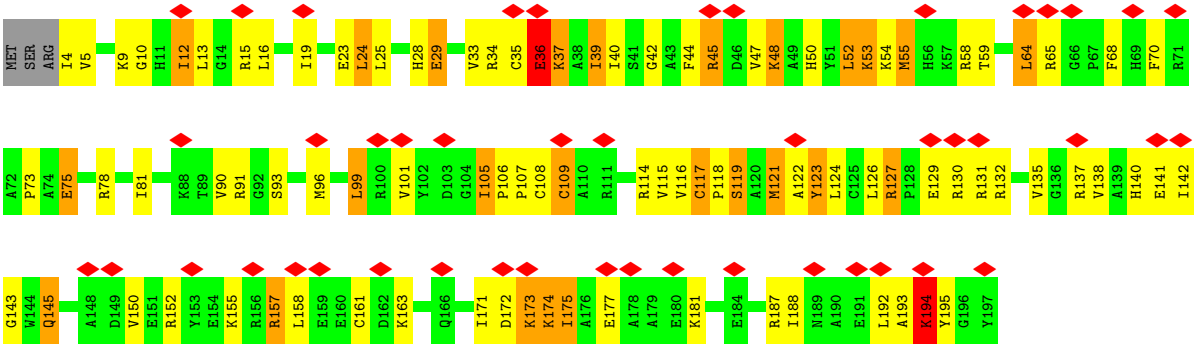

• Molecule 15: Ribosomal protein L15

Chain LO:

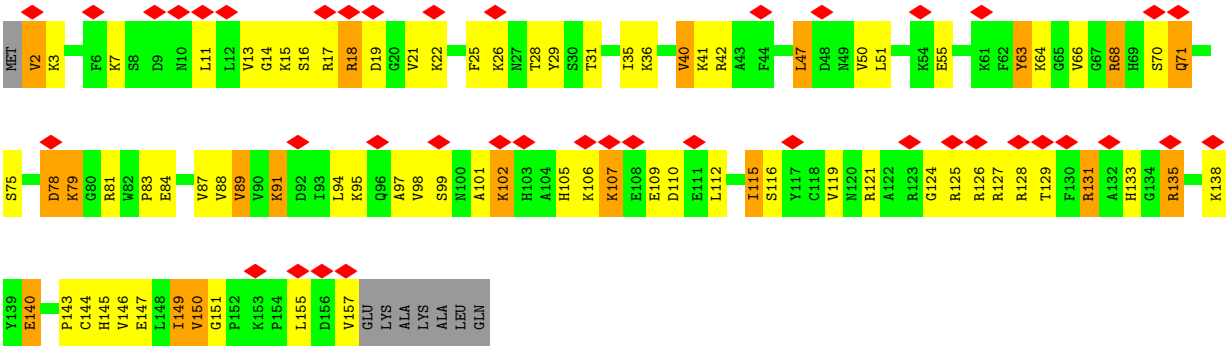




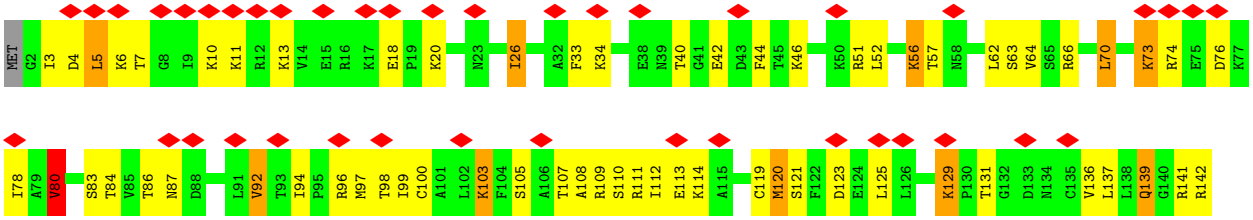

• Molecule 16: Ribosomal protein L13a

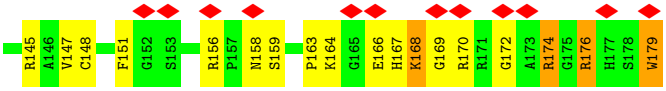



• Molecule 17: Ribosomal protein L17



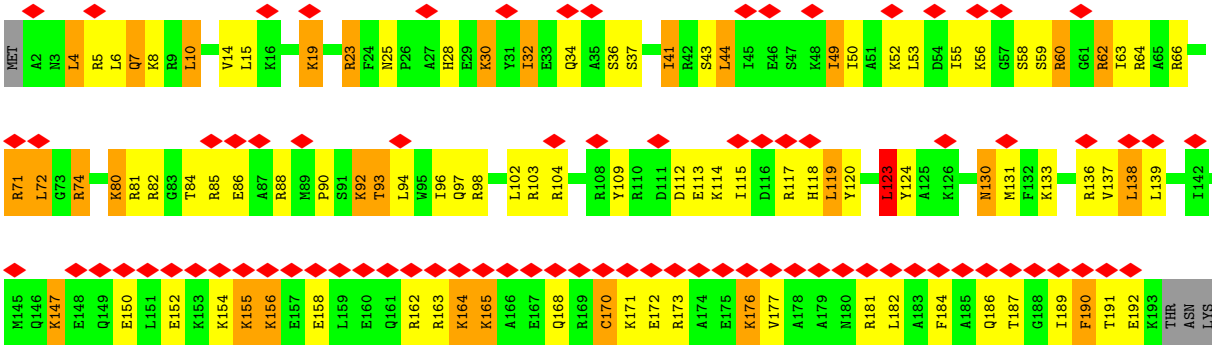

• Molecule 18: Ribosomal protein L18





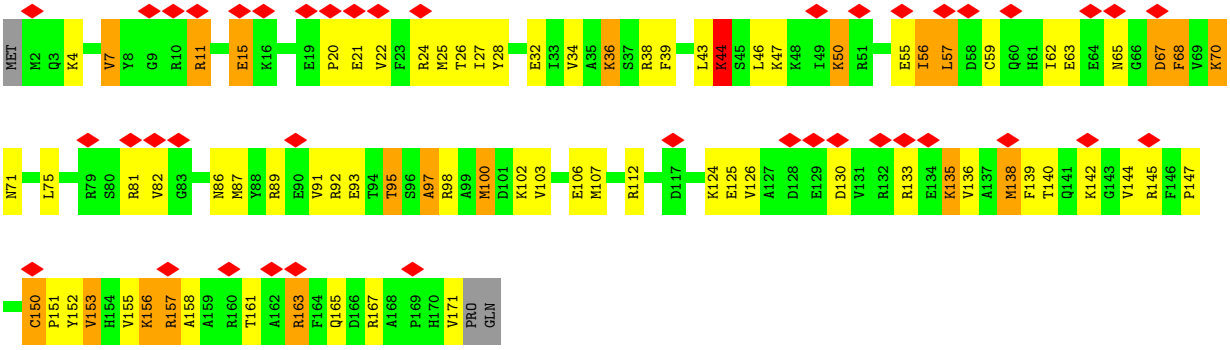

• Molecule 19: Ribosomal protein L19

Chain LS:



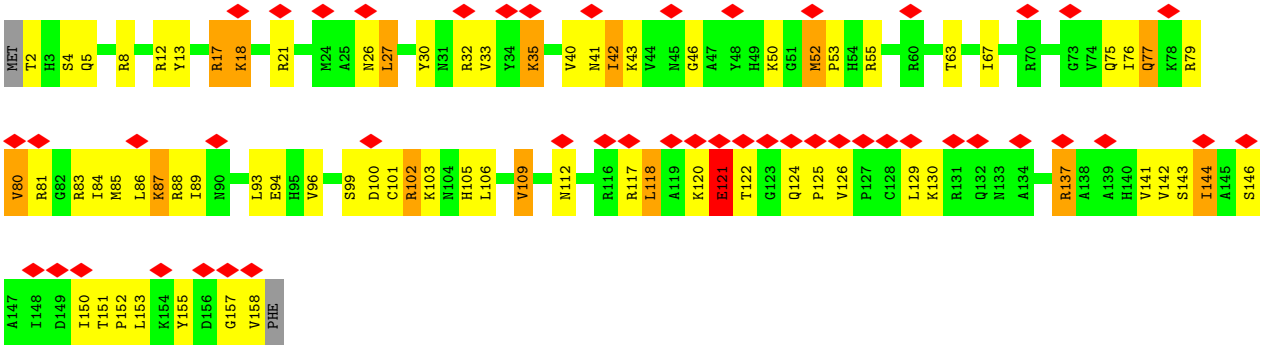

• Molecule 20: Ribosomal protein L18a

Chain LT:

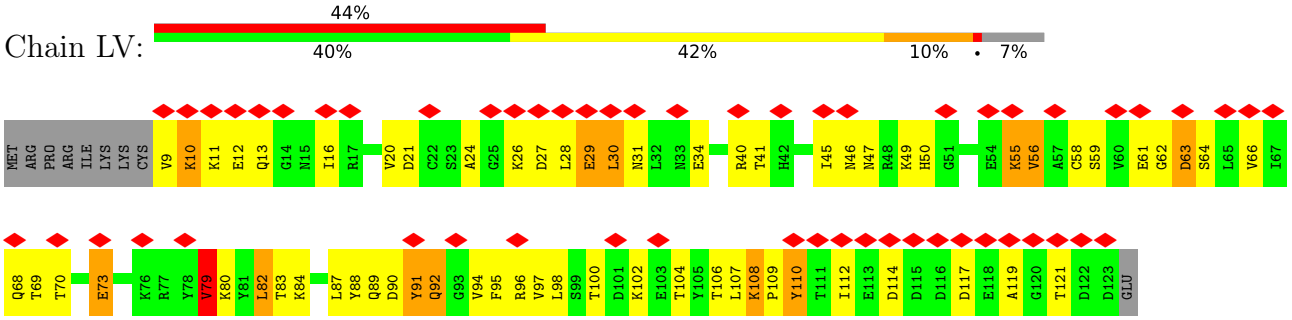



• Molecule 21: Ribosomal protein L21

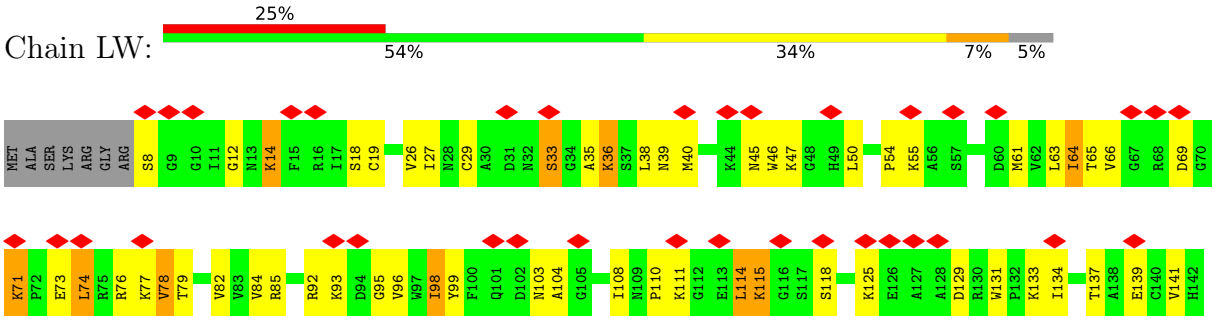
Chain LU:



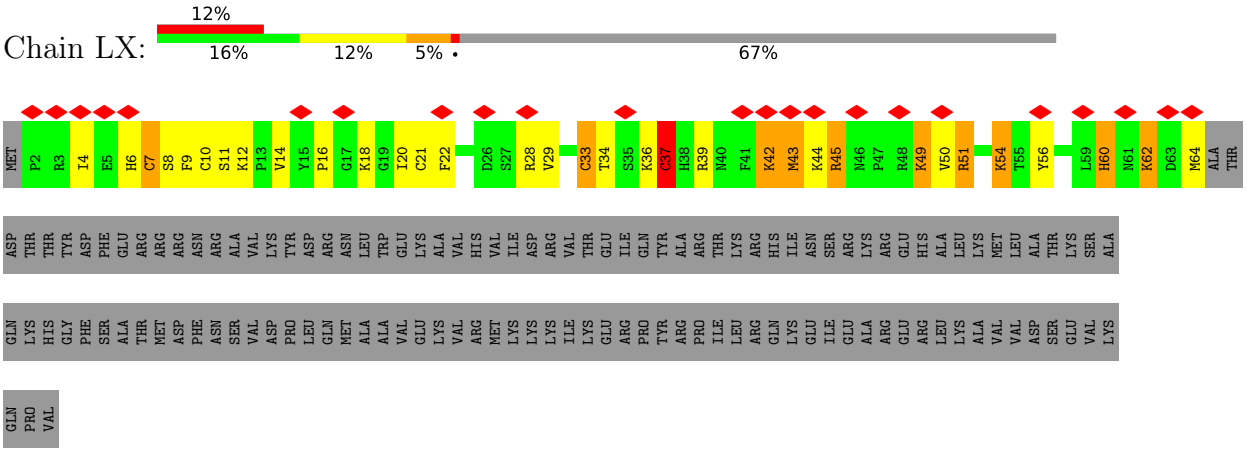

• Molecule 22: Ribosomal protein L22e



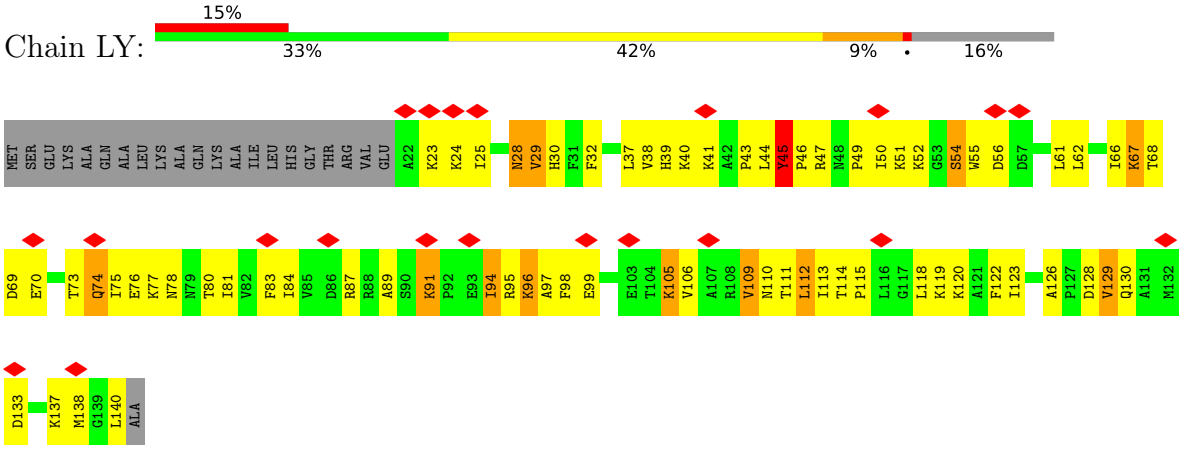

• Molecule 23: Ribosomal protein L23




• Molecule 24: Ribosomal protein L24

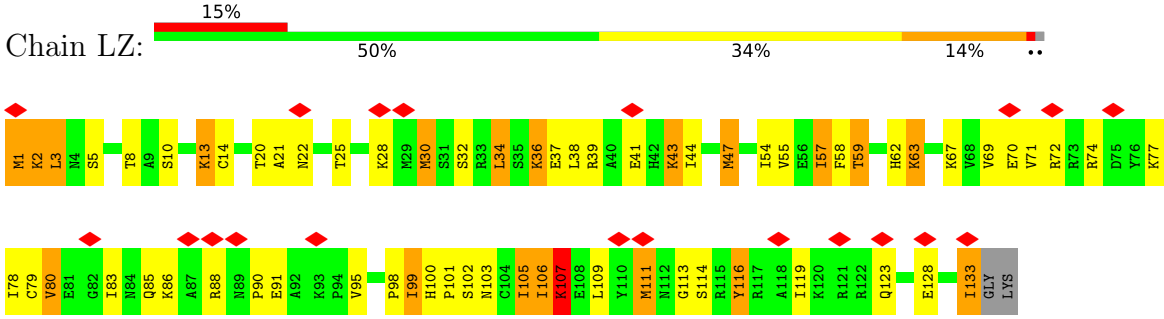



• Molecule 25: Ribosomal protein L23A



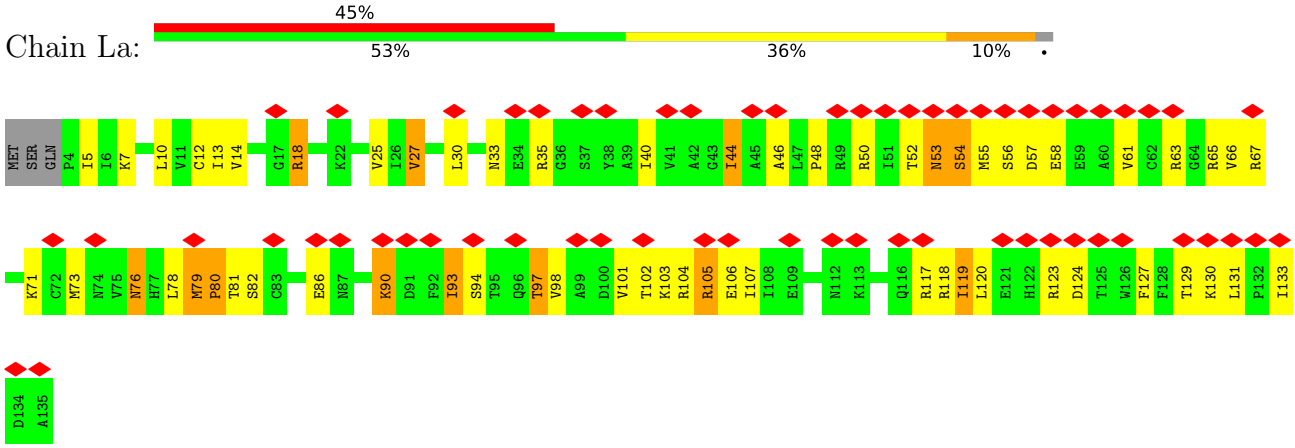
• Molecule 26: Ribosomal protein L26

Chain LZ:



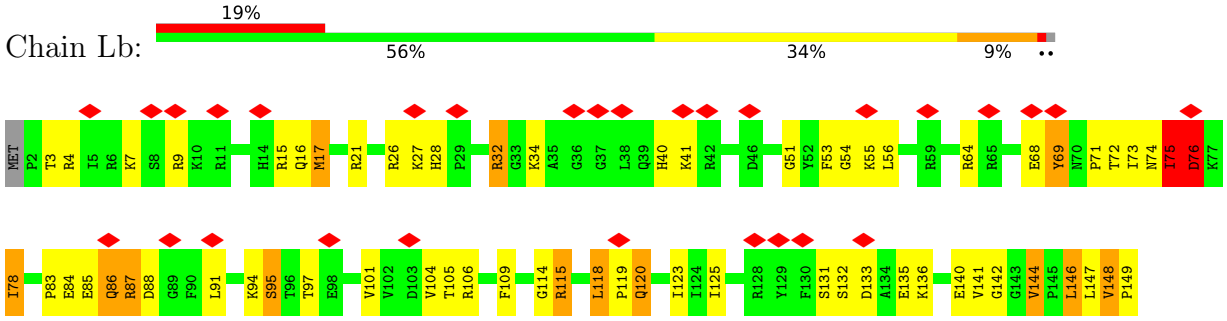

• Molecule 27: Ribosomal protein L27

Chain La:



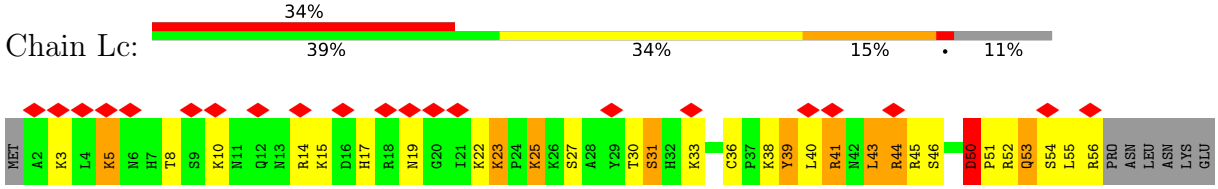

• Molecule 28: Ribosomal protein L27a

Chain Lb:



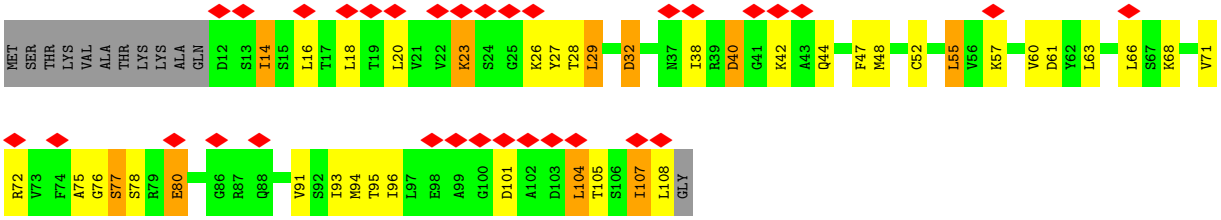

• Molecule 29: Ribosomal protein L29

Chain Lc:




• Molecule 30: Ribosomal protein L30

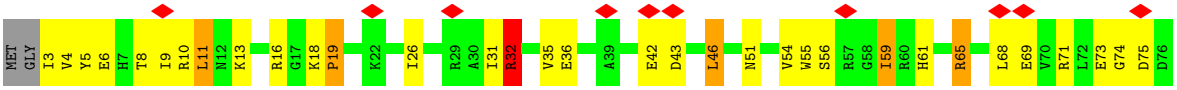
Chain Ld:

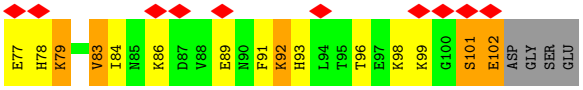




• Molecule 31: Ribosomal protein L31B

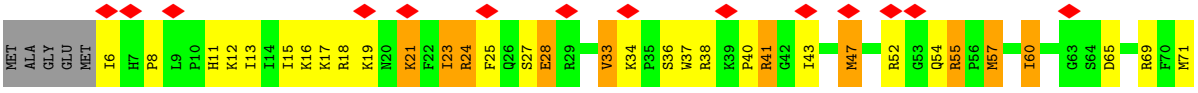
Chain Le:





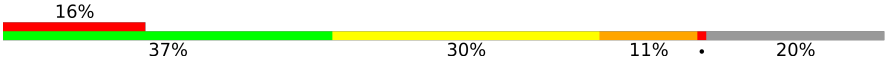
• Molecule 32: Ribosomal protein L32

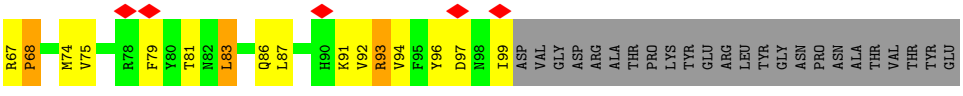
Chain Lf:



• Molecule 33: Ribosomal protein L35a

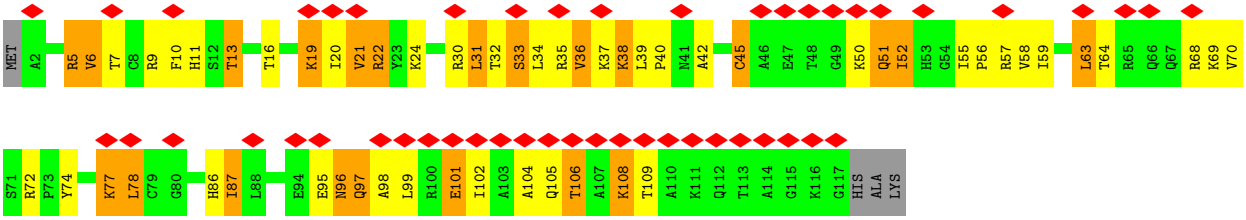
Chain Lg:





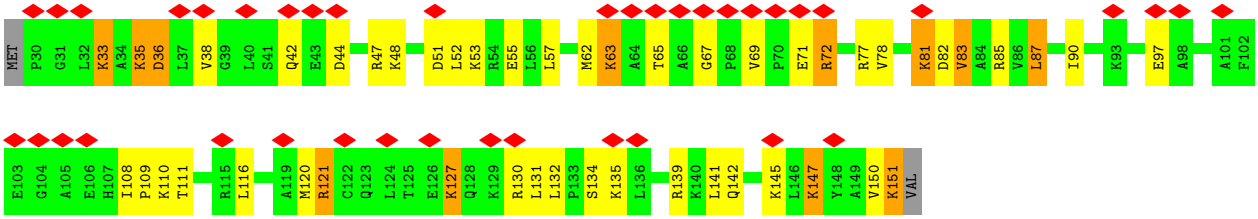
• Molecule 34: Ribosomal protein L34

Chain Lh:



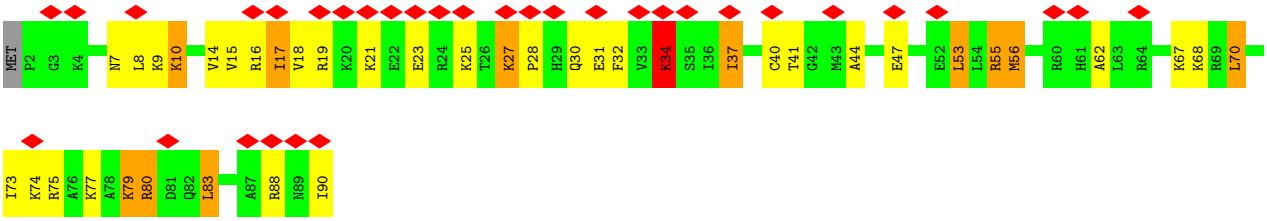

• Molecule 35: Ribosomal protein L29

Chain Li:



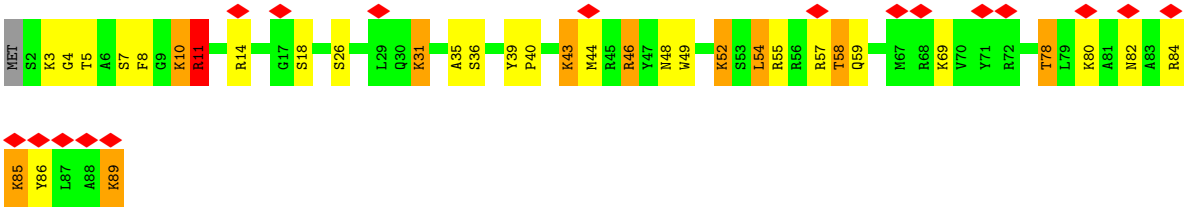

• Molecule 36: Ribosomal protein L36-1

Chain Lj:



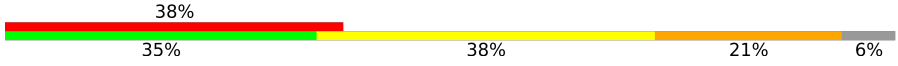

• Molecule 37: Ribosomal protein L37

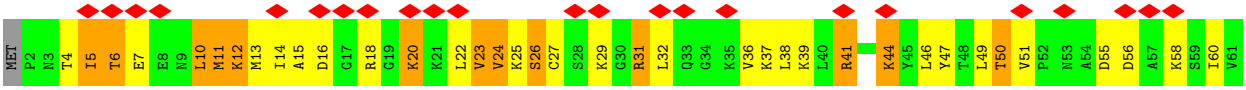
Chain Lk:

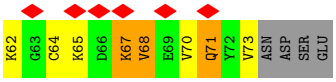



• Molecule 38: Ribosomal protein L38e

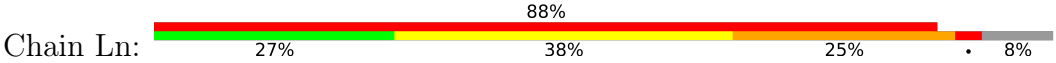
Chain Ll:

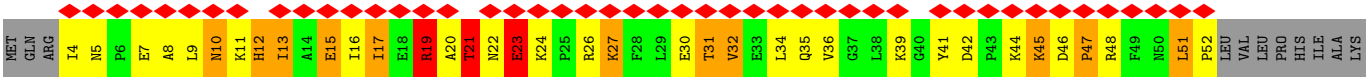


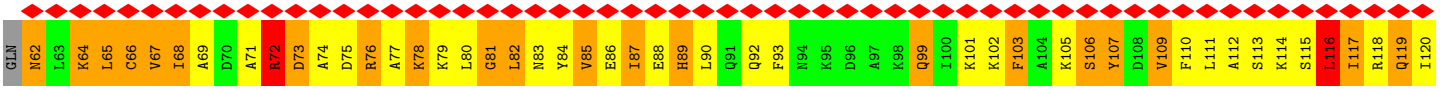



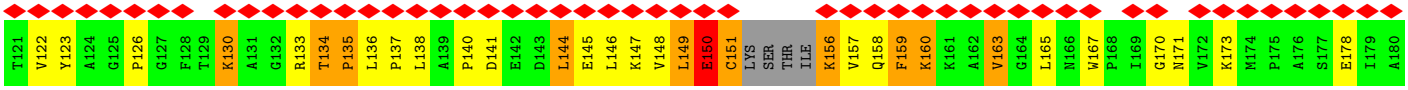


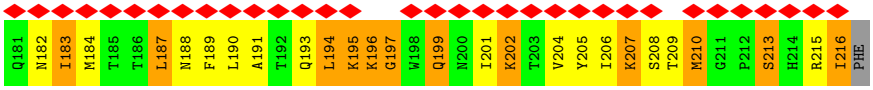

• Molecule 39: Ribosomal protein L10a



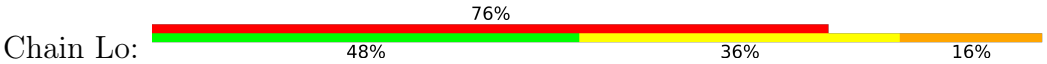



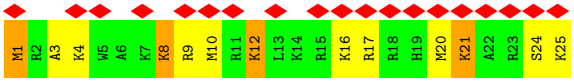



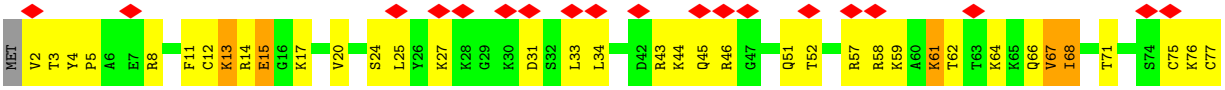




• Molecule 40: Ribosomal protein L41

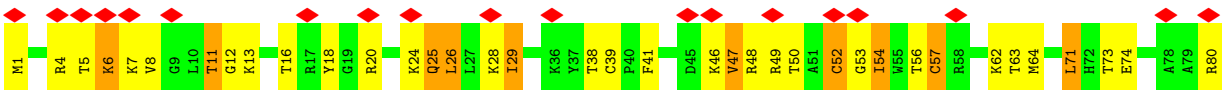


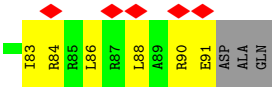




• Molecule 41: Ribosomal protein L44

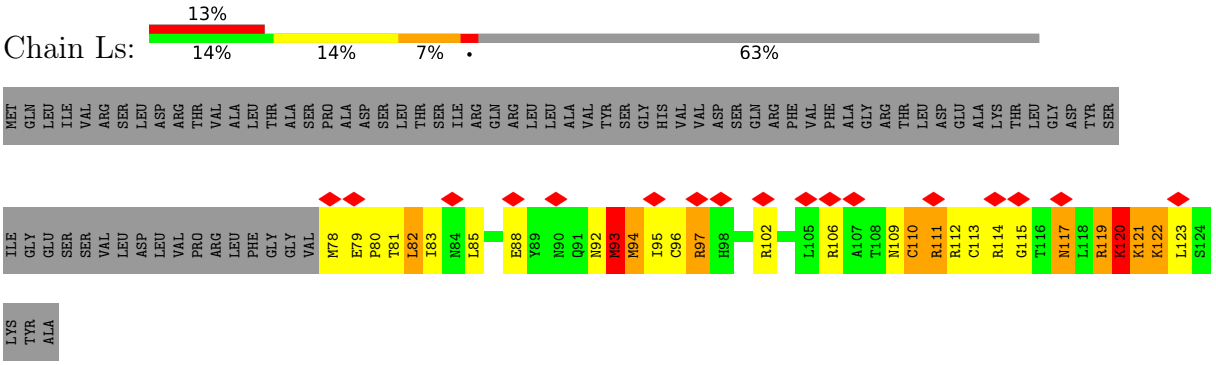


• Molecule 42: Ribosomal protein L37a





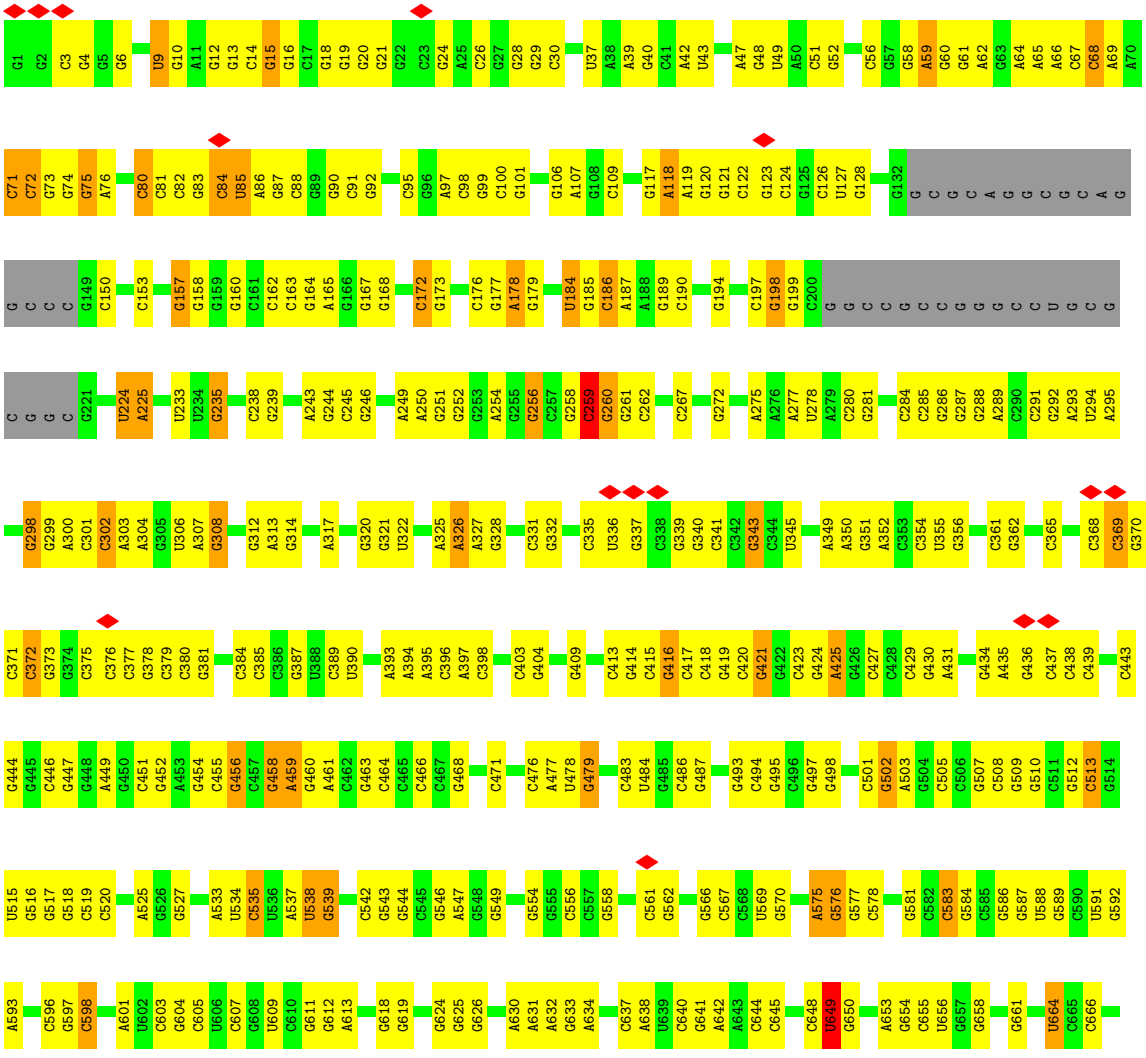

• Molecule 43: Ubiquitin/Ribosomal protein L40e

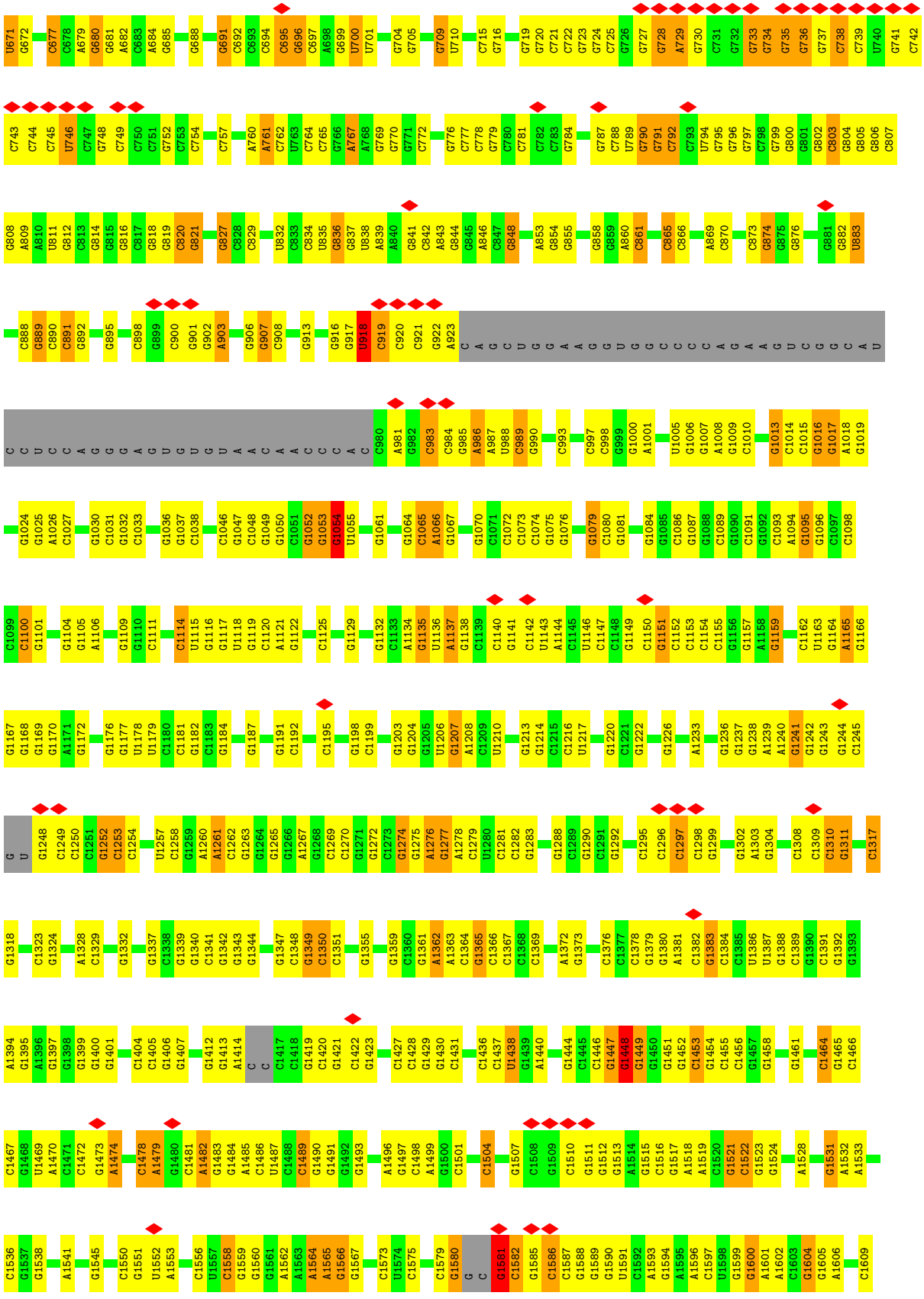


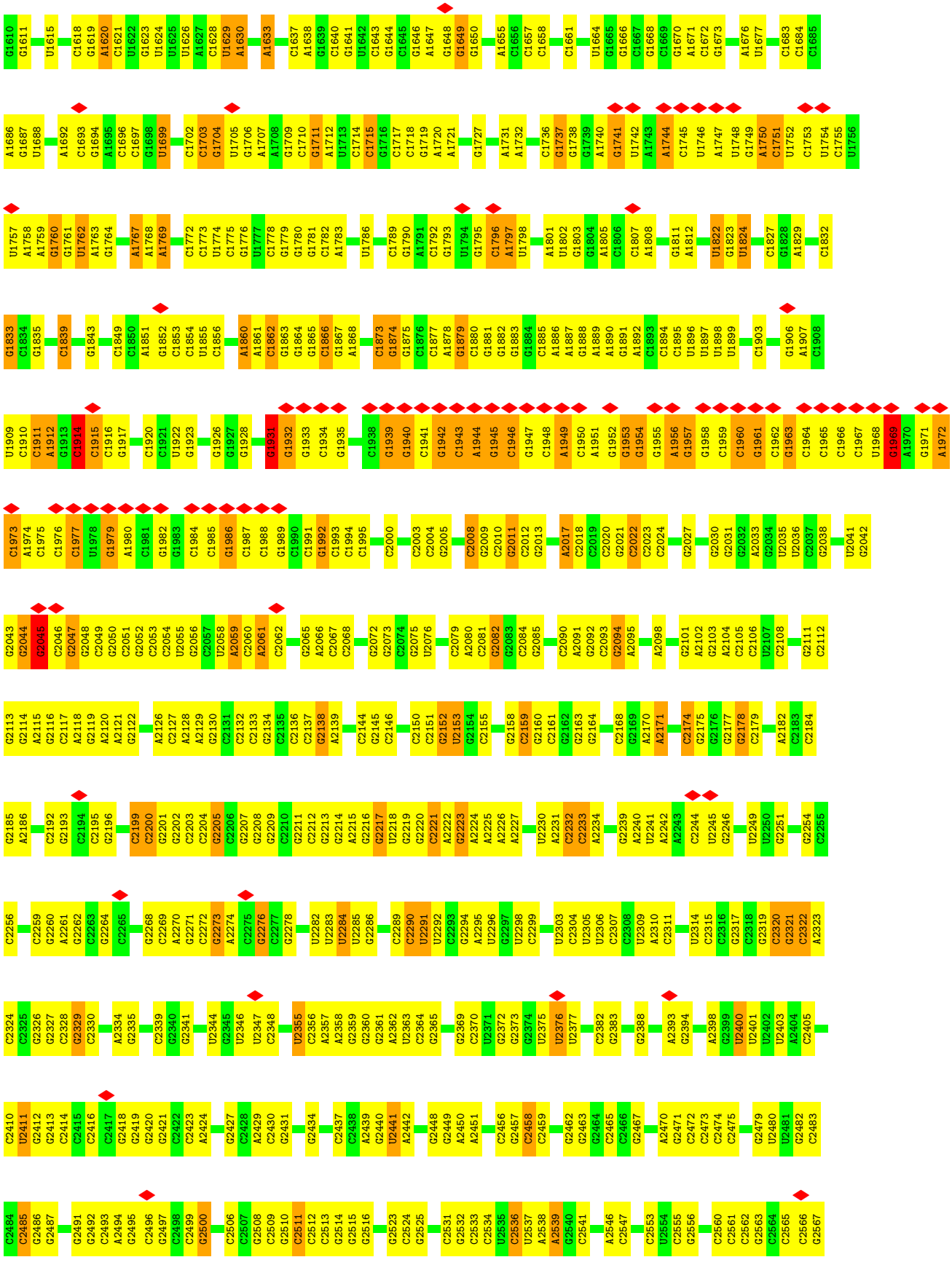


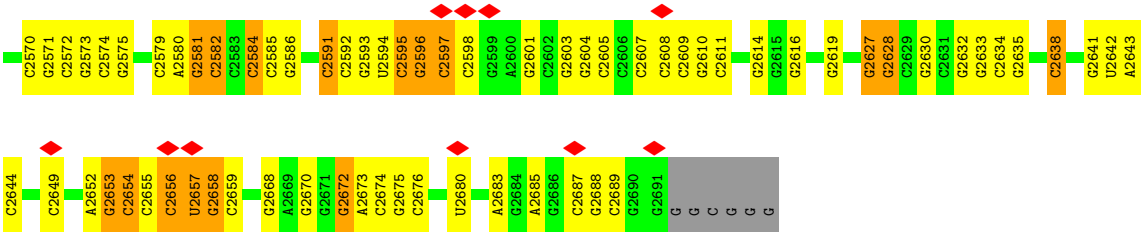


• Molecule 44: Large Subunit rRNA



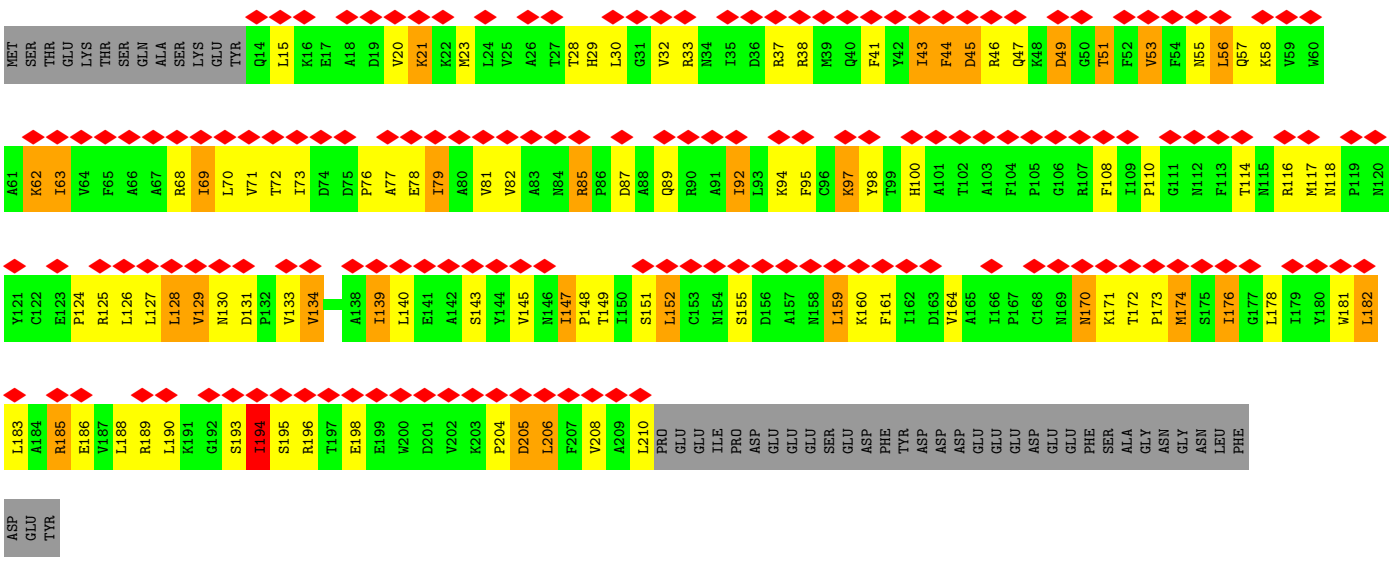






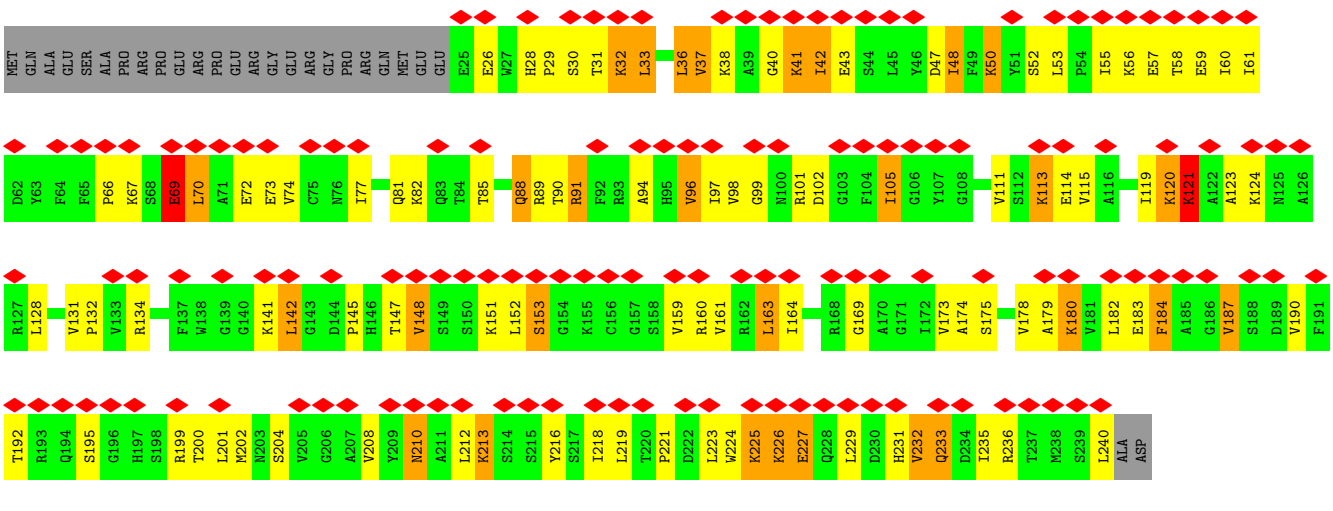
• Molecule 45: Ribosomal protein SA

Chain SA:



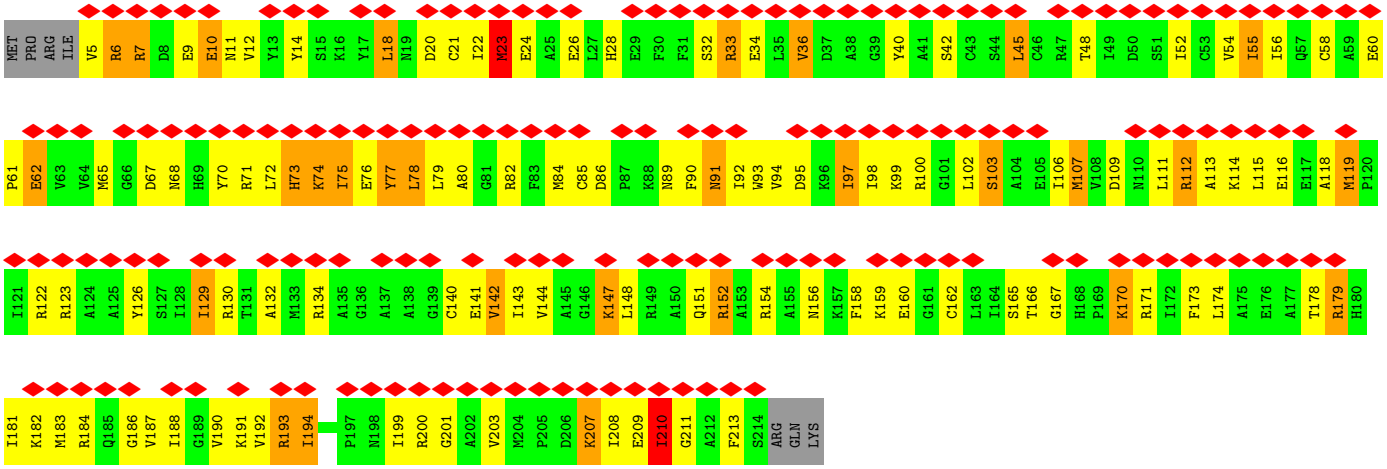
• Molecule 46: Ribosomal protein S2

Chain SB:



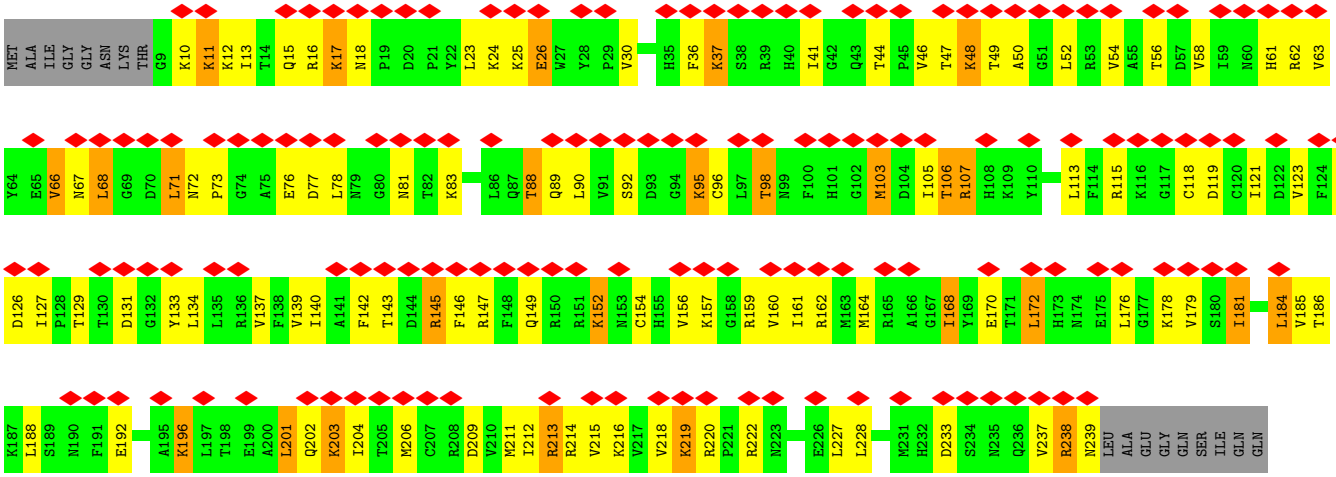
• Molecule 47: Ribosomal protein S3

Chain SC:



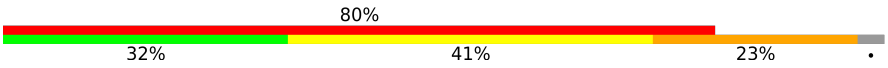
• Molecule 48: Ribosomal protein S3a

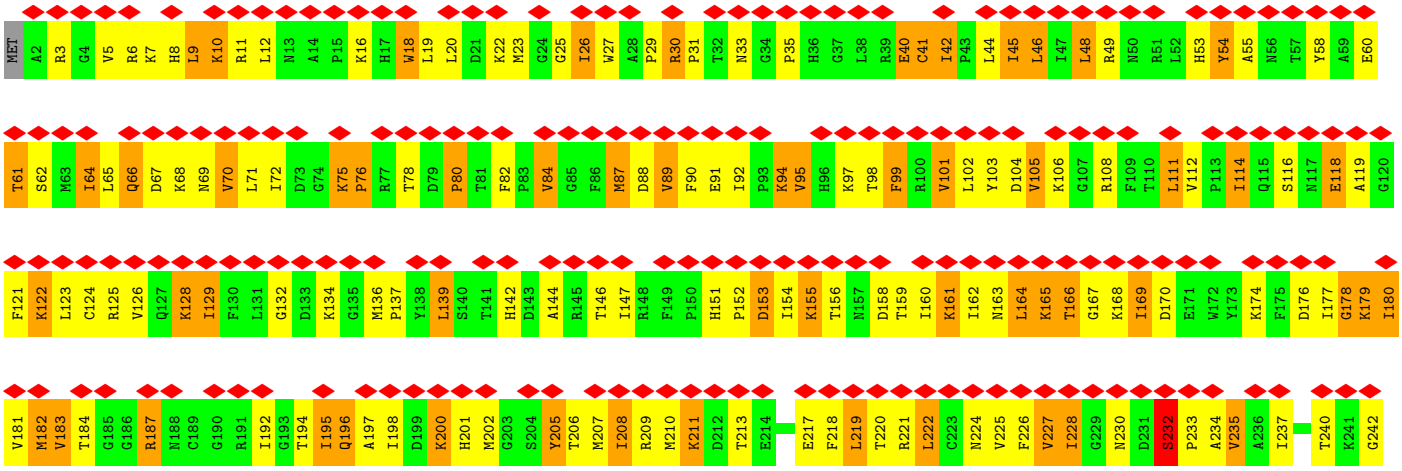
Chain SD:

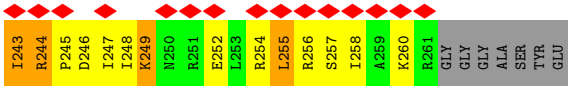


• Molecule 49: Ribosomal protein S4

Chain SE:

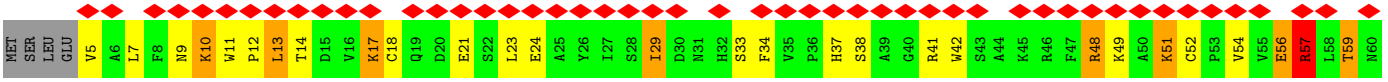


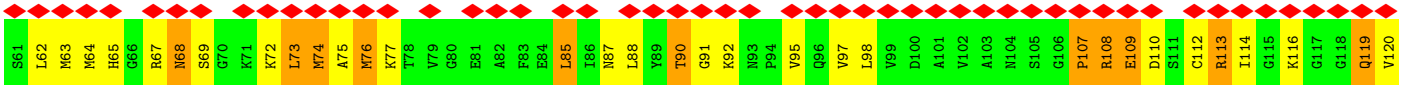



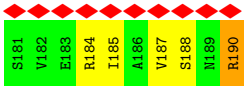



• Molecule 50: Ribosomal protein S5

Chain SF:

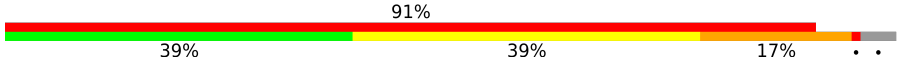


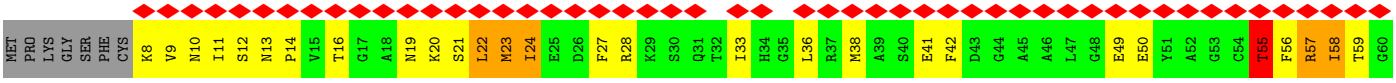



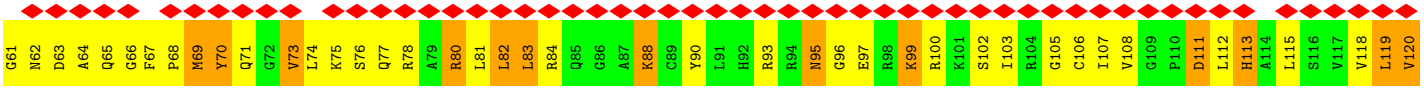


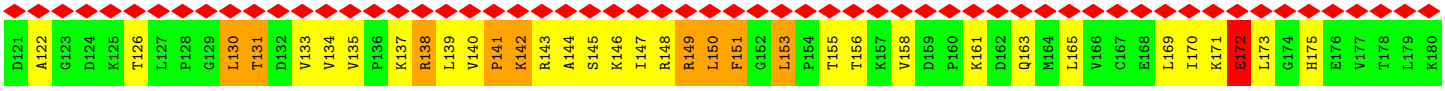

• Molecule 51: Ribosomal protein S6

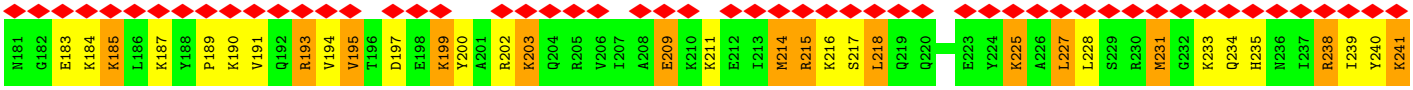
Chain SG:

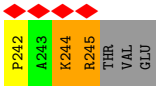


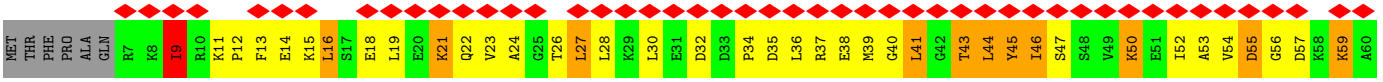



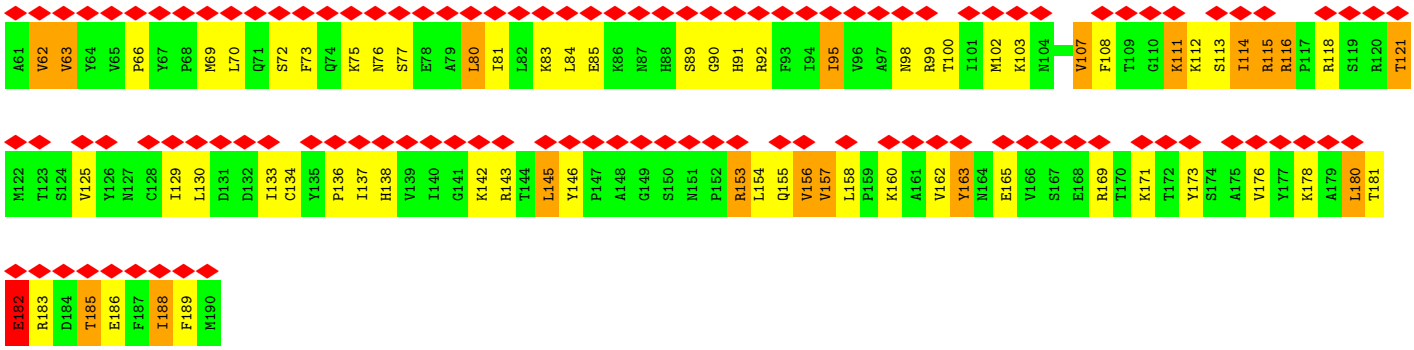



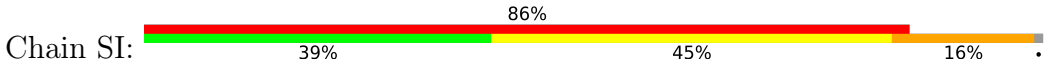

• Molecule 52: Ribosomal protein S7

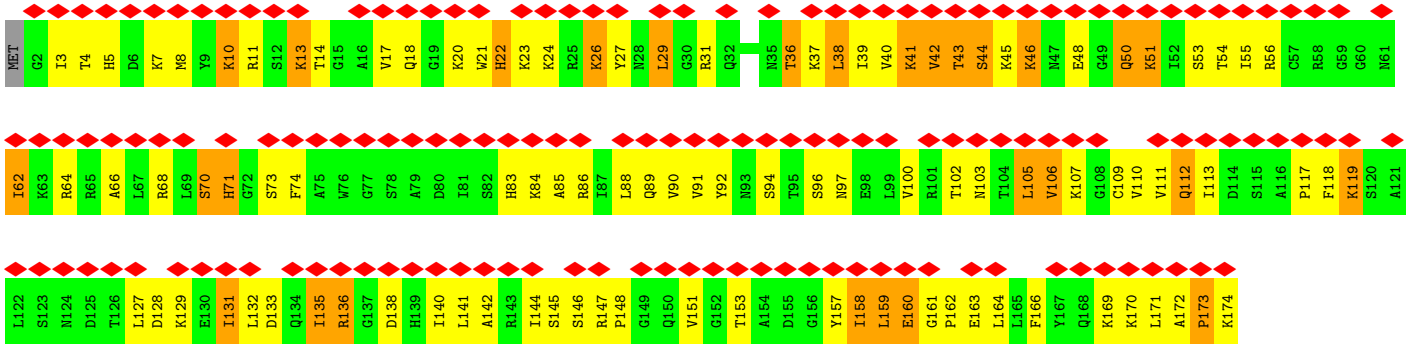
Chain SH:



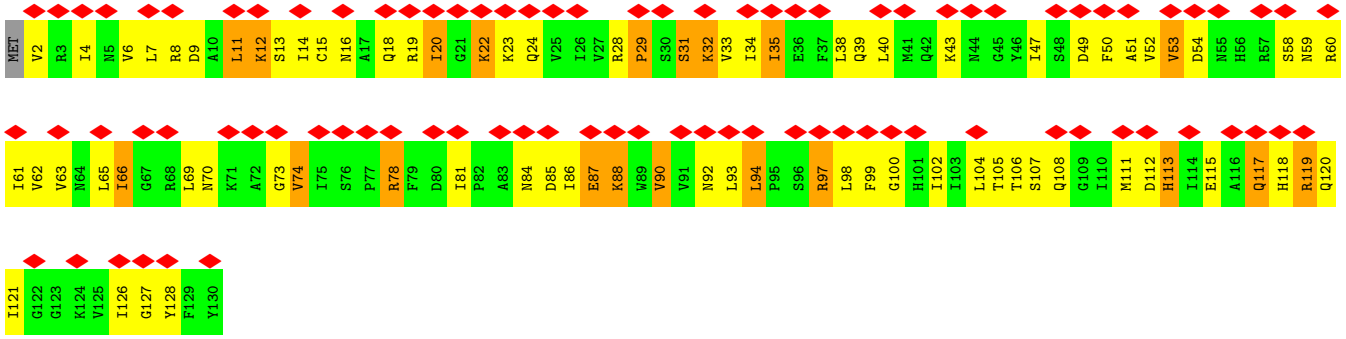



• Molecule 53: Ribosomal protein S8

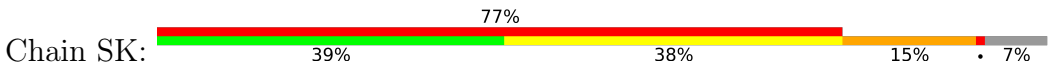


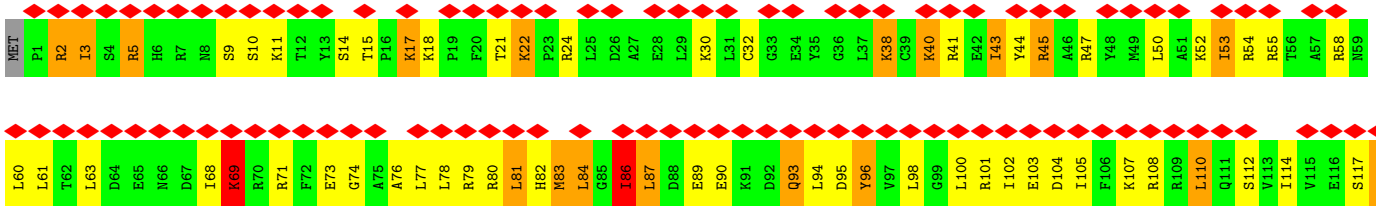



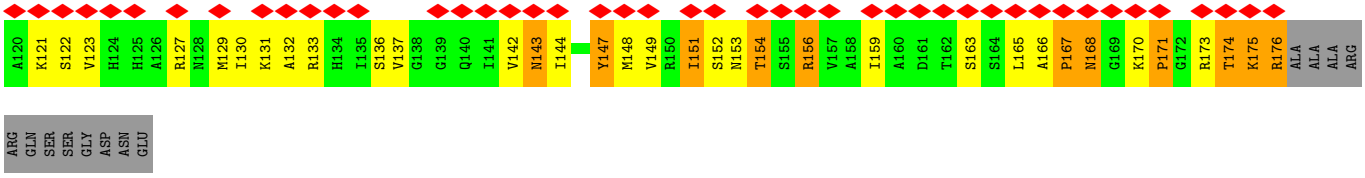

• Molecule 54: Ribosomal protein S15A



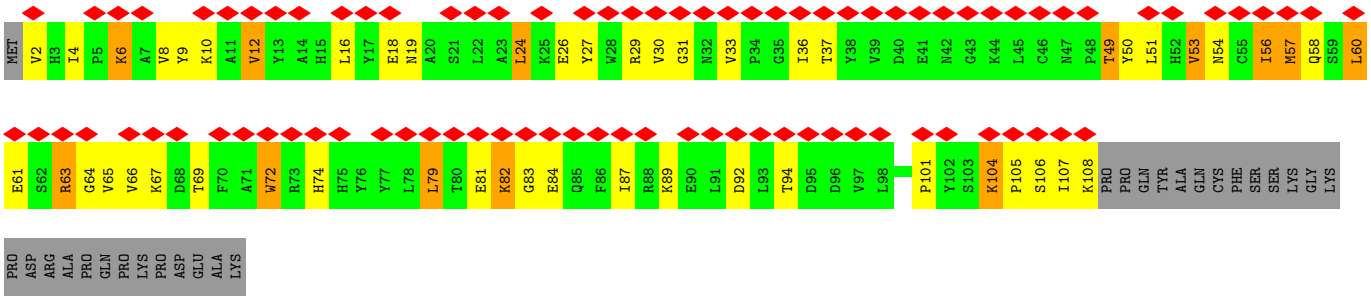

• Molecule 55: Ribosomal protein S9



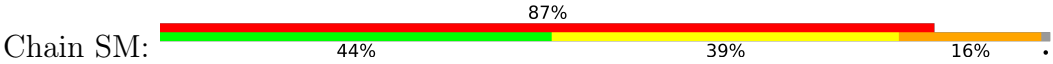



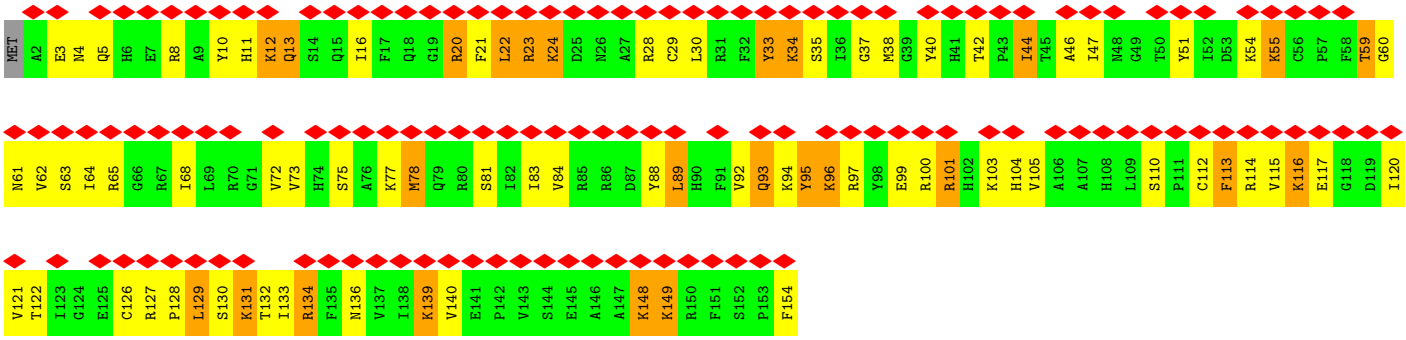



• Molecule 56: Ribosomal protein S10B

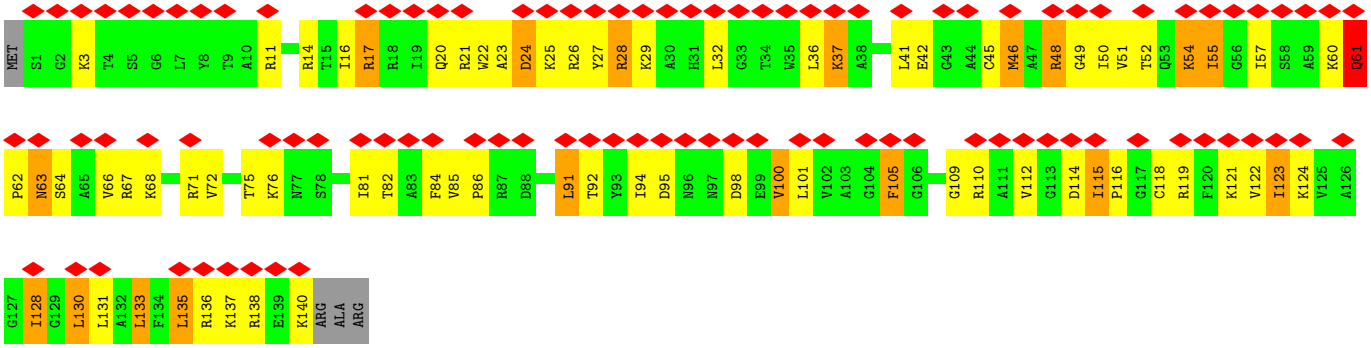



• Molecule 57: Ribosomal protein S11



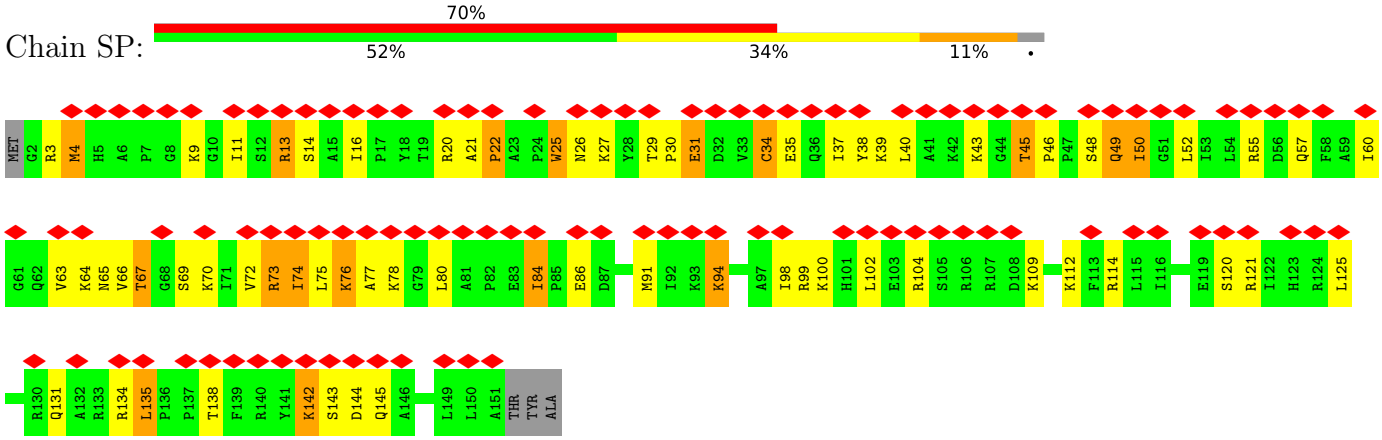




• Molecule 58: Ribosomal protein S23



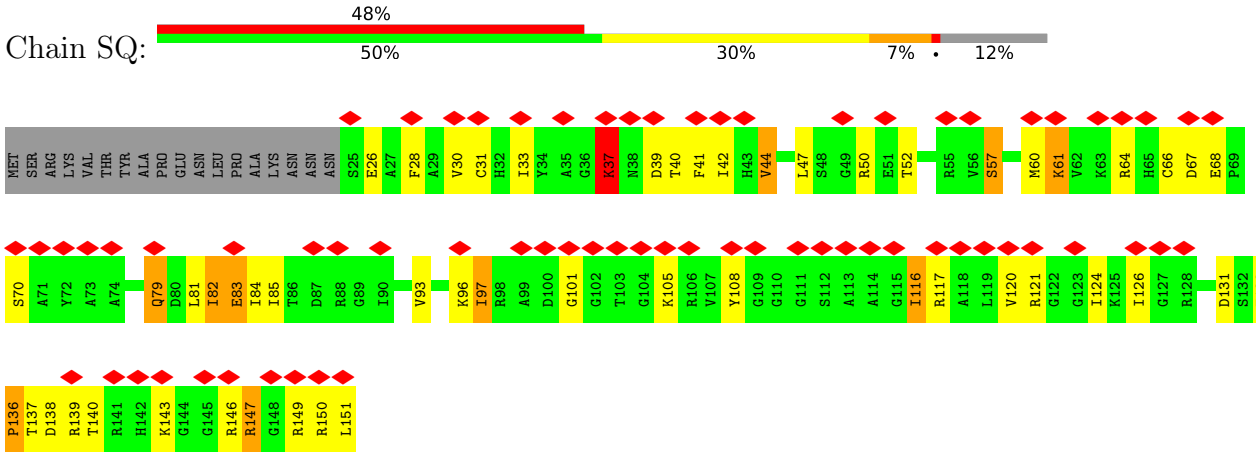

• Molecule 59: Ribosomal protein S13

Chain SP:



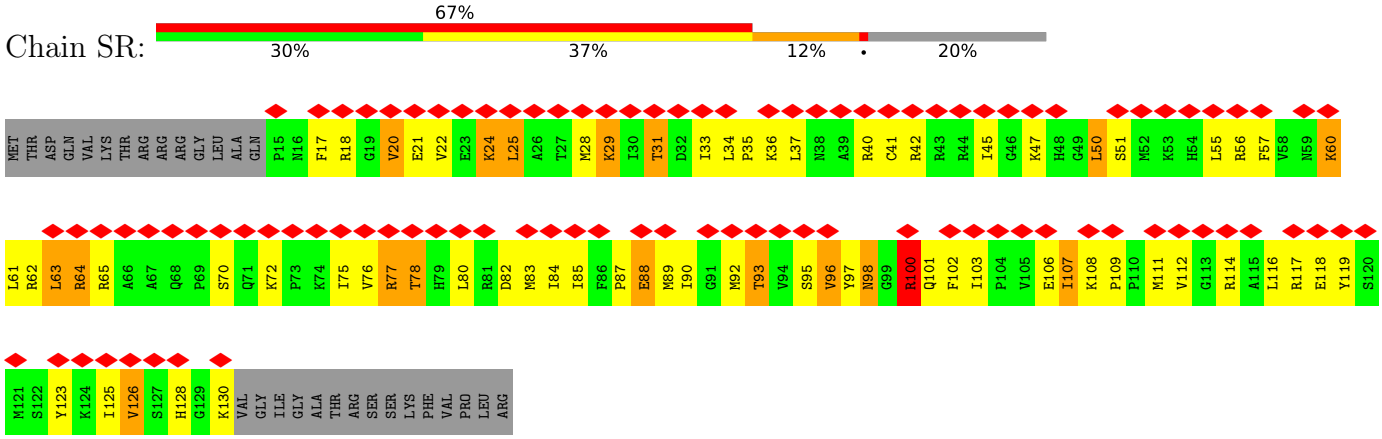

• Molecule 60: Ribosomal protein S14

Chain SQ:



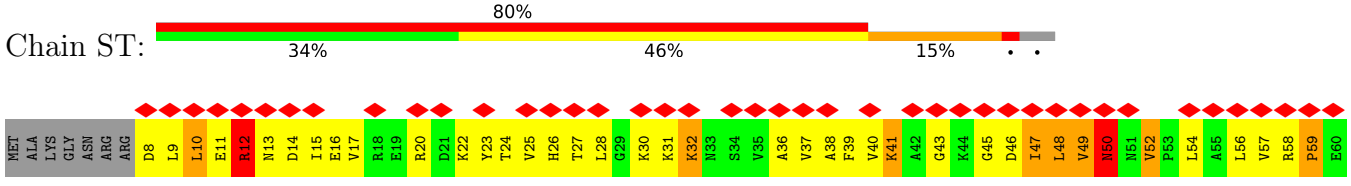

• Molecule 61: Ribosomal protein S15

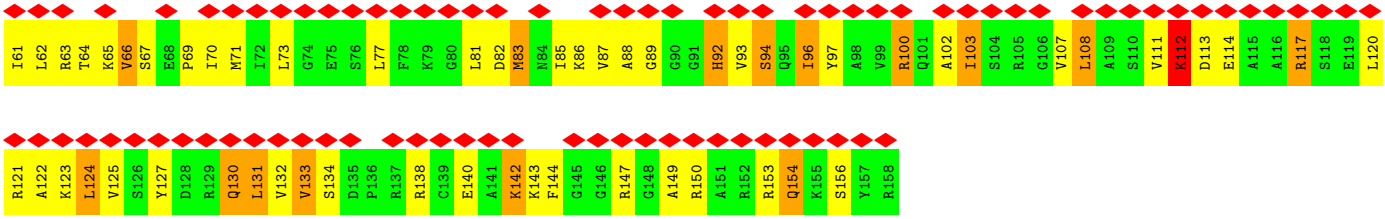
Chain SR:




• Molecule 62: Ribosomal protein S16

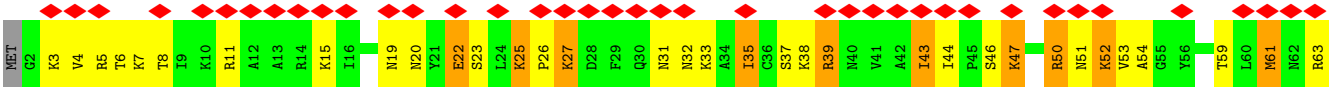
Chain ST:

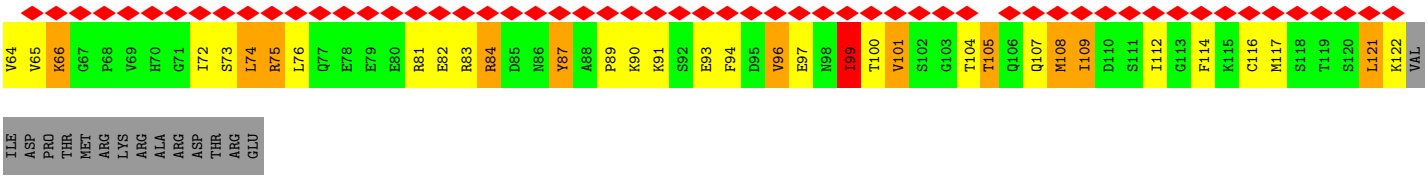





• Molecule 63: Ribosomal protein S17

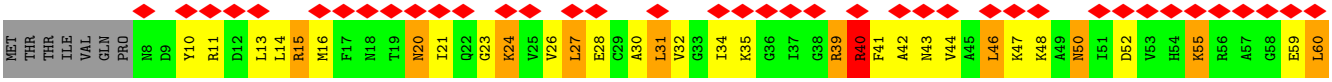
Chain SU:

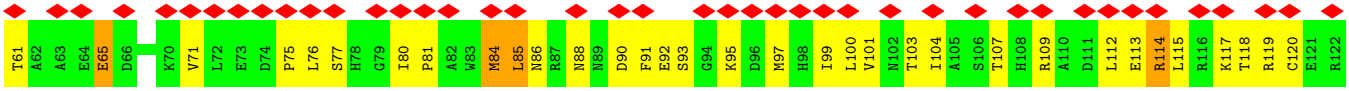


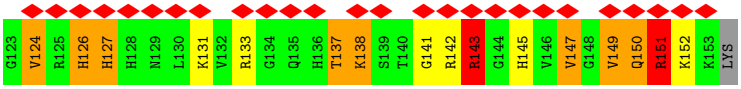




• Molecule 64: Ribosomal protein S18

Chain SV:

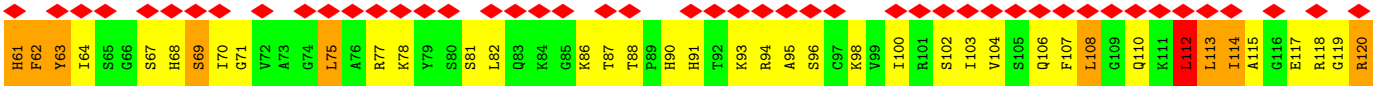


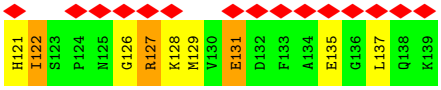




• Molecule 65: Ribosomal protein S19e

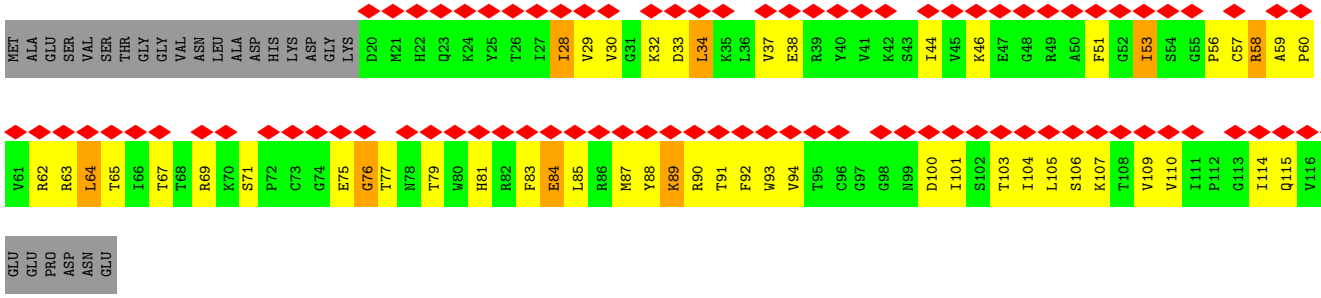
Chain SW:



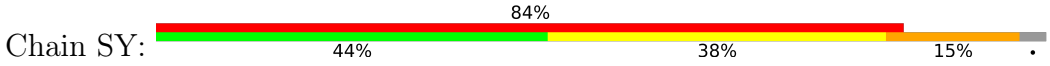
• Molecule 66: Ribosomal protein S20

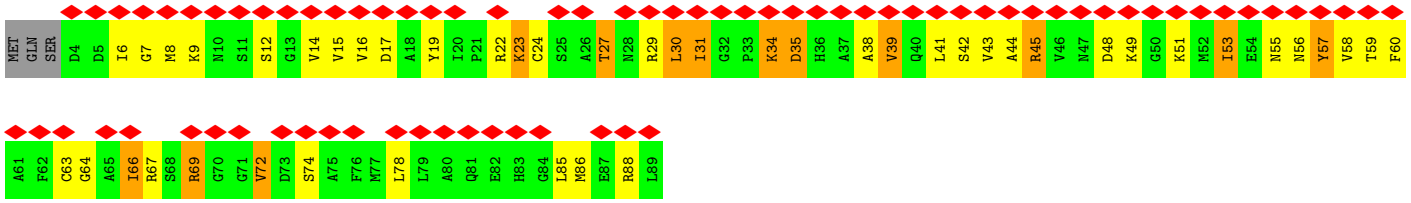
Chain SX:




• Molecule 67: Ribosomal protein S21

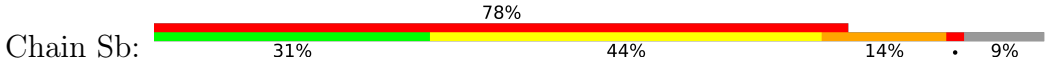
Chain SY:

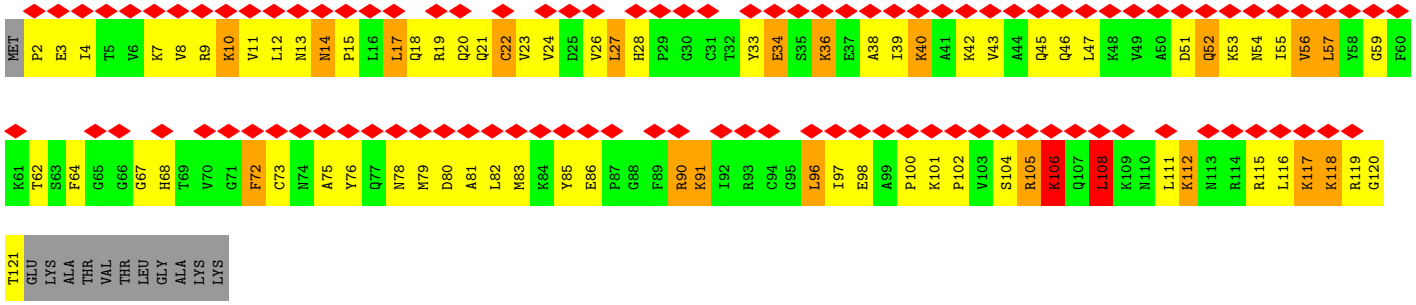



• Molecule 68: Ribosomal protein S24

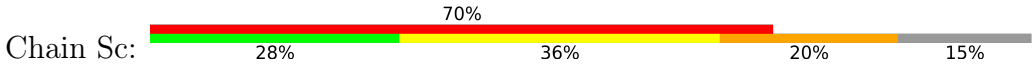
Chain Sb:

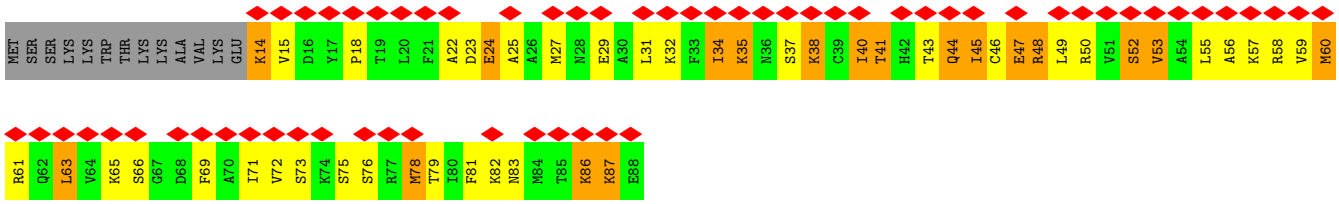



• Molecule 69: Ribosomal protein S25

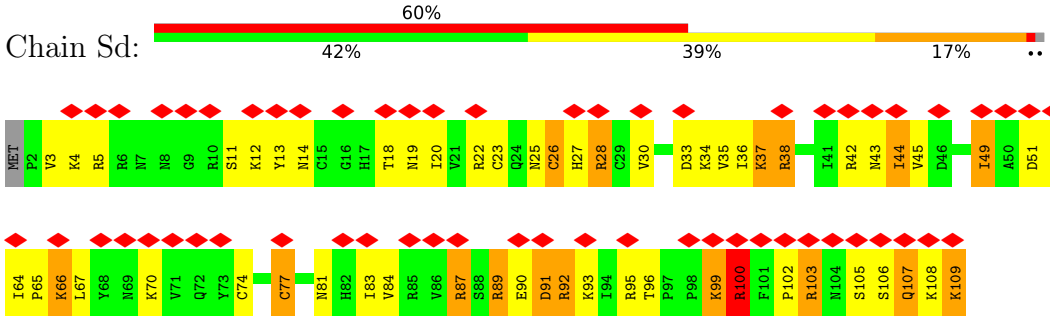
Chain Sc:



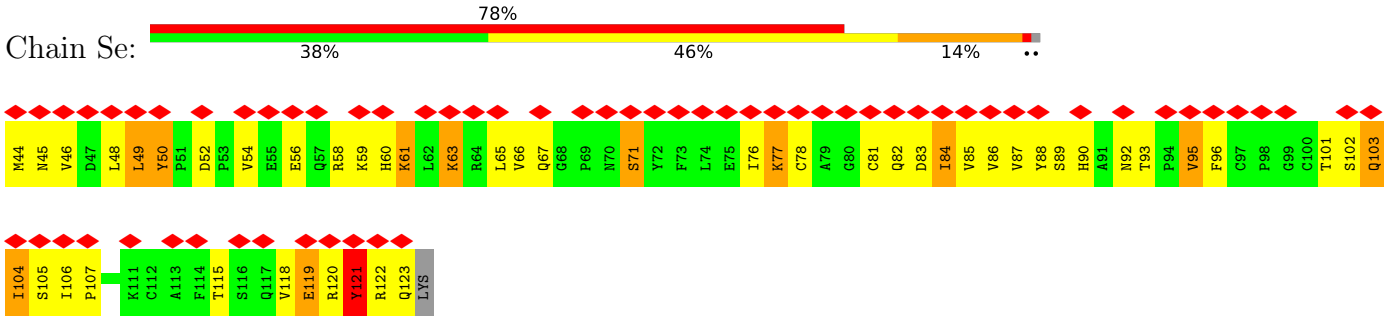

• Molecule 70: Ribosomal protein S26

Chain Sd:



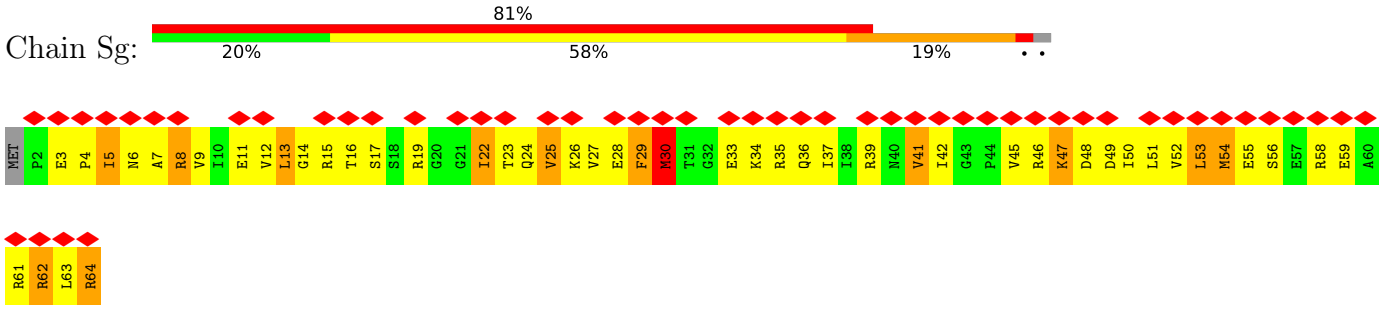

• Molecule 71: Ribosomal protein S27

Chain Se:



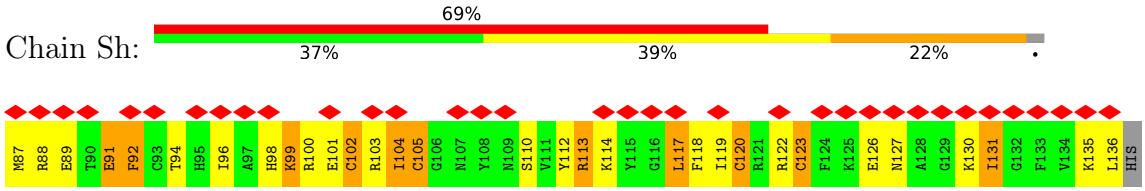

• Molecule 72: Ribosomal protein S28

Chain Sg:



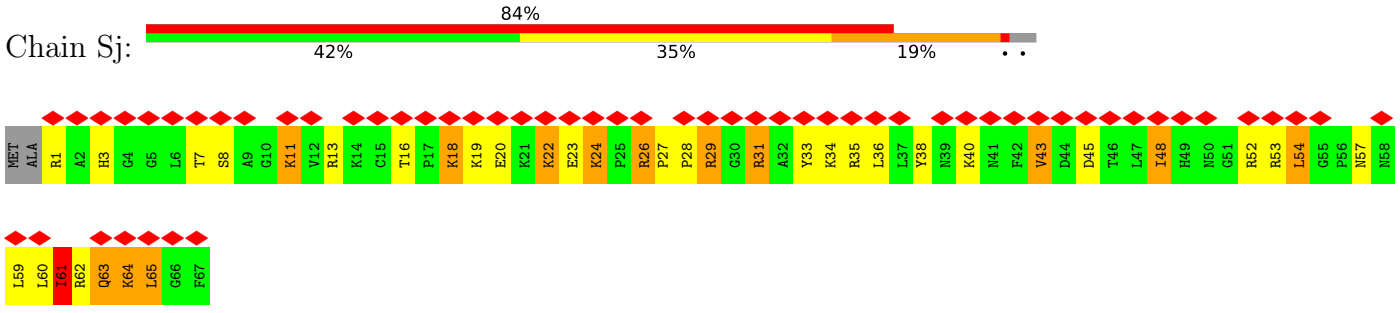

• Molecule 73: Ribosomal protein S29A

Chain Sh:



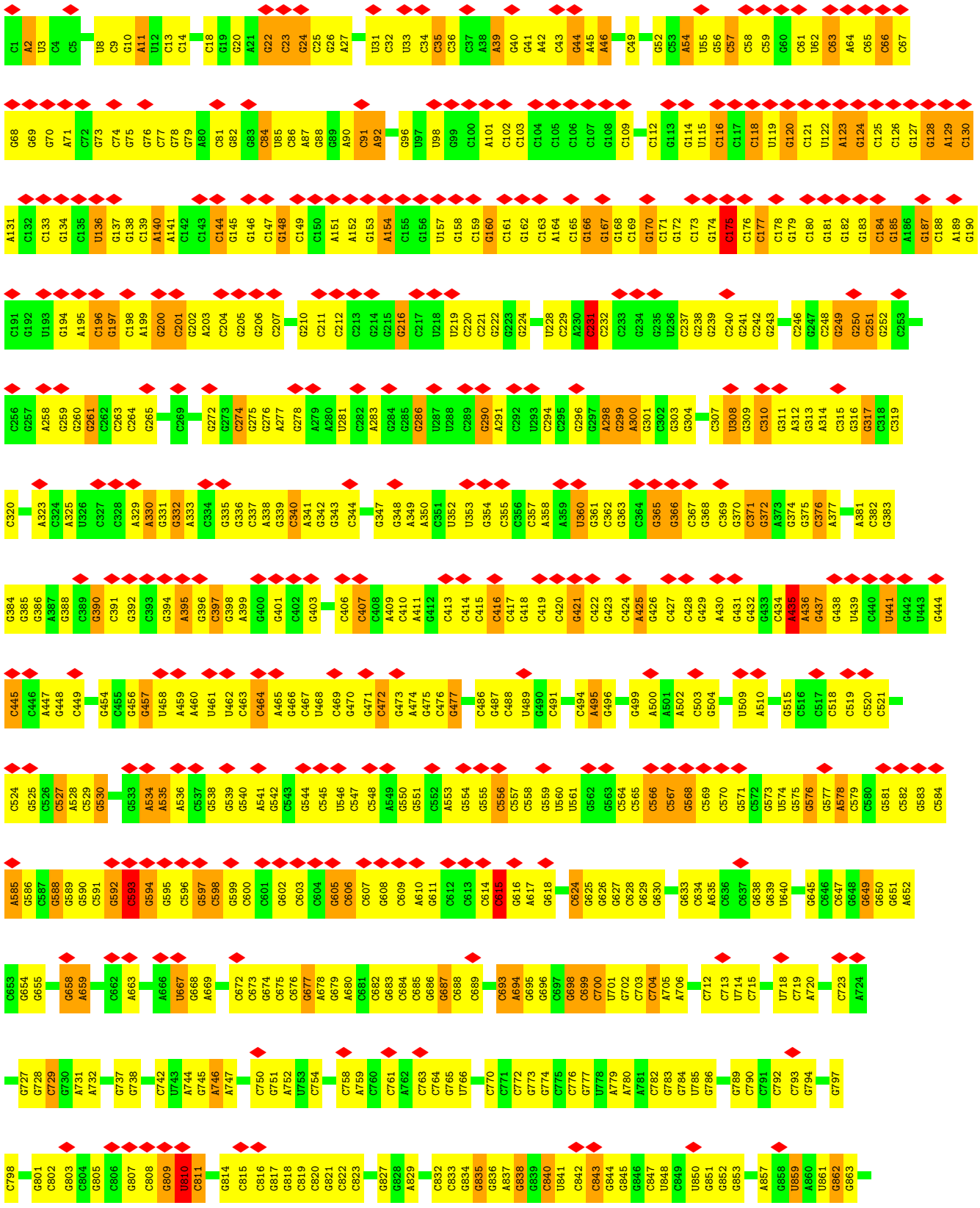

• Molecule 74: Ribosomal protein S30

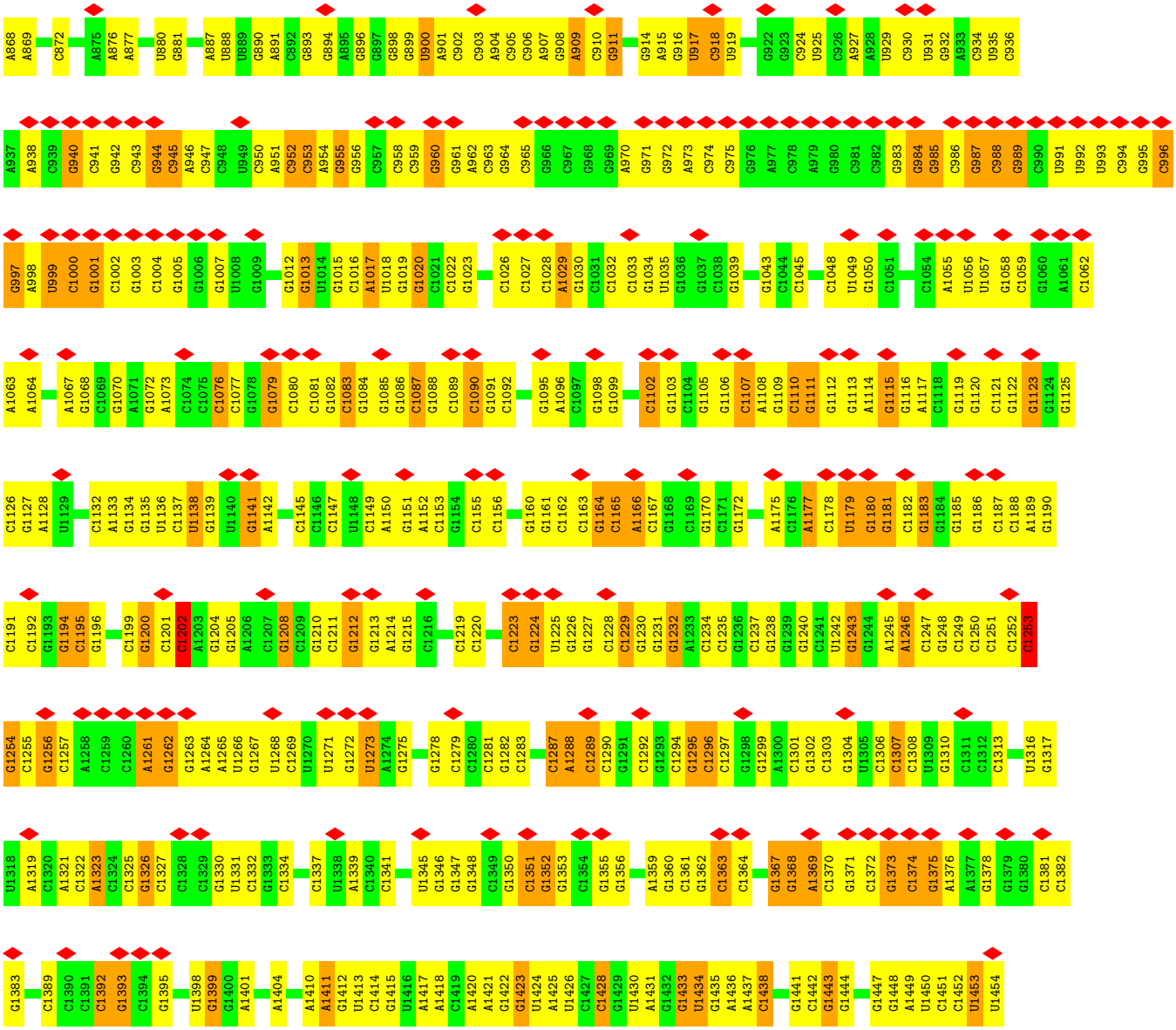
Chain Sj:



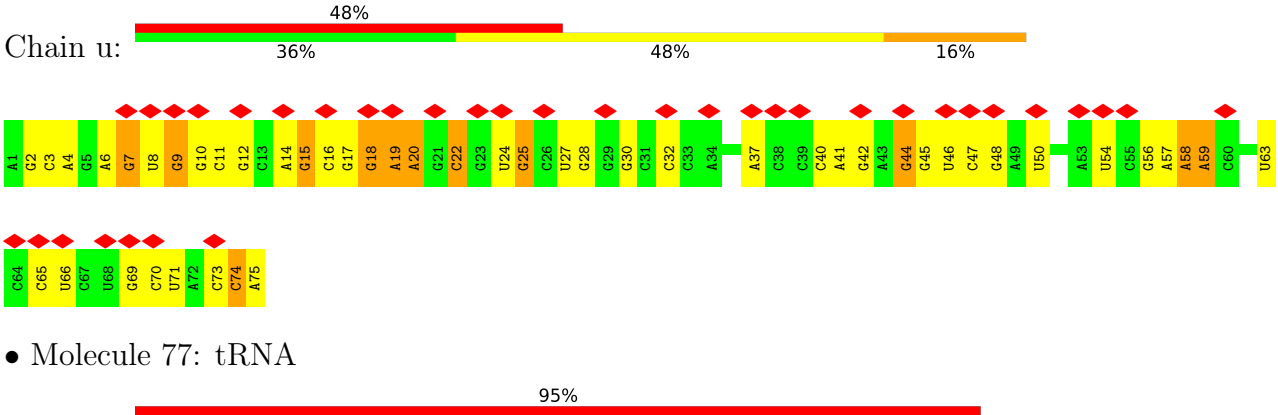
• Molecule 75: Small Subunit rRNA

Chain St:

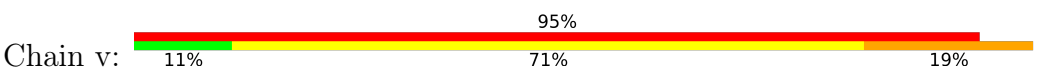


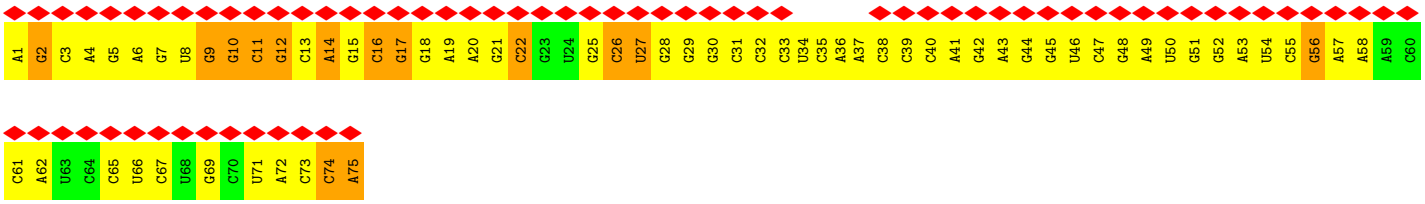


• Molecule 76: tRNA

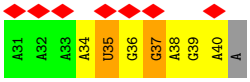



• Molecule 77: tRNA






• Molecule 78: mRNA



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 4500 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 30.0 | Depositor |
| Minimum defocus (nm) | 700 | Depositor |
| Maximum defocus (nm) | 1900 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 BASE (4k x 4k) | Depositor |
| Maximum map value | 13.691 | Depositor |
| Minimum map value | -8.031 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 4 | Depositor |
| Map size (Å) | 410.0, 410.0, 410.0 | wwPDB |
| Map dimensions | 500, 500, 500 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.82, 0.82, 0.82 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | 0.94 | 0/1919 | 1.41 | 4/2577 (0.2%) |
| 2 | LB | 0.91 | 0/3058 | 1.43 | 10/4129 (0.2%) |
| 3 | LC | 0.89 | 0/2506 | 1.42 | 10/3400 (0.3%) |
| 4 | LD | 0.58 | 0/3393 | 0.80 | 1/5292 (0.0%) |
| 5 | LE | 0.55 | 0/2798 | 0.78 | 1/4361 (0.0%) |
| 6 | LF | 0.86 | 0/2398 | 1.42 | 9/3216 (0.3%) |
| 7 | LG | 0.87 | 0/450 | 1.36 | 0/601 |
| 8 | LH | 0.87 | 0/1772 | 1.46 | 10/2389 (0.4%) |
| 9 | LI | 0.89 | 0/1583 | 1.45 | 3/2140 (0.1%) |
| 10 | LJ | 0.89 | 0/1479 | 1.41 | 9/1997 (0.5%) |
| 11 | LK | 0.89 | 0/1708 | 1.38 | 6/2288 (0.3%) |
| 12 | LL | 0.86 | 0/1374 | 1.40 | 10/1845 (0.5%) |
| 13 | LM | 0.89 | 0/1628 | 1.46 | 8/2180 (0.4%) |
| 14 | LN | 0.88 | 0/1037 | 1.40 | 1/1390 (0.1%) |
| 15 | LO | 0.86 | 0/1751 | 1.37 | 6/2346 (0.3%) |
| 16 | LP | 0.87 | 0/1610 | 1.46 | 16/2160 (0.7%) |
| 17 | LQ | 0.88 | 0/1280 | 1.46 | 1/1713 (0.1%) |
| 18 | LR | 0.88 | 0/1425 | 1.39 | 3/1907 (0.2%) |
| 19 | LS | 0.85 | 0/1609 | 1.39 | 7/2129 (0.3%) |
| 20 | LT | 0.88 | 0/1457 | 1.38 | 3/1957 (0.2%) |
| 21 | LU | 0.90 | 0/1290 | 1.38 | 3/1735 (0.2%) |
| 22 | LV | 0.85 | 0/951 | 1.43 | 4/1281 (0.3%) |
| 23 | LW | 0.92 | 0/1049 | 1.42 | 2/1414 (0.1%) |
| 24 | LX | 0.84 | 0/553 | 1.57 | 8/736 (1.1%) |
| 25 | LY | 0.92 | 0/982 | 1.38 | 3/1326 (0.2%) |
| 26 | LZ | 0.88 | 0/1091 | 1.42 | 4/1454 (0.3%) |
| 27 | La | 0.91 | 0/1069 | 1.42 | 6/1442 (0.4%) |
| 28 | Lb | 0.88 | 0/1231 | 1.40 | 3/1647 (0.2%) |
| 29 | Lc | 0.87 | 0/463 | 1.42 | 4/612 (0.7%) |
| 30 | Ld | 0.90 | 0/739 | 1.47 | 7/1000 (0.7%) |
| 31 | Le | 0.89 | 0/832 | 1.38 | 4/1118 (0.4%) |
| 32 | Lf | 0.87 | 0/1101 | 1.35 | 2/1467 (0.1%) |
| 33 | Lg | 0.87 | 0/793 | 1.38 | 4/1062 (0.4%) |
| 34 | Lh | 0.93 | 0/929 | 1.43 | 4/1247 (0.3%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | Li | 0.86 | 0/996 | 1.40 | 2/1328 (0.2%) |
| 36 | Lj | 0.85 | 0/741 | 1.40 | 3/982 (0.3%) |
| 37 | Lk | 0.90 | 0/727 | 1.40 | 4/963 (0.4%) |
| 38 | Ll | 0.85 | 0/562 | 1.38 | 1/749 (0.1%) |
| 39 | Ln | 0.99 | 0/1621 | 1.53 | 19/2183 (0.9%) |
| 40 | Lo | 0.76 | 0/229 | 1.23 | 0/291 |
| 41 | Lp | 0.85 | 0/778 | 1.43 | 4/1029 (0.4%) |
| 42 | Lq | 0.87 | 0/717 | 1.54 | 3/955 (0.3%) |
| 43 | Ls | 0.92 | 0/392 | 1.41 | 1/522 (0.2%) |
| 44 | Lt | 0.58 | 0/62214 | 0.82 | 57/97098 (0.1%) |
| 45 | SA | 0.93 | 0/1612 | 1.44 | 10/2190 (0.5%) |
| 46 | SB | 0.94 | 0/1700 | 1.45 | 6/2293 (0.3%) |
| 47 | SC | 0.92 | 0/1692 | 1.48 | 11/2272 (0.5%) |
| 48 | SD | 0.89 | 0/1903 | 1.38 | 5/2562 (0.2%) |
| 49 | SE | 0.97 | 0/2131 | 1.47 | 14/2874 (0.5%) |
| 50 | SF | 0.89 | 0/1465 | 1.50 | 13/1970 (0.7%) |
| 51 | SG | 0.95 | 0/1915 | 1.45 | 11/2560 (0.4%) |
| 52 | SH | 0.91 | 0/1508 | 1.42 | 8/2032 (0.4%) |
| 53 | SI | 0.95 | 0/1378 | 1.40 | 5/1848 (0.3%) |
| 54 | SJ | 0.92 | 0/1048 | 1.49 | 8/1412 (0.6%) |
| 55 | SK | 0.89 | 0/1443 | 1.44 | 8/1930 (0.4%) |
| 56 | SL | 0.90 | 0/901 | 1.42 | 4/1226 (0.3%) |
| 57 | SM | 0.93 | 0/1294 | 1.36 | 5/1731 (0.3%) |
| 58 | SO | 0.92 | 0/1104 | 1.41 | 5/1478 (0.3%) |
| 59 | SP | 0.90 | 0/1218 | 1.40 | 5/1640 (0.3%) |
| 60 | SQ | 0.95 | 0/938 | 1.45 | 6/1259 (0.5%) |
| 61 | SR | 0.93 | 0/961 | 1.36 | 3/1284 (0.2%) |
| 62 | ST | 0.95 | 0/1192 | 1.44 | 8/1594 (0.5%) |
| 63 | SU | 0.93 | 0/975 | 1.43 | 3/1303 (0.2%) |
| 64 | SV | 0.89 | 0/1178 | 1.48 | 8/1577 (0.5%) |
| 65 | SW | 0.95 | 0/1104 | 1.49 | 9/1484 (0.6%) |
| 66 | SX | 0.91 | 0/817 | 1.40 | 5/1103 (0.5%) |
| 67 | SY | 0.92 | 0/659 | 1.43 | 3/883 (0.3%) |
| 68 | Sb | 0.91 | 0/967 | 1.44 | 5/1294 (0.4%) |
| 69 | Sc | 0.96 | 0/603 | 1.45 | 2/802 (0.2%) |
| 70 | Sd | 0.92 | 0/899 | 1.39 | 3/1205 (0.2%) |
| 71 | Se | 0.93 | 0/643 | 1.38 | 4/871 (0.5%) |
| 72 | Sg | 0.96 | 0/508 | 1.41 | 3/677 (0.4%) |
| 73 | Sh | 0.87 | 0/425 | 1.47 | 3/563 (0.5%) |
| 74 | Sj | 0.88 | 0/553 | 1.38 | 3/736 (0.4%) |
| 75 | St | 0.60 | 0/34858 | 0.84 | 28/54401 (0.1%) |
| 76 | u | 0.57 | 0/1795 | 0.79 | 1/2798 (0.0%) |
| 77 | v | 0.61 | 0/1792 | 0.87 | 0/2793 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 78 | y | 0.58 | 0/249 | 0.94 | 1/387 (0.3%) |
| All | All | 0.74 | 0/191713 | 1.11 | 486/280690 (0.2%) |

There are no bond length outliers.

All (486) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | LC | 204 | VAL | N-CA-C | -11.60 | 102.06 | 113.20 |
| 17 | LQ | 50 | VAL | N-CA-C | -11.15 | 102.22 | 111.81 |
| 9 | LI | 167 | LEU | N-CA-C | -11.12 | 100.26 | 114.04 |
| 16 | LP | 106 | PRO | N-CA-C | 10.38 | 123.36 | 110.70 |
| 24 | LX | 33 | CYS | CB-CA-C | -10.04 | 95.04 | 110.90 |
| 44 | Lt | 1135 | G | C2'-C3'-O3' | 9.92 | 124.37 | 109.50 |
| 51 | SG | 172 | GLU | N-CA-C | 9.69 | 122.20 | 108.54 |
| 51 | SG | 189 | PRO | N-CA-C | -9.19 | 96.80 | 111.14 |
| 19 | LS | 41 | ILE | N-CA-C | -8.88 | 104.17 | 111.81 |
| 46 | SB | 121 | LYS | N-CA-C | -8.87 | 102.59 | 113.41 |
| 44 | Lt | 2022 | C | C2'-C3'-O3' | 8.86 | 126.98 | 113.70 |
| 16 | LP | 73 | PRO | CB-CA-C | -8.84 | 99.21 | 112.11 |
| 56 | SL | 56 | ILE | N-CA-C | -8.35 | 104.63 | 111.81 |
| 44 | Lt | 1349 | G | C2'-C3'-O3' | 8.34 | 126.21 | 113.70 |
| 71 | Se | 121 | TYR | CB-CA-C | -8.32 | 106.98 | 116.54 |
| 12 | LL | 23 | ILE | CA-C-O | -8.31 | 115.40 | 122.63 |
| 44 | Lt | 691 | G | C2'-C3'-O3' | 8.31 | 126.16 | 113.70 |
| 75 | St | 1138 | U | C4'-C3'-O3' | 8.29 | 121.84 | 109.40 |
| 65 | SW | 39 | VAL | N-CA-C | -8.23 | 105.00 | 112.90 |
| 16 | LP | 194 | LYS | CB-CA-C | 8.21 | 117.95 | 109.83 |
| 39 | Ln | 47 | PRO | N-CA-CB | -8.20 | 94.64 | 103.25 |
| 8 | LH | 71 | TYR | CA-C-N | -8.19 | 115.50 | 123.04 |
| 8 | LH | 71 | TYR | C-N-CA | -8.19 | 115.50 | 123.04 |
| 75 | St | 1253 | C | C4'-C3'-O3' | 8.19 | 125.28 | 113.00 |
| 44 | Lt | 2045 | G | C1'-O4'-C4' | -8.04 | 101.66 | 109.70 |
| 44 | Lt | 1079 | G | C2'-C3'-O3' | 8.01 | 121.52 | 109.50 |
| 65 | SW | 20 | LEU | N-CA-C | -7.93 | 102.24 | 112.23 |
| 49 | SE | 80 | PRO | N-CA-C | -7.88 | 105.54 | 114.92 |
| 49 | SE | 166 | THR | N-CA-C | -7.82 | 102.84 | 111.36 |
| 27 | La | 48 | PRO | N-CA-C | 7.80 | 124.62 | 113.47 |
| 25 | LY | 55 | TRP | N-CA-C | -7.77 | 102.86 | 112.88 |
| 33 | Lg | 58 | GLY | N-CA-C | -7.75 | 105.05 | 115.36 |
| 69 | Sc | 32 | LYS | N-CA-C | -7.71 | 101.73 | 112.45 |
| 19 | LS | 120 | TYR | N-CA-C | -7.69 | 102.23 | 111.69 |
| 75 | St | 810 | U | C4'-C3'-O3' | 7.69 | 120.93 | 109.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | LS | 124 | TYR | N-CA-C | -7.64 | 102.52 | 112.68 |
| 23 | LW | 110 | PRO | N-CA-C | -7.64 | 102.91 | 113.53 |
| 1 | LA | 13 | GLY | CA-C-O | -7.60 | 115.58 | 122.57 |
| 75 | St | 1246 | A | C2'-C3'-O3' | -7.60 | 98.11 | 109.50 |
| 44 | Lt | 2284 | U | C2'-C3'-O3' | 7.58 | 125.07 | 113.70 |
| 50 | SF | 107 | PRO | CB-CA-C | -7.57 | 103.31 | 111.56 |
| 44 | Lt | 2591 | C | C2'-C3'-O3' | 7.53 | 120.80 | 109.50 |
| 37 | Lk | 58 | THR | CB-CA-C | -7.53 | 97.40 | 110.95 |
| 75 | St | 599 | G | C2'-C3'-O3' | 7.45 | 124.88 | 113.70 |
| 64 | SV | 142 | ARG | N-CA-C | -7.45 | 103.09 | 111.14 |
| 62 | ST | 12 | ARG | N-CA-C | -7.38 | 104.66 | 112.93 |
| 61 | SR | 60 | LYS | N-CA-C | -7.38 | 103.69 | 114.39 |
| 8 | LH | 200 | PHE | CB-CA-C | -7.37 | 99.81 | 110.06 |
| 39 | Ln | 10 | ASN | N-CA-C | -7.36 | 103.43 | 113.30 |
| 44 | Lt | 1448 | G | C2'-C3'-O3' | 7.36 | 124.74 | 113.70 |
| 50 | SF | 37 | HIS | N-CA-C | -7.36 | 103.20 | 111.07 |
| 75 | St | 1183 | G | C3'-C2'-C1' | -7.34 | 94.16 | 101.50 |
| 45 | SA | 110 | PRO | N-CA-C | 7.33 | 122.73 | 111.15 |
| 42 | Lq | 12 | GLY | N-CA-C | -7.33 | 103.09 | 115.62 |
| 75 | St | 593 | C | C2'-C3'-O3' | 7.33 | 120.49 | 109.50 |
| 49 | SE | 29 | PRO | N-CA-CB | 7.30 | 107.01 | 102.92 |
| 57 | SM | 60 | GLY | CA-C-O | -7.29 | 117.48 | 122.22 |
| 16 | LP | 195 | TYR | N-CA-C | -7.28 | 103.43 | 111.36 |
| 12 | LL | 155 | THR | CB-CA-C | 7.26 | 119.32 | 108.86 |
| 24 | LX | 34 | THR | CB-CA-C | -7.25 | 96.97 | 112.78 |
| 44 | Lt | 1277 | G | C4'-C3'-O3' | 7.24 | 120.27 | 109.40 |
| 75 | St | 365 | G | C3'-C2'-C1' | -7.23 | 94.27 | 101.50 |
| 16 | LP | 181 | LYS | CB-CA-C | -7.22 | 106.68 | 117.07 |
| 48 | SD | 41 | ILE | N-CA-C | -7.21 | 104.35 | 113.22 |
| 49 | SE | 12 | LEU | N-CA-C | -7.21 | 105.67 | 114.75 |
| 44 | Lt | 1277 | G | C2'-C3'-O3' | 7.20 | 120.31 | 109.50 |
| 34 | Lh | 96 | ASN | N-CA-C | -7.19 | 103.18 | 112.23 |
| 46 | SB | 210 | ASN | N-CA-C | -7.18 | 103.99 | 112.89 |
| 47 | SC | 90 | PHE | CA-CB-CG | 7.16 | 120.96 | 113.80 |
| 39 | Ln | 150 | GLU | N-CA-C | -7.16 | 103.52 | 111.82 |
| 2 | LB | 257 | PRO | N-CA-C | -7.15 | 97.74 | 112.47 |
| 64 | SV | 50 | ASN | N-CA-C | -7.15 | 104.02 | 114.39 |
| 13 | LM | 74 | ALA | CA-C-N | -7.13 | 116.19 | 122.96 |
| 13 | LM | 74 | ALA | C-N-CA | -7.13 | 116.19 | 122.96 |
| 3 | LC | 155 | ALA | N-CA-C | -7.07 | 102.63 | 112.45 |
| 29 | Lc | 50 | ASP | CB-CA-C | 7.06 | 124.08 | 110.17 |
| 44 | Lt | 302 | C | C2'-C3'-O3' | 7.06 | 124.28 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 53 | SI | 42 | VAL | N-CA-C | -7.04 | 103.61 | 110.72 |
| 52 | SH | 121 | THR | CB-CA-C | 7.03 | 121.39 | 109.72 |
| 44 | Lt | 2017 | A | C2'-C3'-O3' | 7.01 | 120.01 | 109.50 |
| 46 | SB | 26 | GLU | N-CA-C | -7.00 | 101.73 | 111.39 |
| 20 | LT | 151 | PRO | N-CA-C | -6.99 | 105.43 | 114.03 |
| 44 | Lt | 649 | U | C2'-C3'-O3' | -6.99 | 99.01 | 109.50 |
| 50 | SF | 68 | ASN | CB-CA-C | 6.96 | 122.32 | 110.56 |
| 61 | SR | 64 | ARG | N-CA-C | -6.96 | 104.42 | 113.12 |
| 6 | LF | 100 | ALA | N-CA-C | -6.92 | 104.83 | 113.55 |
| 39 | Ln | 178 | GLU | N-CA-C | -6.88 | 104.15 | 112.54 |
| 12 | LL | 109 | HIS | N-CA-C | -6.87 | 104.16 | 112.54 |
| 27 | La | 48 | PRO | CB-CA-C | -6.84 | 102.19 | 113.06 |
| 44 | Lt | 458 | G | C2'-C3'-O3' | -6.83 | 103.45 | 113.70 |
| 47 | SC | 89 | ASN | N-CA-C | -6.83 | 103.77 | 111.14 |
| 73 | Sh | 99 | LYS | N-CA-C | -6.82 | 102.26 | 111.87 |
| 16 | LP | 36 | GLU | N-CA-C | -6.82 | 104.84 | 113.02 |
| 35 | Li | 83 | VAL | N-CA-C | -6.79 | 103.06 | 112.50 |
| 6 | LF | 142 | ASN | CB-CA-C | -6.77 | 107.32 | 117.07 |
| 2 | LB | 169 | PRO | CB-CA-C | -6.77 | 101.33 | 110.88 |
| 44 | Lt | 2574 | C | C2'-C3'-O3' | 6.77 | 123.86 | 113.70 |
| 10 | LJ | 58 | PRO | CB-CA-C | -6.76 | 104.19 | 111.56 |
| 49 | SE | 230 | ASN | N-CA-C | -6.75 | 103.92 | 111.28 |
| 75 | St | 90 | A | C4'-C3'-O3' | 6.75 | 119.53 | 109.40 |
| 13 | LM | 77 | PRO | CB-CA-C | -6.75 | 102.33 | 113.06 |
| 44 | Lt | 1931 | G | C2'-C3'-O3' | 6.72 | 123.77 | 113.70 |
| 65 | SW | 60 | ARG | N-CA-C | -6.70 | 103.77 | 112.68 |
| 75 | St | 588 | G | C2'-C3'-O3' | 6.69 | 123.74 | 113.70 |
| 44 | Lt | 2627 | G | C2'-C3'-O3' | 6.68 | 123.72 | 113.70 |
| 45 | SA | 21 | LYS | N-CA-C | -6.68 | 104.61 | 112.89 |
| 22 | LV | 47 | ASN | N-CA-C | -6.67 | 103.35 | 113.89 |
| 74 | Sj | 27 | PRO | N-CA-C | -6.67 | 102.57 | 110.70 |
| 16 | LP | 55 | MET | N-CA-C | -6.63 | 105.48 | 113.97 |
| 44 | Lt | 1914 | C | C2'-C3'-O3' | 6.63 | 123.65 | 113.70 |
| 49 | SE | 178 | GLY | N-CA-C | -6.63 | 105.93 | 115.27 |
| 44 | Lt | 1317 | C | C2'-C3'-O3' | 6.62 | 123.64 | 113.70 |
| 62 | ST | 132 | VAL | N-CA-C | -6.61 | 106.79 | 113.47 |
| 60 | SQ | 136 | PRO | CB-CA-C | -6.60 | 100.67 | 111.56 |
| 49 | SE | 137 | PRO | N-CA-C | 6.58 | 121.54 | 111.34 |
| 45 | SA | 139 | ILE | N-CA-C | -6.58 | 104.61 | 111.58 |
| 46 | SB | 40 | GLY | N-CA-C | -6.57 | 106.25 | 115.32 |
| 75 | St | 187 | G | C4'-C3'-O3' | 6.56 | 119.24 | 109.40 |
| 65 | SW | 5 | THR | N-CA-C | -6.54 | 104.93 | 113.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | LI | 162 | ARG | N-CA-C | 6.53 | 120.14 | 109.76 |
| 56 | SL | 6 | LYS | N-CA-C | -6.52 | 104.01 | 112.23 |
| 24 | LX | 60 | HIS | CB-CA-C | 6.52 | 123.47 | 110.17 |
| 13 | LM | 204 | LEU | N-CA-C | -6.52 | 105.34 | 113.55 |
| 44 | Lt | 820 | C | C4'-C3'-O3' | 6.50 | 122.75 | 113.00 |
| 75 | St | 1303 | C | C2'-C3'-O3' | 6.48 | 123.42 | 113.70 |
| 45 | SA | 44 | PHE | N-CA-C | -6.48 | 104.14 | 111.14 |
| 44 | Lt | 694 | C | C1'-C2'-O2' | -6.46 | 98.72 | 108.40 |
| 75 | St | 200 | G | C2'-C3'-O3' | -6.45 | 104.02 | 113.70 |
| 75 | St | 435 | A | C2'-C3'-O3' | 6.45 | 123.37 | 113.70 |
| 50 | SF | 107 | PRO | N-CA-C | 6.43 | 120.59 | 110.50 |
| 6 | LF | 192 | SER | N-CA-C | -6.41 | 102.07 | 110.53 |
| 44 | Lt | 2584 | C | C2'-C3'-O3' | 6.40 | 119.10 | 109.50 |
| 12 | LL | 118 | PRO | N-CA-C | -6.39 | 104.64 | 113.53 |
| 39 | Ln | 72 | ARG | CB-CA-C | -6.38 | 97.73 | 110.42 |
| 75 | St | 1261 | A | C4'-C3'-O3' | 6.37 | 118.95 | 109.40 |
| 8 | LH | 220 | PHE | CA-CB-CG | 6.34 | 120.14 | 113.80 |
| 34 | Lh | 40 | PRO | CB-CA-C | -6.34 | 103.11 | 111.23 |
| 32 | Lf | 73 | PRO | CB-CA-C | -6.34 | 102.33 | 112.21 |
| 75 | St | 1183 | G | C2'-C3'-O3' | -6.33 | 100.00 | 109.50 |
| 31 | Le | 32 | ARG | N-CA-C | -6.32 | 105.22 | 113.12 |
| 11 | LK | 81 | GLY | CA-C-O | -6.32 | 118.11 | 122.22 |
| 59 | SP | 30 | PRO | CB-CA-C | -6.30 | 102.38 | 112.21 |
| 68 | Sb | 36 | LYS | N-CA-C | -6.30 | 106.23 | 114.04 |
| 44 | Lt | 918 | U | C4'-C3'-O3' | -6.27 | 103.59 | 113.00 |
| 39 | Ln | 183 | ILE | N-CA-C | -6.26 | 104.24 | 110.62 |
| 64 | SV | 40 | ARG | CB-CA-C | 6.26 | 119.65 | 110.26 |
| 39 | Ln | 11 | LYS | N-CA-C | -6.25 | 104.92 | 113.30 |
| 50 | SF | 157 | GLU | N-CA-C | -6.25 | 105.15 | 112.89 |
| 11 | LK | 26 | VAL | N-CA-C | -6.24 | 102.84 | 108.95 |
| 12 | LL | 133 | ARG | CA-C-O | -6.21 | 114.72 | 119.32 |
| 56 | SL | 64 | GLY | N-CA-C | -6.21 | 106.85 | 114.92 |
| 3 | LC | 164 | VAL | N-CA-C | -6.21 | 106.69 | 112.83 |
| 75 | St | 1262 | G | C2'-C3'-O3' | -6.20 | 104.40 | 113.70 |
| 10 | LJ | 49 | ASP | N-CA-C | -6.20 | 104.20 | 112.94 |
| 47 | SC | 116 | GLU | N-CA-C | -6.20 | 104.45 | 111.14 |
| 6 | LF | 4 | VAL | N-CA-C | 6.19 | 122.21 | 109.34 |
| 69 | Sc | 35 | LYS | N-CA-C | -6.18 | 105.22 | 112.89 |
| 34 | Lh | 13 | THR | N-CA-C | -6.17 | 106.34 | 114.31 |
| 31 | Le | 78 | HIS | N-CA-C | -6.17 | 105.41 | 113.12 |
| 13 | LM | 172 | GLY | CA-C-O | -6.16 | 117.98 | 122.23 |
| 44 | Lt | 2017 | A | C4'-C3'-O3' | 6.16 | 118.64 | 109.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | SC | 9 | GLU | N-CA-C | -6.14 | 105.77 | 113.20 |
| 28 | Lb | 76 | ASP | N-CA-C | -6.14 | 105.45 | 113.12 |
| 48 | SD | 172 | LEU | N-CA-C | -6.13 | 104.59 | 111.28 |
| 70 | Sd | 102 | PRO | N-CA-C | -6.12 | 108.31 | 114.68 |
| 1 | LA | 52 | ARG | N-CA-C | -6.11 | 103.94 | 111.40 |
| 44 | Lt | 259 | C | C4'-C3'-O3' | 6.11 | 122.16 | 113.00 |
| 66 | SX | 81 | HIS | CB-CA-C | -6.11 | 100.73 | 110.81 |
| 62 | ST | 50 | ASN | N-CA-C | -6.11 | 105.13 | 112.58 |
| 75 | St | 330 | A | C4'-C3'-O3' | 6.10 | 118.56 | 109.40 |
| 26 | LZ | 116 | TYR | N-CA-C | -6.10 | 104.56 | 112.68 |
| 58 | SO | 61 | GLN | CA-C-O | -6.10 | 113.04 | 119.50 |
| 8 | LH | 29 | GLU | N-CA-C | -6.09 | 104.72 | 111.36 |
| 30 | Ld | 32 | ASP | CA-CB-CG | 6.09 | 118.69 | 112.60 |
| 41 | Lp | 87 | HIS | N-CA-C | -6.08 | 104.76 | 111.82 |
| 10 | LJ | 86 | TYR | CB-CA-C | -6.08 | 101.53 | 111.50 |
| 27 | La | 103 | LYS | N-CA-C | -6.08 | 105.81 | 113.72 |
| 51 | SG | 113 | HIS | N-CA-C | 6.07 | 117.69 | 111.14 |
| 52 | SH | 185 | THR | CB-CA-C | -6.07 | 102.69 | 111.91 |
| 54 | SJ | 32 | LYS | N-CA-C | -6.06 | 104.79 | 111.82 |
| 64 | SV | 93 | SER | N-CA-C | -6.06 | 106.14 | 112.93 |
| 29 | Lc | 54 | SER | N-CA-C | -6.04 | 105.62 | 112.87 |
| 50 | SF | 34 | PHE | CA-CB-CG | 6.03 | 119.83 | 113.80 |
| 36 | Lj | 34 | LYS | N-CA-C | -6.03 | 105.19 | 112.54 |
| 16 | LP | 42 | GLY | CA-C-O | -6.02 | 118.31 | 122.22 |
| 39 | Ln | 159 | PHE | CA-C-O | -6.01 | 114.09 | 121.06 |
| 65 | SW | 4 | VAL | N-CA-C | -6.01 | 104.20 | 113.16 |
| 68 | Sb | 106 | LYS | N-CA-C | -6.01 | 104.81 | 111.36 |
| 15 | LO | 167 | ALA | N-CA-C | -6.01 | 105.21 | 112.54 |
| 50 | SF | 12 | PRO | CB-CA-C | -6.01 | 104.01 | 111.64 |
| 57 | SM | 148 | LYS | CB-CA-C | -6.00 | 109.67 | 116.63 |
| 16 | LP | 91 | ARG | N-CA-C | -5.99 | 104.66 | 111.07 |
| 53 | SI | 166 | PHE | CA-CB-CG | 5.99 | 119.78 | 113.80 |
| 26 | LZ | 107 | LYS | N-CA-C | -5.98 | 106.63 | 114.04 |
| 15 | LO | 23 | PHE | N-CA-C | -5.97 | 104.15 | 112.45 |
| 51 | SG | 68 | PRO | N-CA-C | 5.97 | 120.46 | 111.14 |
| 2 | LB | 374 | ARG | N-CA-C | -5.97 | 104.90 | 111.82 |
| 44 | Lt | 71 | C | C2'-C3'-O3' | 5.97 | 122.65 | 113.70 |
| 71 | Se | 50 | TYR | CB-CA-C | 5.96 | 116.07 | 110.17 |
| 11 | LK | 174 | THR | CB-CA-C | -5.96 | 100.61 | 109.90 |
| 60 | SQ | 37 | LYS | N-CA-C | -5.95 | 104.73 | 112.23 |
| 44 | Lt | 1236 | G | C2'-C3'-O3' | 5.95 | 122.62 | 113.70 |
| 60 | SQ | 39 | ASP | CB-CA-C | -5.95 | 100.15 | 109.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 59 | SP | 38 | TYR | N-CA-C | -5.94 | 104.88 | 111.36 |
| 45 | SA | 51 | THR | CB-CA-C | 5.94 | 119.40 | 109.89 |
| 24 | LX | 10 | CYS | CB-CA-C | -5.93 | 100.94 | 110.79 |
| 8 | LH | 158 | ILE | CA-C-O | -5.93 | 117.47 | 122.63 |
| 11 | LK | 29 | PRO | N-CA-C | -5.93 | 101.90 | 111.03 |
| 62 | ST | 89 | GLY | CA-C-O | -5.93 | 118.14 | 122.23 |
| 52 | SH | 90 | GLY | N-CA-C | -5.92 | 107.52 | 115.21 |
| 47 | SC | 119 | MET | CA-C-O | -5.91 | 115.57 | 120.71 |
| 46 | SB | 145 | PRO | N-CA-C | 5.90 | 120.35 | 111.14 |
| 12 | LL | 7 | ASN | CB-CA-C | 5.88 | 119.11 | 109.46 |
| 75 | St | 1202 | C | C2'-C3'-O3' | -5.88 | 104.88 | 113.70 |
| 39 | Ln | 23 | GLU | CB-CA-C | 5.88 | 115.65 | 109.83 |
| 39 | Ln | 19 | ARG | N-CA-C | -5.87 | 104.83 | 112.23 |
| 44 | Lt | 2273 | G | C2'-C3'-O3' | -5.87 | 104.89 | 113.70 |
| 19 | LS | 60 | ARG | N-CA-C | -5.87 | 104.32 | 112.30 |
| 64 | SV | 42 | ALA | N-CA-C | -5.87 | 104.81 | 113.72 |
| 47 | SC | 113 | ALA | N-CA-C | -5.86 | 104.97 | 111.36 |
| 59 | SP | 30 | PRO | N-CA-C | -5.86 | 105.74 | 113.65 |
| 39 | Ln | 21 | THR | CB-CA-C | 5.86 | 122.08 | 110.42 |
| 50 | SF | 187 | VAL | N-CA-C | -5.86 | 105.37 | 111.58 |
| 39 | Ln | 191 | ALA | N-CA-C | -5.85 | 105.40 | 112.54 |
| 33 | Lg | 9 | PHE | CA-CB-CG | 5.84 | 119.64 | 113.80 |
| 51 | SG | 14 | PRO | N-CA-C | 5.84 | 124.51 | 112.47 |
| 6 | LF | 33 | ARG | N-CA-C | -5.84 | 104.92 | 111.28 |
| 2 | LB | 139 | ASP | N-CA-C | -5.83 | 105.82 | 113.17 |
| 5 | LE | 38 | U | C4'-C3'-O3' | 5.83 | 121.74 | 113.00 |
| 42 | Lq | 53 | GLY | CA-C-N | -5.82 | 114.86 | 122.37 |
| 42 | Lq | 53 | GLY | C-N-CA | -5.82 | 114.86 | 122.37 |
| 68 | Sb | 108 | LEU | N-CA-C | -5.82 | 104.94 | 111.28 |
| 71 | Se | 107 | PRO | N-CA-C | 5.81 | 120.21 | 111.14 |
| 75 | St | 170 | G | C4'-C3'-C2' | -5.81 | 96.79 | 102.60 |
| 44 | Lt | 1582 | C | C3'-C2'-O2' | 5.80 | 119.40 | 110.70 |
| 44 | Lt | 1054 | G | C2'-C3'-O3' | -5.80 | 105.00 | 113.70 |
| 44 | Lt | 2045 | G | C1'-C2'-O2' | -5.80 | 103.10 | 111.80 |
| 39 | Ln | 137 | PRO | N-CA-C | 5.80 | 128.75 | 112.92 |
| 57 | SM | 33 | TYR | CB-CA-C | 5.79 | 120.31 | 109.71 |
| 2 | LB | 33 | PRO | N-CA-C | 5.79 | 117.77 | 110.70 |
| 50 | SF | 74 | MET | N-CA-C | -5.79 | 105.71 | 112.89 |
| 15 | LO | 180 | GLY | N-CA-C | -5.79 | 107.69 | 115.21 |
| 49 | SE | 40 | GLU | N-CA-C | 5.78 | 117.58 | 111.28 |
| 58 | SO | 116 | PRO | N-CA-C | 5.78 | 120.56 | 111.38 |
| 31 | Le | 5 | TYR | CB-CA-C | -5.78 | 100.72 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | Ln | 135 | PRO | CB-CA-C | -5.76 | 105.25 | 113.09 |
| 58 | SO | 23 | ALA | N-CA-C | -5.76 | 106.89 | 114.04 |
| 51 | SG | 172 | GLU | CA-C-O | -5.76 | 109.56 | 120.96 |
| 3 | LC | 41 | ARG | N-CA-C | -5.75 | 104.62 | 111.69 |
| 39 | Ln | 116 | LEU | N-CA-C | -5.75 | 104.81 | 113.89 |
| 13 | LM | 195 | GLU | CA-C-N | -5.74 | 117.76 | 123.04 |
| 13 | LM | 195 | GLU | C-N-CA | -5.74 | 117.76 | 123.04 |
| 65 | SW | 61 | HIS | CB-CA-C | 5.73 | 121.23 | 110.63 |
| 24 | LX | 37 | CYS | N-CA-C | -5.73 | 105.04 | 111.28 |
| 16 | LP | 52 | LEU | N-CA-C | -5.72 | 105.19 | 111.82 |
| 10 | LJ | 180 | ARG | N-CA-C | -5.71 | 105.51 | 112.88 |
| 78 | y | 37 | G | C4'-C3'-C2' | -5.71 | 96.89 | 102.60 |
| 44 | Lt | 326 | A | C2'-C3'-O3' | -5.70 | 100.95 | 109.50 |
| 22 | LV | 79 | VAL | N-CA-C | -5.70 | 103.81 | 111.44 |
| 44 | Lt | 1581 | G | C2'-C3'-O3' | -5.69 | 105.17 | 113.70 |
| 54 | SJ | 35 | ILE | N-CA-C | -5.69 | 104.98 | 110.72 |
| 18 | LR | 44 | PHE | N-CA-C | -5.68 | 104.99 | 111.07 |
| 35 | Li | 62 | MET | N-CA-C | -5.67 | 105.86 | 112.89 |
| 44 | Lt | 1751 | C | C2'-C3'-O3' | -5.67 | 100.99 | 109.50 |
| 56 | SL | 92 | ASP | N-CA-C | -5.66 | 106.32 | 113.23 |
| 60 | SQ | 121 | ARG | N-CA-C | -5.66 | 105.11 | 111.28 |
| 30 | Ld | 40 | ASP | N-CA-C | -5.66 | 106.22 | 113.23 |
| 44 | Lt | 918 | U | N1-C1'-C2' | 5.66 | 120.48 | 112.00 |
| 63 | SU | 82 | GLU | N-CA-C | -5.64 | 105.66 | 112.54 |
| 65 | SW | 49 | ASP | N-CA-C | -5.64 | 106.99 | 112.97 |
| 41 | Lp | 11 | PHE | CB-CA-C | -5.63 | 102.21 | 111.68 |
| 44 | Lt | 1013 | G | C2'-C3'-O3' | -5.63 | 105.25 | 113.70 |
| 18 | LR | 80 | VAL | CA-C-O | -5.63 | 117.73 | 122.63 |
| 23 | LW | 12 | GLY | CA-C-O | -5.63 | 118.26 | 122.37 |
| 51 | SG | 27 | PHE | N-CA-C | -5.63 | 105.14 | 112.23 |
| 26 | LZ | 90 | PRO | N-CA-C | -5.62 | 105.72 | 113.53 |
| 51 | SG | 67 | PHE | CB-CA-C | 5.62 | 118.40 | 109.52 |
| 33 | Lg | 86 | GLN | N-CA-C | -5.61 | 105.24 | 111.36 |
| 3 | LC | 21 | PRO | N-CA-C | -5.61 | 102.46 | 111.38 |
| 10 | LJ | 66 | PRO | CB-CA-C | -5.61 | 104.14 | 113.06 |
| 44 | Lt | 1862 | C | C4'-C3'-O3' | 5.61 | 117.81 | 109.40 |
| 6 | LF | 226 | ARG | N-CA-C | -5.61 | 104.56 | 111.40 |
| 66 | SX | 76 | GLY | CA-C-O | -5.59 | 117.76 | 122.29 |
| 37 | Lk | 78 | THR | N-CA-C | -5.59 | 107.00 | 113.88 |
| 1 | LA | 244 | GLY | CA-C-O | -5.59 | 118.10 | 122.52 |
| 22 | LV | 110 | TYR | N-CA-C | -5.59 | 105.28 | 111.71 |
| 1 | LA | 211 | HIS | N-CA-C | -5.59 | 105.29 | 111.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | Lt | 2584 | C | C4'-C3'-O3' | 5.59 | 117.78 | 109.40 |
| 44 | Lt | 259 | C | C2'-C3'-O3' | 5.58 | 122.07 | 113.70 |
| 28 | Lb | 69 | TYR | CB-CA-C | -5.58 | 102.94 | 109.80 |
| 67 | SY | 7 | GLY | CA-C-O | -5.57 | 117.17 | 122.13 |
| 47 | SC | 23 | MET | N-CA-C | -5.57 | 105.21 | 111.28 |
| 49 | SE | 18 | TRP | N-CA-C | -5.57 | 105.75 | 112.54 |
| 55 | SK | 130 | ILE | N-CA-C | -5.57 | 104.93 | 111.00 |
| 44 | Lt | 1014 | C | C2'-C3'-O3' | -5.56 | 105.36 | 113.70 |
| 53 | SI | 162 | PRO | N-CA-C | -5.56 | 106.81 | 113.98 |
| 62 | ST | 47 | ILE | N-CA-C | -5.55 | 106.90 | 112.17 |
| 30 | Ld | 76 | GLY | CA-C-O | -5.54 | 116.51 | 122.05 |
| 12 | LL | 155 | THR | CA-C-O | -5.53 | 115.62 | 120.60 |
| 39 | Ln | 81 | GLY | N-CA-C | 5.53 | 118.08 | 110.56 |
| 55 | SK | 171 | PRO | CB-CA-C | -5.53 | 105.65 | 112.89 |
| 24 | LX | 60 | HIS | CA-CB-CG | 5.51 | 119.31 | 113.80 |
| 29 | Lc | 19 | ASN | N-CA-C | -5.51 | 104.41 | 113.50 |
| 19 | LS | 123 | LEU | N-CA-C | -5.49 | 106.62 | 113.15 |
| 39 | Ln | 112 | ALA | CA-C-O | -5.48 | 115.78 | 122.41 |
| 47 | SC | 78 | LEU | N-CA-C | -5.46 | 105.23 | 111.07 |
| 44 | Lt | 2217 | G | C2'-C3'-O3' | 5.46 | 121.88 | 113.70 |
| 57 | SM | 13 | GLN | N-CA-C | -5.45 | 100.91 | 109.25 |
| 2 | LB | 270 | MET | CA-C-N | -5.44 | 113.87 | 120.51 |
| 2 | LB | 270 | MET | C-N-CA | -5.44 | 113.87 | 120.51 |
| 48 | SD | 50 | ALA | N-CA-C | -5.44 | 105.86 | 112.88 |
| 16 | LP | 193 | ALA | N-CA-C | -5.43 | 106.50 | 113.02 |
| 55 | SK | 45 | ARG | N-CA-C | -5.42 | 105.37 | 111.28 |
| 61 | SR | 98 | ASN | N-CA-C | -5.42 | 102.87 | 110.35 |
| 50 | SF | 177 | SER | N-CA-C | -5.41 | 106.52 | 113.01 |
| 52 | SH | 114 | ILE | CA-C-O | -5.41 | 115.44 | 121.17 |
| 30 | Ld | 75 | ALA | N-CA-C | -5.40 | 105.39 | 111.28 |
| 44 | Lt | 734 | G | C3'-C2'-C1' | -5.40 | 96.10 | 101.50 |
| 32 | Lf | 8 | PRO | N-CA-C | 5.40 | 119.18 | 111.13 |
| 30 | Ld | 32 | ASP | CB-CA-C | 5.39 | 119.74 | 110.79 |
| 37 | Lk | 11 | ARG | CB-CA-C | -5.39 | 103.20 | 111.83 |
| 36 | Lj | 28 | PRO | CB-CA-C | -5.39 | 104.49 | 113.06 |
| 44 | Lt | 1969 | G | C1'-O4'-C4' | -5.38 | 104.52 | 109.90 |
| 54 | SJ | 97 | ARG | N-CA-C | -5.38 | 106.39 | 113.17 |
| 45 | SA | 108 | PHE | CA-C-O | -5.37 | 114.18 | 120.20 |
| 16 | LP | 194 | LYS | N-CA-C | -5.37 | 105.35 | 113.51 |
| 12 | LL | 69 | VAL | CA-C-N | -5.37 | 115.59 | 123.00 |
| 12 | LL | 69 | VAL | C-N-CA | -5.37 | 115.59 | 123.00 |
| 8 | LH | 28 | LYS | N-CA-C | -5.37 | 104.93 | 112.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | LB | 326 | GLY | CA-C-O | -5.36 | 118.53 | 122.23 |
| 18 | LR | 33 | PHE | N-CA-C | -5.35 | 106.26 | 112.89 |
| 76 | u | 54 | U | C2'-C3'-O3' | -5.35 | 105.67 | 113.70 |
| 75 | St | 1200 | G | C4'-C3'-C2' | -5.35 | 97.25 | 102.60 |
| 74 | Sj | 63 | GLN | CB-CA-C | 5.34 | 121.05 | 110.42 |
| 11 | LK | 7 | ARG | N-CA-C | -5.34 | 106.27 | 112.89 |
| 13 | LM | 161 | PRO | N-CA-C | 5.34 | 121.10 | 113.47 |
| 75 | St | 44 | G | C4'-C3'-O3' | 5.34 | 117.40 | 109.40 |
| 39 | Ln | 47 | PRO | CB-CA-C | -5.33 | 102.76 | 111.56 |
| 16 | LP | 172 | ASP | N-CA-C | -5.33 | 105.13 | 111.69 |
| 30 | Ld | 107 | ILE | CA-C-O | -5.33 | 115.49 | 121.36 |
| 52 | SH | 146 | TYR | CA-C-O | -5.33 | 115.39 | 119.71 |
| 55 | SK | 69 | LYS | N-CA-C | -5.33 | 105.47 | 111.28 |
| 29 | Lc | 39 | TYR | CB-CA-C | -5.33 | 101.94 | 110.79 |
| 38 | Ll | 23 | VAL | CA-C-O | -5.33 | 118.00 | 122.63 |
| 27 | La | 76 | ASN | N-CA-C | -5.32 | 106.63 | 113.01 |
| 66 | SX | 60 | PRO | N-CA-C | -5.31 | 102.93 | 111.38 |
| 49 | SE | 54 | TYR | N-CA-C | -5.31 | 105.95 | 112.90 |
| 49 | SE | 132 | GLY | CA-C-O | -5.31 | 116.64 | 121.47 |
| 70 | Sd | 26 | CYS | CA-C-O | -5.31 | 114.92 | 120.55 |
| 45 | SA | 205 | ASP | CA-C-O | -5.31 | 115.94 | 121.99 |
| 6 | LF | 181 | ILE | CA-C-O | -5.30 | 115.42 | 119.98 |
| 44 | Lt | 2597 | C | C2'-C3'-O3' | 5.30 | 117.46 | 109.50 |
| 43 | Ls | 117 | ASN | N-CA-C | -5.30 | 106.49 | 113.17 |
| 31 | Le | 19 | PRO | CB-CA-C | -5.30 | 104.16 | 111.21 |
| 55 | SK | 86 | ILE | N-CA-C | -5.30 | 105.22 | 110.62 |
| 54 | SJ | 53 | VAL | N-CA-C | -5.29 | 102.00 | 109.63 |
| 47 | SC | 132 | ALA | N-CA-C | -5.28 | 105.98 | 112.90 |
| 72 | Sg | 30 | MET | N-CA-C | -5.28 | 105.57 | 112.23 |
| 39 | Ln | 126 | PRO | CB-CA-C | -5.28 | 104.66 | 113.06 |
| 59 | SP | 22 | PRO | CB-CA-C | -5.28 | 104.47 | 111.23 |
| 64 | SV | 40 | ARG | N-CA-C | -5.28 | 101.83 | 109.59 |
| 44 | Lt | 369 | C | C4'-C3'-O3' | 5.28 | 117.32 | 109.40 |
| 54 | SJ | 53 | VAL | CA-C-N | -5.28 | 115.56 | 123.00 |
| 54 | SJ | 53 | VAL | C-N-CA | -5.28 | 115.56 | 123.00 |
| 60 | SQ | 147 | ARG | N-CA-C | -5.28 | 106.68 | 113.02 |
| 54 | SJ | 12 | LYS | N-CA-C | -5.27 | 106.11 | 112.54 |
| 10 | LJ | 52 | SER | CA-C-N | -5.27 | 116.13 | 122.35 |
| 10 | LJ | 52 | SER | C-N-CA | -5.27 | 116.13 | 122.35 |
| 59 | SP | 4 | MET | CB-CA-C | -5.27 | 110.48 | 116.54 |
| 65 | SW | 127 | ARG | N-CA-C | -5.27 | 105.43 | 111.07 |
| 34 | Lh | 97 | GLN | N-CA-C | -5.27 | 106.92 | 113.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 28 | Lb | 142 | GLY | N-CA-C | -5.26 | 107.95 | 113.58 |
| 44 | Lt | 421 | G | C4'-C3'-C2' | -5.26 | 97.34 | 102.60 |
| 75 | St | 1212 | G | C3'-C2'-C1' | -5.26 | 96.24 | 101.50 |
| 68 | Sb | 73 | CYS | CA-C-N | -5.26 | 115.64 | 123.11 |
| 68 | Sb | 73 | CYS | C-N-CA | -5.26 | 115.64 | 123.11 |
| 53 | SI | 133 | ASP | N-CA-C | -5.23 | 105.64 | 112.23 |
| 3 | LC | 236 | LEU | CA-C-N | -5.23 | 116.29 | 123.14 |
| 3 | LC | 236 | LEU | C-N-CA | -5.23 | 116.29 | 123.14 |
| 44 | Lt | 157 | G | C3'-C2'-C1' | -5.23 | 96.27 | 101.50 |
| 10 | LJ | 53 | VAL | N-CA-C | -5.22 | 107.32 | 111.81 |
| 67 | SY | 48 | ASP | CB-CA-C | -5.22 | 110.58 | 116.63 |
| 50 | SF | 176 | ILE | N-CA-C | -5.21 | 105.00 | 112.35 |
| 27 | La | 80 | PRO | N-CA-C | 5.21 | 119.67 | 111.38 |
| 20 | LT | 44 | LYS | N-CA-C | -5.21 | 105.28 | 111.69 |
| 21 | LU | 46 | GLY | N-CA-C | -5.21 | 106.97 | 115.46 |
| 44 | Lt | 74 | G | C2'-C3'-O3' | -5.21 | 105.89 | 113.70 |
| 67 | SY | 31 | ILE | N-CA-C | -5.21 | 102.13 | 109.21 |
| 3 | LC | 201 | THR | CB-CA-C | 5.21 | 117.56 | 110.06 |
| 46 | SB | 232 | VAL | N-CA-C | -5.21 | 104.46 | 111.44 |
| 52 | SH | 62 | VAL | CA-C-O | -5.21 | 118.10 | 122.63 |
| 55 | SK | 83 | MET | N-CA-C | -5.21 | 105.61 | 111.28 |
| 57 | SM | 113 | PHE | CA-CB-CG | 5.21 | 119.00 | 113.80 |
| 70 | Sd | 11 | SER | N-CA-C | -5.21 | 106.24 | 112.59 |
| 55 | SK | 168 | ASN | N-CA-C | -5.20 | 105.61 | 111.28 |
| 50 | SF | 34 | PHE | CB-CA-C | -5.20 | 101.33 | 109.70 |
| 16 | LP | 47 | VAL | N-CA-C | -5.20 | 106.24 | 113.00 |
| 24 | LX | 45 | ARG | N-CA-C | -5.20 | 102.22 | 109.96 |
| 60 | SQ | 137 | THR | CA-C-O | -5.19 | 116.08 | 122.36 |
| 48 | SD | 52 | LEU | N-CA-C | -5.19 | 105.71 | 111.36 |
| 64 | SV | 114 | ARG | N-CA-C | -5.18 | 105.53 | 111.07 |
| 49 | SE | 222 | LEU | N-CA-C | -5.18 | 106.94 | 113.20 |
| 2 | LB | 329 | PRO | CB-CA-C | -5.17 | 104.61 | 111.23 |
| 72 | Sg | 62 | ARG | CA-C-N | -5.17 | 115.54 | 122.42 |
| 72 | Sg | 62 | ARG | C-N-CA | -5.17 | 115.54 | 122.42 |
| 8 | LH | 126 | ASP | N-CA-C | -5.17 | 106.66 | 113.12 |
| 48 | SD | 170 | GLU | CA-C-O | -5.17 | 115.88 | 121.87 |
| 3 | LC | 156 | LEU | N-CA-C | -5.17 | 105.08 | 111.33 |
| 37 | Lk | 5 | THR | N-CA-C | 5.17 | 116.91 | 111.28 |
| 54 | SJ | 66 | ILE | N-CA-C | -5.16 | 106.00 | 113.07 |
| 14 | LN | 19 | PRO | N-CA-C | -5.16 | 106.36 | 113.53 |
| 47 | SC | 109 | ASP | N-CA-C | -5.16 | 105.74 | 111.36 |
| 58 | SO | 123 | ILE | N-CA-C | -5.16 | 108.48 | 113.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | SA | 110 | PRO | CB-CA-C | -5.15 | 105.02 | 111.56 |
| 62 | ST | 131 | LEU | N-CA-C | -5.15 | 106.25 | 112.54 |
| 6 | LF | 127 | PRO | N-CA-C | -5.14 | 106.38 | 113.53 |
| 44 | Lt | 1931 | G | C4'-C3'-O3' | 5.14 | 120.71 | 113.00 |
| 62 | ST | 111 | VAL | N-CA-C | -5.12 | 105.50 | 110.42 |
| 22 | LV | 62 | GLY | N-CA-C | -5.12 | 108.60 | 114.69 |
| 30 | Ld | 78 | SER | N-CA-C | -5.12 | 105.70 | 111.28 |
| 45 | SA | 194 | ILE | N-CA-C | 5.12 | 115.84 | 110.62 |
| 16 | LP | 177 | GLU | N-CA-C | -5.12 | 105.70 | 111.28 |
| 75 | St | 175 | C | C4'-C3'-O3' | 5.12 | 117.07 | 109.40 |
| 44 | Lt | 861 | C | C2'-C3'-O3' | -5.11 | 106.03 | 113.70 |
| 50 | SF | 57 | ARG | N-CA-C | -5.11 | 105.71 | 111.28 |
| 75 | St | 57 | C | C2'-C3'-O3' | -5.11 | 106.03 | 113.70 |
| 8 | LH | 22 | ALA | N-CA-C | -5.11 | 106.89 | 113.02 |
| 58 | SO | 36 | LEU | N-CA-C | -5.11 | 105.41 | 111.69 |
| 8 | LH | 186 | CYS | CB-CA-C | 5.11 | 118.70 | 111.86 |
| 16 | LP | 140 | HIS | N-CA-C | -5.11 | 106.56 | 112.89 |
| 44 | Lt | 1699 | U | C2'-C3'-O3' | -5.11 | 106.04 | 113.70 |
| 52 | SH | 55 | ASP | N-CA-C | -5.10 | 107.06 | 113.28 |
| 20 | LT | 97 | ALA | N-CA-C | -5.10 | 105.42 | 111.69 |
| 15 | LO | 186 | PRO | N-CA-C | -5.10 | 101.97 | 112.47 |
| 25 | LY | 45 | TYR | CB-CA-C | 5.09 | 117.66 | 109.51 |
| 44 | Lt | 512 | G | C4'-C3'-C2' | -5.09 | 97.51 | 102.60 |
| 52 | SH | 45 | TYR | N-CA-C | -5.09 | 103.61 | 110.68 |
| 19 | LS | 109 | TYR | N-CA-C | -5.07 | 105.75 | 111.28 |
| 51 | SG | 88 | LYS | CA-C-O | -5.07 | 115.99 | 121.87 |
| 44 | Lt | 1252 | G | C4'-C3'-O3' | 5.06 | 120.59 | 113.00 |
| 21 | LU | 100 | ASP | N-CA-C | -5.06 | 105.67 | 111.14 |
| 51 | SG | 225 | LYS | N-CA-C | -5.06 | 105.76 | 111.28 |
| 41 | Lp | 92 | SER | CA-C-N | -5.06 | 115.69 | 122.42 |
| 41 | Lp | 92 | SER | C-N-CA | -5.06 | 115.69 | 122.42 |
| 53 | SI | 169 | LYS | N-CA-C | -5.06 | 105.77 | 111.28 |
| 49 | SE | 90 | PHE | CA-C-N | -5.06 | 115.87 | 123.00 |
| 49 | SE | 90 | PHE | C-N-CA | -5.06 | 115.87 | 123.00 |
| 26 | LZ | 123 | GLN | CB-CA-C | 5.05 | 119.18 | 110.79 |
| 44 | Lt | 343 | G | C2'-C3'-O3' | -5.05 | 106.12 | 113.70 |
| 71 | Se | 89 | SER | N-CA-C | -5.05 | 105.77 | 111.28 |
| 75 | St | 22 | G | C2'-C3'-O3' | 5.05 | 121.28 | 113.70 |
| 47 | SC | 10 | GLU | N-CA-C | -5.05 | 107.27 | 112.93 |
| 24 | LX | 16 | PRO | CB-CA-C | -5.05 | 104.95 | 111.46 |
| 33 | Lg | 68 | PRO | CB-CA-C | -5.05 | 104.95 | 111.46 |
| 4 | LD | 79 | C | C2'-C3'-O3' | -5.05 | 106.13 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 36 | Lj | 19 | ARG | CB-CA-C | -5.05 | 100.93 | 110.16 |
| 15 | LO | 10 | LEU | N-CA-C | -5.04 | 106.39 | 112.54 |
| 11 | LK | 181 | TYR | CB-CA-C | -5.04 | 102.11 | 110.68 |
| 3 | LC | 56 | VAL | N-CA-C | -5.04 | 107.00 | 112.80 |
| 63 | SU | 53 | VAL | N-CA-C | -5.04 | 105.63 | 110.72 |
| 44 | Lt | 1472 | C | C4'-C3'-O3' | 5.04 | 120.56 | 113.00 |
| 66 | SX | 83 | PHE | CA-C-N | -5.04 | 115.38 | 122.94 |
| 66 | SX | 83 | PHE | C-N-CA | -5.04 | 115.38 | 122.94 |
| 12 | LL | 21 | ILE | CA-C-O | -5.04 | 116.38 | 121.67 |
| 25 | LY | 115 | PRO | CB-CA-C | -5.04 | 104.31 | 112.62 |
| 6 | LF | 105 | CYS | CB-CA-C | -5.04 | 102.33 | 110.79 |
| 15 | LO | 15 | GLN | N-CA-C | -5.03 | 107.18 | 113.72 |
| 73 | Sh | 127 | ASN | CB-CA-C | -5.03 | 104.65 | 111.95 |
| 75 | St | 231 | C | C2'-C3'-O3' | -5.03 | 106.15 | 113.70 |
| 10 | LJ | 70 | CYS | N-CA-C | -5.03 | 107.27 | 113.41 |
| 55 | SK | 143 | ASN | CB-CA-C | 5.03 | 118.00 | 109.55 |
| 63 | SU | 50 | ARG | N-CA-C | -5.03 | 105.80 | 111.28 |
| 62 | ST | 52 | VAL | CB-CA-C | 5.02 | 114.25 | 109.33 |
| 19 | LS | 36 | SER | N-CA-C | -5.02 | 107.28 | 113.41 |
| 27 | La | 97 | THR | CA-C-O | -5.02 | 116.26 | 121.99 |
| 64 | SV | 23 | GLY | N-CA-C | -5.02 | 107.82 | 115.66 |
| 74 | Sj | 61 | ILE | N-CA-C | -5.02 | 105.50 | 110.62 |
| 45 | SA | 76 | PRO | N-CA-C | -5.01 | 106.88 | 113.65 |
| 73 | Sh | 118 | PHE | N-CA-C | -5.01 | 107.00 | 113.02 |
| 2 | LB | 54 | THR | CA-C-O | -5.01 | 113.34 | 120.51 |
| 9 | LI | 141 | LEU | N-CA-C | -5.01 | 106.42 | 112.54 |
| 51 | SG | 55 | THR | CB-CA-C | 5.01 | 117.91 | 109.89 |
| 65 | SW | 112 | LEU | N-CA-C | -5.01 | 105.90 | 111.36 |
| 44 | Lt | 1963 | G | C1'-O4'-C4' | -5.01 | 104.89 | 109.90 |
| 75 | St | 615 | C | C2'-C3'-O3' | -5.01 | 106.19 | 113.70 |
| 21 | LU | 118 | LEU | N-CA-C | -5.00 | 105.83 | 111.28 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | LA | 1886 | 0 | 1948 | 37 | 0 |
| 2 | LB | 2987 | 0 | 3024 | 58 | 0 |
| 3 | LC | 2454 | 0 | 2541 | 48 | 0 |
| 4 | LD | 3038 | 0 | 1556 | 16 | 0 |
| 5 | LE | 2502 | 0 | 1268 | 15 | 0 |
| 6 | LF | 2355 | 0 | 2416 | 49 | 0 |
| 7 | LG | 439 | 0 | 479 | 6 | 0 |
| 8 | LH | 1742 | 0 | 1776 | 28 | 0 |
| 9 | LI | 1554 | 0 | 1636 | 30 | 0 |
| 10 | LJ | 1452 | 0 | 1495 | 23 | 0 |
| 11 | LK | 1671 | 0 | 1689 | 29 | 0 |
| 12 | LL | 1349 | 0 | 1362 | 31 | 0 |
| 13 | LM | 1605 | 0 | 1704 | 30 | 0 |
| 14 | LN | 1024 | 0 | 1091 | 24 | 0 |
| 15 | LO | 1708 | 0 | 1785 | 31 | 0 |
| 16 | LP | 1578 | 0 | 1616 | 35 | 0 |
| 17 | LQ | 1254 | 0 | 1289 | 29 | 0 |
| 18 | LR | 1402 | 0 | 1478 | 26 | 0 |
| 19 | LS | 1592 | 0 | 1697 | 40 | 0 |
| 20 | LT | 1423 | 0 | 1426 | 36 | 0 |
| 21 | LU | 1264 | 0 | 1303 | 26 | 0 |
| 22 | LV | 935 | 0 | 902 | 18 | 0 |
| 23 | LW | 1029 | 0 | 1068 | 18 | 0 |
| 24 | LX | 538 | 0 | 547 | 13 | 0 |
| 25 | LY | 962 | 0 | 1021 | 23 | 0 |
| 26 | LZ | 1076 | 0 | 1140 | 25 | 0 |
| 27 | La | 1051 | 0 | 1083 | 17 | 0 |
| 28 | Lb | 1201 | 0 | 1233 | 22 | 0 |
| 29 | Lc | 456 | 0 | 482 | 11 | 0 |
| 30 | Ld | 731 | 0 | 762 | 8 | 0 |
| 31 | Le | 818 | 0 | 857 | 11 | 0 |
| 32 | Lf | 1077 | 0 | 1133 | 34 | 0 |
| 33 | Lg | 778 | 0 | 816 | 15 | 0 |
| 34 | Lh | 914 | 0 | 956 | 22 | 0 |
| 35 | Li | 983 | 0 | 1081 | 16 | 0 |
| 36 | Lj | 731 | 0 | 794 | 15 | 0 |
| 37 | Lk | 711 | 0 | 712 | 16 | 0 |
| 38 | Ll | 558 | 0 | 612 | 17 | 0 |
| 39 | Ln | 1592 | 0 | 1667 | 61 | 0 |
| 40 | Lo | 227 | 0 | 272 | 6 | 0 |
| 41 | Lp | 767 | 0 | 822 | 13 | 0 |
| 42 | Lq | 708 | 0 | 753 | 14 | 0 |
| 43 | Ls | 388 | 0 | 401 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 44 | Lt | 55643 | 0 | 28280 | 345 | 0 |
| 45 | SA | 1578 | 0 | 1618 | 39 | 0 |
| 46 | SB | 1667 | 0 | 1713 | 45 | 0 |
| 47 | SC | 1665 | 0 | 1705 | 43 | 0 |
| 48 | SD | 1868 | 0 | 1927 | 30 | 0 |
| 49 | SE | 2085 | 0 | 2174 | 79 | 0 |
| 50 | SF | 1442 | 0 | 1469 | 34 | 0 |
| 51 | SG | 1889 | 0 | 2011 | 71 | 0 |
| 52 | SH | 1481 | 0 | 1544 | 31 | 0 |
| 53 | SI | 1357 | 0 | 1421 | 42 | 0 |
| 54 | SJ | 1031 | 0 | 1082 | 24 | 0 |
| 55 | SK | 1423 | 0 | 1515 | 41 | 0 |
| 56 | SL | 876 | 0 | 869 | 18 | 0 |
| 57 | SM | 1265 | 0 | 1298 | 29 | 0 |
| 58 | SO | 1089 | 0 | 1177 | 24 | 0 |
| 59 | SP | 1193 | 0 | 1258 | 23 | 0 |
| 60 | SQ | 926 | 0 | 933 | 13 | 0 |
| 61 | SR | 943 | 0 | 1020 | 27 | 0 |
| 62 | ST | 1180 | 0 | 1250 | 46 | 0 |
| 63 | SU | 965 | 0 | 1017 | 25 | 0 |
| 64 | SV | 1162 | 0 | 1195 | 33 | 0 |
| 65 | SW | 1080 | 0 | 1106 | 26 | 0 |
| 66 | SX | 802 | 0 | 840 | 20 | 0 |
| 67 | SY | 651 | 0 | 655 | 27 | 0 |
| 68 | Sb | 952 | 0 | 1013 | 35 | 0 |
| 69 | Sc | 597 | 0 | 636 | 25 | 0 |
| 70 | Sd | 884 | 0 | 917 | 25 | 0 |
| 71 | Se | 629 | 0 | 623 | 15 | 0 |
| 72 | Sg | 505 | 0 | 540 | 18 | 0 |
| 73 | Sh | 417 | 0 | 416 | 12 | 0 |
| 74 | Sj | 543 | 0 | 587 | 16 | 0 |
| 75 | St | 31176 | 0 | 15856 | 275 | 0 |
| 76 | u | 1604 | 0 | 816 | 11 | 0 |
| 77 | v | 1602 | 0 | 816 | 18 | 0 |
| 78 | y | 221 | 0 | 110 | 1 | 0 |
| All | All | 178901 | 0 | 135100 | 2357 | 0 |

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

All (2357) 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) |
|---|---|---|---|
| 66:SX:93:TRP:CH2 | 75:St:1087:C:OP1 | 1.81 | 1.32 |
| 50:SF:145:ARG:NH1 | 50:SF:145:ARG:HG3 | 1.55 | 1.07 |
| 66:SX:93:TRP:CZ3 | 75:St:1087:C:OP1 | 2.10 | 1.04 |
| 50:SF:145:ARG:HH11 | 50:SF:145:ARG:CG | 1.72 | 1.02 |
| 50:SF:145:ARG:HG3 | 50:SF:145:ARG:HH11 | 0.83 | 0.98 |
| 66:SX:93:TRP:HH2 | 75:St:1087:C:OP1 | 1.54 | 0.88 |
| 75:St:1362:G:O2' | 75:St:1363:C:H5' | 1.77 | 0.85 |
| 51:SG:76:SER:HA | 51:SG:105:GLY:HA3 | 1.57 | 0.85 |
| 49:SE:181:VAL:HG21 | 49:SE:195:ILE:HD13 | 1.57 | 0.84 |
| 69:Sc:83:ASN:HB2 | 69:Sc:86:LYS:HB2 | 1.60 | 0.83 |
| 16:LP:117:CYS:HB3 | 20:LT:163:ARG:HB3 | 1.61 | 0.82 |
| 69:Sc:38:LYS:HA | 69:Sc:86:LYS:HD2 | 1.62 | 0.82 |
| 30:Ld:20:LEU:HD11 | 30:Ld:101:ASP:HB2 | 1.63 | 0.81 |
| 51:SG:245:ARG:HB3 | 51:SG:245:ARG:CZ | 2.10 | 0.81 |
| 27:La:53:ASN:HB2 | 27:La:57:ASP:HB2 | 1.62 | 0.80 |
| 49:SE:99:PHE:HB2 | 49:SE:111:LEU:HD12 | 1.65 | 0.79 |
| 50:SF:113:ARG:HA | 50:SF:122:ARG:HA | 1.65 | 0.79 |
| 70:Sd:23:CYS:HB2 | 70:Sd:74:CYS:HB3 | 1.63 | 0.79 |
| 39:Ln:207:LYS:HB2 | 44:Lt:1977:C:H4' | 1.64 | 0.79 |
| 47:SC:55:ILE:HA | 47:SC:93:TRP:HB2 | 1.64 | 0.79 |
| 45:SA:145:VAL:HG13 | 45:SA:147:ILE:HG12 | 1.65 | 0.79 |
| 66:SX:62:ARG:HB2 | 66:SX:87:MET:HB2 | 1.66 | 0.78 |
| 75:St:1373:G:H4' | 75:St:1374:C:H5' | 1.65 | 0.78 |
| 3:LC:39:GLN:HG3 | 3:LC:103:ARG:HB3 | 1.64 | 0.77 |
| 75:St:1115:G:H3' | 75:St:1116:G:H8 | 1.50 | 0.77 |
| 57:SM:46:ALA:HA | 57:SM:112:CYS:HB2 | 1.66 | 0.77 |
| 21:LU:42:ILE:HD11 | 21:LU:53:PRO:HG3 | 1.66 | 0.77 |
| 72:Sg:12:VAL:HA | 72:Sg:25:VAL:HG22 | 1.66 | 0.77 |
| 45:SA:81:VAL:HG13 | 45:SA:128:LEU:HB3 | 1.67 | 0.77 |
| 3:LC:8:PHE:HA | 3:LC:13:THR:HA | 1.66 | 0.77 |
| 65:SW:4:VAL:HG21 | 65:SW:131:GLU:HG3 | 1.66 | 0.77 |
| 51:SG:42:PHE:HB2 | 51:SG:58:ILE:HG12 | 1.67 | 0.77 |
| 75:St:75:G:H4' | 75:St:154:A:H4' | 1.68 | 0.76 |
| 62:ST:150:ARG:HD2 | 75:St:1273:U:H4' | 1.68 | 0.76 |
| 44:Lt:2441:U:H2' | 44:Lt:2442:A:H8 | 1.51 | 0.75 |
| 65:SW:3:SER:HA | 65:SW:6:ARG:HB2 | 1.67 | 0.75 |
| 49:SE:89:VAL:HG11 | 49:SE:119:ALA:HA | 1.67 | 0.75 |
| 44:Lt:1972:A:H1' | 44:Lt:1973:C:H2' | 1.69 | 0.75 |
| 11:LK:30:LYS:HG3 | 11:LK:63:GLU:HG2 | 1.69 | 0.74 |
| 30:Ld:77:SER:HB2 | 30:Ld:80:GLU:HB2 | 1.69 | 0.74 |
| 11:LK:170:ASN:HA | 11:LK:177:THR:HA | 1.69 | 0.74 |
| 55:SK:171:PRO:HD2 | 55:SK:175:LYS:HB2 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:SG:195:VAL:HG23 | 51:SG:199:LYS:HB3 | 1.69 | 0.74 |
| 10:LJ:65:LEU:HD11 | 44:Lt:2539:A:H1' | 1.68 | 0.74 |
| 73:Sh:89:GLU:HA | 73:Sh:92:PHE:HB2 | 1.68 | 0.74 |
| 32:Lf:81:ILE:HG12 | 32:Lf:99:ALA:HB1 | 1.69 | 0.74 |
| 44:Lt:1958:G:H22 | 44:Lt:1960:C:H2' | 1.51 | 0.74 |
| 47:SC:209:GLU:HB2 | 63:SU:43:ILE:HG23 | 1.68 | 0.73 |
| 44:Lt:695:C:H2' | 44:Lt:696:G:H4' | 1.68 | 0.73 |
| 21:LU:88:ARG:HH22 | 29:Lc:31:SER:H | 1.36 | 0.73 |
| 34:Lh:56:PRO:HA | 44:Lt:1404:C:H5" | 1.71 | 0.73 |
| 19:LS:44:LEU:HB3 | 19:LS:50:ILE:HG13 | 1.70 | 0.72 |
| 72:Sg:17:SER:HB3 | 72:Sg:22:ILE:HB | 1.70 | 0.72 |
| 62:ST:25:VAL:HB | 62:ST:40:VAL:HB | 1.69 | 0.72 |
| 70:Sd:87:ARG:HB2 | 70:Sd:91:ASP:HB2 | 1.71 | 0.72 |
| 48:SD:145:ARG:HA | 48:SD:154:CYS:HB3 | 1.70 | 0.72 |
| 65:SW:28:CYS:HB3 | 65:SW:51:PHE:HB3 | 1.72 | 0.72 |
| 67:SY:66:ILE:HB | 67:SY:72:VAL:HG13 | 1.70 | 0.72 |
| 45:SA:15:LEU:HD21 | 45:SA:57:GLN:HA | 1.71 | 0.72 |
| 67:SY:23:LYS:HA | 67:SY:30:LEU:HA | 1.71 | 0.72 |
| 62:ST:38:ALA:HA | 62:ST:85:ILE:HG13 | 1.72 | 0.71 |
| 62:ST:45:GLY:H | 62:ST:81:LEU:H | 1.37 | 0.71 |
| 77:v:12:G:H1 | 77:v:22:C:H42 | 1.38 | 0.71 |
| 49:SE:26:ILE:HB | 55:SK:3:ILE:HG21 | 1.72 | 0.71 |
| 77:v:25:G:H1 | 77:v:43:A:H61 | 1.37 | 0.71 |
| 62:ST:122:ALA:HA | 62:ST:125:VAL:HG23 | 1.73 | 0.71 |
| 69:Sc:44:GLN:HG2 | 69:Sc:48:ARG:HE | 1.56 | 0.70 |
| 1:LA:42:ARG:HG2 | 1:LA:87:GLU:HG2 | 1.72 | 0.70 |
| 76:u:12:G:H1 | 76:u:22:C:H42 | 1.40 | 0.70 |
| 12:LL:7:ASN:HD21 | 12:LL:9:MET:HG3 | 1.55 | 0.70 |
| 44:Lt:403:C:H2' | 44:Lt:404:G:C8 | 2.25 | 0.70 |
| 51:SG:141:PRO:HB3 | 51:SG:146:LYS:HB3 | 1.71 | 0.70 |
| 19:LS:186:GLN:HA | 52:SH:38:GLU:HB2 | 1.74 | 0.70 |
| 39:Ln:22:ASN:HA | 44:Lt:1958:G:H5" | 1.73 | 0.70 |
| 53:SI:51:LYS:H | 53:SI:68:ARG:HB2 | 1.56 | 0.70 |
| 3:LC:92:ALA:HB1 | 44:Lt:520:C:H5" | 1.73 | 0.70 |
| 28:Lb:118:LEU:HD22 | 28:Lb:119:PRO:HD2 | 1.73 | 0.70 |
| 39:Ln:184:MET:HA | 39:Ln:187:LEU:HB2 | 1.73 | 0.70 |
| 39:Ln:65:LEU:HA | 39:Ln:109:VAL:HB | 1.73 | 0.70 |
| 6:LF:4:VAL:HG11 | 44:Lt:2094:G:H5' | 1.74 | 0.69 |
| 12:LL:53:THR:HB | 12:LL:60:ARG:HA | 1.73 | 0.69 |
| 13:LM:29:MET:HG3 | 44:Lt:513:C:H4' | 1.74 | 0.69 |
| 51:SG:175:HIS:CD2 | 75:St:66:C:H5' | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 66:SX:65:THR:HG22 | 66:SX:84:GLU:HB2 | 1.74 | 0.69 |
| 44:Lt:157:G:H1 | 44:Lt:172:C:H5 | 1.38 | 0.69 |
| 49:SE:35:PRO:HA | 49:SE:144:ALA:HB3 | 1.72 | 0.69 |
| 13:LM:189:ILE:HD13 | 28:Lb:144:VAL:HG23 | 1.73 | 0.69 |
| 22:LV:13:GLN:HB3 | 22:LV:73:GLU:HB2 | 1.74 | 0.69 |
| 39:Ln:23:GLU:HB2 | 44:Lt:1957:G:H4' | 1.74 | 0.69 |
| 39:Ln:117:ILE:HG21 | 39:Ln:135:PRO:HB3 | 1.75 | 0.69 |
| 64:SV:15:ARG:HB2 | 64:SV:20:ASN:HA | 1.75 | 0.69 |
| 58:SO:49:GLY:HA2 | 58:SO:75:THR:HG23 | 1.74 | 0.69 |
| 2:LB:90:ILE:HD11 | 2:LB:160:VAL:HG23 | 1.74 | 0.69 |
| 47:SC:60:GLU:OE2 | 47:SC:62:GLU:OE2 | 2.11 | 0.68 |
| 47:SC:71:ARG:HA | 47:SC:74:LYS:HB3 | 1.75 | 0.68 |
| 45:SA:68:ARG:HB3 | 67:SY:44:ALA:H | 1.59 | 0.68 |
| 54:SJ:86:ILE:HG21 | 54:SJ:117:GLN:HB3 | 1.75 | 0.68 |
| 8:LH:215:ALA:HA | 20:LT:34:VAL:HG22 | 1.75 | 0.68 |
| 52:SH:53:ALA:HA | 52:SH:59:LYS:HG3 | 1.75 | 0.68 |
| 22:LV:56:VAL:HG23 | 22:LV:69:THR:HG22 | 1.74 | 0.68 |
| 44:Lt:2058:U:H3' | 44:Lt:2059:A:H5" | 1.73 | 0.68 |
| 51:SG:73:VAL:HB | 51:SG:105:GLY:HA2 | 1.75 | 0.68 |
| 57:SM:37:GLY:HA3 | 75:St:185:G:H21 | 1.59 | 0.68 |
| 60:SQ:79:GLN:HA | 60:SQ:82:ILE:HB | 1.75 | 0.68 |
| 12:LL:110:ILE:HG12 | 12:LL:116:TYR:HA | 1.76 | 0.67 |
| 6:LF:60:ILE:H | 6:LF:80:SER:HB3 | 1.59 | 0.67 |
| 39:Ln:45:LYS:HD2 | 39:Ln:195:LYS:HB2 | 1.76 | 0.67 |
| 49:SE:42:ILE:HG22 | 49:SE:46:LEU:HD21 | 1.75 | 0.67 |
| 66:SX:76:GLY:HA3 | 75:St:1023:G:H4' | 1.76 | 0.67 |
| 45:SA:129:VAL:HG22 | 45:SA:151:SER:HB2 | 1.75 | 0.67 |
| 51:SG:144:ALA:HB3 | 51:SG:193:ARG:HB3 | 1.74 | 0.67 |
| 44:Lt:413:C:H2' | 44:Lt:414:G:H8 | 1.60 | 0.67 |
| 14:LN:100:LEU:HD22 | 16:LP:194:LYS:HG2 | 1.77 | 0.67 |
| 44:Lt:2656:C:H2' | 44:Lt:2657:U:H4' | 1.77 | 0.67 |
| 77:v:36:A:C2' | 77:v:37:A:H5' | 2.25 | 0.67 |
| 4:LD:139:U:H3 | 44:Lt:4:G:H1 | 1.41 | 0.67 |
| 39:Ln:90:LEU:HB3 | 39:Ln:93:PHE:HB2 | 1.76 | 0.67 |
| 32:Lf:84:VAL:HG12 | 32:Lf:113:ILE:HG13 | 1.75 | 0.66 |
| 49:SE:162:ILE:HG22 | 49:SE:164:LEU:H | 1.60 | 0.66 |
| 53:SI:106:VAL:HG12 | 53:SI:109:CYS:HB3 | 1.76 | 0.66 |
| 51:SG:245:ARG:CB | 51:SG:245:ARG:NH1 | 2.58 | 0.66 |
| 53:SI:14:THR:HG23 | 75:St:261:G:H1' | 1.77 | 0.66 |
| 48:SD:103:MET:HG2 | 48:SD:215:VAL:HG12 | 1.78 | 0.66 |
| 55:SK:110:LEU:HD12 | 55:SK:149:VAL:HB | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:SB:173:VAL:HG11 | 75:St:2:A:H5' | 1.78 | 0.66 |
| 58:SO:94:ILE:HD11 | 58:SO:130:LEU:HD11 | 1.78 | 0.66 |
| 3:LC:160:LYS:HA | 3:LC:165:LEU:HB3 | 1.78 | 0.66 |
| 21:LU:13:TYR:HB2 | 44:Lt:709:G:H5" | 1.77 | 0.66 |
| 47:SC:141:GLU:HB2 | 47:SC:193:ARG:HB2 | 1.78 | 0.66 |
| 3:LC:63:TRP:HB3 | 3:LC:69:VAL:HG21 | 1.78 | 0.66 |
| 49:SE:182:MET:HB2 | 49:SE:228:ILE:HG12 | 1.79 | 0.65 |
| 75:St:1249:C:H4' | 75:St:1287:C:H4' | 1.79 | 0.65 |
| 6:LF:34:LYS:HD2 | 21:LU:27:LEU:HD22 | 1.78 | 0.65 |
| 10:LJ:124:CYS:HB3 | 10:LJ:128:VAL:HG22 | 1.77 | 0.65 |
| 39:Ln:39:LYS:HB2 | 39:Ln:202:LYS:HB3 | 1.77 | 0.65 |
| 53:SI:83:HIS:HB3 | 53:SI:117:PRO:HG2 | 1.79 | 0.65 |
| 62:ST:59:PRO:HG2 | 62:ST:62:LEU:HD22 | 1.79 | 0.65 |
| 1:LA:50:HIS:HB2 | 42:Lq:54:ILE:HD11 | 1.79 | 0.65 |
| 5:LE:75:A:H61 | 5:LE:101:A:H5" | 1.62 | 0.65 |
| 44:Lt:306:U:H2' | 44:Lt:307:A:H8 | 1.60 | 0.64 |
| 44:Lt:355:U:H4' | 44:Lt:1104:G:H4' | 1.79 | 0.64 |
| 44:Lt:2221:C:H5' | 44:Lt:2223:G:H5' | 1.79 | 0.64 |
| 14:LN:9:ALA:HB1 | 14:LN:64:ILE:HD11 | 1.79 | 0.64 |
| 9:LI:120:ILE:HD12 | 9:LI:178:SER:HB2 | 1.79 | 0.64 |
| 11:LK:140:CYS:HB2 | 11:LK:144:ALA:HB3 | 1.79 | 0.64 |
| 44:Lt:2441:U:H2' | 44:Lt:2442:A:C8 | 2.31 | 0.64 |
| 55:SK:86:ILE:HB | 55:SK:104:ASP:HB3 | 1.78 | 0.64 |
| 1:LA:177:LYS:HB2 | 42:Lq:29:ILE:HG21 | 1.80 | 0.64 |
| 32:Lf:60:ILE:HD12 | 44:Lt:1052:G:H21 | 1.62 | 0.64 |
| 75:St:541:A:H3' | 75:St:542:G:H8 | 1.61 | 0.64 |
| 22:LV:24:ALA:HB2 | 22:LV:30:LEU:HD23 | 1.78 | 0.64 |
| 27:La:27:VAL:HG21 | 27:La:93:ILE:HB | 1.80 | 0.64 |
| 14:LN:53:ARG:HB3 | 20:LT:153:VAL:HG11 | 1.79 | 0.63 |
| 46:SB:96:VAL:HG11 | 46:SB:123:ALA:HA | 1.80 | 0.63 |
| 53:SI:88:LEU:HB2 | 53:SI:112:GLN:HB3 | 1.80 | 0.63 |
| 11:LK:20:SER:H | 11:LK:23:CYS:HB3 | 1.62 | 0.63 |
| 62:ST:108:LEU:HD11 | 62:ST:121:ARG:HB2 | 1.79 | 0.63 |
| 75:St:567:C:H3' | 75:St:568:G:H4' | 1.80 | 0.63 |
| 50:SF:145:ARG:NH1 | 50:SF:145:ARG:CG | 2.41 | 0.63 |
| 10:LJ:166:LYS:HG2 | 44:Lt:2324:C:H5" | 1.79 | 0.63 |
| 26:LZ:30:MET:HA | 26:LZ:101:PRO:HG3 | 1.80 | 0.63 |
| 27:La:46:ALA:HB3 | 27:La:67:ARG:HB2 | 1.80 | 0.63 |
| 51:SG:13:ASN:HB2 | 51:SG:131:THR:HG22 | 1.80 | 0.63 |
| 53:SI:71:HIS:HA | 53:SI:86:ARG:HA | 1.80 | 0.63 |
| 75:St:1362:G:C2' | 75:St:1363:C:H5' | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:SB:152:LEU:HB2 | 46:SB:163:LEU:HB2 | 1.81 | 0.63 |
| 69:Sc:34:ILE:HD11 | 69:Sc:45:ILE:HG21 | 1.79 | 0.63 |
| 45:SA:131:ASP:HB3 | 45:SA:134:VAL:HG12 | 1.81 | 0.63 |
| 14:LN:106:PHE:H | 33:Lg:44:LYS:HE2 | 1.64 | 0.62 |
| 54:SJ:50:PHE:HB3 | 54:SJ:63:VAL:HG13 | 1.80 | 0.62 |
| 39:Ln:68:ILE:HG12 | 39:Ln:85:VAL:HB | 1.81 | 0.62 |
| 51:SG:241:LYS:N | 51:SG:242:PRO:HD2 | 2.15 | 0.62 |
| 23:LW:38:LEU:HD22 | 23:LW:64:ILE:HD13 | 1.81 | 0.62 |
| 39:Ln:41:TYR:HA | 39:Ln:45:LYS:HD3 | 1.81 | 0.62 |
| 67:SY:9:LYS:HA | 67:SY:16:VAL:H | 1.63 | 0.62 |
| 12:LL:15:GLU:HB2 | 12:LL:132:SER:HB3 | 1.81 | 0.62 |
| 6:LF:217:LEU:HB3 | 6:LF:225:TYR:HB2 | 1.80 | 0.62 |
| 15:LO:4:TYR:HB3 | 15:LO:46:GLU:HG2 | 1.81 | 0.62 |
| 26:LZ:80:VAL:HG22 | 26:LZ:83:ILE:HG12 | 1.81 | 0.62 |
| 65:SW:62:PHE:HZ | 65:SW:120:ARG:HB3 | 1.64 | 0.62 |
| 10:LJ:89:ARG:HG2 | 43:Ls:82:LEU:HD22 | 1.82 | 0.62 |
| 49:SE:122:LYS:HG3 | 49:SE:162:ILE:HB | 1.80 | 0.62 |
| 75:St:909:A:H2' | 75:St:910:C:C6 | 2.35 | 0.62 |
| 25:LY:91:LYS:HD2 | 44:Lt:1465:G:H5" | 1.82 | 0.62 |
| 44:Lt:2289:C:H1' | 44:Lt:2290:C:H5 | 1.65 | 0.62 |
| 45:SA:72:THR:HG21 | 67:SY:42:SER:HB3 | 1.82 | 0.62 |
| 46:SB:105:ILE:HG21 | 46:SB:212:LEU:HD13 | 1.81 | 0.61 |
| 48:SD:129:THR:HG22 | 48:SD:131:ASP:H | 1.65 | 0.61 |
| 16:LP:118:PRO:HD2 | 20:LT:163:ARG:HA | 1.81 | 0.61 |
| 44:Lt:2150:C:H1' | 44:Lt:2153:U:H5 | 1.64 | 0.61 |
| 58:SO:67:ARG:HH12 | 75:St:449:C:H41 | 1.48 | 0.61 |
| 75:St:591:C:H2' | 75:St:592:G:N2 | 2.16 | 0.61 |
| 1:LA:18:ALA:HB2 | 44:Lt:1661:C:H5" | 1.81 | 0.61 |
| 6:LF:223:GLU:HA | 6:LF:226:ARG:HE | 1.64 | 0.61 |
| 20:LT:86:ASN:HD21 | 21:LU:155:TYR:H | 1.48 | 0.61 |
| 45:SA:124:PRO:HB2 | 45:SA:126:LEU:O | 2.00 | 0.61 |
| 49:SE:161:LYS:HB3 | 49:SE:170:ASP:HB2 | 1.81 | 0.61 |
| 62:ST:49:VAL:HB | 62:ST:85:ILE:HD13 | 1.82 | 0.61 |
| 2:LB:283:PHE:HB3 | 2:LB:353:LEU:HD21 | 1.83 | 0.61 |
| 60:SQ:67:ASP:HA | 60:SQ:70:SER:HB3 | 1.81 | 0.61 |
| 20:LT:7:VAL:HG21 | 20:LT:39:PHE:HB2 | 1.81 | 0.61 |
| 32:Lf:25:PHE:HB2 | 32:Lf:47:MET:HE3 | 1.82 | 0.61 |
| 61:SR:119:TYR:HD1 | 64:SV:120:CYS:HB3 | 1.65 | 0.61 |
| 69:Sc:23:ASP:HA | 69:Sc:27:MET:HB2 | 1.82 | 0.61 |
| 10:LJ:5:SER:HB2 | 10:LJ:66:PRO:HG3 | 1.83 | 0.61 |
| 62:ST:25:VAL:O | 62:ST:39:PHE:HA | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 76:u:7:G:H1 | 76:u:65:C:H42 | 1.49 | 0.61 |
| 15:LO:186:PRO:HB3 | 44:Lt:61:G:H21 | 1.66 | 0.60 |
| 25:LY:94:ILE:HG13 | 25:LY:109:VAL:HG21 | 1.82 | 0.60 |
| 52:SH:54:VAL:HG12 | 52:SH:56:GLY:H | 1.63 | 0.60 |
| 59:SP:45:THR:HG22 | 59:SP:49:GLN:HB3 | 1.83 | 0.60 |
| 59:SP:55:ARG:HH12 | 71:Se:92:ASN:HB2 | 1.64 | 0.60 |
| 68:Sb:20:GLN:HB2 | 68:Sb:75:ALA:HB3 | 1.83 | 0.60 |
| 75:St:1281:C:H2' | 75:St:1282:G:C8 | 2.36 | 0.60 |
| 75:St:128:G:H1 | 75:St:154:A:H61 | 1.48 | 0.60 |
| 49:SE:159:THR:HG21 | 49:SE:227:VAL:HB | 1.84 | 0.60 |
| 64:SV:41:PHE:C | 64:SV:43:ASN:H | 2.09 | 0.60 |
| 8:LH:61:ARG:HH22 | 8:LH:70:LEU:HG | 1.65 | 0.60 |
| 14:LN:130:ILE:HD11 | 16:LP:175:ILE:HG12 | 1.82 | 0.60 |
| 49:SE:178:GLY:H | 49:SE:195:ILE:HG22 | 1.67 | 0.60 |
| 57:SM:128:PRO:HA | 57:SM:134:ARG:HG3 | 1.84 | 0.60 |
| 44:Lt:2084:C:H2' | 44:Lt:2085:G:C8 | 2.35 | 0.60 |
| 51:SG:64:ALA:HA | 51:SG:113:HIS:HB2 | 1.84 | 0.60 |
| 75:St:944:G:H1 | 75:St:1288:A:H5' | 1.66 | 0.60 |
| 6:LF:117:ILE:HG21 | 6:LF:121:ALA:HB3 | 1.83 | 0.60 |
| 55:SK:81:LEU:HB3 | 55:SK:87:LEU:HB2 | 1.83 | 0.60 |
| 10:LJ:33:LEU:HD22 | 10:LJ:146:SER:HB3 | 1.84 | 0.60 |
| 55:SK:147:TYR:HD2 | 55:SK:147:TYR:H | 1.49 | 0.60 |
| 20:LT:70:LYS:HB3 | 20:LT:125:GLU:HG3 | 1.84 | 0.60 |
| 75:St:1107:C:H2' | 75:St:1108:A:C8 | 2.37 | 0.60 |
| 1:LA:132:THR:HG21 | 44:Lt:1666:G:H5" | 1.84 | 0.60 |
| 15:LO:164:LEU:HD21 | 44:Lt:61:G:H5" | 1.83 | 0.60 |
| 28:Lb:83:PRO:HG2 | 28:Lb:86:GLN:HG3 | 1.83 | 0.60 |
| 38:Ll:29:LYS:C | 38:Ll:31:ARG:H | 2.09 | 0.60 |
| 55:SK:30:LYS:HA | 74:Sj:38:TYR:HE2 | 1.67 | 0.60 |
| 75:St:1081:C:H2' | 75:St:1082:G:H8 | 1.67 | 0.60 |
| 25:LY:126:ALA:HB3 | 25:LY:129:VAL:HG23 | 1.84 | 0.59 |
| 44:Lt:1446:C:H2' | 44:Lt:1447:G:C8 | 2.37 | 0.59 |
| 10:LJ:3:LEU:HB3 | 10:LJ:58:PRO:HD2 | 1.84 | 0.59 |
| 38:Ll:5:ILE:HB | 38:Ll:47:TYR:HB3 | 1.84 | 0.59 |
| 45:SA:148:PRO:HA | 67:SY:39:VAL:HG22 | 1.83 | 0.59 |
| 51:SG:82:LEU:HA | 51:SG:100:ARG:HA | 1.84 | 0.59 |
| 55:SK:82:HIS:HB3 | 55:SK:89:GLU:HG3 | 1.84 | 0.59 |
| 4:LD:135:C:H41 | 9:LI:34:TRP:HE1 | 1.50 | 0.59 |
| 27:La:10:LEU:HD21 | 27:La:80:PRO:HB3 | 1.84 | 0.59 |
| 75:St:687:G:H1 | 75:St:698:G:H1 | 1.49 | 0.59 |
| 24:LX:7:CYS:SG | 24:LX:33:CYS:N | 2.74 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:SG:245:ARG:O | 51:SG:245:ARG:HG2 | 2.03 | 0.59 |
| 51:SG:245:ARG:CZ | 51:SG:245:ARG:CB | 2.78 | 0.59 |
| 47:SC:60:GLU:OE2 | 47:SC:62:GLU:CD | 2.45 | 0.59 |
| 53:SI:36:THR:HB | 53:SI:105:LEU:H | 1.67 | 0.59 |
| 39:Ln:202:LYS:HD3 | 44:Lt:1979:G:H5" | 1.85 | 0.59 |
| 44:Lt:1448:G:H2' | 44:Lt:1449:G:C8 | 2.38 | 0.59 |
| 57:SM:78:MET:HB2 | 57:SM:81:SER:HB2 | 1.84 | 0.59 |
| 58:SO:54:LYS:HG2 | 58:SO:91:LEU:HD11 | 1.85 | 0.59 |
| 75:St:624:C:H2' | 75:St:625:G:C8 | 2.37 | 0.59 |
| 44:Lt:403:C:H2' | 44:Lt:404:G:H8 | 1.68 | 0.59 |
| 51:SG:143:ARG:HE | 51:SG:193:ARG:HG3 | 1.66 | 0.59 |
| 53:SI:160:GLU:HB2 | 57:SM:22:LEU:HD21 | 1.85 | 0.59 |
| 70:Sd:38:ARG:HG3 | 75:St:1453:U:H2' | 1.84 | 0.59 |
| 75:St:1022:C:H2' | 75:St:1023:G:H8 | 1.68 | 0.59 |
| 16:LP:24:LEU:HD21 | 16:LP:99:LEU:HB2 | 1.85 | 0.59 |
| 62:ST:46:ASP:HB2 | 62:ST:82:ASP:HA | 1.85 | 0.59 |
| 75:St:918:C:H4' | 75:St:1289:C:H42 | 1.67 | 0.59 |
| 4:LD:133:G:H1 | 44:Lt:9:U:H3 | 1.50 | 0.58 |
| 44:Lt:1446:C:H2' | 44:Lt:1447:G:H8 | 1.68 | 0.58 |
| 64:SV:30:ALA:O | 64:SV:34:ILE:HG12 | 2.03 | 0.58 |
| 44:Lt:243:A:H2' | 44:Lt:244:G:C8 | 2.38 | 0.58 |
| 49:SE:18:TRP:HH2 | 49:SE:31:PRO:HD3 | 1.68 | 0.58 |
| 23:LW:63:LEU:HB3 | 23:LW:78:VAL:HG12 | 1.85 | 0.58 |
| 28:Lb:84:GLU:HA | 28:Lb:87:ARG:HB2 | 1.84 | 0.58 |
| 44:Lt:1580:G:H1 | 44:Lt:1587:C:H42 | 1.50 | 0.58 |
| 47:SC:186:GLY:HA3 | 75:St:1017:A:H2 | 1.67 | 0.58 |
| 4:LD:4:C:H4' | 17:LQ:63:TYR:HE1 | 1.68 | 0.58 |
| 11:LK:109:ASP:HA | 44:Lt:2047:G:C8 | 2.38 | 0.58 |
| 48:SD:66:VAL:HB | 48:SD:71:LEU:HD22 | 1.86 | 0.58 |
| 43:Ls:115:GLY:HA3 | 44:Lt:907:G:H5" | 1.85 | 0.58 |
| 51:SG:245:ARG:HH11 | 51:SG:245:ARG:CG | 2.16 | 0.58 |
| 52:SH:13:PHE:HB2 | 52:SH:45:TYR:HB3 | 1.86 | 0.58 |
| 61:SR:50:LEU:HB3 | 61:SR:55:LEU:HG | 1.84 | 0.58 |
| 9:LI:139:ASP:HB2 | 44:Lt:127:U:H3 | 1.68 | 0.58 |
| 45:SA:47:GLN:HE21 | 45:SA:49:ASP:HB3 | 1.69 | 0.58 |
| 68:Sb:76:TYR:CE2 | 68:Sb:85:TYR:HB2 | 2.38 | 0.58 |
| 70:Sd:74:CYS:SG | 70:Sd:77:CYS:N | 2.75 | 0.58 |
| 44:Lt:985:G:H2' | 44:Lt:986:A:H8 | 1.68 | 0.58 |
| 1:LA:116:VAL:HA | 1:LA:164:ALA:HB2 | 1.83 | 0.58 |
| 38:Ll:26:SER:HB2 | 38:Ll:29:LYS:HB2 | 1.85 | 0.58 |
| 44:Lt:413:C:H2' | 44:Lt:414:G:C8 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 68:Sb:34:GLU:HB3 | 68:Sb:38:ALA:HB3 | 1.86 | 0.58 |
| 3:LC:7:VAL:HB | 3:LC:16:ALA:HB3 | 1.85 | 0.58 |
| 37:Lk:10:LYS:HB3 | 44:Lt:535:C:H5" | 1.85 | 0.58 |
| 76:u:19:A:H2' | 76:u:20:A:H4' | 1.85 | 0.58 |
| 19:LS:190:PHE:HB3 | 52:SH:41:LEU:H | 1.68 | 0.58 |
| 32:Lf:88:LYS:HA | 32:Lf:91:PHE:HB3 | 1.85 | 0.58 |
| 65:SW:55:ALA:HB2 | 65:SW:103:ILE:HD11 | 1.86 | 0.58 |
| 47:SC:61:PRO:HA | 47:SC:94:VAL:HG22 | 1.86 | 0.57 |
| 75:St:988:C:H3' | 75:St:989:G:H8 | 1.68 | 0.57 |
| 27:La:101:VAL:HG13 | 27:La:102:THR:HG23 | 1.85 | 0.57 |
| 46:SB:147:THR:HA | 46:SB:187:VAL:HG13 | 1.86 | 0.57 |
| 49:SE:206:THR:HB | 49:SE:222:LEU:HD22 | 1.85 | 0.57 |
| 25:LY:74:GLN:HG2 | 25:LY:80:THR:HB | 1.85 | 0.57 |
| 55:SK:151:ILE:HA | 55:SK:154:THR:HG23 | 1.86 | 0.57 |
| 71:Se:60:HIS:HB3 | 71:Se:63:LYS:HB2 | 1.87 | 0.57 |
| 44:Lt:51:C:H2' | 44:Lt:52:G:H8 | 1.69 | 0.57 |
| 16:LP:105:ILE:HG22 | 16:LP:109:CYS:HB2 | 1.86 | 0.57 |
| 44:Lt:1796:C:H5" | 44:Lt:1797:A:H2' | 1.87 | 0.57 |
| 49:SE:35:PRO:HD3 | 75:St:109:C:H4' | 1.86 | 0.57 |
| 75:St:177:C:H42 | 75:St:598:C:H42 | 1.50 | 0.57 |
| 49:SE:233:PRO:C | 49:SE:235:VAL:H | 2.12 | 0.57 |
| 50:SF:107:PRO:HD3 | 50:SF:135:ILE:HG12 | 1.87 | 0.57 |
| 51:SG:57:ARG:HB2 | 51:SG:120:VAL:HG22 | 1.87 | 0.57 |
| 61:SR:85:ILE:HG23 | 61:SR:112:VAL:HG23 | 1.87 | 0.57 |
| 70:Sd:44:ILE:HB | 70:Sd:65:PRO:HB2 | 1.87 | 0.57 |
| 50:SF:124:SER:HB2 | 50:SF:190:ARG:HA | 1.87 | 0.57 |
| 55:SK:114:ILE:HG23 | 55:SK:119:LEU:HB2 | 1.87 | 0.57 |
| 24:LX:7:CYS:HB3 | 24:LX:11:SER:H | 1.70 | 0.57 |
| 44:Lt:1736:C:H4' | 44:Lt:1760:G:H8 | 1.69 | 0.57 |
| 49:SE:105:VAL:HG11 | 49:SE:245:PRO:HD2 | 1.87 | 0.57 |
| 58:SO:71:ARG:HA | 58:SO:82:THR:HA | 1.86 | 0.57 |
| 74:Sj:29:ARG:HA | 74:Sj:33:TYR:HB2 | 1.87 | 0.57 |
| 76:u:58:A:H3' | 76:u:59:A:H8 | 1.69 | 0.57 |
| 19:LS:28:HIS:HB2 | 19:LS:49:ILE:HD13 | 1.87 | 0.57 |
| 19:LS:63:ILE:HG21 | 44:Lt:1493:G:H5" | 1.86 | 0.57 |
| 47:SC:80:ALA:HA | 47:SC:85:CYS:H | 1.70 | 0.57 |
| 61:SR:20:VAL:HG12 | 61:SR:24:LYS:HB3 | 1.87 | 0.57 |
| 66:SX:57:CYS:HB3 | 66:SX:91:THR:HB | 1.87 | 0.57 |
| 2:LB:90:ILE:HG23 | 2:LB:104:THR:HG22 | 1.86 | 0.57 |
| 46:SB:210:ASN:HA | 46:SB:213:LYS:HD2 | 1.87 | 0.57 |
| 51:SG:244:LYS:O | 51:SG:244:LYS:NZ | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 60:SQ:41:PHE:HD1 | 60:SQ:57:SER:HB2 | 1.70 | 0.57 |
| 47:SC:147:LYS:HD3 | 47:SC:151:GLN:HG3 | 1.87 | 0.56 |
| 54:SJ:7:LEU:HG | 54:SJ:34:ILE:HG22 | 1.87 | 0.56 |
| 57:SM:88:TYR:CE2 | 57:SM:101:ARG:HB2 | 2.40 | 0.56 |
| 51:SG:172:GLU:H | 75:St:66:C:H5" | 1.70 | 0.56 |
| 61:SR:90:ILE:HG12 | 61:SR:109:PRO:HA | 1.87 | 0.56 |
| 68:Sb:8:VAL:HG21 | 68:Sb:46:GLN:HB3 | 1.86 | 0.56 |
| 69:Sc:45:ILE:HD13 | 69:Sc:60:MET:HE3 | 1.86 | 0.56 |
| 69:Sc:53:VAL:HB | 75:St:1224:G:N7 | 2.19 | 0.56 |
| 12:LL:138:VAL:HA | 12:LL:141:ARG:HE | 1.70 | 0.56 |
| 14:LN:14:TYR:HE1 | 14:LN:22:GLY:HA2 | 1.70 | 0.56 |
| 44:Lt:1945:G:H1' | 44:Lt:1949:A:H61 | 1.70 | 0.56 |
| 44:Lt:2245:U:H2' | 44:Lt:2246:G:H8 | 1.69 | 0.56 |
| 68:Sb:26:VAL:HG11 | 68:Sb:39:ILE:HD12 | 1.87 | 0.56 |
| 75:St:340:C:H1' | 75:St:372:G:H1' | 1.87 | 0.56 |
| 8:LH:24:ARG:O | 8:LH:28:LYS:HB3 | 2.05 | 0.56 |
| 19:LS:90:PRO:HB2 | 19:LS:93:THR:HB | 1.85 | 0.56 |
| 39:Ln:72:ARG:HB2 | 39:Ln:140:PRO:HB3 | 1.87 | 0.56 |
| 44:Lt:2043:G:H1 | 77:v:75:A:H61 | 1.53 | 0.56 |
| 46:SB:169:GLY:HA2 | 55:SK:98:LEU:HD22 | 1.88 | 0.56 |
| 44:Lt:1629:U:H1' | 44:Lt:2400:U:H5' | 1.88 | 0.56 |
| 11:LK:109:ASP:HB2 | 44:Lt:2047:G:H5' | 1.87 | 0.56 |
| 45:SA:69:ILE:HG22 | 67:SY:43:VAL:HG12 | 1.88 | 0.56 |
| 47:SC:210:ILE:HG22 | 47:SC:211:GLY:H | 1.71 | 0.56 |
| 54:SJ:31:SER:HB3 | 54:SJ:34:ILE:HG23 | 1.86 | 0.56 |
| 57:SM:88:TYR:HE1 | 57:SM:103:LYS:HB2 | 1.68 | 0.56 |
| 2:LB:232:ARG:CZ | 2:LB:268:GLY:HA3 | 2.36 | 0.56 |
| 43:Ls:115:GLY:HA3 | 44:Lt:907:G:H4' | 1.87 | 0.56 |
| 44:Lt:2375:U:H2' | 44:Lt:2376:U:H2' | 1.88 | 0.56 |
| 51:SG:24:ILE:HB | 51:SG:112:LEU:HD11 | 1.87 | 0.56 |
| 10:LJ:19:ILE:HG23 | 10:LJ:24:VAL:HG22 | 1.87 | 0.56 |
| 18:LR:172:GLY:HA2 | 18:LR:179:TRP:HB3 | 1.88 | 0.56 |
| 40:Lo:10:MET:HE2 | 75:St:859:U:H4' | 1.87 | 0.56 |
| 54:SJ:51:ALA:HB3 | 71:Se:49:LEU:HD11 | 1.88 | 0.56 |
| 61:SR:85:ILE:HG12 | 61:SR:107:ILE:HG21 | 1.87 | 0.56 |
| 18:LR:64:VAL:HG23 | 18:LR:87:ASN:HA | 1.87 | 0.56 |
| 18:LR:92:VAL:HG21 | 28:Lb:119:PRO:HB3 | 1.87 | 0.56 |
| 51:SG:80:ARG:HA | 51:SG:102:SER:HA | 1.87 | 0.56 |
| 53:SI:70:SER:HB2 | 53:SI:86:ARG:HD2 | 1.87 | 0.56 |
| 75:St:469:C:H2' | 75:St:470:G:H8 | 1.70 | 0.56 |
| 41:Lp:44:LYS:HB3 | 41:Lp:52:THR:HG21 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:575:A:H2' | 44:Lt:576:G:C8 | 2.41 | 0.55 |
| 44:Lt:1943:C:H1' | 44:Lt:1944:A:N7 | 2.22 | 0.55 |
| 47:SC:186:GLY:HA3 | 75:St:1017:A:C2 | 2.41 | 0.55 |
| 55:SK:38:LYS:HA | 74:Sj:31:ARG:HB2 | 1.89 | 0.55 |
| 49:SE:41:CYS:HB3 | 49:SE:84:VAL:H | 1.71 | 0.55 |
| 57:SM:16:ILE:HG22 | 57:SM:20:ARG:HH22 | 1.70 | 0.55 |
| 63:SU:25:LYS:HG2 | 63:SU:31:ASN:HB3 | 1.88 | 0.55 |
| 75:St:850:U:H2' | 75:St:851:G:H8 | 1.72 | 0.55 |
| 44:Lt:1873:C:H3' | 44:Lt:1874:G:H8 | 1.71 | 0.55 |
| 44:Lt:2291:U:H2' | 44:Lt:2292:U:C6 | 2.41 | 0.55 |
| 1:LA:207:VAL:HG23 | 44:Lt:1903:C:H5' | 1.88 | 0.55 |
| 6:LF:111:GLU:HG2 | 6:LF:257:PRO:HG2 | 1.89 | 0.55 |
| 44:Lt:1348:C:H4' | 44:Lt:1350:C:H41 | 1.71 | 0.55 |
| 5:LE:28:C:H5" | 12:LL:137:ARG:HB3 | 1.89 | 0.55 |
| 6:LF:95:TYR:CZ | 6:LF:169:ALA:HB2 | 2.42 | 0.55 |
| 6:LF:144:ASN:HD21 | 6:LF:149:ALA:H | 1.55 | 0.55 |
| 49:SE:64:ILE:HB | 49:SE:69:ASN:HD22 | 1.71 | 0.55 |
| 16:LP:127:ARG:HB2 | 44:Lt:1016:G:H5' | 1.88 | 0.55 |
| 43:Ls:95:ILE:HG21 | 44:Lt:2319:G:H4' | 1.87 | 0.55 |
| 43:Ls:110:CYS:SG | 43:Ls:113:CYS:N | 2.79 | 0.55 |
| 44:Lt:259:C:H2' | 44:Lt:260:G:C8 | 2.42 | 0.55 |
| 48:SD:83:LYS:HD2 | 48:SD:106:THR:HG23 | 1.87 | 0.55 |
| 75:St:428:C:H4' | 75:St:477:G:H4' | 1.87 | 0.55 |
| 75:St:469:C:H2' | 75:St:470:G:C8 | 2.42 | 0.55 |
| 27:La:27:VAL:HG23 | 27:La:90:LYS:HA | 1.88 | 0.55 |
| 61:SR:130:LYS:HD3 | 75:St:924:C:H4' | 1.89 | 0.55 |
| 2:LB:73:ILE:HG12 | 23:LW:95:GLY:HA3 | 1.89 | 0.55 |
| 10:LJ:116:GLN:HB3 | 10:LJ:120:ARG:HH22 | 1.71 | 0.55 |
| 49:SE:114:ILE:HG13 | 49:SE:118:GLU:HB3 | 1.88 | 0.55 |
| 42:Lq:11:THR:HG21 | 42:Lq:26:LEU:HB3 | 1.89 | 0.55 |
| 44:Lt:418:C:H2' | 44:Lt:419:G:C8 | 2.42 | 0.55 |
| 44:Lt:700:U:H2' | 44:Lt:701:U:C6 | 2.42 | 0.55 |
| 47:SC:75:ILE:HA | 47:SC:78:LEU:HD12 | 1.89 | 0.55 |
| 13:LM:95:ASN:HD21 | 44:Lt:72:C:H2' | 1.72 | 0.54 |
| 25:LY:112:LEU:CD2 | 25:LY:122:PHE:HE1 | 2.19 | 0.54 |
| 44:Lt:2245:U:H2' | 44:Lt:2246:G:C8 | 2.42 | 0.54 |
| 49:SE:11:ARG:HG2 | 49:SE:25:GLY:HA3 | 1.88 | 0.54 |
| 75:St:23:C:H2' | 75:St:24:G:H8 | 1.72 | 0.54 |
| 47:SC:21:CYS:HB3 | 73:Sh:131:ILE:HA | 1.88 | 0.54 |
| 49:SE:99:PHE:HA | 49:SE:114:ILE:HB | 1.89 | 0.54 |
| 43:Ls:79:GLU:HG3 | 43:Ls:82:LEU:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:648:C:H3' | 44:Lt:649:U:H2' | 1.89 | 0.54 |
| 51:SG:138:ARG:HH12 | 75:St:148:G:H21 | 1.53 | 0.54 |
| 1:LA:117:GLU:HG2 | 1:LA:124:GLY:H | 1.73 | 0.54 |
| 45:SA:188:LEU:HB3 | 45:SA:194:ILE:HB | 1.89 | 0.54 |
| 77:v:41:A:H2' | 77:v:42:G:C8 | 2.42 | 0.54 |
| 16:LP:10:GLY:HA2 | 16:LP:39:ILE:HD11 | 1.89 | 0.54 |
| 44:Lt:2121:A:H2' | 44:Lt:2122:G:C8 | 2.42 | 0.54 |
| 72:Sg:51:LEU:HG | 72:Sg:53:LEU:HD12 | 1.89 | 0.54 |
| 2:LB:205:ILE:HD13 | 2:LB:322:ILE:HG21 | 1.89 | 0.54 |
| 2:LB:282:VAL:HG12 | 2:LB:324:ILE:HG22 | 1.89 | 0.54 |
| 12:LL:138:VAL:HG23 | 12:LL:141:ARG:HH21 | 1.71 | 0.54 |
| 44:Lt:1633:A:H1' | 44:Lt:1769:A:H61 | 1.73 | 0.54 |
| 53:SI:26:LYS:HD3 | 75:St:312:A:H2' | 1.90 | 0.54 |
| 64:SV:60:LEU:HD21 | 64:SV:65:GLU:HB2 | 1.89 | 0.54 |
| 1:LA:200:ARG:HH21 | 1:LA:203:ALA:HB2 | 1.73 | 0.54 |
| 52:SH:63:VAL:HG22 | 52:SH:95:ILE:HG22 | 1.90 | 0.54 |
| 44:Lt:671:U:H2' | 44:Lt:672:G:H8 | 1.73 | 0.54 |
| 44:Lt:1914:C:H2' | 44:Lt:1915:C:C6 | 2.43 | 0.54 |
| 45:SA:63:ILE:HG21 | 45:SA:182:LEU:HD12 | 1.90 | 0.54 |
| 54:SJ:87:GLU:HA | 54:SJ:90:VAL:HG13 | 1.88 | 0.54 |
| 44:Lt:1267:A:H1' | 44:Lt:1288:G:H1' | 1.90 | 0.54 |
| 68:Sb:11:VAL:HA | 68:Sb:22:CYS:HB3 | 1.90 | 0.54 |
| 6:LF:64:VAL:HG21 | 6:LF:109:LEU:HD22 | 1.89 | 0.54 |
| 70:Sd:37:LYS:HG2 | 70:Sd:70:LYS:HE2 | 1.89 | 0.54 |
| 38:Ll:16:ASP:HA | 38:Ll:65:LYS:HD3 | 1.90 | 0.53 |
| 2:LB:126:GLU:HB2 | 2:LB:128:THR:HG23 | 1.90 | 0.53 |
| 10:LJ:130:ILE:HD11 | 10:LJ:140:LEU:HB3 | 1.89 | 0.53 |
| 16:LP:70:PHE:HB3 | 16:LP:75:GLU:HG3 | 1.90 | 0.53 |
| 46:SB:159:VAL:HG11 | 46:SB:204:SER:HA | 1.89 | 0.53 |
| 63:SU:26:PRO:HA | 63:SU:61:MET:HB3 | 1.90 | 0.53 |
| 75:St:401:G:H1 | 75:St:419:C:H42 | 1.57 | 0.53 |
| 2:LB:285:ILE:HD12 | 2:LB:322:ILE:HD13 | 1.91 | 0.53 |
| 15:LO:4:TYR:HA | 15:LO:7:VAL:HG23 | 1.90 | 0.53 |
| 55:SK:5:ARG:HB2 | 75:St:39:A:H5" | 1.90 | 0.53 |
| 56:SL:31:GLY:HA3 | 56:SL:50:TYR:HB2 | 1.89 | 0.53 |
| 74:Sj:31:ARG:HA | 74:Sj:34:LYS:HB2 | 1.91 | 0.53 |
| 3:LC:123:ASN:HD22 | 3:LC:126:LEU:HD12 | 1.74 | 0.53 |
| 18:LR:169:GLY:HA2 | 28:Lb:54:GLY:O | 2.08 | 0.53 |
| 44:Lt:733:G:H1 | 44:Lt:746:U:H3 | 1.55 | 0.53 |
| 44:Lt:1581:G:H2' | 44:Lt:1586:C:N4 | 2.23 | 0.53 |
| 55:SK:76:ALA:HB1 | 55:SK:80:ARG:HH21 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:SA:188:LEU:HD13 | 45:SA:194:ILE:HG12 | 1.90 | 0.53 |
| 61:SR:78:THR:HA | 75:St:984:G:H4' | 1.91 | 0.53 |
| 77:v:36:A:O2' | 77:v:37:A:H5' | 2.08 | 0.53 |
| 2:LB:227:GLU:HB2 | 2:LB:270:MET:HB2 | 1.90 | 0.53 |
| 44:Lt:224:U:H2' | 44:Lt:225:A:C8 | 2.43 | 0.53 |
| 49:SE:129:ILE:HG13 | 49:SE:139:LEU:HD13 | 1.90 | 0.53 |
| 68:Sb:104:SER:C | 68:Sb:106:LYS:H | 2.17 | 0.53 |
| 3:LC:297:PRO:HA | 3:LC:303:ALA:HB3 | 1.91 | 0.53 |
| 35:Li:33:LYS:HD3 | 35:Li:36:ASP:HB3 | 1.90 | 0.53 |
| 39:Ln:71:ALA:HB3 | 39:Ln:140:PRO:HG3 | 1.91 | 0.53 |
| 61:SR:93:THR:HB | 61:SR:106:GLU:HG2 | 1.89 | 0.53 |
| 62:ST:130:GLN:HG2 | 62:ST:133:VAL:HG12 | 1.91 | 0.53 |
| 75:St:10:G:H2' | 75:St:11:A:C8 | 2.43 | 0.53 |
| 32:Lf:120:MET:HB3 | 32:Lf:122:VAL:HG23 | 1.91 | 0.53 |
| 44:Lt:51:C:H2' | 44:Lt:52:G:C8 | 2.44 | 0.53 |
| 49:SE:45:ILE:HA | 49:SE:61:THR:HG21 | 1.90 | 0.53 |
| 60:SQ:52:THR:HG21 | 75:St:649:G:H21 | 1.74 | 0.53 |
| 60:SQ:117:ARG:HB2 | 70:Sd:49:ILE:HG21 | 1.90 | 0.53 |
| 75:St:906:C:H2' | 75:St:907:A:H8 | 1.73 | 0.53 |
| 2:LB:17:LEU:HG | 2:LB:18:PRO:HA | 1.91 | 0.53 |
| 18:LR:73:LYS:HE2 | 18:LR:73:LYS:H | 1.72 | 0.53 |
| 25:LY:32:PHE:HZ | 44:Lt:1253:C:H4' | 1.74 | 0.53 |
| 53:SI:128:ASP:HB3 | 53:SI:131:ILE:HB | 1.90 | 0.53 |
| 75:St:597:G:H2' | 75:St:598:C:O4' | 2.09 | 0.53 |
| 12:LL:54:ILE:HD11 | 12:LL:57:PHE:HB3 | 1.90 | 0.53 |
| 44:Lt:533:A:H5" | 44:Lt:637:C:H41 | 1.73 | 0.53 |
| 44:Lt:842:C:H2' | 44:Lt:843:A:H8 | 1.74 | 0.53 |
| 44:Lt:1581:G:H21 | 44:Lt:1586:C:H5 | 1.56 | 0.53 |
| 51:SG:175:HIS:HD2 | 75:St:66:C:H5' | 1.73 | 0.53 |
| 75:St:955:G:H21 | 75:St:984:G:H22 | 1.56 | 0.53 |
| 9:LI:53:VAL:HB | 9:LI:213:GLY:HA3 | 1.91 | 0.52 |
| 45:SA:152:LEU:HD23 | 45:SA:170:ASN:HD21 | 1.74 | 0.52 |
| 49:SE:26:ILE:HG23 | 75:St:360:U:H1' | 1.90 | 0.52 |
| 54:SJ:31:SER:H | 54:SJ:34:ILE:HG12 | 1.73 | 0.52 |
| 65:SW:115:ALA:HB1 | 65:SW:120:ARG:HA | 1.91 | 0.52 |
| 15:LO:179:ILE:HB | 44:Lt:68:C:H5' | 1.91 | 0.52 |
| 16:LP:119:SER:HB2 | 20:LT:158:ALA:HB1 | 1.91 | 0.52 |
| 44:Lt:243:A:H2' | 44:Lt:244:G:H8 | 1.72 | 0.52 |
| 44:Lt:415:C:H2' | 44:Lt:416:G:C8 | 2.44 | 0.52 |
| 75:St:120:G:H21 | 75:St:158:G:H5" | 1.74 | 0.52 |
| 3:LC:129:ALA:C | 3:LC:131:GLY:H | 2.17 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:LD:17:G:N2 | 44:Lt:356:G:H1' | 2.24 | 0.52 |
| 48:SD:13:ILE:HG21 | 48:SD:26:GLU:HA | 1.91 | 0.52 |
| 51:SG:95:ASN:HB2 | 75:St:308:U:H4' | 1.92 | 0.52 |
| 73:Sh:102:CYS:HB2 | 73:Sh:120:CYS:CA | 2.39 | 0.52 |
| 14:LN:28:VAL:HG12 | 14:LN:68:PRO:HD2 | 1.89 | 0.52 |
| 28:Lb:148:VAL:HG22 | 28:Lb:149:PRO:HD2 | 1.90 | 0.52 |
| 39:Ln:208:SER:H | 39:Ln:210:MET:HE2 | 1.75 | 0.52 |
| 47:SC:170:LYS:O | 47:SC:174:LEU:HB2 | 2.10 | 0.52 |
| 55:SK:60:LEU:HB3 | 55:SK:94:LEU:HD11 | 1.91 | 0.52 |
| 57:SM:131:LYS:HB2 | 75:St:250:G:H3' | 1.90 | 0.52 |
| 62:ST:13:ASN:HA | 62:ST:16:GLU:HB2 | 1.91 | 0.52 |
| 2:LB:67:LEU:HD12 | 2:LB:72:ALA:HB2 | 1.91 | 0.52 |
| 14:LN:67:LYS:HD2 | 20:LT:68:PHE:HB3 | 1.92 | 0.52 |
| 22:LV:95:PHE:HA | 22:LV:109:PRO:HA | 1.92 | 0.52 |
| 46:SB:50:LYS:HA | 67:SY:19:TYR:HE1 | 1.75 | 0.52 |
| 52:SH:77:SER:HB2 | 52:SH:136:PRO:HG3 | 1.91 | 0.52 |
| 2:LB:54:THR:O | 2:LB:55:HIS:HB2 | 2.08 | 0.52 |
| 20:LT:46:LEU:HD11 | 21:LU:152:PRO:HA | 1.92 | 0.52 |
| 54:SJ:86:ILE:HD11 | 54:SJ:113:HIS:HB2 | 1.92 | 0.52 |
| 59:SP:57:GLN:HA | 71:Se:95:VAL:HG13 | 1.90 | 0.52 |
| 64:SV:124:VAL:HA | 64:SV:127:HIS:HD2 | 1.75 | 0.52 |
| 33:Lg:46:LEU:HD11 | 33:Lg:68:PRO:HD3 | 1.92 | 0.52 |
| 44:Lt:2441:U:C5 | 44:Lt:2449:G:C2 | 2.97 | 0.52 |
| 48:SD:176:LEU:HA | 48:SD:179:VAL:HG22 | 1.92 | 0.52 |
| 37:Lk:4:GLY:HA3 | 44:Lt:1628:C:H41 | 1.73 | 0.52 |
| 42:Lq:6:LYS:HB3 | 44:Lt:1558:C:H3' | 1.92 | 0.52 |
| 44:Lt:1767:A:H2 | 44:Lt:1774:U:H3 | 1.55 | 0.52 |
| 59:SP:50:ILE:HD12 | 59:SP:75:LEU:HD11 | 1.92 | 0.52 |
| 65:SW:7:VAL:HG11 | 65:SW:12:PHE:HD1 | 1.75 | 0.52 |
| 9:LI:124:VAL:HG13 | 9:LI:156:VAL:HG21 | 1.91 | 0.52 |
| 22:LV:31:ASN:HB3 | 22:LV:34:GLU:H | 1.74 | 0.52 |
| 46:SB:37:VAL:HG11 | 46:SB:60:ILE:HA | 1.91 | 0.52 |
| 47:SC:142:VAL:HG23 | 47:SC:158:PHE:HB2 | 1.91 | 0.52 |
| 66:SX:53:ILE:HG13 | 66:SX:94:VAL:HG22 | 1.92 | 0.52 |
| 67:SY:27:THR:C | 67:SY:29:ARG:H | 2.18 | 0.52 |
| 67:SY:64:GLY:HA2 | 67:SY:67:ARG:HD3 | 1.92 | 0.52 |
| 75:St:658:G:H2' | 75:St:659:A:C8 | 2.45 | 0.52 |
| 75:St:1115:G:H3' | 75:St:1116:G:C8 | 2.37 | 0.52 |
| 1:LA:62:GLN:HG3 | 1:LA:71:ARG:HB2 | 1.91 | 0.52 |
| 2:LB:240:ARG:HG2 | 44:Lt:1824:U:H5" | 1.92 | 0.52 |
| 45:SA:173:PRO:HA | 45:SA:176:ILE:HB | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:SE:3:ARG:HA | 75:St:312:A:H4' | 1.91 | 0.52 |
| 75:St:1442:C:H2' | 75:St:1443:G:C8 | 2.45 | 0.52 |
| 6:LF:39:GLN:HG2 | 6:LF:48:ARG:HH11 | 1.75 | 0.51 |
| 32:Lf:87:LEU:HD21 | 32:Lf:117:ALA:HB2 | 1.93 | 0.51 |
| 39:Ln:208:SER:N | 39:Ln:210:MET:HE2 | 2.25 | 0.51 |
| 44:Lt:84:C:H1' | 44:Lt:85:U:C5 | 2.45 | 0.51 |
| 77:v:36:A:H2' | 77:v:37:A:H5' | 1.92 | 0.51 |
| 3:LC:310:SER:HB2 | 8:LH:40:VAL:HA | 1.93 | 0.51 |
| 31:Le:10:ARG:HA | 31:Le:65:ARG:HG3 | 1.91 | 0.51 |
| 44:Lt:2192:C:H2' | 44:Lt:2193:G:C8 | 2.44 | 0.51 |
| 46:SB:36:LEU:HD13 | 46:SB:41:LYS:HB3 | 1.92 | 0.51 |
| 51:SG:83:LEU:HD13 | 51:SG:90:TYR:HB2 | 1.91 | 0.51 |
| 14:LN:60:GLN:HB3 | 14:LN:82:ALA:HB1 | 1.91 | 0.51 |
| 20:LT:27:ILE:HG12 | 20:LT:38:ARG:HB2 | 1.92 | 0.51 |
| 26:LZ:57:ILE:HB | 26:LZ:63:LYS:HA | 1.92 | 0.51 |
| 27:La:18:ARG:HB2 | 44:Lt:1302:G:H1 | 1.75 | 0.51 |
| 44:Lt:2441:U:C5 | 44:Lt:2449:G:N2 | 2.78 | 0.51 |
| 49:SE:163:ASN:H | 49:SE:167:GLY:HA2 | 1.76 | 0.51 |
| 51:SG:144:ALA:HA | 51:SG:147:ILE:HB | 1.92 | 0.51 |
| 70:Sd:23:CYS:HB3 | 70:Sd:27:HIS:H | 1.75 | 0.51 |
| 12:LL:30:LEU:HD12 | 12:LL:64:LYS:HB2 | 1.92 | 0.51 |
| 34:Lh:104:ALA:C | 34:Lh:106:THR:N | 2.67 | 0.51 |
| 44:Lt:2199:C:H5' | 44:Lt:2200:C:H5' | 1.92 | 0.51 |
| 50:SF:56:GLU:HA | 50:SF:59:THR:HB | 1.92 | 0.51 |
| 51:SG:245:ARG:O | 51:SG:245:ARG:CG | 2.55 | 0.51 |
| 54:SJ:105:THR:HB | 54:SJ:126:ILE:HD11 | 1.92 | 0.51 |
| 6:LF:186:LYS:HA | 6:LF:191:TYR:CG | 2.45 | 0.51 |
| 10:LJ:73:ILE:HA | 10:LJ:76:MET:HG3 | 1.93 | 0.51 |
| 19:LS:173:ARG:HB2 | 59:SP:34:CYS:SG | 2.50 | 0.51 |
| 49:SE:152:PRO:HG2 | 51:SG:227:LEU:HG | 1.93 | 0.51 |
| 55:SK:132:ALA:HA | 75:St:397:C:H4' | 1.92 | 0.51 |
| 61:SR:17:PHE:HB3 | 61:SR:25:LEU:HD22 | 1.92 | 0.51 |
| 62:ST:112:LYS:HA | 62:ST:117:ARG:HH21 | 1.76 | 0.51 |
| 75:St:667:U:O2 | 75:St:667:U:O4' | 2.26 | 0.51 |
| 75:St:905:C:H1' | 75:St:1307:C:H42 | 1.76 | 0.51 |
| 19:LS:4:LEU:HD23 | 19:LS:7:GLN:HG3 | 1.93 | 0.51 |
| 44:Lt:735:G:H3' | 44:Lt:736:G:H8 | 1.75 | 0.51 |
| 49:SE:160:ILE:HD12 | 49:SE:169:ILE:HB | 1.93 | 0.51 |
| 51:SG:10:ASN:HA | 51:SG:21:SER:HA | 1.92 | 0.51 |
| 51:SG:90:TYR:CE1 | 51:SG:99:LYS:HB2 | 2.46 | 0.51 |
| 52:SH:145:LEU:HD12 | 54:SJ:51:ALA:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 65:SW:122:ILE:HB | 65:SW:127:ARG:HG2 | 1.91 | 0.51 |
| 66:SX:28:ILE:HA | 66:SX:90:ARG:O | 2.11 | 0.51 |
| 75:St:73:G:H2' | 75:St:74:C:C6 | 2.45 | 0.51 |
| 26:LZ:32:SER:HB2 | 26:LZ:106:ILE:HG12 | 1.91 | 0.51 |
| 26:LZ:57:ILE:HD12 | 26:LZ:99:ILE:HG21 | 1.92 | 0.51 |
| 29:Lc:53:GLN:C | 29:Lc:55:LEU:N | 2.66 | 0.51 |
| 58:SO:128:ILE:HG13 | 58:SO:133:LEU:HD11 | 1.92 | 0.51 |
| 1:LA:36:GLU:HG3 | 1:LA:91:GLY:HA2 | 1.93 | 0.51 |
| 53:SI:90:VAL:HA | 53:SI:111:VAL:HG12 | 1.92 | 0.51 |
| 75:St:1122:G:H2' | 75:St:1123:G:H2' | 1.93 | 0.51 |
| 7:LG:4:ASN:HB3 | 44:Lt:1261:A:C5 | 2.46 | 0.51 |
| 9:LI:28:LEU:HG | 25:LY:29:VAL:HG13 | 1.93 | 0.51 |
| 13:LM:112:VAL:HG21 | 13:LM:145:LEU:HB3 | 1.92 | 0.51 |
| 20:LT:22:VAL:HG11 | 21:LU:144:ILE:HG22 | 1.93 | 0.51 |
| 44:Lt:2082:G:H5" | 44:Lt:2178:G:H1' | 1.92 | 0.51 |
| 46:SB:77:ILE:HB | 46:SB:94:ALA:HB2 | 1.93 | 0.51 |
| 49:SE:9:LEU:HD13 | 49:SE:30:ARG:HB2 | 1.92 | 0.51 |
| 75:St:274:C:H2' | 75:St:275:G:C8 | 2.45 | 0.51 |
| 64:SV:40:ARG:HA | 75:St:1254:G:C4' | 2.41 | 0.51 |
| 66:SX:29:VAL:O | 66:SX:89:LYS:HA | 2.11 | 0.51 |
| 70:Sd:13:TYR:CE2 | 75:St:688:C:H1' | 2.45 | 0.51 |
| 75:St:624:C:H2' | 75:St:625:G:H8 | 1.76 | 0.51 |
| 75:St:1022:C:H2' | 75:St:1023:G:C8 | 2.45 | 0.51 |
| 75:St:1079:G:H2' | 75:St:1117:A:H8 | 1.76 | 0.51 |
| 75:St:1368:G:N2 | 75:St:1375:G:H2' | 2.26 | 0.51 |
| 3:LC:159:ILE:HG23 | 3:LC:164:VAL:HB | 1.92 | 0.50 |
| 9:LI:163:THR:HG21 | 44:Lt:6:G:H21 | 1.76 | 0.50 |
| 44:Lt:842:C:H2' | 44:Lt:843:A:C8 | 2.46 | 0.50 |
| 47:SC:45:LEU:HB2 | 47:SC:54:VAL:HG22 | 1.92 | 0.50 |
| 75:St:77:C:H2' | 75:St:78:G:H8 | 1.76 | 0.50 |
| 18:LR:80:VAL:HB | 18:LR:137:LEU:HD12 | 1.92 | 0.50 |
| 19:LS:60:ARG:HH12 | 44:Lt:1337:G:H5" | 1.75 | 0.50 |
| 19:LS:117:ARG:HB3 | 44:Lt:1383:G:H5' | 1.94 | 0.50 |
| 37:Lk:39:TYR:CG | 37:Lk:40:PRO:HA | 2.46 | 0.50 |
| 44:Lt:1630:A:H8 | 44:Lt:2398:A:H2 | 1.59 | 0.50 |
| 46:SB:29:PRO:HG3 | 46:SB:38:LYS:HD3 | 1.93 | 0.50 |
| 62:ST:73:LEU:HB2 | 62:ST:124:LEU:HD21 | 1.93 | 0.50 |
| 75:St:277:A:C5 | 75:St:278:G:H1' | 2.47 | 0.50 |
| 2:LB:215:ILE:HG12 | 2:LB:282:VAL:HG13 | 1.93 | 0.50 |
| 19:LS:102:LEU:HD22 | 19:LS:138:LEU:HD22 | 1.93 | 0.50 |
| 19:LS:115:ILE:HG12 | 19:LS:119:LEU:HB3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:LV:61:GLU:HB3 | 22:LV:64:SER:HB2 | 1.94 | 0.50 |
| 26:LZ:59:THR:HB | 26:LZ:103:ASN:HB3 | 1.93 | 0.50 |
| 32:Lf:37:TRP:HZ3 | 32:Lf:47:MET:HE1 | 1.77 | 0.50 |
| 39:Ln:20:ALA:O | 39:Ln:21:THR:C | 2.53 | 0.50 |
| 44:Lt:285:C:H2' | 44:Lt:286:G:C8 | 2.46 | 0.50 |
| 45:SA:85:ARG:HB2 | 45:SA:130:ASN:ND2 | 2.27 | 0.50 |
| 54:SJ:94:LEU:HG | 54:SJ:100:GLY:HA2 | 1.92 | 0.50 |
| 67:SY:43:VAL:HG22 | 67:SY:60:PHE:HE2 | 1.76 | 0.50 |
| 75:St:23:C:H2' | 75:St:24:G:C8 | 2.46 | 0.50 |
| 75:St:654:G:H3' | 75:St:655:G:H21 | 1.76 | 0.50 |
| 8:LH:46:TYR:HE2 | 8:LH:178:ASP:HA | 1.77 | 0.50 |
| 9:LI:146:TRP:HB3 | 36:Lj:37:ILE:HD11 | 1.94 | 0.50 |
| 11:LK:171:TRP:HB2 | 11:LK:178:LYS:HA | 1.93 | 0.50 |
| 24:LX:51:ARG:HA | 24:LX:56:TYR:HD2 | 1.76 | 0.50 |
| 44:Lt:2138:G:H4' | 44:Lt:2139:A:H5" | 1.92 | 0.50 |
| 72:Sg:13:LEU:HB3 | 72:Sg:64:ARG:HH22 | 1.76 | 0.50 |
| 75:St:1413:U:H2' | 75:St:1414:C:C6 | 2.46 | 0.50 |
| 13:LM:28:ALA:HA | 44:Lt:821:G:OP1 | 2.11 | 0.50 |
| 15:LO:120:TRP:HE1 | 15:LO:123:GLN:HB3 | 1.77 | 0.50 |
| 18:LR:87:ASN:HB3 | 18:LR:108:ALA:HA | 1.94 | 0.50 |
| 25:LY:112:LEU:HB3 | 44:Lt:1207:G:H5' | 1.94 | 0.50 |
| 39:Ln:67:VAL:HG21 | 39:Ln:138:LEU:HD23 | 1.93 | 0.50 |
| 44:Lt:1953:G:H2' | 44:Lt:1954:G:C8 | 2.46 | 0.50 |
| 49:SE:159:THR:HG21 | 49:SE:227:VAL:H | 1.77 | 0.50 |
| 55:SK:69:LYS:O | 55:SK:73:GLU:HB2 | 2.11 | 0.50 |
| 75:St:184:C:H2' | 75:St:185:G:H3' | 1.94 | 0.50 |
| 45:SA:73:ILE:HG13 | 45:SA:125:ARG:HD3 | 1.93 | 0.50 |
| 4:LD:92:C:H2' | 4:LD:93:A:C8 | 2.46 | 0.50 |
| 15:LO:174:LEU:HD21 | 44:Lt:62:A:H5" | 1.94 | 0.50 |
| 32:Lf:91:PHE:HB2 | 32:Lf:120:MET:CG | 2.42 | 0.50 |
| 44:Lt:1341:C:H2' | 44:Lt:1342:G:C8 | 2.46 | 0.50 |
| 57:SM:88:TYR:CE1 | 57:SM:103:LYS:HB2 | 2.47 | 0.50 |
| 62:ST:36:ALA:HB2 | 62:ST:87:VAL:HG13 | 1.94 | 0.50 |
| 69:Sc:45:ILE:HD12 | 69:Sc:56:ALA:HB1 | 1.93 | 0.50 |
| 3:LC:51:SER:HB3 | 3:LC:54:ALA:HB2 | 1.93 | 0.50 |
| 32:Lf:72:LEU:HD11 | 32:Lf:78:LYS:HB2 | 1.94 | 0.50 |
| 44:Lt:583:C:H3' | 44:Lt:584:G:H8 | 1.77 | 0.50 |
| 44:Lt:1146:U:C2 | 44:Lt:1159:G:C2 | 3.00 | 0.50 |
| 51:SG:70:TYR:HB3 | 51:SG:103:ILE:HG21 | 1.94 | 0.50 |
| 53:SI:22:HIS:HB3 | 75:St:298:A:H4' | 1.94 | 0.50 |
| 75:St:441:U:H3 | 75:St:464:C:H42 | 1.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:LC:38:THR:HG21 | 44:Lt:1114:C:H5' | 1.94 | 0.50 |
| 44:Lt:1945:G:H2' | 44:Lt:1946:C:H2' | 1.92 | 0.50 |
| 52:SH:66:PRO:HB2 | 52:SH:69:MET:HG3 | 1.94 | 0.50 |
| 55:SK:117:SER:HB2 | 55:SK:119:LEU:HG | 1.94 | 0.50 |
| 8:LH:69:GLN:HA | 21:LU:143:SER:HA | 1.92 | 0.49 |
| 42:Lq:18:TYR:HA | 44:Lt:1620:A:H61 | 1.77 | 0.49 |
| 44:Lt:1146:U:C2 | 44:Lt:1159:G:N2 | 2.79 | 0.49 |
| 46:SB:134:ARG:HA | 46:SB:216:TYR:CZ | 2.47 | 0.49 |
| 51:SG:61:GLY:HA3 | 51:SG:69:MET:HE3 | 1.93 | 0.49 |
| 63:SU:32:ASN:HA | 63:SU:35:ILE:HG22 | 1.94 | 0.49 |
| 64:SV:41:PHE:C | 64:SV:43:ASN:N | 2.70 | 0.49 |
| 29:Lc:53:GLN:C | 29:Lc:55:LEU:H | 2.19 | 0.49 |
| 42:Lq:6:LYS:HG2 | 42:Lq:8:VAL:H | 1.76 | 0.49 |
| 44:Lt:235:G:H1 | 44:Lt:256:G:H21 | 1.60 | 0.49 |
| 45:SA:41:PHE:HB3 | 71:Se:44:MET:HE2 | 1.95 | 0.49 |
| 51:SG:90:TYR:HA | 75:St:144:C:H5' | 1.93 | 0.49 |
| 75:St:894:G:H3' | 75:St:1423:G:H21 | 1.77 | 0.49 |
| 2:LB:169:PRO:HG3 | 2:LB:315:GLY:H | 1.77 | 0.49 |
| 6:LF:65:THR:HG22 | 6:LF:74:VAL:HA | 1.95 | 0.49 |
| 44:Lt:790:G:N2 | 44:Lt:792:C:H3' | 2.28 | 0.49 |
| 44:Lt:2458:C:H2' | 44:Lt:2459:C:C6 | 2.48 | 0.49 |
| 62:ST:12:ARG:HH22 | 75:St:1087:C:H4' | 1.76 | 0.49 |
| 12:LL:23:ILE:O | 12:LL:24:GLY:C | 2.54 | 0.49 |
| 19:LS:23:ARG:HG3 | 44:Lt:1157:G:H5" | 1.94 | 0.49 |
| 42:Lq:49:ARG:HE | 42:Lq:52:CYS:HA | 1.77 | 0.49 |
| 44:Lt:2195:C:H42 | 44:Lt:2211:G:H1 | 1.60 | 0.49 |
| 57:SM:122:THR:HG22 | 57:SM:139:LYS:H | 1.77 | 0.49 |
| 75:St:1033:C:H2' | 75:St:1034:G:C8 | 2.48 | 0.49 |
| 3:LC:158:ILE:O | 3:LC:162:VAL:HG22 | 2.13 | 0.49 |
| 9:LI:131:LEU:HB3 | 9:LI:181:PHE:HB2 | 1.94 | 0.49 |
| 12:LL:117:ASP:HB3 | 12:LL:120:MET:H | 1.76 | 0.49 |
| 17:LQ:81:ARG:O | 17:LQ:83:PRO:HD3 | 2.11 | 0.49 |
| 24:LX:43:MET:HB2 | 24:LX:45:ARG:HD3 | 1.93 | 0.49 |
| 44:Lt:306:U:H2' | 44:Lt:307:A:C8 | 2.43 | 0.49 |
| 44:Lt:430:G:H2' | 44:Lt:431:A:C8 | 2.47 | 0.49 |
| 44:Lt:1522:C:H2' | 44:Lt:1523:G:C8 | 2.48 | 0.49 |
| 53:SI:172:ALA:HB3 | 53:SI:173:PRO:HD3 | 1.93 | 0.49 |
| 55:SK:53:ILE:HG13 | 55:SK:81:LEU:HD21 | 1.94 | 0.49 |
| 73:Sh:102:CYS:SG | 73:Sh:105:CYS:N | 2.85 | 0.49 |
| 75:St:746:A:H2 | 75:St:766:U:H3 | 1.59 | 0.49 |
| 75:St:1083:C:H2' | 75:St:1084:G:C8 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:LB:169:PRO:HG3 | 2:LB:315:GLY:N | 2.27 | 0.49 |
| 2:LB:363:GLY:HA3 | 44:Lt:2638:C:H4' | 1.94 | 0.49 |
| 11:LK:48:TYR:HE2 | 11:LK:142:ALA:HA | 1.77 | 0.49 |
| 16:LP:12:ILE:HG12 | 16:LP:122:ALA:HB2 | 1.95 | 0.49 |
| 16:LP:44:PHE:CZ | 16:LP:141:GLU:HG3 | 2.48 | 0.49 |
| 16:LP:119:SER:HB3 | 20:LT:163:ARG:HG2 | 1.95 | 0.49 |
| 48:SD:26:GLU:HG2 | 48:SD:48:LYS:HG3 | 1.94 | 0.49 |
| 75:St:495:A:H61 | 75:St:850:U:H3 | 1.60 | 0.49 |
| 75:St:1164:G:H2' | 75:St:1164:G:N3 | 2.27 | 0.49 |
| 3:LC:297:PRO:HB2 | 3:LC:304:LEU:HD13 | 1.94 | 0.49 |
| 5:LE:118:U:H2' | 6:LF:264:PHE:HB3 | 1.94 | 0.49 |
| 8:LH:97:ILE:HB | 8:LH:125:VAL:HG21 | 1.95 | 0.49 |
| 23:LW:45:ASN:HA | 44:Lt:2355:U:H5' | 1.95 | 0.49 |
| 46:SB:36:LEU:HB3 | 46:SB:42:ILE:HG12 | 1.94 | 0.49 |
| 50:SF:139:ASN:HD22 | 50:SF:175:ALA:HA | 1.78 | 0.49 |
| 68:Sb:105:ARG:HA | 68:Sb:108:LEU:HB2 | 1.94 | 0.49 |
| 75:St:299:G:H2' | 75:St:300:A:C8 | 2.47 | 0.49 |
| 75:St:1294:C:H2' | 75:St:1295:G:C8 | 2.48 | 0.49 |
| 77:v:8:U:H3 | 77:v:14:A:H8 | 1.58 | 0.49 |
| 3:LC:229:PRO:HG3 | 3:LC:235:ARG:HH11 | 1.78 | 0.49 |
| 16:LP:118:PRO:HA | 16:LP:121:MET:HE2 | 1.94 | 0.49 |
| 32:Lf:81:ILE:HG21 | 32:Lf:87:LEU:HD13 | 1.94 | 0.49 |
| 52:SH:130:LEU:HD11 | 52:SH:156:VAL:HG21 | 1.94 | 0.49 |
| 62:ST:142:LYS:HA | 62:ST:149:ALA:HA | 1.95 | 0.49 |
| 75:St:242:C:H2' | 75:St:243:G:C8 | 2.48 | 0.49 |
| 75:St:772:C:H2' | 75:St:773:G:C8 | 2.48 | 0.49 |
| 16:LP:121:MET:HE2 | 16:LP:121:MET:HB2 | 1.61 | 0.49 |
| 28:Lb:115:ARG:HG2 | 44:Lt:459:A:H3' | 1.95 | 0.49 |
| 31:Le:68:LEU:HD13 | 31:Le:83:VAL:HG21 | 1.95 | 0.49 |
| 35:Li:71:GLU:O | 35:Li:72:ARG:HB3 | 2.13 | 0.49 |
| 44:Lt:245:C:H2' | 44:Lt:246:G:C8 | 2.48 | 0.49 |
| 44:Lt:259:C:H1' | 44:Lt:1711:G:H21 | 1.76 | 0.49 |
| 44:Lt:1643:C:H2' | 44:Lt:1644:G:C8 | 2.48 | 0.49 |
| 44:Lt:1744:A:H61 | 75:St:1411:A:H2' | 1.77 | 0.49 |
| 47:SC:73:HIS:CG | 56:SL:105:PRO:HB3 | 2.48 | 0.49 |
| 49:SE:101:VAL:HG13 | 49:SE:111:LEU:HD22 | 1.94 | 0.49 |
| 56:SL:31:GLY:HA3 | 56:SL:50:TYR:HD2 | 1.78 | 0.49 |
| 73:Sh:104:ILE:HD12 | 73:Sh:123:CYS:HB3 | 1.95 | 0.49 |
| 73:Sh:114:LYS:HB2 | 75:St:1282:G:H5" | 1.94 | 0.49 |
| 5:LE:62:G:H4' | 6:LF:275:LEU:HD12 | 1.95 | 0.49 |
| 11:LK:57:LYS:HG2 | 11:LK:130:SER:HA | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Lg:38:THR:HG23 | 33:Lg:41:GLU:HB2 | 1.95 | 0.49 |
| 53:SI:113:ILE:HB | 53:SI:140:ILE:HB | 1.95 | 0.49 |
| 55:SK:174:THR:HG21 | 75:St:395:A:H5" | 1.95 | 0.49 |
| 2:LB:218:ILE:HB | 2:LB:337:VAL:HG13 | 1.94 | 0.48 |
| 17:LQ:29:TYR:HB2 | 17:LQ:119:VAL:HG11 | 1.94 | 0.48 |
| 23:LW:33:SER:HB2 | 23:LW:115:LYS:HB3 | 1.94 | 0.48 |
| 26:LZ:133:ILE:HG12 | 44:Lt:198:G:H1' | 1.94 | 0.48 |
| 41:Lp:15:GLU:HB3 | 41:Lp:75:CYS:HB3 | 1.94 | 0.48 |
| 45:SA:56:LEU:HD13 | 63:SU:108:MET:HE2 | 1.95 | 0.48 |
| 54:SJ:115:GLU:HB3 | 54:SJ:119:ARG:HH21 | 1.78 | 0.48 |
| 57:SM:44:ILE:H | 57:SM:44:ILE:HG12 | 1.32 | 0.48 |
| 62:ST:48:LEU:HD22 | 65:SW:6:ARG:HH12 | 1.78 | 0.48 |
| 75:St:676:C:H2' | 75:St:677:G:C8 | 2.48 | 0.48 |
| 1:LA:34:PHE:HB2 | 44:Lt:2011:G:H2' | 1.95 | 0.48 |
| 15:LO:33:LEU:HD13 | 15:LO:33:LEU:HA | 1.72 | 0.48 |
| 23:LW:114:LEU:H | 23:LW:114:LEU:HG | 1.47 | 0.48 |
| 26:LZ:62:HIS:HB3 | 26:LZ:83:ILE:HB | 1.95 | 0.48 |
| 29:Lc:5:LYS:HG2 | 44:Lt:827:G:P | 2.53 | 0.48 |
| 44:Lt:1053:G:H3' | 44:Lt:1054:G:H8 | 1.78 | 0.48 |
| 44:Lt:2628:G:H1' | 44:Lt:2685:A:H5' | 1.94 | 0.48 |
| 47:SC:62:GLU:H | 47:SC:62:GLU:HG3 | 1.38 | 0.48 |
| 48:SD:196:LYS:HB3 | 48:SD:196:LYS:HE2 | 1.51 | 0.48 |
| 49:SE:92:ILE:HB | 49:SE:95:VAL:HG12 | 1.95 | 0.48 |
| 50:SF:90:THR:HB | 50:SF:92:LYS:HG2 | 1.95 | 0.48 |
| 74:Sj:48:ILE:HA | 74:Sj:61:ILE:HD11 | 1.95 | 0.48 |
| 75:St:1194:G:H1' | 75:St:1211:C:H6 | 1.78 | 0.48 |
| 5:LE:17:C:H2' | 5:LE:18:G:C8 | 2.48 | 0.48 |
| 7:LG:50:LYS:O | 7:LG:51:LEU:C | 2.56 | 0.48 |
| 15:LO:101:LEU:HD13 | 15:LO:101:LEU:HA | 1.73 | 0.48 |
| 16:LP:64:LEU:HD12 | 16:LP:68:PHE:HE1 | 1.77 | 0.48 |
| 26:LZ:13:LYS:HB2 | 26:LZ:13:LYS:HE3 | 1.63 | 0.48 |
| 37:Lk:35:ALA:HB1 | 44:Lt:313:A:H5' | 1.95 | 0.48 |
| 44:Lt:2653:G:H2' | 44:Lt:2654:C:C6 | 2.48 | 0.48 |
| 49:SE:18:TRP:CH2 | 49:SE:31:PRO:HD3 | 2.48 | 0.48 |
| 49:SE:45:ILE:HB | 49:SE:80:PRO:HB2 | 1.95 | 0.48 |
| 51:SG:203:LYS:HB2 | 51:SG:203:LYS:HE3 | 1.51 | 0.48 |
| 54:SJ:107:SER:HA | 75:St:578:A:C8 | 2.48 | 0.48 |
| 68:Sb:28:HIS:HB2 | 68:Sb:67:GLY:HA3 | 1.94 | 0.48 |
| 75:St:66:C:H2' | 75:St:67:C:O4' | 2.13 | 0.48 |
| 75:St:1307:C:H2' | 75:St:1308:C:C6 | 2.48 | 0.48 |
| 75:St:1398:U:H2' | 75:St:1399:G:H8 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:LC:255:GLN:H | 3:LC:255:GLN:HG3 | 1.36 | 0.48 |
| 6:LF:109:LEU:HD23 | 6:LF:179:LEU:HD11 | 1.94 | 0.48 |
| 8:LH:27:GLU:HA | 8:LH:30:LYS:HB2 | 1.94 | 0.48 |
| 44:Lt:1165:A:H62 | 44:Lt:1504:C:H42 | 1.60 | 0.48 |
| 44:Lt:1531:G:H1 | 44:Lt:1822:U:H3' | 1.78 | 0.48 |
| 51:SG:16:THR:HB | 51:SG:134:VAL:HA | 1.95 | 0.48 |
| 75:St:593:C:O2' | 75:St:594:G:H4' | 2.14 | 0.48 |
| 5:LE:117:C:H2' | 5:LE:118:U:C6 | 2.49 | 0.48 |
| 12:LL:50:SER:HB2 | 12:LL:59:ILE:HD12 | 1.96 | 0.48 |
| 44:Lt:1162:C:H2' | 44:Lt:1163:U:C6 | 2.49 | 0.48 |
| 44:Lt:1750:A:N6 | 75:St:1413:U:H4' | 2.28 | 0.48 |
| 45:SA:70:LEU:HD22 | 45:SA:79:ILE:HD13 | 1.96 | 0.48 |
| 47:SC:65:MET:HG3 | 47:SC:72:LEU:HD13 | 1.94 | 0.48 |
| 51:SG:64:ALA:HB2 | 51:SG:111:ASP:HB2 | 1.96 | 0.48 |
| 8:LH:27:GLU:O | 8:LH:31:ARG:HB2 | 2.13 | 0.48 |
| 12:LL:167:PHE:HB2 | 12:LL:169:VAL:HG13 | 1.95 | 0.48 |
| 25:LY:67:LYS:HZ2 | 35:Li:65:THR:HG22 | 1.79 | 0.48 |
| 44:Lt:1146:U:H2' | 44:Lt:1147:C:C6 | 2.48 | 0.48 |
| 45:SA:174:MET:H | 45:SA:174:MET:HG2 | 1.33 | 0.48 |
| 46:SB:69:GLU:HG2 | 46:SB:70:LEU:H | 1.77 | 0.48 |
| 49:SE:122:LYS:HG2 | 49:SE:164:LEU:HD12 | 1.95 | 0.48 |
| 51:SG:175:HIS:HB2 | 75:St:66:C:P | 2.53 | 0.48 |
| 62:ST:120:LEU:HA | 62:ST:123:LYS:HD3 | 1.95 | 0.48 |
| 64:SV:24:LYS:HB2 | 69:Sc:18:PRO:HB2 | 1.95 | 0.48 |
| 75:St:704:C:H2' | 75:St:705:A:C8 | 2.49 | 0.48 |
| 75:St:900:U:H2' | 75:St:901:A:C8 | 2.48 | 0.48 |
| 6:LF:33:ARG:HH11 | 6:LF:37:ILE:HG21 | 1.78 | 0.48 |
| 6:LF:185:MET:HA | 6:LF:188:PHE:CD1 | 2.49 | 0.48 |
| 10:LJ:143:ARG:HH11 | 10:LJ:184:GLU:HB3 | 1.78 | 0.48 |
| 14:LN:47:ARG:HD3 | 20:LT:67:ASP:HA | 1.95 | 0.48 |
| 44:Lt:2328:C:H2' | 44:Lt:2329:G:C8 | 2.48 | 0.48 |
| 58:SO:63:ASN:HD21 | 58:SO:114:ASP:HB2 | 1.78 | 0.48 |
| 59:SP:21:ALA:HB1 | 59:SP:22:PRO:HD2 | 1.96 | 0.48 |
| 65:SW:4:VAL:HB | 65:SW:63:TYR:CZ | 2.48 | 0.48 |
| 74:Sj:64:LYS:HE3 | 74:Sj:64:LYS:HB3 | 1.49 | 0.48 |
| 75:St:130:C:H2' | 75:St:131:A:H8 | 1.78 | 0.48 |
| 17:LQ:81:ARG:HG2 | 44:Lt:1839:C:H5" | 1.95 | 0.48 |
| 21:LU:17:ARG:H | 21:LU:17:ARG:HG2 | 1.44 | 0.48 |
| 23:LW:82:VAL:HG21 | 23:LW:131:TRP:CD1 | 2.49 | 0.48 |
| 28:Lb:32:ARG:HD3 | 44:Lt:37:U:H5" | 1.95 | 0.48 |
| 44:Lt:372:C:H2' | 44:Lt:373:G:C8 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:478:U:H2' | 44:Lt:479:G:C8 | 2.48 | 0.48 |
| 44:Lt:1464:C:H5" | 44:Lt:1465:G:H5' | 1.96 | 0.48 |
| 58:SO:135:LEU:HB3 | 58:SO:137:LYS:HG3 | 1.96 | 0.48 |
| 62:ST:43:GLY:H | 62:ST:82:ASP:HB2 | 1.79 | 0.48 |
| 66:SX:28:ILE:HG23 | 66:SX:89:LYS:HG3 | 1.96 | 0.48 |
| 75:St:890:G:H2' | 75:St:891:A:C8 | 2.49 | 0.48 |
| 9:LI:55:PRO:HD3 | 9:LI:212:TYR:HA | 1.95 | 0.48 |
| 17:LQ:97:ALA:HB1 | 17:LQ:150:VAL:HG22 | 1.96 | 0.48 |
| 17:LQ:135:ARG:HE | 17:LQ:135:ARG:HB3 | 1.42 | 0.48 |
| 26:LZ:43:LYS:HE2 | 26:LZ:43:LYS:HB2 | 1.70 | 0.48 |
| 32:Lf:41:ARG:HE | 32:Lf:41:ARG:HB2 | 1.50 | 0.48 |
| 39:Ln:77:ALA:HB1 | 39:Ln:82:LEU:HD23 | 1.96 | 0.48 |
| 44:Lt:2595:C:H1' | 44:Lt:2596:G:H8 | 1.79 | 0.48 |
| 55:SK:17:LYS:HB2 | 55:SK:17:LYS:HE2 | 1.62 | 0.48 |
| 63:SU:27:LYS:HB2 | 63:SU:27:LYS:HE2 | 1.70 | 0.48 |
| 75:St:565:C:H2' | 75:St:566:C:H4' | 1.95 | 0.48 |
| 3:LC:27:PRO:HD3 | 3:LC:262:SER:HA | 1.96 | 0.48 |
| 3:LC:50:VAL:HG21 | 3:LC:91:MET:SD | 2.54 | 0.48 |
| 10:LJ:106:LYS:HB2 | 10:LJ:106:LYS:HE2 | 1.67 | 0.48 |
| 15:LO:182:MET:HG3 | 44:Lt:98:C:H4' | 1.96 | 0.48 |
| 32:Lf:79:HIS:HB3 | 32:Lf:90:LEU:HD11 | 1.96 | 0.48 |
| 34:Lh:5:ARG:O | 44:Lt:1489:C:H1' | 2.14 | 0.48 |
| 35:Li:121:ARG:HE | 35:Li:121:ARG:HB2 | 1.55 | 0.48 |
| 36:Lj:34:LYS:HB2 | 36:Lj:34:LYS:HE2 | 1.62 | 0.48 |
| 36:Lj:55:ARG:HB2 | 36:Lj:55:ARG:HH11 | 1.78 | 0.48 |
| 51:SG:93:ARG:HH12 | 75:St:317:G:H4' | 1.78 | 0.48 |
| 52:SH:24:ALA:O | 52:SH:27:LEU:HB2 | 2.14 | 0.48 |
| 75:St:906:C:H2' | 75:St:907:A:C8 | 2.48 | 0.48 |
| 1:LA:226:PRO:HG2 | 1:LA:229:ALA:HB2 | 1.96 | 0.47 |
| 2:LB:237:ARG:HG3 | 2:LB:246:ASN:HD22 | 1.78 | 0.47 |
| 2:LB:296:THR:H | 2:LB:299:ASP:HB2 | 1.79 | 0.47 |
| 16:LP:78:ARG:HH21 | 16:LP:101:VAL:HG22 | 1.79 | 0.47 |
| 17:LQ:25:PHE:HA | 17:LQ:144:CYS:HB3 | 1.96 | 0.47 |
| 28:Lb:74:ASN:C | 28:Lb:76:ASP:H | 2.22 | 0.47 |
| 39:Ln:187:LEU:HD13 | 39:Ln:187:LEU:HA | 1.74 | 0.47 |
| 42:Lq:47:VAL:HG12 | 42:Lq:57:CYS:HB2 | 1.95 | 0.47 |
| 44:Lt:2232:C:H2' | 44:Lt:2233:C:H4' | 1.96 | 0.47 |
| 48:SD:181:ILE:HA | 48:SD:184:LEU:HB2 | 1.95 | 0.47 |
| 75:St:1316:U:H2' | 75:St:1317:G:C8 | 2.49 | 0.47 |
| 78:y:35:U:H3' | 78:y:36:G:C8 | 2.49 | 0.47 |
| 16:LP:157:ARG:HE | 16:LP:157:ARG:HB3 | 1.31 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:LS:172:GLU:HG2 | 19:LS:176:LYS:HE2 | 1.96 | 0.47 |
| 36:Lj:27:LYS:HE2 | 36:Lj:27:LYS:HB3 | 1.43 | 0.47 |
| 39:Ln:69:ALA:O | 39:Ln:73:ASP:HB3 | 2.14 | 0.47 |
| 39:Ln:75:ASP:O | 39:Ln:79:LYS:HB3 | 2.14 | 0.47 |
| 44:Lt:2044:G:H3' | 44:Lt:2045:G:H4' | 1.95 | 0.47 |
| 44:Lt:2581:G:H1' | 44:Lt:2582:C:C5 | 2.50 | 0.47 |
| 67:SY:39:VAL:HG21 | 67:SY:67:ARG:HD2 | 1.95 | 0.47 |
| 8:LH:23:GLU:H | 8:LH:23:GLU:HG2 | 1.38 | 0.47 |
| 44:Lt:245:C:H2' | 44:Lt:246:G:H8 | 1.79 | 0.47 |
| 44:Lt:1877:C:H2' | 44:Lt:1878:A:C8 | 2.48 | 0.47 |
| 44:Lt:2133:C:H2' | 44:Lt:2134:G:C8 | 2.49 | 0.47 |
| 63:SU:61:MET:HA | 63:SU:61:MET:HE3 | 1.96 | 0.47 |
| 65:SW:17:ALA:HA | 65:SW:20:LEU:HB2 | 1.96 | 0.47 |
| 70:Sd:14:ASN:HB2 | 75:St:819:C:H4' | 1.96 | 0.47 |
| 70:Sd:23:CYS:HB3 | 70:Sd:26:CYS:HB2 | 1.95 | 0.47 |
| 20:LT:156:LYS:C | 20:LT:158:ALA:H | 2.22 | 0.47 |
| 44:Lt:177:G:C5 | 44:Lt:197:C:H4' | 2.48 | 0.47 |
| 44:Lt:1048:C:H2' | 44:Lt:1049:G:C8 | 2.49 | 0.47 |
| 44:Lt:1448:G:H2' | 44:Lt:1449:G:H8 | 1.80 | 0.47 |
| 51:SG:245:ARG:NH1 | 51:SG:245:ARG:CG | 2.76 | 0.47 |
| 57:SM:78:MET:SD | 75:St:260:G:H5' | 2.55 | 0.47 |
| 57:SM:95:TYR:C | 57:SM:97:ARG:H | 2.21 | 0.47 |
| 58:SO:67:ARG:HG3 | 58:SO:115:ILE:HG21 | 1.96 | 0.47 |
| 2:LB:266:ARG:HE | 2:LB:266:ARG:HB3 | 1.46 | 0.47 |
| 6:LF:209:HIS:CD2 | 6:LF:210:VAL:HG23 | 2.49 | 0.47 |
| 22:LV:79:VAL:O | 22:LV:83:THR:HG23 | 2.14 | 0.47 |
| 39:Ln:52:PRO:HA | 39:Ln:156:LYS:N | 2.30 | 0.47 |
| 46:SB:69:GLU:HG2 | 46:SB:70:LEU:HG | 1.96 | 0.47 |
| 50:SF:76:MET:HE2 | 50:SF:76:MET:HB2 | 1.65 | 0.47 |
| 75:St:861:U:H2' | 75:St:862:G:C8 | 2.50 | 0.47 |
| 10:LJ:24:VAL:HG11 | 10:LJ:73:ILE:HD11 | 1.97 | 0.47 |
| 13:LM:83:LEU:HD22 | 13:LM:148:TYR:HB2 | 1.96 | 0.47 |
| 19:LS:190:PHE:HB3 | 52:SH:40:GLY:HA2 | 1.97 | 0.47 |
| 39:Ln:5:ASN:HB3 | 39:Ln:8:ALA:HB3 | 1.95 | 0.47 |
| 44:Lt:566:G:H2' | 44:Lt:567:C:C6 | 2.50 | 0.47 |
| 48:SD:107:ARG:H | 48:SD:107:ARG:HG2 | 1.38 | 0.47 |
| 49:SE:55:ALA:HB1 | 49:SE:60:GLU:HB2 | 1.96 | 0.47 |
| 50:SF:172:LYS:HE3 | 50:SF:172:LYS:HB3 | 1.63 | 0.47 |
| 52:SH:115:ARG:HE | 52:SH:116:ARG:H | 1.63 | 0.47 |
| 53:SI:27:TYR:HB2 | 75:St:246:C:H41 | 1.79 | 0.47 |
| 64:SV:31:LEU:HD22 | 64:SV:46:LEU:HD21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 69:Sc:48:ARG:HD3 | 69:Sc:48:ARG:HA | 1.57 | 0.47 |
| 75:St:445:C:H2' | 75:St:457:G:C4 | 2.49 | 0.47 |
| 2:LB:56:VAL:HG21 | 2:LB:353:LEU:HD23 | 1.97 | 0.47 |
| 3:LC:254:LYS:HB2 | 3:LC:257:TYR:HB3 | 1.96 | 0.47 |
| 6:LF:209:HIS:HD2 | 6:LF:210:VAL:HG23 | 1.80 | 0.47 |
| 17:LQ:18:ARG:HD3 | 17:LQ:18:ARG:HA | 1.66 | 0.47 |
| 19:LS:190:PHE:O | 52:SH:43:THR:HB | 2.15 | 0.47 |
| 27:La:124:ASP:HB3 | 27:La:127:PHE:HB3 | 1.97 | 0.47 |
| 38:Ll:24:VAL:HG13 | 38:Ll:71:GLN:HB2 | 1.95 | 0.47 |
| 39:Ln:45:LYS:HB3 | 39:Ln:45:LYS:HE3 | 1.42 | 0.47 |
| 39:Ln:196:LYS:O | 39:Ln:197:GLY:C | 2.58 | 0.47 |
| 42:Lq:26:LEU:HD13 | 42:Lq:26:LEU:HA | 1.71 | 0.47 |
| 44:Lt:1586:C:H2' | 44:Lt:1587:C:O4' | 2.15 | 0.47 |
| 44:Lt:2320:C:H2' | 44:Lt:2322:C:H5' | 1.95 | 0.47 |
| 46:SB:36:LEU:HD22 | 46:SB:36:LEU:HA | 1.80 | 0.47 |
| 49:SE:155:LYS:HE3 | 49:SE:155:LYS:HB2 | 1.67 | 0.47 |
| 51:SG:153:LEU:HD13 | 51:SG:153:LEU:HA | 1.78 | 0.47 |
| 57:SM:23:ARG:HA | 57:SM:23:ARG:HD2 | 1.63 | 0.47 |
| 58:SO:105:PHE:CE2 | 58:SO:121:LYS:HB2 | 2.50 | 0.47 |
| 59:SP:40:LEU:HD12 | 59:SP:50:ILE:HG23 | 1.97 | 0.47 |
| 61:SR:107:ILE:H | 61:SR:107:ILE:HG12 | 1.56 | 0.47 |
| 62:ST:124:LEU:HD13 | 62:ST:124:LEU:HA | 1.77 | 0.47 |
| 75:St:406:C:H2' | 75:St:407:C:O4' | 2.15 | 0.47 |
| 77:v:37:A:H2' | 77:v:38:C:O4' | 2.14 | 0.47 |
| 2:LB:249:VAL:HG21 | 2:LB:265:ALA:HB3 | 1.97 | 0.47 |
| 3:LC:71:ARG:H | 3:LC:71:ARG:HG3 | 1.54 | 0.47 |
| 3:LC:162:VAL:HG23 | 3:LC:164:VAL:HG23 | 1.97 | 0.47 |
| 11:LK:157:PHE:CD2 | 44:Lt:2259:C:H4' | 2.50 | 0.47 |
| 17:LQ:124:GLY:HA2 | 17:LQ:143:PRO:HG2 | 1.97 | 0.47 |
| 39:Ln:23:GLU:HG3 | 44:Lt:1956:A:H4' | 1.96 | 0.47 |
| 45:SA:205:ASP:O | 45:SA:206:LEU:HB2 | 2.13 | 0.47 |
| 46:SB:142:LEU:H | 46:SB:142:LEU:HG | 1.44 | 0.47 |
| 46:SB:226:LYS:HD3 | 46:SB:226:LYS:HA | 1.61 | 0.47 |
| 48:SD:37:LYS:HG3 | 48:SD:72:ASN:HB2 | 1.97 | 0.47 |
| 49:SE:121:PHE:HB2 | 49:SE:161:LYS:HG2 | 1.97 | 0.47 |
| 49:SE:243:ILE:HD12 | 49:SE:243:ILE:HA | 1.68 | 0.47 |
| 63:SU:66:LYS:HB3 | 63:SU:66:LYS:HE3 | 1.39 | 0.47 |
| 75:St:251:C:H2' | 75:St:252:G:C8 | 2.50 | 0.47 |
| 6:LF:131:LYS:HB2 | 6:LF:131:LYS:HE3 | 1.46 | 0.47 |
| 15:LO:36:ILE:HG23 | 15:LO:106:VAL:HG12 | 1.96 | 0.47 |
| 20:LT:133:ARG:HD3 | 20:LT:133:ARG:HA | 1.66 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:LZ:36:LYS:HA | 26:LZ:36:LYS:HD2 | 1.49 | 0.47 |
| 34:Lh:22:ARG:HB3 | 34:Lh:36:VAL:HG23 | 1.96 | 0.47 |
| 39:Ln:209:THR:HB | 44:Lt:1954:G:H21 | 1.80 | 0.47 |
| 41:Lp:59:LYS:HB2 | 41:Lp:59:LYS:HE2 | 1.66 | 0.47 |
| 44:Lt:478:U:H2' | 44:Lt:479:G:H8 | 1.79 | 0.47 |
| 52:SH:39:MET:HG2 | 52:SH:75:LYS:HB2 | 1.97 | 0.47 |
| 62:ST:58:ARG:HD3 | 62:ST:58:ARG:HA | 1.71 | 0.47 |
| 75:St:251:C:H2' | 75:St:252:G:H8 | 1.79 | 0.47 |
| 75:St:1029:A:H5" | 75:St:1055:A:H4' | 1.96 | 0.47 |
| 5:LE:23:A:H2' | 5:LE:24:A:C8 | 2.50 | 0.47 |
| 8:LH:100:LEU:HD23 | 44:Lt:812:G:H1' | 1.97 | 0.47 |
| 19:LS:112:ASP:HB3 | 19:LS:114:LYS:HG3 | 1.96 | 0.47 |
| 19:LS:156:LYS:HA | 19:LS:156:LYS:HD2 | 1.50 | 0.47 |
| 25:LY:95:ARG:HB2 | 25:LY:109:VAL:HG11 | 1.97 | 0.47 |
| 26:LZ:58:PHE:HE2 | 26:LZ:105:ILE:HG13 | 1.80 | 0.47 |
| 43:Ls:97:ARG:HE | 43:Ls:97:ARG:HB2 | 1.47 | 0.47 |
| 44:Lt:1519:A:C2 | 44:Lt:1879:G:H4' | 2.50 | 0.47 |
| 44:Lt:2303:U:H2' | 44:Lt:2304:C:C6 | 2.49 | 0.47 |
| 44:Lt:2560:C:H2' | 44:Lt:2561:C:C6 | 2.50 | 0.47 |
| 47:SC:20:ASP:HA | 47:SC:23:MET:HE3 | 1.96 | 0.47 |
| 56:SL:24:LEU:HB2 | 56:SL:50:TYR:HE1 | 1.80 | 0.47 |
| 58:SO:25:LYS:HA | 58:SO:28:ARG:HD2 | 1.97 | 0.47 |
| 59:SP:109:LYS:HD3 | 75:St:729:C:H4' | 1.97 | 0.47 |
| 67:SY:45:ARG:H | 67:SY:45:ARG:HG2 | 1.51 | 0.47 |
| 68:Sb:76:TYR:HE2 | 68:Sb:85:TYR:HB2 | 1.79 | 0.47 |
| 75:St:140:A:H61 | 75:St:332:G:H1' | 1.80 | 0.47 |
| 75:St:1081:C:H2' | 75:St:1082:G:C8 | 2.47 | 0.47 |
| 1:LA:134:CYS:SG | 1:LA:151:PRO:HD3 | 2.56 | 0.46 |
| 18:LR:70:LEU:HD12 | 18:LR:70:LEU:HA | 1.69 | 0.46 |
| 21:LU:121:GLU:HB2 | 21:LU:122:THR:H | 1.63 | 0.46 |
| 22:LV:87:LEU:HD11 | 22:LV:107:LEU:HD21 | 1.97 | 0.46 |
| 25:LY:45:TYR:HD2 | 35:Li:109:PRO:HA | 1.80 | 0.46 |
| 39:Ln:87:ILE:HG12 | 39:Ln:116:LEU:HB2 | 1.97 | 0.46 |
| 44:Lt:598:C:H1' | 44:Lt:1482:A:H5" | 1.97 | 0.46 |
| 44:Lt:1709:G:H21 | 44:Lt:1712:A:H2 | 1.62 | 0.46 |
| 44:Lt:1866:C:H2' | 44:Lt:1867:G:C8 | 2.50 | 0.46 |
| 46:SB:221:PRO:HA | 46:SB:224:TRP:CD2 | 2.50 | 0.46 |
| 48:SD:95:LYS:HB3 | 48:SD:95:LYS:HE2 | 1.73 | 0.46 |
| 52:SH:50:LYS:HD2 | 52:SH:50:LYS:HA | 1.50 | 0.46 |
| 55:SK:118:LYS:HE2 | 55:SK:118:LYS:HB2 | 1.51 | 0.46 |
| 58:SO:67:ARG:HB3 | 58:SO:84:PHE:CE1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 62:ST:62:LEU:HD23 | 62:ST:96:ILE:HG12 | 1.98 | 0.46 |
| 75:St:1434:U:H2' | 75:St:1436:A:OP2 | 2.15 | 0.46 |
| 9:LI:49:ARG:HE | 9:LI:49:ARG:HB2 | 1.62 | 0.46 |
| 18:LR:176:ARG:HB2 | 18:LR:176:ARG:HH11 | 1.80 | 0.46 |
| 44:Lt:1296:C:H2' | 44:Lt:1297:C:C2 | 2.50 | 0.46 |
| 46:SB:33:LEU:HD13 | 46:SB:48:ILE:HG21 | 1.97 | 0.46 |
| 62:ST:38:ALA:HB2 | 62:ST:102:ALA:HB1 | 1.96 | 0.46 |
| 64:SV:40:ARG:HB2 | 75:St:1253:C:O2' | 2.14 | 0.46 |
| 65:SW:108:LEU:HA | 65:SW:113:LEU:O | 2.15 | 0.46 |
| 68:Sb:116:LEU:HD12 | 68:Sb:116:LEU:HA | 1.81 | 0.46 |
| 1:LA:114:CYS:HB2 | 1:LA:169:VAL:HG23 | 1.96 | 0.46 |
| 3:LC:29:ARG:HD2 | 3:LC:32:ILE:HG13 | 1.97 | 0.46 |
| 8:LH:66:LYS:HE2 | 8:LH:66:LYS:HB3 | 1.55 | 0.46 |
| 13:LM:84:ARG:HB3 | 13:LM:101:GLY:O | 2.15 | 0.46 |
| 13:LM:99:ARG:HE | 13:LM:99:ARG:HB3 | 1.59 | 0.46 |
| 18:LR:5:LEU:H | 18:LR:5:LEU:HG | 1.50 | 0.46 |
| 23:LW:98:ILE:HA | 24:LX:21:CYS:O | 2.15 | 0.46 |
| 34:Lh:38:LYS:H | 34:Lh:38:LYS:HG2 | 1.41 | 0.46 |
| 38:Ll:29:LYS:C | 38:Ll:31:ARG:N | 2.73 | 0.46 |
| 43:Ls:88:GLU:HA | 43:Ls:92:ASN:HB3 | 1.98 | 0.46 |
| 44:Lt:1545:G:N3 | 44:Lt:1609:C:H2' | 2.30 | 0.46 |
| 44:Lt:1604:G:H22 | 44:Lt:1609:C:H1' | 1.80 | 0.46 |
| 45:SA:159:LEU:HD22 | 45:SA:159:LEU:HA | 1.74 | 0.46 |
| 48:SD:37:LYS:HE2 | 48:SD:37:LYS:HB2 | 1.42 | 0.46 |
| 52:SH:163:TYR:HB2 | 52:SH:189:PHE:CD1 | 2.51 | 0.46 |
| 58:SO:61:GLN:HG2 | 58:SO:62:PRO:HA | 1.98 | 0.46 |
| 63:SU:15:LYS:HA | 63:SU:15:LYS:HD2 | 1.75 | 0.46 |
| 63:SU:84:ARG:HA | 63:SU:87:TYR:HB3 | 1.97 | 0.46 |
| 68:Sb:18:GLN:HB3 | 68:Sb:78:ASN:HB2 | 1.96 | 0.46 |
| 71:Se:121:TYR:HB3 | 71:Se:122:ARG:H | 1.47 | 0.46 |
| 75:St:983:G:N2 | 75:St:985:G:H3' | 2.30 | 0.46 |
| 75:St:1223:C:H4' | 75:St:1229:C:H42 | 1.80 | 0.46 |
| 75:St:1243:G:N2 | 75:St:1245:A:H3' | 2.30 | 0.46 |
| 76:u:74:C:H6 | 76:u:74:C:H2' | 1.59 | 0.46 |
| 4:LD:80:C:O2' | 4:LD:81:G:H8 | 1.98 | 0.46 |
| 6:LF:34:LYS:HA | 6:LF:34:LYS:HE3 | 1.98 | 0.46 |
| 8:LH:155:ARG:HG3 | 8:LH:198:TRP:CD2 | 2.50 | 0.46 |
| 9:LI:153:LYS:HG2 | 36:Lj:32:PHE:HE1 | 1.80 | 0.46 |
| 9:LI:163:THR:HG22 | 9:LI:165:GLY:H | 1.81 | 0.46 |
| 17:LQ:28:THR:HA | 17:LQ:31:THR:HG22 | 1.96 | 0.46 |
| 21:LU:35:LYS:HD3 | 21:LU:35:LYS:HA | 1.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:729:A:H61 | 44:Lt:749:C:H42 | 1.63 | 0.46 |
| 51:SG:62:ASN:HB3 | 51:SG:66:GLY:HA2 | 1.96 | 0.46 |
| 54:SJ:74:VAL:HA | 54:SJ:127:GLY:HA2 | 1.97 | 0.46 |
| 55:SK:80:ARG:HA | 55:SK:83:MET:HE3 | 1.96 | 0.46 |
| 61:SR:90:ILE:HG21 | 61:SR:109:PRO:HG3 | 1.96 | 0.46 |
| 62:ST:31:LYS:HG2 | 62:ST:97:TYR:HB3 | 1.97 | 0.46 |
| 68:Sb:33:TYR:HE1 | 75:St:416:C:H1' | 1.80 | 0.46 |
| 69:Sc:83:ASN:HB2 | 69:Sc:86:LYS:CB | 2.38 | 0.46 |
| 8:LH:92:PRO:HD3 | 44:Lt:848:G:O3' | 2.16 | 0.46 |
| 17:LQ:68:ARG:HG3 | 17:LQ:78:ASP:HB3 | 1.97 | 0.46 |
| 32:Lf:23:ILE:H | 32:Lf:23:ILE:HG12 | 1.43 | 0.46 |
| 35:Li:33:LYS:HB2 | 35:Li:33:LYS:HE3 | 1.68 | 0.46 |
| 44:Lt:1384:C:H4' | 44:Lt:1397:G:H4' | 1.98 | 0.46 |
| 47:SC:194:ILE:HD12 | 47:SC:194:ILE:HA | 1.72 | 0.46 |
| 51:SG:96:GLY:HA2 | 75:St:307:C:O2' | 2.15 | 0.46 |
| 61:SR:119:TYR:CD1 | 64:SV:120:CYS:HB3 | 2.47 | 0.46 |
| 64:SV:141:GLY:HA2 | 64:SV:143:ARG:HG2 | 1.98 | 0.46 |
| 72:Sg:52:VAL:C | 72:Sg:53:LEU:HG | 2.41 | 0.46 |
| 75:St:1033:C:H2' | 75:St:1034:G:H8 | 1.81 | 0.46 |
| 75:St:1249:C:H2' | 75:St:1250:C:C6 | 2.51 | 0.46 |
| 2:LB:206:LYS:H | 2:LB:206:LYS:HG2 | 1.43 | 0.46 |
| 3:LC:264:ILE:H | 3:LC:264:ILE:HG13 | 1.68 | 0.46 |
| 6:LF:8:LYS:HE2 | 6:LF:8:LYS:HB2 | 1.50 | 0.46 |
| 6:LF:151:LYS:HE3 | 6:LF:151:LYS:HB3 | 1.48 | 0.46 |
| 17:LQ:16:SER:HB3 | 17:LQ:97:ALA:HB2 | 1.97 | 0.46 |
| 18:LR:174:ARG:H | 18:LR:174:ARG:HG2 | 1.54 | 0.46 |
| 25:LY:30:HIS:CE1 | 44:Lt:2008:C:H1' | 2.50 | 0.46 |
| 32:Lf:21:LYS:HZ2 | 32:Lf:21:LYS:HG2 | 1.54 | 0.46 |
| 44:Lt:298:G:H2' | 44:Lt:299:G:C8 | 2.51 | 0.46 |
| 44:Lt:1181:C:H2' | 44:Lt:1182:G:C8 | 2.51 | 0.46 |
| 49:SE:54:TYR:HA | 68:Sb:14:ASN:HD21 | 1.80 | 0.46 |
| 62:ST:66:VAL:HG13 | 62:ST:100:ARG:HB2 | 1.98 | 0.46 |
| 65:SW:75:LEU:H | 65:SW:75:LEU:HG | 1.37 | 0.46 |
| 70:Sd:107:GLN:HE21 | 70:Sd:109:LYS:HB2 | 1.79 | 0.46 |
| 72:Sg:4:PRO:HB2 | 72:Sg:52:VAL:O | 2.15 | 0.46 |
| 5:LE:95:C:H2' | 5:LE:96:G:C8 | 2.51 | 0.46 |
| 6:LF:182:PRO:HB2 | 44:Lt:2171:A:H4' | 1.97 | 0.46 |
| 8:LH:90:VAL:HG13 | 8:LH:95:ARG:HE | 1.81 | 0.46 |
| 13:LM:39:ARG:HA | 13:LM:39:ARG:HD3 | 1.70 | 0.46 |
| 13:LM:210:ALA:HA | 13:LM:213:ARG:HH21 | 1.79 | 0.46 |
| 17:LQ:71:GLN:H | 17:LQ:71:GLN:HG2 | 1.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:LY:28:ASN:HD21 | 25:LY:30:HIS:HB2 | 1.79 | 0.46 |
| 28:Lb:71:PRO:HB2 | 28:Lb:109:PHE:HA | 1.98 | 0.46 |
| 29:Lc:50:ASP:HB3 | 29:Lc:51:PRO:HD3 | 1.98 | 0.46 |
| 44:Lt:1736:C:H4' | 44:Lt:1760:G:C8 | 2.50 | 0.46 |
| 44:Lt:1789:C:H2' | 44:Lt:1790:G:H8 | 1.80 | 0.46 |
| 48:SD:36:PHE:CG | 48:SD:71:LEU:HG | 2.51 | 0.46 |
| 49:SE:187:ARG:HD2 | 49:SE:187:ARG:HA | 1.73 | 0.46 |
| 57:SM:116:LYS:HA | 57:SM:116:LYS:HD2 | 1.55 | 0.46 |
| 60:SQ:83:GLU:H | 60:SQ:83:GLU:HG2 | 1.42 | 0.46 |
| 61:SR:57:PHE:HD2 | 61:SR:80:LEU:HD22 | 1.79 | 0.46 |
| 61:SR:63:LEU:HD22 | 61:SR:63:LEU:HA | 1.76 | 0.46 |
| 74:Sj:62:ARG:HA | 74:Sj:65:LEU:HD23 | 1.96 | 0.46 |
| 75:St:166:G:H2' | 75:St:167:G:C8 | 2.50 | 0.46 |
| 8:LH:168:LEU:HB3 | 8:LH:173:ILE:HB | 1.97 | 0.46 |
| 9:LI:117:ILE:HD13 | 9:LI:117:ILE:HA | 1.73 | 0.46 |
| 31:Le:19:PRO:HA | 44:Lt:1833:G:OP1 | 2.16 | 0.46 |
| 34:Lh:87:ILE:HD13 | 34:Lh:87:ILE:HA | 1.83 | 0.46 |
| 34:Lh:108:LYS:HE3 | 34:Lh:108:LYS:HB3 | 1.62 | 0.46 |
| 35:Li:81:LYS:HD3 | 35:Li:81:LYS:HA | 1.57 | 0.46 |
| 36:Lj:80:ARG:HE | 36:Lj:80:ARG:HB3 | 1.45 | 0.46 |
| 44:Lt:1274:G:H21 | 44:Lt:1276:A:H8 | 1.64 | 0.46 |
| 44:Lt:1478:C:H3' | 44:Lt:1479:A:H8 | 1.81 | 0.46 |
| 44:Lt:1944:A:N3 | 44:Lt:1969:G:H1' | 2.31 | 0.46 |
| 46:SB:148:VAL:HG11 | 46:SB:152:LEU:HD11 | 1.97 | 0.46 |
| 47:SC:112:ARG:HG2 | 47:SC:179:ARG:HG2 | 1.98 | 0.46 |
| 48:SD:152:LYS:H | 48:SD:152:LYS:HG3 | 1.32 | 0.46 |
| 49:SE:75:LYS:HE2 | 49:SE:75:LYS:HB3 | 1.68 | 0.46 |
| 50:SF:17:LYS:HD2 | 50:SF:17:LYS:HA | 1.67 | 0.46 |
| 53:SI:131:ILE:HG23 | 53:SI:135:ILE:HD12 | 1.98 | 0.46 |
| 55:SK:2:ARG:HB3 | 55:SK:5:ARG:HG2 | 1.98 | 0.46 |
| 62:ST:38:ALA:HA | 62:ST:85:ILE:CG1 | 2.45 | 0.46 |
| 65:SW:25:ILE:HG12 | 65:SW:110:GLN:HG2 | 1.97 | 0.46 |
| 67:SY:53:ILE:HG12 | 67:SY:55:ASN:H | 1.80 | 0.46 |
| 71:Se:84:ILE:H | 71:Se:84:ILE:HG13 | 1.53 | 0.46 |
| 75:St:1232:G:H1 | 75:St:1256:G:H1' | 1.81 | 0.46 |
| 6:LF:34:LYS:HZ3 | 21:LU:30:TYR:HB2 | 1.80 | 0.46 |
| 16:LP:24:LEU:HD12 | 16:LP:24:LEU:HA | 1.77 | 0.46 |
| 16:LP:45:ARG:H | 16:LP:45:ARG:HG3 | 1.41 | 0.46 |
| 20:LT:11:ARG:HG2 | 20:LT:20:PRO:HB3 | 1.98 | 0.46 |
| 39:Ln:51:LEU:HD12 | 39:Ln:51:LEU:HA | 1.71 | 0.46 |
| 44:Lt:1065:C:H2' | 44:Lt:1066:A:C8 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:1931:G:H3' | 44:Lt:1932:G:H8 | 1.80 | 0.46 |
| 50:SF:164:MET:HE3 | 50:SF:164:MET:HB3 | 1.60 | 0.46 |
| 52:SH:80:LEU:HD22 | 52:SH:80:LEU:HA | 1.65 | 0.46 |
| 55:SK:74:GLY:HA3 | 55:SK:94:LEU:HD12 | 1.97 | 0.46 |
| 75:St:471:G:H2' | 75:St:472:C:C6 | 2.51 | 0.46 |
| 75:St:984:G:H5' | 75:St:985:G:C8 | 2.50 | 0.46 |
| 6:LF:193:LYS:H | 6:LF:193:LYS:HG2 | 1.51 | 0.46 |
| 12:LL:24:GLY:O | 12:LL:65:ILE:HA | 2.16 | 0.46 |
| 22:LV:10:LYS:HD2 | 22:LV:10:LYS:HA | 1.52 | 0.46 |
| 23:LW:74:LEU:H | 23:LW:74:LEU:HG | 1.44 | 0.46 |
| 27:La:12:CYS:HA | 27:La:81:THR:HG23 | 1.98 | 0.46 |
| 33:Lg:7:LYS:HG3 | 33:Lg:97:ASP:HB2 | 1.96 | 0.46 |
| 41:Lp:4:TYR:CD2 | 41:Lp:5:PRO:HD2 | 2.51 | 0.46 |
| 42:Lq:71:LEU:HD23 | 42:Lq:71:LEU:HA | 1.73 | 0.46 |
| 44:Lt:1960:C:H1' | 44:Lt:1961:G:H2' | 1.98 | 0.46 |
| 47:SC:73:HIS:HA | 47:SC:76:GLU:HG3 | 1.98 | 0.46 |
| 49:SE:10:LYS:HA | 49:SE:27:TRP:HD1 | 1.81 | 0.46 |
| 51:SG:69:MET:SD | 51:SG:106:CYS:HA | 2.56 | 0.46 |
| 58:SO:17:ARG:HD3 | 58:SO:17:ARG:HA | 1.67 | 0.46 |
| 62:ST:50:ASN:HD22 | 62:ST:50:ASN:HA | 1.36 | 0.46 |
| 62:ST:124:LEU:HB3 | 62:ST:131:LEU:HD22 | 1.97 | 0.46 |
| 68:Sb:40:LYS:HD3 | 68:Sb:52:GLN:HB2 | 1.98 | 0.46 |
| 72:Sg:7:ALA:HA | 72:Sg:30:MET:H | 1.81 | 0.46 |
| 1:LA:52:ARG:HE | 1:LA:52:ARG:HB3 | 1.30 | 0.45 |
| 3:LC:72:LEU:HD21 | 3:LC:80:GLY:HA2 | 1.96 | 0.45 |
| 11:LK:63:GLU:HB3 | 44:Lt:2276:G:H5' | 1.98 | 0.45 |
| 14:LN:37:LEU:HD21 | 14:LN:47:ARG:HE | 1.80 | 0.45 |
| 15:LO:143:ARG:HE | 15:LO:143:ARG:HB3 | 1.58 | 0.45 |
| 20:LT:50:LYS:HB3 | 20:LT:50:LYS:HE3 | 1.69 | 0.45 |
| 29:Lc:23:LYS:HE2 | 29:Lc:23:LYS:HB2 | 1.43 | 0.45 |
| 31:Le:32:ARG:HE | 31:Le:32:ARG:HB2 | 1.55 | 0.45 |
| 32:Lf:60:ILE:HG12 | 44:Lt:664:U:H5' | 1.97 | 0.45 |
| 35:Li:151:LYS:HB2 | 35:Li:151:LYS:HE2 | 1.72 | 0.45 |
| 44:Lt:455:C:C5 | 44:Lt:456:G:H1' | 2.51 | 0.45 |
| 44:Lt:1911:C:H2' | 44:Lt:1912:A:H8 | 1.81 | 0.45 |
| 44:Lt:2658:G:H2' | 44:Lt:2659:C:C6 | 2.50 | 0.45 |
| 47:SC:23:MET:HE2 | 47:SC:23:MET:HB2 | 1.83 | 0.45 |
| 47:SC:36:VAL:HG23 | 47:SC:40:TYR:HD2 | 1.80 | 0.45 |
| 48:SD:11:LYS:H | 48:SD:11:LYS:HG2 | 1.42 | 0.45 |
| 57:SM:10:TYR:HE2 | 57:SM:12:LYS:HB3 | 1.80 | 0.45 |
| 61:SR:100:ARG:HG3 | 75:St:927:A:C4 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 62:ST:108:LEU:HD12 | 62:ST:108:LEU:HA | 1.81 | 0.45 |
| 63:SU:51:ASN:HA | 63:SU:54:ALA:HB3 | 1.98 | 0.45 |
| 74:Sj:62:ARG:HH22 | 75:St:437:G:H1' | 1.81 | 0.45 |
| 75:St:527:C:H2' | 75:St:528:A:C8 | 2.51 | 0.45 |
| 75:St:541:A:H3' | 75:St:542:G:C8 | 2.47 | 0.45 |
| 20:LT:22:VAL:HG21 | 21:LU:144:ILE:HA | 1.98 | 0.45 |
| 24:LX:51:ARG:HA | 24:LX:56:TYR:CD2 | 2.51 | 0.45 |
| 39:Ln:146:LEU:HD23 | 39:Ln:146:LEU:HA | 1.77 | 0.45 |
| 39:Ln:150:GLU:H | 39:Ln:150:GLU:HG2 | 1.21 | 0.45 |
| 44:Lt:538:U:H2' | 44:Lt:539:G:C8 | 2.50 | 0.45 |
| 44:Lt:2020:C:H2' | 44:Lt:2021:G:C8 | 2.51 | 0.45 |
| 44:Lt:2044:G:C3' | 44:Lt:2045:G:H4' | 2.47 | 0.45 |
| 48:SD:68:LEU:HD23 | 48:SD:68:LEU:HA | 1.70 | 0.45 |
| 51:SG:19:ASN:ND2 | 75:St:136:U:H1' | 2.31 | 0.45 |
| 51:SG:238:ARG:HA | 51:SG:238:ARG:HD2 | 1.70 | 0.45 |
| 52:SH:21:LYS:HB3 | 52:SH:21:LYS:HE2 | 1.49 | 0.45 |
| 59:SP:84:ILE:HA | 59:SP:135:LEU:HD21 | 1.97 | 0.45 |
| 61:SR:87:PRO:HA | 61:SR:112:VAL:HG21 | 1.98 | 0.45 |
| 62:ST:9:LEU:C | 62:ST:10:LEU:HG | 2.41 | 0.45 |
| 64:SV:81:PRO:HD2 | 65:SW:34:TYR:CZ | 2.51 | 0.45 |
| 74:Sj:18:LYS:H | 74:Sj:18:LYS:HG2 | 1.36 | 0.45 |
| 75:St:77:C:H2' | 75:St:78:G:C8 | 2.51 | 0.45 |
| 4:LD:68:U:H2' | 4:LD:69:G:C8 | 2.51 | 0.45 |
| 13:LM:201:PHE:CD1 | 28:Lb:132:SER:HB2 | 2.51 | 0.45 |
| 22:LV:61:GLU:CB | 22:LV:64:SER:HB2 | 2.46 | 0.45 |
| 27:La:105:ARG:HD3 | 27:La:105:ARG:HA | 1.65 | 0.45 |
| 33:Lg:52:ILE:HG21 | 33:Lg:83:LEU:HD11 | 1.98 | 0.45 |
| 44:Lt:778:C:H2' | 44:Lt:779:G:C8 | 2.50 | 0.45 |
| 44:Lt:1580:G:H1 | 44:Lt:1587:C:N4 | 2.11 | 0.45 |
| 46:SB:219:LEU:HG | 46:SB:224:TRP:CD1 | 2.51 | 0.45 |
| 47:SC:33:ARG:HD3 | 47:SC:33:ARG:HA | 1.48 | 0.45 |
| 52:SH:44:LEU:H | 52:SH:44:LEU:HG | 1.18 | 0.45 |
| 53:SI:119:LYS:HA | 53:SI:135:ILE:HG23 | 1.98 | 0.45 |
| 75:St:130:C:H2' | 75:St:131:A:C8 | 2.51 | 0.45 |
| 1:LA:134:CYS:HB3 | 1:LA:148:ILE:HD11 | 1.98 | 0.45 |
| 1:LA:154:GLN:H | 1:LA:154:GLN:HG2 | 1.43 | 0.45 |
| 14:LN:117:ARG:HA | 14:LN:117:ARG:HD2 | 1.78 | 0.45 |
| 26:LZ:107:LYS:HB3 | 26:LZ:107:LYS:HE2 | 1.46 | 0.45 |
| 34:Lh:96:ASN:C | 34:Lh:98:ALA:H | 2.25 | 0.45 |
| 36:Lj:44:ALA:HB3 | 36:Lj:47:GLU:HG3 | 1.99 | 0.45 |
| 44:Lt:1866:C:H2' | 44:Lt:1867:G:H8 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:2304:C:H2' | 44:Lt:2305:U:C6 | 2.52 | 0.45 |
| 46:SB:32:LYS:HD2 | 46:SB:32:LYS:HA | 1.54 | 0.45 |
| 47:SC:207:LYS:HB2 | 47:SC:207:LYS:HE2 | 1.77 | 0.45 |
| 48:SD:140:ILE:HB | 48:SD:213:ARG:HD3 | 1.99 | 0.45 |
| 50:SF:62:LEU:HD22 | 50:SF:155:PHE:HE2 | 1.82 | 0.45 |
| 51:SG:55:THR:HB | 51:SG:120:VAL:HB | 1.98 | 0.45 |
| 53:SI:62:ILE:H | 53:SI:62:ILE:HG13 | 1.56 | 0.45 |
| 61:SR:116:LEU:HD23 | 61:SR:116:LEU:HA | 1.85 | 0.45 |
| 62:ST:32:LYS:HB3 | 62:ST:94:SER:HB3 | 1.98 | 0.45 |
| 66:SX:93:TRP:HH2 | 75:St:1087:C:P | 2.37 | 0.45 |
| 68:Sb:21:GLN:HB2 | 68:Sb:72:PHE:HE2 | 1.81 | 0.45 |
| 70:Sd:44:ILE:HD13 | 70:Sd:44:ILE:HA | 1.77 | 0.45 |
| 75:St:535:A:H3' | 75:St:536:A:H8 | 1.80 | 0.45 |
| 2:LB:102:VAL:HG23 | 2:LB:154:ALA:HB2 | 1.99 | 0.45 |
| 3:LC:301:LYS:HD2 | 3:LC:301:LYS:HA | 1.44 | 0.45 |
| 6:LF:161:ALA:HB1 | 6:LF:168:PHE:HZ | 1.82 | 0.45 |
| 8:LH:119:LEU:HD22 | 8:LH:119:LEU:HA | 1.74 | 0.45 |
| 9:LI:139:ASP:HB3 | 15:LO:41:HIS:CE1 | 2.52 | 0.45 |
| 17:LQ:14:GLY:HA3 | 17:LQ:101:ALA:HB2 | 1.97 | 0.45 |
| 20:LT:15:GLU:H | 20:LT:15:GLU:HG3 | 1.48 | 0.45 |
| 21:LU:77:GLN:HE21 | 21:LU:77:GLN:HB3 | 1.49 | 0.45 |
| 27:La:27:VAL:HG11 | 27:La:93:ILE:HD12 | 1.98 | 0.45 |
| 29:Lc:50:ASP:HB3 | 29:Lc:51:PRO:CD | 2.46 | 0.45 |
| 34:Lh:45:CYS:HB3 | 34:Lh:52:ILE:HD11 | 1.97 | 0.45 |
| 44:Lt:2328:C:H2' | 44:Lt:2329:G:H8 | 1.81 | 0.45 |
| 69:Sc:41:THR:O | 69:Sc:45:ILE:HG13 | 2.16 | 0.45 |
| 75:St:538:G:H22 | 75:St:566:C:H1' | 1.82 | 0.45 |
| 1:LA:180:LEU:HD23 | 1:LA:180:LEU:HA | 1.74 | 0.45 |
| 1:LA:234:LYS:HB2 | 1:LA:234:LYS:HE3 | 1.47 | 0.45 |
| 2:LB:292:ARG:H | 2:LB:292:ARG:HG3 | 1.61 | 0.45 |
| 8:LH:58:LYS:HA | 8:LH:58:LYS:HD2 | 1.71 | 0.45 |
| 8:LH:94:VAL:HG13 | 8:LH:125:VAL:HG13 | 1.98 | 0.45 |
| 15:LO:27:THR:HG22 | 15:LO:122:ALA:HB1 | 1.99 | 0.45 |
| 18:LR:169:GLY:HA3 | 28:Lb:51:GLY:O | 2.17 | 0.45 |
| 36:Lj:7:ASN:O | 36:Lj:8:LEU:C | 2.59 | 0.45 |
| 50:SF:97:VAL:HG12 | 50:SF:163:ILE:HG22 | 1.98 | 0.45 |
| 51:SG:214:MET:HE3 | 51:SG:214:MET:HB2 | 1.73 | 0.45 |
| 51:SG:214:MET:O | 51:SG:218:LEU:HB2 | 2.16 | 0.45 |
| 58:SO:128:ILE:H | 58:SO:128:ILE:HG12 | 1.68 | 0.45 |
| 60:SQ:31:CYS:HA | 60:SQ:44:VAL:HA | 1.99 | 0.45 |
| 63:SU:74:LEU:HD12 | 63:SU:74:LEU:HA | 1.74 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 68:Sb:118:LYS:HG3 | 68:Sb:121:THR:HB | 1.98 | 0.45 |
| 70:Sd:109:LYS:HD3 | 70:Sd:109:LYS:HA | 1.73 | 0.45 |
| 75:St:425:A:N1 | 75:St:473:G:H2' | 2.31 | 0.45 |
| 75:St:1392:C:H2' | 75:St:1393:G:C8 | 2.51 | 0.45 |
| 1:LA:246:SER:HB3 | 1:LA:247:GLY:H | 1.59 | 0.45 |
| 2:LB:185:GLY:HA3 | 2:LB:191:LYS:HG2 | 1.98 | 0.45 |
| 3:LC:107:LEU:HA | 3:LC:110:ARG:HE | 1.80 | 0.45 |
| 4:LD:14:G:H2' | 4:LD:15:C:C6 | 2.52 | 0.45 |
| 6:LF:263:LYS:HA | 6:LF:263:LYS:HD2 | 1.62 | 0.45 |
| 11:LK:14:ASN:HD22 | 11:LK:14:ASN:HA | 1.67 | 0.45 |
| 20:LT:56:ILE:H | 20:LT:56:ILE:HG13 | 1.48 | 0.45 |
| 20:LT:138:MET:HE2 | 20:LT:138:MET:HB2 | 1.64 | 0.45 |
| 24:LX:33:CYS:HB2 | 24:LX:37:CYS:HB2 | 1.60 | 0.45 |
| 25:LY:61:LEU:HD22 | 25:LY:89:ALA:HB2 | 1.98 | 0.45 |
| 29:Lc:43:LEU:HD12 | 29:Lc:43:LEU:HA | 1.73 | 0.45 |
| 34:Lh:97:GLN:O | 34:Lh:102:ILE:HB | 2.16 | 0.45 |
| 37:Lk:8:PHE:O | 37:Lk:11:ARG:HB2 | 2.16 | 0.45 |
| 41:Lp:13:LYS:H | 41:Lp:13:LYS:HG2 | 1.42 | 0.45 |
| 44:Lt:361:C:H2' | 44:Lt:362:G:H8 | 1.81 | 0.45 |
| 44:Lt:2643:A:H2' | 44:Lt:2644:C:C6 | 2.52 | 0.45 |
| 46:SB:120:LYS:HD2 | 46:SB:120:LYS:HA | 1.40 | 0.45 |
| 49:SE:151:HIS:HD2 | 49:SE:154:ILE:HG23 | 1.80 | 0.45 |
| 75:St:310:C:H2' | 75:St:311:G:C8 | 2.50 | 0.45 |
| 75:St:529:C:H2' | 75:St:530:G:C8 | 2.52 | 0.45 |
| 75:St:628:C:H2' | 75:St:629:G:C8 | 2.52 | 0.45 |
| 75:St:915:A:H2' | 75:St:916:G:C8 | 2.51 | 0.45 |
| 75:St:1433:G:H1 | 75:St:1438:C:H42 | 1.65 | 0.45 |
| 2:LB:168:THR:HG23 | 2:LB:170:LEU:H | 1.81 | 0.45 |
| 2:LB:290:ASN:HB2 | 2:LB:293:CYS:HB3 | 1.99 | 0.45 |
| 14:LN:46:LYS:HE2 | 14:LN:46:LYS:HB2 | 1.54 | 0.45 |
| 21:LU:12:ARG:HH22 | 44:Lt:762:C:H5' | 1.82 | 0.45 |
| 26:LZ:63:LYS:HE3 | 26:LZ:63:LYS:HB3 | 1.53 | 0.45 |
| 32:Lf:40:PRO:HG2 | 32:Lf:47:MET:HB3 | 1.97 | 0.45 |
| 44:Lt:224:U:H2' | 44:Lt:225:A:H8 | 1.81 | 0.45 |
| 44:Lt:1714:C:H2' | 44:Lt:1715:C:C6 | 2.52 | 0.45 |
| 44:Lt:2264:G:H2' | 44:Lt:2321:G:N2 | 2.32 | 0.45 |
| 44:Lt:2305:U:H2' | 44:Lt:2306:U:C6 | 2.52 | 0.45 |
| 47:SC:40:TYR:HD1 | 47:SC:56:ILE:HG23 | 1.82 | 0.45 |
| 48:SD:203:LYS:HE2 | 48:SD:203:LYS:HB2 | 1.32 | 0.45 |
| 49:SE:180:ILE:HG13 | 49:SE:232:SER:H | 1.82 | 0.45 |
| 50:SF:85:LEU:HD13 | 50:SF:85:LEU:HA | 1.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 69:Sc:24:GLU:HB2 | 69:Sc:25:ALA:H | 1.52 | 0.45 |
| 75:St:582:C:H2' | 75:St:583:G:C8 | 2.51 | 0.45 |
| 75:St:1110:C:H2' | 75:St:1111:G:C8 | 2.52 | 0.45 |
| 3:LC:311:GLY:O | 3:LC:314:MET:HG3 | 2.17 | 0.45 |
| 8:LH:24:ARG:HA | 8:LH:28:LYS:HD3 | 1.99 | 0.45 |
| 9:LI:48:GLN:HB2 | 15:LO:25:LEU:HD11 | 1.99 | 0.45 |
| 15:LO:148:ILE:HD12 | 15:LO:148:ILE:HA | 1.88 | 0.45 |
| 17:LQ:79:LYS:H | 17:LQ:79:LYS:HG2 | 1.48 | 0.45 |
| 27:La:98:VAL:HA | 27:La:104:ARG:HG3 | 1.98 | 0.45 |
| 31:Le:74:GLY:HA3 | 31:Le:79:LYS:HA | 1.99 | 0.45 |
| 32:Lf:24:ARG:HD2 | 32:Lf:33:VAL:HG12 | 1.99 | 0.45 |
| 34:Lh:101:GLU:H | 34:Lh:101:GLU:HG3 | 1.33 | 0.45 |
| 35:Li:65:THR:C | 35:Li:67:GLY:N | 2.74 | 0.45 |
| 37:Lk:46:ARG:HD2 | 37:Lk:54:LEU:HD11 | 1.98 | 0.45 |
| 39:Ln:138:LEU:HD11 | 39:Ln:145:GLU:H | 1.81 | 0.45 |
| 40:Lo:1:MET:H1 | 40:Lo:1:MET:HG2 | 1.68 | 0.45 |
| 44:Lt:586:G:H3' | 44:Lt:587:G:H8 | 1.81 | 0.45 |
| 44:Lt:1421:G:H2' | 44:Lt:1422:C:C6 | 2.52 | 0.45 |
| 47:SC:7:ARG:HE | 47:SC:7:ARG:HB2 | 1.31 | 0.45 |
| 47:SC:40:TYR:O | 47:SC:106:ILE:HD11 | 2.17 | 0.45 |
| 50:SF:146:LYS:HA | 50:SF:146:LYS:HD3 | 1.46 | 0.45 |
| 55:SK:38:LYS:HB2 | 55:SK:38:LYS:HE2 | 1.37 | 0.45 |
| 56:SL:9:TYR:HE2 | 75:St:999:U:H4' | 1.82 | 0.45 |
| 58:SO:37:LYS:H | 58:SO:37:LYS:HG2 | 1.53 | 0.45 |
| 63:SU:25:LYS:HA | 63:SU:26:PRO:HD3 | 1.88 | 0.45 |
| 64:SV:10:TYR:HE1 | 69:Sc:22:ALA:HB2 | 1.82 | 0.45 |
| 65:SW:112:LEU:O | 65:SW:126:GLY:HA3 | 2.17 | 0.45 |
| 73:Sh:91:GLU:H | 73:Sh:91:GLU:HG3 | 1.59 | 0.45 |
| 77:v:10:G:H2' | 77:v:10:G:N3 | 2.31 | 0.45 |
| 2:LB:58:ARG:HH22 | 2:LB:349:PRO:HB2 | 1.82 | 0.45 |
| 8:LH:198:TRP:O | 8:LH:199:PRO:C | 2.59 | 0.45 |
| 12:LL:9:MET:HE2 | 12:LL:9:MET:HB3 | 1.80 | 0.45 |
| 13:LM:108:GLU:H | 13:LM:108:GLU:HG2 | 1.56 | 0.45 |
| 14:LN:31:LEU:HD11 | 20:LT:93:GLU:HA | 1.99 | 0.45 |
| 32:Lf:111:LYS:HB2 | 32:Lf:111:LYS:HE2 | 1.47 | 0.45 |
| 39:Ln:16:ILE:HD11 | 39:Ln:213:SER:HB2 | 1.97 | 0.45 |
| 39:Ln:196:LYS:HB3 | 39:Ln:199:GLN:HB2 | 1.98 | 0.45 |
| 44:Lt:1958:G:N2 | 44:Lt:1960:C:H2' | 2.26 | 0.45 |
| 46:SB:121:LYS:HD2 | 46:SB:121:LYS:HA | 1.46 | 0.45 |
| 49:SE:179:LYS:O | 49:SE:181:VAL:HG13 | 2.17 | 0.45 |
| 49:SE:255:LEU:HD22 | 49:SE:255:LEU:HA | 1.69 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 53:SI:13:LYS:HD3 | 57:SM:132:THR:HG23 | 1.99 | 0.45 |
| 62:ST:138:ARG:HH22 | 75:St:1295:G:H5' | 1.82 | 0.45 |
| 63:SU:101:VAL:HG13 | 63:SU:105:THR:HB | 1.99 | 0.45 |
| 67:SY:67:ARG:HA | 67:SY:72:VAL:HG21 | 1.98 | 0.45 |
| 71:Se:71:SER:HB2 | 71:Se:88:TYR:CZ | 2.52 | 0.45 |
| 71:Se:77:LYS:HB2 | 71:Se:119:GLU:HB2 | 1.98 | 0.45 |
| 75:St:160:G:H1 | 75:St:201:C:H42 | 1.65 | 0.45 |
| 75:St:575:G:H2' | 75:St:576:G:C8 | 2.52 | 0.45 |
| 75:St:764:C:H3' | 75:St:765:G:H8 | 1.82 | 0.45 |
| 75:St:840:C:H1' | 75:St:843:C:H4' | 1.99 | 0.45 |
| 9:LI:169:LYS:HE2 | 9:LI:169:LYS:HB2 | 1.57 | 0.44 |
| 15:LO:41:HIS:CE1 | 15:LO:43:THR:HA | 2.51 | 0.44 |
| 16:LP:131:ARG:HD3 | 16:LP:131:ARG:HA | 1.62 | 0.44 |
| 27:La:118:ARG:HG2 | 27:La:123:ARG:HD3 | 1.99 | 0.44 |
| 35:Li:63:LYS:HB2 | 35:Li:63:LYS:HE2 | 1.40 | 0.44 |
| 38:Ll:71:GLN:HE21 | 38:Ll:71:GLN:HB3 | 1.61 | 0.44 |
| 42:Lq:64:MET:HE2 | 42:Lq:64:MET:HB2 | 1.83 | 0.44 |
| 44:Lt:2084:C:H2' | 44:Lt:2085:G:H8 | 1.78 | 0.44 |
| 45:SA:129:VAL:CG2 | 45:SA:151:SER:HB2 | 2.47 | 0.44 |
| 63:SU:22:GLU:HB3 | 63:SU:23:SER:H | 1.71 | 0.44 |
| 70:Sd:37:LYS:HE2 | 70:Sd:37:LYS:HB2 | 1.41 | 0.44 |
| 2:LB:316:ARG:HE | 2:LB:318:GLN:HA | 1.82 | 0.44 |
| 13:LM:38:MET:HE1 | 44:Lt:515:U:H1' | 1.99 | 0.44 |
| 13:LM:184:ILE:H | 13:LM:184:ILE:HG13 | 1.39 | 0.44 |
| 18:LR:56:LYS:H | 18:LR:56:LYS:HG3 | 1.64 | 0.44 |
| 19:LS:19:LYS:HB3 | 19:LS:19:LYS:HE2 | 1.80 | 0.44 |
| 26:LZ:34:LEU:HD21 | 26:LZ:47:MET:HB2 | 1.99 | 0.44 |
| 30:Ld:14:ILE:H | 30:Ld:14:ILE:HG12 | 1.56 | 0.44 |
| 34:Lh:74:TYR:HB3 | 34:Lh:78:LEU:HB2 | 1.99 | 0.44 |
| 44:Lt:418:C:H2' | 44:Lt:419:G:H8 | 1.82 | 0.44 |
| 44:Lt:1939:G:H2' | 44:Lt:1940:G:C8 | 2.52 | 0.44 |
| 47:SC:199:ILE:HG22 | 47:SC:201:GLY:H | 1.81 | 0.44 |
| 49:SE:205:TYR:HB3 | 49:SE:221:ARG:HD2 | 1.99 | 0.44 |
| 57:SM:13:GLN:HE22 | 57:SM:59:THR:HG23 | 1.82 | 0.44 |
| 58:SO:48:ARG:HE | 58:SO:48:ARG:HB2 | 1.35 | 0.44 |
| 65:SW:38:GLY:HA2 | 65:SW:95:ALA:HA | 1.99 | 0.44 |
| 68:Sb:91:LYS:HB2 | 68:Sb:91:LYS:HE2 | 1.73 | 0.44 |
| 75:St:1019:G:H3' | 75:St:1020:G:H8 | 1.82 | 0.44 |
| 1:LA:210:PRO:HD2 | 1:LA:235:VAL:HG21 | 1.99 | 0.44 |
| 3:LC:40:LEU:HD23 | 3:LC:40:LEU:HA | 1.73 | 0.44 |
| 11:LK:22:PHE:CE1 | 44:Lt:761:A:H2' | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:LP:53:LYS:HB2 | 16:LP:53:LYS:HE3 | 1.30 | 0.44 |
| 17:LQ:107:LYS:HB2 | 17:LQ:107:LYS:HE2 | 1.56 | 0.44 |
| 21:LU:130:LYS:HB2 | 21:LU:130:LYS:HE2 | 1.77 | 0.44 |
| 22:LV:55:LYS:HA | 22:LV:55:LYS:HD2 | 1.61 | 0.44 |
| 29:Lc:41:ARG:HA | 29:Lc:44:ARG:HD2 | 1.99 | 0.44 |
| 31:Le:92:LYS:HD3 | 31:Le:92:LYS:HA | 1.47 | 0.44 |
| 32:Lf:91:PHE:HB2 | 32:Lf:120:MET:HG2 | 2.00 | 0.44 |
| 44:Lt:2499:C:H2' | 44:Lt:2500:G:H8 | 1.81 | 0.44 |
| 53:SI:50:GLN:H | 53:SI:50:GLN:HG3 | 1.53 | 0.44 |
| 60:SQ:97:ILE:HD13 | 60:SQ:116:ILE:HD11 | 1.99 | 0.44 |
| 75:St:1166:A:H3' | 75:St:1167:C:H6 | 1.83 | 0.44 |
| 76:u:65:C:H2' | 76:u:66:U:O4' | 2.17 | 0.44 |
| 11:LK:124:GLY:O | 11:LK:125:THR:C | 2.60 | 0.44 |
| 13:LM:202:MET:HE2 | 13:LM:202:MET:HB2 | 1.72 | 0.44 |
| 14:LN:94:LYS:HD3 | 14:LN:94:LYS:HA | 1.71 | 0.44 |
| 18:LR:46:LYS:HE3 | 18:LR:46:LYS:HB3 | 1.68 | 0.44 |
| 28:Lb:28:HIS:CE1 | 28:Lb:32:ARG:HE | 2.34 | 0.44 |
| 28:Lb:120:GLN:H | 28:Lb:120:GLN:HG2 | 1.52 | 0.44 |
| 32:Lf:117:ALA:HA | 32:Lf:120:MET:HB2 | 2.00 | 0.44 |
| 36:Lj:83:LEU:HD12 | 36:Lj:83:LEU:HA | 1.75 | 0.44 |
| 38:Ll:11:MET:HB3 | 38:Ll:11:MET:HE3 | 1.42 | 0.44 |
| 51:SG:130:LEU:HB3 | 51:SG:131:THR:H | 1.58 | 0.44 |
| 57:SM:55:LYS:H | 57:SM:55:LYS:HG2 | 1.50 | 0.44 |
| 61:SR:108:LYS:HD3 | 64:SV:118:THR:HG22 | 1.99 | 0.44 |
| 64:SV:27:LEU:HD13 | 64:SV:27:LEU:HA | 1.73 | 0.44 |
| 69:Sc:40:ILE:HD13 | 69:Sc:40:ILE:HA | 1.75 | 0.44 |
| 77:v:1:A:H3' | 77:v:2:G:H8 | 1.81 | 0.44 |
| 1:LA:53:GLY:HA2 | 1:LA:191:ALA:HB1 | 1.99 | 0.44 |
| 6:LF:242:LEU:HD13 | 6:LF:242:LEU:HA | 1.73 | 0.44 |
| 18:LR:120:MET:HE2 | 18:LR:120:MET:HB2 | 1.75 | 0.44 |
| 20:LT:155:VAL:C | 20:LT:157:ARG:N | 2.75 | 0.44 |
| 21:LU:80:VAL:HG21 | 21:LU:85:MET:HE2 | 1.99 | 0.44 |
| 36:Lj:10:LYS:HB2 | 36:Lj:10:LYS:HE2 | 1.69 | 0.44 |
| 39:Ln:74:ALA:HA | 39:Ln:78:LYS:HB3 | 1.99 | 0.44 |
| 41:Lp:51:GLN:HE22 | 44:Lt:1909:U:H4' | 1.82 | 0.44 |
| 43:Ls:112:ARG:H | 43:Ls:112:ARG:HG2 | 1.60 | 0.44 |
| 43:Ls:121:LYS:HD2 | 43:Ls:121:LYS:HA | 1.71 | 0.44 |
| 44:Lt:163:C:H1' | 44:Lt:186:C:N4 | 2.32 | 0.44 |
| 44:Lt:903:A:N6 | 44:Lt:1000:G:H2' | 2.33 | 0.44 |
| 44:Lt:1100:C:H2' | 44:Lt:1101:G:C8 | 2.53 | 0.44 |
| 44:Lt:1364:C:H2' | 44:Lt:1365:G:H8 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:SB:174:ALA:HB3 | 46:SB:179:ALA:HB2 | 2.00 | 0.44 |
| 48:SD:17:LYS:H | 48:SD:17:LYS:HG3 | 1.52 | 0.44 |
| 55:SK:84:LEU:HB3 | 55:SK:86:ILE:HG23 | 1.99 | 0.44 |
| 55:SK:176:ARG:HH12 | 75:St:421:G:H8 | 1.65 | 0.44 |
| 57:SM:149:LYS:HE2 | 57:SM:149:LYS:HB2 | 1.41 | 0.44 |
| 58:SO:100:VAL:HG13 | 58:SO:122:VAL:HG23 | 1.99 | 0.44 |
| 62:ST:23:TYR:HA | 62:ST:41:LYS:HG3 | 2.00 | 0.44 |
| 64:SV:147:VAL:O | 64:SV:149:VAL:HG22 | 2.18 | 0.44 |
| 66:SX:34:LEU:HD13 | 66:SX:34:LEU:HA | 1.83 | 0.44 |
| 66:SX:58:ARG:HB2 | 75:St:1090:C:H4' | 1.99 | 0.44 |
| 68:Sb:56:VAL:HG21 | 68:Sb:86:GLU:HG2 | 1.99 | 0.44 |
| 72:Sg:39:ARG:HA | 72:Sg:39:ARG:HD2 | 1.81 | 0.44 |
| 73:Sh:98:HIS:HB2 | 73:Sh:100:ARG:HG3 | 1.98 | 0.44 |
| 74:Sj:54:LEU:HD12 | 74:Sj:54:LEU:HA | 1.79 | 0.44 |
| 5:LE:21:G:H2' | 5:LE:22:G:C8 | 2.52 | 0.44 |
| 13:LM:50:LEU:HD23 | 13:LM:50:LEU:HA | 1.67 | 0.44 |
| 18:LR:56:LYS:NZ | 44:Lt:419:G:H3' | 2.33 | 0.44 |
| 18:LR:62:LEU:HD12 | 18:LR:62:LEU:HA | 1.84 | 0.44 |
| 26:LZ:2:LYS:HB3 | 26:LZ:2:LYS:HE2 | 1.38 | 0.44 |
| 34:Lh:31:LEU:HD22 | 34:Lh:31:LEU:HA | 1.74 | 0.44 |
| 36:Lj:70:LEU:HD12 | 36:Lj:70:LEU:HA | 1.75 | 0.44 |
| 39:Ln:88:GLU:HB3 | 39:Ln:89:HIS:H | 1.66 | 0.44 |
| 42:Lq:25:GLN:HE21 | 42:Lq:29:ILE:HD13 | 1.82 | 0.44 |
| 45:SA:81:VAL:HG11 | 45:SA:92:ILE:HD11 | 2.00 | 0.44 |
| 47:SC:103:SER:O | 47:SC:107:MET:HB3 | 2.17 | 0.44 |
| 48:SD:238:ARG:O | 48:SD:239:ASN:C | 2.60 | 0.44 |
| 57:SM:94:LYS:HA | 75:St:286:G:OP1 | 2.17 | 0.44 |
| 59:SP:74:ILE:H | 59:SP:74:ILE:HG12 | 1.47 | 0.44 |
| 64:SV:151:ARG:HD3 | 64:SV:151:ARG:HA | 1.31 | 0.44 |
| 72:Sg:8:ARG:HA | 72:Sg:8:ARG:HD2 | 1.54 | 0.44 |
| 74:Sj:26:ARG:HE | 74:Sj:26:ARG:HB2 | 1.20 | 0.44 |
| 75:St:147:C:H2' | 75:St:148:G:C8 | 2.53 | 0.44 |
| 3:LC:28:LEU:H | 3:LC:28:LEU:HG | 1.55 | 0.44 |
| 11:LK:101:LYS:HD3 | 11:LK:101:LYS:HA | 1.58 | 0.44 |
| 30:Ld:104:LEU:H | 30:Ld:104:LEU:HG | 1.36 | 0.44 |
| 32:Lf:28:GLU:HG3 | 44:Lt:371:C:H5' | 1.99 | 0.44 |
| 34:Lh:64:THR:HB | 44:Lt:1310:C:H5 | 1.81 | 0.44 |
| 36:Lj:56:MET:HB3 | 36:Lj:56:MET:HE3 | 1.53 | 0.44 |
| 44:Lt:235:G:H1 | 44:Lt:256:G:N2 | 2.16 | 0.44 |
| 44:Lt:736:G:H2' | 44:Lt:738:C:H5 | 1.83 | 0.44 |
| 44:Lt:1311:G:H1 | 44:Lt:1453:C:H5 | 1.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:2204:C:H2' | 44:Lt:2205:G:C8 | 2.52 | 0.44 |
| 44:Lt:2570:C:H2' | 44:Lt:2571:G:H8 | 1.82 | 0.44 |
| 49:SE:68:LYS:HA | 49:SE:76:PRO:HG3 | 1.99 | 0.44 |
| 50:SF:59:THR:HA | 50:SF:75:ALA:HB1 | 1.99 | 0.44 |
| 51:SG:214:MET:HG3 | 51:SG:215:ARG:N | 2.33 | 0.44 |
| 51:SG:215:ARG:H | 51:SG:215:ARG:HG3 | 1.64 | 0.44 |
| 52:SH:181:THR:O | 52:SH:182:GLU:HB2 | 2.17 | 0.44 |
| 56:SL:82:LYS:H | 56:SL:82:LYS:HG3 | 1.49 | 0.44 |
| 58:SO:46:MET:HE3 | 58:SO:46:MET:HB3 | 1.65 | 0.44 |
| 63:SU:25:LYS:HA | 63:SU:25:LYS:HD3 | 1.47 | 0.44 |
| 63:SU:47:LYS:HD2 | 63:SU:47:LYS:HA | 1.70 | 0.44 |
| 65:SW:71:GLY:HA3 | 75:St:1196:G:H5" | 1.99 | 0.44 |
| 67:SY:42:SER:HB2 | 67:SY:59:THR:HG23 | 2.00 | 0.44 |
| 76:u:58:A:H3' | 76:u:59:A:C8 | 2.51 | 0.44 |
| 2:LB:21:ARG:HG2 | 2:LB:272:TYR:HD2 | 1.82 | 0.44 |
| 3:LC:111:ARG:NH2 | 3:LC:254:LYS:HB3 | 2.32 | 0.44 |
| 5:LE:7:G:H4' | 6:LF:33:ARG:HH21 | 1.83 | 0.44 |
| 8:LH:101:LEU:HD22 | 8:LH:101:LEU:HA | 1.82 | 0.44 |
| 9:LI:196:LEU:HD23 | 9:LI:196:LEU:HA | 1.72 | 0.44 |
| 12:LL:45:PRO:HA | 12:LL:69:VAL:HG13 | 1.99 | 0.44 |
| 12:LL:54:ILE:HD11 | 12:LL:57:PHE:CB | 2.48 | 0.44 |
| 15:LO:84:PRO:HA | 15:LO:87:ILE:HG13 | 2.00 | 0.44 |
| 19:LS:23:ARG:HD3 | 19:LS:23:ARG:HA | 1.69 | 0.44 |
| 39:Ln:149:LEU:HD13 | 39:Ln:149:LEU:HA | 1.83 | 0.44 |
| 39:Ln:205:TYR:HB3 | 39:Ln:207:LYS:HE3 | 1.99 | 0.44 |
| 44:Lt:380:C:H2' | 44:Lt:381:G:C8 | 2.53 | 0.44 |
| 44:Lt:735:G:C2 | 44:Lt:736:G:H1' | 2.53 | 0.44 |
| 44:Lt:1762:U:H2' | 44:Lt:1763:A:H8 | 1.82 | 0.44 |
| 45:SA:62:LYS:HD2 | 45:SA:62:LYS:HA | 1.72 | 0.44 |
| 46:SB:180:LYS:HA | 46:SB:180:LYS:HD2 | 1.80 | 0.44 |
| 50:SF:152:VAL:HG21 | 69:Sc:47:GLU:HB2 | 2.00 | 0.44 |
| 51:SG:71:GLN:HG3 | 75:St:1369:A:H2' | 1.99 | 0.44 |
| 60:SQ:101:GLY:HA3 | 60:SQ:134:PRO:HD2 | 1.99 | 0.44 |
| 61:SR:29:LYS:HE3 | 61:SR:29:LYS:HB3 | 1.48 | 0.44 |
| 65:SW:12:PHE:CD2 | 65:SW:60:ARG:HG3 | 2.53 | 0.44 |
| 67:SY:78:LEU:HD12 | 67:SY:78:LEU:HA | 1.75 | 0.44 |
| 73:Sh:117:LEU:H | 73:Sh:117:LEU:HG | 1.40 | 0.44 |
| 75:St:1141:G:H2' | 75:St:1141:G:N3 | 2.33 | 0.44 |
| 4:LD:13:G:H5" | 17:LQ:2:VAL:HA | 1.99 | 0.44 |
| 18:LR:129:LYS:HE3 | 18:LR:129:LYS:HB3 | 1.44 | 0.44 |
| 23:LW:71:LYS:HB3 | 23:LW:71:LYS:HE2 | 1.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:Ln:10:ASN:HA | 39:Ln:13:ILE:HD11 | 2.00 | 0.44 |
| 44:Lt:778:C:H2' | 44:Lt:779:G:H8 | 1.83 | 0.44 |
| 47:SC:18:LEU:H | 47:SC:18:LEU:HG | 1.59 | 0.44 |
| 54:SJ:88:LYS:HA | 54:SJ:88:LYS:HD2 | 1.33 | 0.44 |
| 59:SP:13:ARG:H | 59:SP:13:ARG:HG2 | 1.42 | 0.44 |
| 59:SP:94:LYS:HB2 | 59:SP:94:LYS:HE2 | 1.60 | 0.44 |
| 65:SW:113:LEU:HD21 | 65:SW:120:ARG:HG2 | 1.99 | 0.44 |
| 67:SY:35:ASP:HB3 | 67:SY:38:ALA:HB2 | 1.99 | 0.44 |
| 68:Sb:36:LYS:HG2 | 75:St:406:C:H5" | 2.00 | 0.44 |
| 75:St:1273:U:H3 | 75:St:1299:G:H8 | 1.66 | 0.44 |
| 3:LC:9:GLY:H | 3:LC:13:THR:HA | 1.83 | 0.43 |
| 7:LG:34:LYS:HB3 | 7:LG:34:LYS:HE3 | 1.59 | 0.43 |
| 9:LI:52:LYS:H | 9:LI:52:LYS:HG3 | 1.49 | 0.43 |
| 10:LJ:3:LEU:HD12 | 10:LJ:3:LEU:HA | 1.82 | 0.43 |
| 10:LJ:111:ARG:HG3 | 10:LJ:119:THR:HB | 1.99 | 0.43 |
| 15:LO:48:ALA:HB1 | 15:LO:53:TYR:HB3 | 1.99 | 0.43 |
| 16:LP:145:GLN:H | 16:LP:145:GLN:HG2 | 1.51 | 0.43 |
| 21:LU:112:ASN:HB3 | 21:LU:129:LEU:HD13 | 1.98 | 0.43 |
| 32:Lf:57:MET:HB3 | 32:Lf:57:MET:HE3 | 1.70 | 0.43 |
| 32:Lf:118:LYS:HB3 | 32:Lf:118:LYS:HE3 | 1.37 | 0.43 |
| 35:Li:83:VAL:O | 35:Li:87:LEU:HB2 | 2.18 | 0.43 |
| 35:Li:116:LEU:HB3 | 35:Li:120:MET:HB2 | 1.99 | 0.43 |
| 44:Lt:1350:C:H2' | 44:Lt:1351:C:C6 | 2.53 | 0.43 |
| 44:Lt:1649:G:H2' | 44:Lt:1650:G:C8 | 2.52 | 0.43 |
| 44:Lt:1649:G:H2' | 44:Lt:1650:G:H8 | 1.83 | 0.43 |
| 46:SB:88:GLN:H | 46:SB:88:GLN:HG3 | 1.43 | 0.43 |
| 51:SG:245:ARG:HH11 | 51:SG:245:ARG:HG3 | 1.81 | 0.43 |
| 53:SI:127:LEU:HD12 | 53:SI:127:LEU:HA | 1.89 | 0.43 |
| 57:SM:34:LYS:HZ2 | 57:SM:34:LYS:HG3 | 1.43 | 0.43 |
| 62:ST:43:GLY:H | 62:ST:81:LEU:C | 2.26 | 0.43 |
| 62:ST:154:GLN:HE21 | 62:ST:154:GLN:HB3 | 1.63 | 0.43 |
| 64:SV:31:LEU:HB2 | 64:SV:46:LEU:HD11 | 1.98 | 0.43 |
| 64:SV:41:PHE:H | 75:St:1254:G:H4' | 1.83 | 0.43 |
| 75:St:538:G:H2' | 75:St:539:G:H8 | 1.83 | 0.43 |
| 75:St:1234:C:H2' | 75:St:1235:C:O4' | 2.18 | 0.43 |
| 1:LA:155:LYS:HB3 | 1:LA:155:LYS:HE2 | 1.48 | 0.43 |
| 2:LB:14:LEU:HD22 | 2:LB:14:LEU:HA | 1.72 | 0.43 |
| 2:LB:252:ILE:HA | 2:LB:264:VAL:HG11 | 2.00 | 0.43 |
| 6:LF:118:LYS:HD3 | 6:LF:118:LYS:HA | 1.42 | 0.43 |
| 17:LQ:47:LEU:HA | 17:LQ:47:LEU:HD22 | 1.69 | 0.43 |
| 19:LS:80:LYS:HA | 19:LS:80:LYS:HD3 | 1.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:La:54:SER:HB3 | 27:La:55:MET:H | 1.73 | 0.43 |
| 30:Ld:29:LEU:HD12 | 30:Ld:91:VAL:HG11 | 1.99 | 0.43 |
| 44:Lt:1362:A:H2' | 44:Lt:1363:A:C8 | 2.53 | 0.43 |
| 53:SI:119:LYS:HD3 | 53:SI:136:ARG:HA | 2.00 | 0.43 |
| 64:SV:147:VAL:HB | 75:St:1166:A:H5' | 1.99 | 0.43 |
| 74:Sj:22:LYS:HB3 | 74:Sj:22:LYS:HE2 | 1.61 | 0.43 |
| 75:St:74:C:H2' | 75:St:75:G:O4' | 2.18 | 0.43 |
| 75:St:1035:U:H3 | 75:St:1064:A:H61 | 1.65 | 0.43 |
| 75:St:1201:C:H2' | 75:St:1202:C:O4' | 2.17 | 0.43 |
| 3:LC:113:ALA:HB3 | 3:LC:224:LEU:HD21 | 2.00 | 0.43 |
| 6:LF:231:LYS:HD3 | 6:LF:231:LYS:HA | 1.62 | 0.43 |
| 8:LH:227:ILE:HD13 | 8:LH:227:ILE:HA | 1.77 | 0.43 |
| 15:LO:13:LYS:HE3 | 15:LO:13:LYS:HB3 | 1.51 | 0.43 |
| 17:LQ:115:ILE:HD12 | 17:LQ:115:ILE:HA | 1.70 | 0.43 |
| 19:LS:147:LYS:HA | 19:LS:147:LYS:HD3 | 1.47 | 0.43 |
| 23:LW:50:LEU:HD12 | 23:LW:50:LEU:HA | 1.79 | 0.43 |
| 29:Lc:36:CYS:HB3 | 29:Lc:39:TYR:HB2 | 2.00 | 0.43 |
| 30:Ld:72:ARG:HD2 | 30:Ld:107:ILE:HB | 1.99 | 0.43 |
| 32:Lf:101:ILE:HD11 | 32:Lf:124:VAL:HG21 | 2.00 | 0.43 |
| 36:Lj:17:ILE:H | 36:Lj:17:ILE:HG13 | 1.45 | 0.43 |
| 37:Lk:89:LYS:HA | 37:Lk:89:LYS:HD3 | 1.55 | 0.43 |
| 43:Ls:94:MET:HE3 | 43:Ls:119:ARG:HG2 | 2.00 | 0.43 |
| 49:SE:87:MET:HE2 | 49:SE:87:MET:HB3 | 1.91 | 0.43 |
| 49:SE:197:ALA:O | 49:SE:208:ILE:HA | 2.18 | 0.43 |
| 55:SK:40:LYS:HB2 | 55:SK:40:LYS:HE3 | 1.74 | 0.43 |
| 55:SK:93:GLN:HB2 | 55:SK:96:TYR:HD1 | 1.83 | 0.43 |
| 56:SL:8:VAL:O | 56:SL:12:VAL:HB | 2.17 | 0.43 |
| 58:SO:55:ILE:HD12 | 58:SO:55:ILE:HA | 1.77 | 0.43 |
| 61:SR:37:LEU:HD23 | 61:SR:37:LEU:HA | 1.85 | 0.43 |
| 61:SR:95:SER:O | 61:SR:96:VAL:C | 2.61 | 0.43 |
| 63:SU:99:ILE:HG23 | 63:SU:121:LEU:HB3 | 1.99 | 0.43 |
| 65:SW:68:HIS:O | 65:SW:69:SER:HB2 | 2.18 | 0.43 |
| 68:Sb:64:PHE:CD2 | 75:St:415:C:H5" | 2.53 | 0.43 |
| 68:Sb:64:PHE:HD2 | 75:St:415:C:H5" | 1.83 | 0.43 |
| 75:St:876:A:H2' | 75:St:877:A:C8 | 2.53 | 0.43 |
| 75:St:1367:G:H2' | 75:St:1368:G:C4 | 2.53 | 0.43 |
| 2:LB:240:ARG:HD3 | 2:LB:240:ARG:HA | 1.33 | 0.43 |
| 6:LF:208:LYS:HD2 | 6:LF:208:LYS:HA | 1.53 | 0.43 |
| 12:LL:108:GLU:HB2 | 12:LL:111:ASP:HB2 | 2.01 | 0.43 |
| 15:LO:19:LEU:HD22 | 15:LO:19:LEU:HA | 1.64 | 0.43 |
| 15:LO:160:GLU:H | 15:LO:160:GLU:HG3 | 1.25 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:LR:163:PRO:HB2 | 18:LR:167:HIS:CD2 | 2.54 | 0.43 |
| 21:LU:121:GLU:H | 21:LU:121:GLU:HG2 | 1.44 | 0.43 |
| 31:Le:46:LEU:HD13 | 31:Le:46:LEU:HA | 1.89 | 0.43 |
| 36:Lj:53:LEU:HD13 | 36:Lj:62:ALA:HA | 2.01 | 0.43 |
| 39:Ln:194:LEU:HD12 | 39:Ln:194:LEU:HA | 1.79 | 0.43 |
| 44:Lt:1137:A:H62 | 44:Lt:1843:G:H21 | 1.67 | 0.43 |
| 44:Lt:1213:G:H3' | 44:Lt:1214:G:H8 | 1.83 | 0.43 |
| 51:SG:22:LEU:HD13 | 51:SG:22:LEU:HA | 1.77 | 0.43 |
| 62:ST:69:PRO:HA | 62:ST:124:LEU:HD11 | 1.99 | 0.43 |
| 75:St:679:G:H21 | 75:St:742:C:H1' | 1.83 | 0.43 |
| 75:St:930:C:H4' | 75:St:952:C:H1' | 1.99 | 0.43 |
| 75:St:1177:A:H2 | 75:St:1181:G:H1' | 1.83 | 0.43 |
| 6:LF:16:PHE:HD1 | 6:LF:16:PHE:HA | 1.75 | 0.43 |
| 6:LF:142:ASN:HB2 | 6:LF:143:GLU:H | 1.48 | 0.43 |
| 10:LJ:29:LYS:HG3 | 10:LJ:81:THR:HA | 2.00 | 0.43 |
| 13:LM:76:PHE:N | 13:LM:77:PRO:HD2 | 2.33 | 0.43 |
| 16:LP:188:ILE:H | 16:LP:188:ILE:HG13 | 1.69 | 0.43 |
| 17:LQ:21:VAL:HG11 | 17:LQ:89:VAL:HG11 | 2.01 | 0.43 |
| 17:LQ:40:VAL:HG11 | 17:LQ:98:VAL:HG21 | 1.99 | 0.43 |
| 19:LS:92:LYS:HG2 | 19:LS:96:ILE:HD11 | 1.99 | 0.43 |
| 19:LS:92:LYS:O | 19:LS:96:ILE:HG12 | 2.19 | 0.43 |
| 23:LW:14:LYS:HE3 | 23:LW:14:LYS:HB3 | 1.44 | 0.43 |
| 25:LY:38:VAL:HG13 | 44:Lt:13:G:H4' | 2.01 | 0.43 |
| 39:Ln:106:SER:HB3 | 39:Ln:107:TYR:H | 1.67 | 0.43 |
| 54:SJ:11:LEU:HD12 | 54:SJ:11:LEU:HA | 1.77 | 0.43 |
| 56:SL:31:GLY:O | 56:SL:49:THR:HA | 2.19 | 0.43 |
| 56:SL:60:LEU:HD23 | 56:SL:60:LEU:HA | 1.72 | 0.43 |
| 57:SM:134:ARG:HE | 57:SM:134:ARG:HB2 | 1.65 | 0.43 |
| 63:SU:75:ARG:HD2 | 63:SU:75:ARG:HA | 1.68 | 0.43 |
| 64:SV:40:ARG:HA | 75:St:1254:G:H4' | 2.00 | 0.43 |
| 64:SV:138:LYS:HD2 | 75:St:1165:C:C5 | 2.54 | 0.43 |
| 75:St:745:G:H4' | 75:St:1441:G:H4' | 2.00 | 0.43 |
| 75:St:1250:C:H2' | 75:St:1251:C:C6 | 2.53 | 0.43 |
| 3:LC:62:SER:HA | 3:LC:73:PRO:HA | 2.01 | 0.43 |
| 11:LK:99:ILE:HB | 11:LK:123:GLN:HG2 | 2.00 | 0.43 |
| 12:LL:110:ILE:HG12 | 12:LL:116:TYR:CA | 2.46 | 0.43 |
| 19:LS:32:ILE:HG12 | 19:LS:49:ILE:HD11 | 2.00 | 0.43 |
| 21:LU:105:HIS:O | 21:LU:109:VAL:HG12 | 2.18 | 0.43 |
| 26:LZ:21:ALA:HB1 | 26:LZ:25:THR:HB | 2.00 | 0.43 |
| 31:Le:11:LEU:HD13 | 31:Le:11:LEU:HA | 1.73 | 0.43 |
| 32:Lf:80:ARG:HD2 | 44:Lt:1098:C:H4' | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:Lh:42:ALA:HB3 | 34:Lh:51:GLN:HG3 | 1.99 | 0.43 |
| 37:Lk:43:LYS:HB3 | 37:Lk:43:LYS:HE3 | 1.60 | 0.43 |
| 38:Ll:41:ARG:HA | 38:Ll:41:ARG:HD2 | 1.68 | 0.43 |
| 44:Lt:1741:G:H2' | 44:Lt:1741:G:N3 | 2.33 | 0.43 |
| 44:Lt:1916:C:H2' | 44:Lt:1917:G:C8 | 2.53 | 0.43 |
| 46:SB:219:LEU:HD12 | 46:SB:219:LEU:HA | 1.82 | 0.43 |
| 49:SE:183:VAL:HA | 49:SE:225:VAL:HA | 1.99 | 0.43 |
| 51:SG:148:ARG:HA | 51:SG:153:LEU:O | 2.19 | 0.43 |
| 67:SY:44:ALA:HB2 | 67:SY:57:TYR:HD1 | 1.83 | 0.43 |
| 72:Sg:4:PRO:HA | 72:Sg:54:MET:O | 2.19 | 0.43 |
| 74:Sj:11:LYS:H | 74:Sj:11:LYS:HG3 | 1.39 | 0.43 |
| 76:u:14:A:H3' | 76:u:15:G:C8 | 2.54 | 0.43 |
| 77:v:9:G:H2' | 77:v:11:C:H41 | 1.83 | 0.43 |
| 77:v:42:G:H2' | 77:v:43:A:C8 | 2.54 | 0.43 |
| 2:LB:282:VAL:HB | 2:LB:322:ILE:HD11 | 2.00 | 0.43 |
| 3:LC:165:LEU:HG | 3:LC:166:ARG:N | 2.33 | 0.43 |
| 5:LE:35:U:H2' | 5:LE:36:C:O4' | 2.18 | 0.43 |
| 5:LE:101:A:H3' | 5:LE:102:A:H8 | 1.83 | 0.43 |
| 12:LL:96:PHE:HB2 | 12:LL:160:ARG:HH21 | 1.84 | 0.43 |
| 21:LU:41:ASN:H | 21:LU:99:SER:HB2 | 1.82 | 0.43 |
| 21:LU:52:MET:HE2 | 21:LU:52:MET:HB2 | 1.81 | 0.43 |
| 23:LW:36:LYS:HB3 | 23:LW:36:LYS:HE2 | 1.66 | 0.43 |
| 23:LW:85:ARG:HG3 | 23:LW:104:ALA:HB3 | 2.00 | 0.43 |
| 32:Lf:100:GLN:HB2 | 32:Lf:125:LEU:HD12 | 1.99 | 0.43 |
| 44:Lt:677:C:H4' | 44:Lt:680:G:N1 | 2.33 | 0.43 |
| 44:Lt:811:U:H2' | 44:Lt:812:G:C8 | 2.53 | 0.43 |
| 44:Lt:1207:G:C2 | 44:Lt:1281:C:H4' | 2.53 | 0.43 |
| 44:Lt:1703:C:H3' | 44:Lt:1704:G:H8 | 1.83 | 0.43 |
| 45:SA:182:LEU:HA | 45:SA:185:ARG:HD2 | 2.00 | 0.43 |
| 49:SE:128:LYS:HE3 | 49:SE:128:LYS:HB3 | 1.61 | 0.43 |
| 49:SE:256:ARG:HE | 49:SE:256:ARG:HB2 | 1.31 | 0.43 |
| 57:SM:55:LYS:HE3 | 57:SM:55:LYS:HB3 | 1.71 | 0.43 |
| 67:SY:69:ARG:HD3 | 67:SY:69:ARG:HA | 1.38 | 0.43 |
| 68:Sb:26:VAL:O | 68:Sb:68:HIS:HA | 2.18 | 0.43 |
| 68:Sb:91:LYS:HG2 | 68:Sb:96:LEU:HD23 | 2.00 | 0.43 |
| 75:St:54:A:H5' | 75:St:371:C:H5" | 2.01 | 0.43 |
| 75:St:1242:U:H2' | 75:St:1243:G:C8 | 2.54 | 0.43 |
| 76:u:9:G:H21 | 76:u:44:G:H5" | 1.83 | 0.43 |
| 3:LC:151:LYS:HA | 3:LC:151:LYS:HD3 | 1.57 | 0.43 |
| 6:LF:41:LYS:HD2 | 6:LF:41:LYS:HA | 1.75 | 0.43 |
| 7:LG:5:LYS:HB2 | 7:LG:5:LYS:HE2 | 1.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:LL:49:LYS:HB3 | 12:LL:49:LYS:HE3 | 1.38 | 0.43 |
| 13:LM:77:PRO:HG3 | 35:Li:147:LYS:HB3 | 1.99 | 0.43 |
| 15:LO:115:VAL:HG13 | 15:LO:160:GLU:HG2 | 2.01 | 0.43 |
| 15:LO:202:ARG:H | 15:LO:202:ARG:HG3 | 1.61 | 0.43 |
| 16:LP:123:TYR:CZ | 16:LP:124:LEU:HG | 2.54 | 0.43 |
| 18:LR:84:THR:HG23 | 18:LR:103:LYS:HB3 | 2.00 | 0.43 |
| 19:LS:155:LYS:HB3 | 19:LS:155:LYS:HE2 | 1.73 | 0.43 |
| 20:LT:4:LYS:HG3 | 20:LT:28:TYR:CZ | 2.54 | 0.43 |
| 21:LU:87:LYS:HE3 | 21:LU:87:LYS:HB3 | 1.31 | 0.43 |
| 37:Lk:52:LYS:HB2 | 37:Lk:52:LYS:HE3 | 1.48 | 0.43 |
| 42:Lq:6:LYS:HG2 | 42:Lq:6:LYS:HZ3 | 1.59 | 0.43 |
| 44:Lt:883:U:H1' | 44:Lt:889:G:H2' | 2.01 | 0.43 |
| 44:Lt:988:U:H2' | 44:Lt:989:C:C6 | 2.54 | 0.43 |
| 46:SB:99:GLY:HA2 | 46:SB:184:PHE:HB3 | 2.00 | 0.43 |
| 52:SH:45:TYR:O | 52:SH:46:ILE:C | 2.62 | 0.43 |
| 53:SI:41:LYS:HD2 | 53:SI:41:LYS:HA | 1.52 | 0.43 |
| 59:SP:135:LEU:HD13 | 59:SP:135:LEU:HA | 1.86 | 0.43 |
| 62:ST:59:PRO:HB2 | 62:ST:62:LEU:HB2 | 1.99 | 0.43 |
| 63:SU:52:LYS:HA | 63:SU:52:LYS:HD3 | 1.60 | 0.43 |
| 64:SV:10:TYR:CE1 | 69:Sc:22:ALA:HB2 | 2.54 | 0.43 |
| 70:Sd:26:CYS:HB3 | 70:Sd:28:ARG:HB2 | 2.01 | 0.43 |
| 75:St:676:C:H2' | 75:St:677:G:H8 | 1.82 | 0.43 |
| 75:St:699:C:H2' | 75:St:700:C:C6 | 2.53 | 0.43 |
| 75:St:987:G:H1 | 75:St:992:U:H3 | 1.66 | 0.43 |
| 75:St:1232:G:N1 | 75:St:1256:G:H1' | 2.33 | 0.43 |
| 2:LB:205:ILE:HG23 | 2:LB:285:ILE:HD11 | 2.01 | 0.43 |
| 2:LB:314:TYR:O | 44:Lt:2676:C:H5" | 2.19 | 0.43 |
| 8:LH:59:LYS:HD3 | 8:LH:59:LYS:HA | 1.29 | 0.43 |
| 8:LH:233:ARG:HG3 | 8:LH:234:MET:HG3 | 2.00 | 0.43 |
| 10:LJ:85:GLU:HG2 | 10:LJ:183:GLN:H | 1.84 | 0.43 |
| 17:LQ:126:ARG:HG3 | 17:LQ:140:GLU:HG2 | 2.00 | 0.43 |
| 28:Lb:17:MET:HE3 | 28:Lb:17:MET:HB3 | 1.72 | 0.43 |
| 32:Lf:71:MET:HE3 | 32:Lf:71:MET:HB2 | 1.79 | 0.43 |
| 32:Lf:101:ILE:HG13 | 32:Lf:126:ASN:HB2 | 2.00 | 0.43 |
| 36:Lj:79:LYS:HD2 | 36:Lj:79:LYS:HA | 1.60 | 0.43 |
| 37:Lk:31:LYS:HE3 | 37:Lk:31:LYS:HB2 | 1.65 | 0.43 |
| 39:Ln:64:LYS:HE2 | 39:Ln:64:LYS:HB2 | 1.63 | 0.43 |
| 39:Ln:206:ILE:HG13 | 39:Ln:216:ILE:HG22 | 2.01 | 0.43 |
| 44:Lt:2174:C:H2' | 44:Lt:2175:G:C8 | 2.54 | 0.43 |
| 48:SD:201:LEU:HD13 | 48:SD:201:LEU:HA | 1.78 | 0.43 |
| 53:SI:38:LEU:HB2 | 53:SI:103:ASN:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:SJ:20:ILE:HD12 | 54:SJ:20:ILE:HA | 1.69 | 0.43 |
| 65:SW:128:LYS:HE2 | 65:SW:128:LYS:HB2 | 1.57 | 0.43 |
| 70:Sd:66:LYS:HD3 | 70:Sd:66:LYS:HA | 1.83 | 0.43 |
| 70:Sd:99:LYS:O | 70:Sd:100:ARG:C | 2.61 | 0.43 |
| 72:Sg:14:GLY:H | 72:Sg:64:ARG:NH2 | 2.17 | 0.43 |
| 75:St:84:C:H2' | 75:St:85:U:C6 | 2.53 | 0.43 |
| 75:St:1251:C:H2' | 75:St:1252:C:C6 | 2.53 | 0.43 |
| 16:LP:36:GLU:H | 16:LP:36:GLU:HG3 | 1.53 | 0.43 |
| 18:LR:168:LYS:HE3 | 18:LR:168:LYS:HB3 | 1.39 | 0.43 |
| 20:LT:95:THR:HG22 | 20:LT:97:ALA:H | 1.83 | 0.43 |
| 23:LW:66:VAL:HG21 | 23:LW:74:LEU:HB2 | 2.01 | 0.43 |
| 33:Lg:59:LYS:HA | 33:Lg:60:PRO:HD3 | 1.88 | 0.43 |
| 39:Ln:77:ALA:HB2 | 39:Ln:144:LEU:HD22 | 2.01 | 0.43 |
| 44:Lt:259:C:H2' | 44:Lt:260:G:H8 | 1.83 | 0.43 |
| 44:Lt:1991:C:H2' | 44:Lt:1992:G:C8 | 2.53 | 0.43 |
| 44:Lt:2511:C:H2' | 44:Lt:2512:C:C6 | 2.54 | 0.43 |
| 44:Lt:2672:G:H2' | 44:Lt:2673:A:C8 | 2.54 | 0.43 |
| 45:SA:79:ILE:H | 45:SA:79:ILE:HG13 | 1.65 | 0.43 |
| 46:SB:163:LEU:HD21 | 46:SB:208:VAL:HG13 | 2.00 | 0.43 |
| 49:SE:64:ILE:HB | 49:SE:69:ASN:ND2 | 2.34 | 0.43 |
| 49:SE:153:ASP:HB3 | 51:SG:231:MET:SD | 2.59 | 0.43 |
| 51:SG:241:LYS:N | 51:SG:242:PRO:CD | 2.80 | 0.43 |
| 56:SL:82:LYS:HE3 | 56:SL:82:LYS:HB2 | 1.70 | 0.43 |
| 59:SP:66:VAL:HG13 | 59:SP:67:THR:HG22 | 2.00 | 0.43 |
| 66:SX:56:PRO:HB3 | 66:SX:92:PHE:CE1 | 2.53 | 0.43 |
| 69:Sc:58:ARG:HA | 69:Sc:61:ARG:HH11 | 1.84 | 0.43 |
| 75:St:693:C:H2' | 75:St:694:A:C8 | 2.54 | 0.43 |
| 75:St:1281:C:H2' | 75:St:1282:G:H8 | 1.84 | 0.43 |
| 77:v:9:G:H1' | 77:v:44:G:H2' | 2.00 | 0.43 |
| 12:LL:75:LYS:HE2 | 12:LL:75:LYS:HB2 | 1.87 | 0.42 |
| 13:LM:146:LYS:HD3 | 13:LM:146:LYS:HA | 1.84 | 0.42 |
| 13:LM:149:LEU:HD22 | 13:LM:149:LEU:HA | 1.83 | 0.42 |
| 18:LR:129:LYS:H | 18:LR:129:LYS:HG2 | 1.74 | 0.42 |
| 20:LT:44:LYS:HE3 | 20:LT:44:LYS:HB3 | 1.39 | 0.42 |
| 22:LV:29:GLU:H | 22:LV:29:GLU:HG3 | 1.53 | 0.42 |
| 22:LV:92:GLN:H | 22:LV:92:GLN:HG2 | 1.58 | 0.42 |
| 26:LZ:3:LEU:HD13 | 26:LZ:3:LEU:HA | 1.76 | 0.42 |
| 37:Lk:10:LYS:HE2 | 37:Lk:10:LYS:HB2 | 1.50 | 0.42 |
| 37:Lk:85:LYS:HA | 37:Lk:85:LYS:HD2 | 1.37 | 0.42 |
| 44:Lt:14:C:H2' | 44:Lt:15:G:C8 | 2.54 | 0.42 |
| 44:Lt:80:C:H2' | 44:Lt:81:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:1860:A:H1' | 44:Lt:2291:U:H5" | 2.00 | 0.42 |
| 47:SC:97:ILE:HD13 | 47:SC:97:ILE:HA | 1.72 | 0.42 |
| 49:SE:10:LYS:H | 49:SE:10:LYS:HG2 | 1.64 | 0.42 |
| 50:SF:126:ASP:O | 72:Sg:41:VAL:HA | 2.18 | 0.42 |
| 52:SH:173:TYR:HA | 52:SH:176:VAL:HG22 | 2.00 | 0.42 |
| 53:SI:36:THR:CB | 53:SI:105:LEU:H | 2.32 | 0.42 |
| 57:SM:93:GLN:O | 57:SM:94:LYS:C | 2.62 | 0.42 |
| 66:SX:51:PHE:CE1 | 66:SX:100:ASP:HB3 | 2.54 | 0.42 |
| 75:St:231:C:H2' | 75:St:232:C:C6 | 2.54 | 0.42 |
| 4:LD:126:C:H2' | 4:LD:127:C:C6 | 2.54 | 0.42 |
| 5:LE:64:C:H5" | 11:LK:206:LEU:H | 1.85 | 0.42 |
| 14:LN:2:SER:HB3 | 20:LT:147:PRO:HB3 | 2.00 | 0.42 |
| 15:LO:118:SER:HB3 | 15:LO:132:VAL:HG22 | 2.01 | 0.42 |
| 19:LS:71:ARG:HE | 19:LS:71:ARG:HB3 | 1.42 | 0.42 |
| 20:LT:36:LYS:HG2 | 20:LT:56:ILE:HG21 | 2.01 | 0.42 |
| 20:LT:161:THR:HG23 | 20:LT:163:ARG:H | 1.83 | 0.42 |
| 33:Lg:3:GLU:H | 33:Lg:3:GLU:HG2 | 1.50 | 0.42 |
| 39:Ln:76:ARG:HB3 | 39:Ln:144:LEU:HB2 | 2.02 | 0.42 |
| 44:Lt:2121:A:H2' | 44:Lt:2122:G:H8 | 1.82 | 0.42 |
| 53:SI:51:LYS:N | 53:SI:68:ARG:HB2 | 2.27 | 0.42 |
| 54:SJ:86:ILE:HD13 | 54:SJ:104:LEU:HD11 | 2.01 | 0.42 |
| 55:SK:22:LYS:HA | 55:SK:22:LYS:HD2 | 1.36 | 0.42 |
| 64:SV:55:LYS:HA | 64:SV:55:LYS:HD3 | 1.65 | 0.42 |
| 74:Sj:28:PRO:HG3 | 75:St:390:G:H5' | 2.00 | 0.42 |
| 1:LA:114:CYS:HB2 | 1:LA:169:VAL:CG2 | 2.48 | 0.42 |
| 2:LB:86:CYS:HB3 | 2:LB:198:LEU:O | 2.18 | 0.42 |
| 2:LB:169:PRO:HB3 | 2:LB:315:GLY:HA3 | 2.02 | 0.42 |
| 11:LK:57:LYS:HE3 | 11:LK:57:LYS:HB3 | 1.84 | 0.42 |
| 12:LL:37:LEU:HD13 | 12:LL:37:LEU:HA | 1.69 | 0.42 |
| 13:LM:29:MET:H | 44:Lt:821:G:H5' | 1.85 | 0.42 |
| 15:LO:56:LYS:HB3 | 15:LO:56:LYS:HE3 | 1.78 | 0.42 |
| 18:LR:139:GLN:HE21 | 18:LR:142:ARG:HE | 1.67 | 0.42 |
| 19:LS:30:LYS:HA | 19:LS:30:LYS:HD2 | 1.77 | 0.42 |
| 24:LX:42:LYS:HA | 24:LX:42:LYS:HD2 | 1.79 | 0.42 |
| 26:LZ:34:LEU:HD13 | 26:LZ:34:LEU:HA | 1.80 | 0.42 |
| 26:LZ:100:HIS:CG | 44:Lt:184:U:H4' | 2.54 | 0.42 |
| 44:Lt:767:A:H5' | 44:Lt:2061:A:H61 | 1.83 | 0.42 |
| 44:Lt:2055:U:H2' | 44:Lt:2056:G:C8 | 2.55 | 0.42 |
| 44:Lt:2159:C:H2' | 44:Lt:2160:G:C8 | 2.55 | 0.42 |
| 48:SD:149:GLN:HE22 | 48:SD:154:CYS:HA | 1.84 | 0.42 |
| 50:SF:88:LEU:HD23 | 50:SF:88:LEU:HA | 1.91 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:SG:147:ILE:HG12 | 51:SG:151:PHE:HD1 | 1.84 | 0.42 |
| 53:SI:26:LYS:O | 53:SI:29:LEU:HB3 | 2.20 | 0.42 |
| 54:SJ:78:ARG:H | 54:SJ:78:ARG:HG2 | 1.48 | 0.42 |
| 56:SL:63:ARG:HE | 56:SL:63:ARG:HB2 | 1.36 | 0.42 |
| 62:ST:43:GLY:N | 62:ST:82:ASP:HB2 | 2.33 | 0.42 |
| 65:SW:23:ARG:HD2 | 65:SW:23:ARG:HA | 1.74 | 0.42 |
| 75:St:605:G:H4' | 75:St:606:C:H5' | 2.01 | 0.42 |
| 75:St:818:G:H5" | 75:St:835:G:H22 | 1.83 | 0.42 |
| 75:St:1102:C:H2' | 75:St:1103:G:C8 | 2.54 | 0.42 |
| 1:LA:71:ARG:H | 1:LA:71:ARG:HG2 | 1.35 | 0.42 |
| 2:LB:230:VAL:HG11 | 2:LB:247:ARG:HE | 1.84 | 0.42 |
| 10:LJ:122:ILE:HG21 | 10:LJ:157:ILE:HG13 | 2.01 | 0.42 |
| 11:LK:91:VAL:HG23 | 11:LK:135:LEU:HA | 2.02 | 0.42 |
| 16:LP:45:ARG:HE | 16:LP:45:ARG:HB2 | 1.28 | 0.42 |
| 22:LV:108:LYS:HE2 | 22:LV:108:LYS:HB2 | 1.39 | 0.42 |
| 23:LW:29:CYS:HB3 | 23:LW:35:ALA:O | 2.20 | 0.42 |
| 23:LW:46:TRP:CE2 | 23:LW:54:PRO:HA | 2.54 | 0.42 |
| 28:Lb:75:ILE:HA | 28:Lb:78:ILE:HG13 | 2.02 | 0.42 |
| 40:Lo:21:LYS:HE2 | 40:Lo:21:LYS:HB2 | 1.30 | 0.42 |
| 44:Lt:307:A:H3' | 44:Lt:308:G:H8 | 1.84 | 0.42 |
| 44:Lt:1241:G:C5 | 44:Lt:1254:C:H4' | 2.55 | 0.42 |
| 44:Lt:1789:C:H2' | 44:Lt:1790:G:C8 | 2.54 | 0.42 |
| 46:SB:113:LYS:HE2 | 46:SB:113:LYS:HB2 | 1.76 | 0.42 |
| 49:SE:70:VAL:HA | 49:SE:91:GLU:O | 2.19 | 0.42 |
| 50:SF:119:GLN:HE21 | 50:SF:119:GLN:HB2 | 1.49 | 0.42 |
| 51:SG:241:LYS:HB3 | 51:SG:241:LYS:HE3 | 1.83 | 0.42 |
| 52:SH:70:LEU:HA | 52:SH:70:LEU:HD12 | 1.83 | 0.42 |
| 53:SI:43:THR:HB | 53:SI:44:SER:H | 1.57 | 0.42 |
| 54:SJ:22:LYS:HD3 | 54:SJ:22:LYS:HA | 1.54 | 0.42 |
| 59:SP:20:ARG:HD3 | 75:St:615:C:H5' | 2.01 | 0.42 |
| 60:SQ:135:ILE:HA | 60:SQ:136:PRO:HD3 | 1.82 | 0.42 |
| 67:SY:23:LYS:HB3 | 67:SY:23:LYS:HE2 | 1.42 | 0.42 |
| 67:SY:30:LEU:H | 67:SY:30:LEU:HG | 1.68 | 0.42 |
| 75:St:91:C:H4' | 75:St:92:A:C8 | 2.54 | 0.42 |
| 75:St:988:C:H6 | 75:St:988:C:H2' | 1.64 | 0.42 |
| 76:u:24:U:H2' | 76:u:25:G:C8 | 2.55 | 0.42 |
| 2:LB:243:ARG:HG3 | 2:LB:244:ARG:HD2 | 2.01 | 0.42 |
| 6:LF:138:HIS:HB2 | 6:LF:141:GLU:HB3 | 2.00 | 0.42 |
| 11:LK:78:LYS:HE3 | 11:LK:78:LYS:HB3 | 1.70 | 0.42 |
| 12:LL:21:ILE:HD11 | 12:LL:123:TYR:HB3 | 2.01 | 0.42 |
| 17:LQ:91:LYS:HB3 | 17:LQ:91:LYS:HE3 | 1.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Lg:63:GLY:HA3 | 33:Lg:79:PHE:HA | 2.00 | 0.42 |
| 39:Ln:31:THR:H | 39:Ln:210:MET:HB3 | 1.83 | 0.42 |
| 43:Ls:93:MET:HB2 | 43:Ls:93:MET:HE2 | 1.81 | 0.42 |
| 43:Ls:119:ARG:O | 43:Ls:120:LYS:HB3 | 2.19 | 0.42 |
| 44:Lt:446:C:O2' | 44:Lt:505:C:H5" | 2.20 | 0.42 |
| 44:Lt:1942:G:H1' | 76:u:18:G:N3 | 2.34 | 0.42 |
| 46:SB:47:ASP:HB3 | 46:SB:233:GLN:HE22 | 1.84 | 0.42 |
| 49:SE:121:PHE:HA | 49:SE:162:ILE:O | 2.19 | 0.42 |
| 49:SE:192:ILE:HG23 | 49:SE:242:GLY:HA3 | 2.01 | 0.42 |
| 56:SL:66:VAL:HG13 | 56:SL:79:LEU:HA | 2.01 | 0.42 |
| 57:SM:89:LEU:HD13 | 57:SM:89:LEU:HA | 1.83 | 0.42 |
| 59:SP:25:TRP:CD1 | 59:SP:25:TRP:H | 2.37 | 0.42 |
| 62:ST:12:ARG:HG3 | 75:St:1086:G:H22 | 1.85 | 0.42 |
| 66:SX:64:LEU:HB2 | 66:SX:85:LEU:O | 2.19 | 0.42 |
| 75:St:1076:C:H2' | 75:St:1077:C:C6 | 2.54 | 0.42 |
| 3:LC:84:ASN:HB3 | 3:LC:92:ALA:H | 1.84 | 0.42 |
| 8:LH:186:CYS:O | 8:LH:186:CYS:SG | 2.77 | 0.42 |
| 14:LN:53:ARG:HG2 | 20:LT:150:CYS:SG | 2.60 | 0.42 |
| 26:LZ:98:PRO:HG2 | 44:Lt:325:A:H4' | 2.01 | 0.42 |
| 33:Lg:19:ARG:HG2 | 33:Lg:20:SER:O | 2.19 | 0.42 |
| 33:Lg:44:LYS:HD2 | 33:Lg:44:LYS:HA | 1.65 | 0.42 |
| 34:Lh:96:ASN:C | 34:Lh:98:ALA:N | 2.77 | 0.42 |
| 34:Lh:104:ALA:C | 34:Lh:106:THR:H | 2.27 | 0.42 |
| 39:Ln:88:GLU:HB2 | 39:Ln:119:GLN:HE22 | 1.85 | 0.42 |
| 39:Ln:99:GLN:H | 39:Ln:99:GLN:HG3 | 1.59 | 0.42 |
| 43:Ls:111:ARG:H | 43:Ls:111:ARG:HG3 | 1.29 | 0.42 |
| 44:Lt:98:C:H2' | 44:Lt:99:G:C8 | 2.55 | 0.42 |
| 44:Lt:803:C:H2' | 44:Lt:804:G:C8 | 2.55 | 0.42 |
| 44:Lt:803:C:H2' | 44:Lt:804:G:H8 | 1.83 | 0.42 |
| 44:Lt:1094:A:H2' | 44:Lt:1095:G:C8 | 2.54 | 0.42 |
| 44:Lt:1429:G:H2' | 44:Lt:1430:G:C8 | 2.55 | 0.42 |
| 45:SA:77:ALA:HA | 45:SA:100:HIS:O | 2.20 | 0.42 |
| 47:SC:213:PHE:HB2 | 63:SU:20:ASN:HA | 2.01 | 0.42 |
| 48:SD:238:ARG:H | 48:SD:238:ARG:HG2 | 1.60 | 0.42 |
| 51:SG:149:ARG:HB3 | 51:SG:150:LEU:H | 1.39 | 0.42 |
| 52:SH:180:LEU:HD12 | 52:SH:180:LEU:HA | 1.88 | 0.42 |
| 55:SK:74:GLY:CA | 55:SK:94:LEU:HD12 | 2.49 | 0.42 |
| 59:SP:46:PRO:HB2 | 59:SP:86:GLU:HG3 | 2.02 | 0.42 |
| 68:Sb:112:LYS:HE3 | 68:Sb:112:LYS:HB3 | 1.51 | 0.42 |
| 75:St:413:C:H2' | 75:St:414:C:C6 | 2.55 | 0.42 |
| 75:St:988:C:H3' | 75:St:989:G:C8 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 77:v:17:G:H1 | 77:v:56:G:H2' | 1.84 | 0.42 |
| 3:LC:247:LEU:HD12 | 3:LC:247:LEU:HA | 1.76 | 0.42 |
| 4:LD:42:A:H4' | 37:Lk:59:GLN:HG2 | 2.00 | 0.42 |
| 9:LI:221:GLU:H | 9:LI:221:GLU:HG2 | 1.56 | 0.42 |
| 11:LK:169:ARG:HD2 | 11:LK:169:ARG:HA | 1.63 | 0.42 |
| 17:LQ:131:ARG:HD3 | 17:LQ:131:ARG:HA | 1.67 | 0.42 |
| 19:LS:164:LYS:HB3 | 19:LS:165:LYS:H | 1.58 | 0.42 |
| 35:Li:35:LYS:H | 35:Li:35:LYS:HG2 | 1.36 | 0.42 |
| 39:Ln:78:LYS:HA | 39:Ln:81:GLY:O | 2.20 | 0.42 |
| 39:Ln:130:LYS:HD3 | 39:Ln:130:LYS:HA | 1.76 | 0.42 |
| 44:Lt:1049:G:H2' | 44:Lt:1050:G:C8 | 2.55 | 0.42 |
| 44:Lt:2053:C:H2' | 44:Lt:2054:C:C6 | 2.54 | 0.42 |
| 47:SC:167:GLY:O | 47:SC:170:LYS:HB3 | 2.20 | 0.42 |
| 49:SE:94:LYS:HB3 | 68:Sb:15:PRO:HB2 | 2.02 | 0.42 |
| 49:SE:182:MET:HE3 | 49:SE:182:MET:HB3 | 1.62 | 0.42 |
| 53:SI:159:LEU:HD23 | 53:SI:159:LEU:HA | 1.81 | 0.42 |
| 55:SK:142:VAL:HB | 55:SK:147:TYR:CE1 | 2.54 | 0.42 |
| 56:SL:10:LYS:HE3 | 56:SL:10:LYS:HB3 | 1.73 | 0.42 |
| 58:SO:46:MET:HB2 | 58:SO:101:LEU:HD23 | 2.00 | 0.42 |
| 62:ST:8:ASP:HA | 62:ST:88:ALA:HB1 | 2.00 | 0.42 |
| 70:Sd:54:LEU:HD22 | 70:Sd:54:LEU:HA | 1.82 | 0.42 |
| 71:Se:96:PHE:HA | 71:Se:103:GLN:HA | 2.00 | 0.42 |
| 72:Sg:54:MET:HE3 | 72:Sg:54:MET:HB3 | 1.71 | 0.42 |
| 75:St:1351:C:H2' | 75:St:1352:G:C8 | 2.55 | 0.42 |
| 3:LC:98:ILE:H | 3:LC:98:ILE:HG12 | 1.61 | 0.42 |
| 3:LC:285:LYS:HD2 | 3:LC:285:LYS:HA | 1.79 | 0.42 |
| 6:LF:14:LYS:HB2 | 6:LF:14:LYS:HE2 | 1.70 | 0.42 |
| 9:LI:28:LEU:HD11 | 25:LY:29:VAL:HG22 | 2.00 | 0.42 |
| 9:LI:82:GLU:HB3 | 9:LI:86:GLU:HB3 | 2.00 | 0.42 |
| 10:LJ:182:LEU:H | 10:LJ:182:LEU:HG | 1.50 | 0.42 |
| 14:LN:20:ASP:HB3 | 14:LN:23:LYS:HG3 | 2.02 | 0.42 |
| 15:LO:27:THR:CG2 | 15:LO:122:ALA:HB1 | 2.50 | 0.42 |
| 15:LO:172:ARG:HD3 | 15:LO:174:LEU:HD22 | 2.02 | 0.42 |
| 24:LX:45:ARG:HB3 | 44:Lt:1600:G:H2' | 2.02 | 0.42 |
| 25:LY:96:LYS:HD2 | 25:LY:96:LYS:HA | 1.59 | 0.42 |
| 28:Lb:146:LEU:HD22 | 28:Lb:146:LEU:HA | 1.84 | 0.42 |
| 32:Lf:47:MET:HG2 | 32:Lf:54:GLN:HB3 | 2.02 | 0.42 |
| 35:Li:127:LYS:HE2 | 35:Li:127:LYS:HB2 | 1.95 | 0.42 |
| 38:Ll:44:LYS:HA | 38:Ll:44:LYS:HD2 | 1.86 | 0.42 |
| 38:Ll:67:LYS:HD3 | 38:Ll:67:LYS:HA | 1.64 | 0.42 |
| 43:Ls:109:ASN:HB3 | 43:Ls:115:GLY:CA | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:Lt:835:U:H2' | 44:Lt:836:G:C8 | 2.55 | 0.42 |
| 44:Lt:865:C:H2' | 44:Lt:866:C:C6 | 2.55 | 0.42 |
| 44:Lt:1953:G:H2' | 44:Lt:1954:G:H8 | 1.84 | 0.42 |
| 44:Lt:2524:C:H3' | 44:Lt:2536:C:H41 | 1.85 | 0.42 |
| 55:SK:87:LEU:HD22 | 55:SK:87:LEU:HA | 1.69 | 0.42 |
| 58:SO:60:LYS:HB2 | 58:SO:60:LYS:HE2 | 1.84 | 0.42 |
| 64:SV:24:LYS:HZ2 | 64:SV:24:LYS:HG2 | 1.79 | 0.42 |
| 65:SW:46:ARG:HG2 | 65:SW:46:ARG:HH11 | 1.84 | 0.42 |
| 72:Sg:5:ILE:H | 72:Sg:5:ILE:HG12 | 1.64 | 0.42 |
| 72:Sg:29:PHE:HD1 | 72:Sg:29:PHE:HA | 1.72 | 0.42 |
| 75:St:46:A:N1 | 75:St:299:G:H1' | 2.34 | 0.42 |
| 75:St:435:A:H2' | 75:St:436:A:C8 | 2.54 | 0.42 |
| 75:St:527:C:H42 | 75:St:575:G:H1 | 1.68 | 0.42 |
| 75:St:705:A:H2' | 75:St:706:A:O4' | 2.20 | 0.42 |
| 1:LA:48:ILE:O | 42:Lq:54:ILE:HG21 | 2.19 | 0.42 |
| 2:LB:168:THR:OG1 | 2:LB:169:PRO:HD2 | 2.20 | 0.42 |
| 2:LB:216:ASP:HB2 | 2:LB:339:ARG:HG2 | 2.01 | 0.42 |
| 2:LB:297:GLU:H | 2:LB:297:GLU:HG3 | 1.47 | 0.42 |
| 6:LF:257:PRO:O | 6:LF:258:GLN:C | 2.63 | 0.42 |
| 8:LH:85:ARG:HB2 | 8:LH:128:TYR:CD1 | 2.54 | 0.42 |
| 9:LI:102:LYS:H | 9:LI:103:PRO:HD3 | 1.84 | 0.42 |
| 12:LL:96:PHE:HE2 | 12:LL:163:VAL:HG21 | 1.84 | 0.42 |
| 21:LU:124:GLN:N | 21:LU:125:PRO:HD2 | 2.35 | 0.42 |
| 39:Ln:138:LEU:HG | 39:Ln:144:LEU:HD23 | 2.02 | 0.42 |
| 44:Lt:118:A:H2' | 44:Lt:126:C:N4 | 2.35 | 0.42 |
| 45:SA:43:ILE:HD13 | 45:SA:43:ILE:HA | 1.66 | 0.42 |
| 45:SA:194:ILE:HD12 | 45:SA:194:ILE:HA | 1.69 | 0.42 |
| 53:SI:66:ALA:HB2 | 53:SI:148:PRO:HB2 | 2.01 | 0.42 |
| 58:SO:54:LYS:HB2 | 58:SO:54:LYS:HE3 | 1.78 | 0.42 |
| 60:SQ:61:LYS:HZ2 | 60:SQ:61:LYS:HG2 | 1.78 | 0.42 |
| 66:SX:59:ALA:HB3 | 66:SX:89:LYS:H | 1.84 | 0.42 |
| 4:LD:129:C:H2' | 4:LD:130:C:C6 | 2.55 | 0.42 |
| 9:LI:92:LEU:O | 9:LI:96:ASP:HB2 | 2.20 | 0.42 |
| 9:LI:143:LEU:HD12 | 9:LI:177:THR:HG21 | 2.02 | 0.42 |
| 11:LK:36:LEU:HD23 | 11:LK:36:LEU:HA | 1.88 | 0.42 |
| 14:LN:73:LEU:HD12 | 14:LN:73:LEU:HA | 1.87 | 0.42 |
| 16:LP:9:LYS:HA | 16:LP:37:LYS:HB3 | 2.00 | 0.42 |
| 44:Lt:1551:G:H1' | 44:Lt:1566:G:N2 | 2.35 | 0.42 |
| 44:Lt:1951:A:H2' | 44:Lt:1952:G:C8 | 2.55 | 0.42 |
| 46:SB:225:LYS:HG2 | 67:SY:6:ILE:HG13 | 2.01 | 0.42 |
| 49:SE:49:ARG:HA | 49:SE:55:ALA:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:SE:249:LYS:HE2 | 49:SE:249:LYS:HB2 | 1.35 | 0.42 |
| 50:SF:29:ILE:H | 50:SF:29:ILE:HG13 | 1.78 | 0.42 |
| 53:SI:7:LYS:H | 53:SI:7:LYS:HG2 | 1.61 | 0.42 |
| 69:Sc:63:LEU:HD22 | 69:Sc:63:LEU:HA | 1.89 | 0.42 |
| 75:St:776:C:H4' | 75:St:869:A:H61 | 1.84 | 0.42 |
| 75:St:908:G:H1 | 75:St:1269:C:H42 | 1.68 | 0.42 |
| 1:LA:49:LEU:H | 1:LA:49:LEU:HG | 1.60 | 0.41 |
| 3:LC:144:VAL:HG21 | 3:LC:238:LEU:HD23 | 2.02 | 0.41 |
| 4:LD:2:C:N4 | 44:Lt:1873:C:H41 | 2.18 | 0.41 |
| 9:LI:143:LEU:HD22 | 9:LI:143:LEU:HA | 1.67 | 0.41 |
| 11:LK:186:GLU:HG2 | 11:LK:187:ARG:N | 2.34 | 0.41 |
| 13:LM:218:LYS:HE3 | 13:LM:218:LYS:HB3 | 1.61 | 0.41 |
| 14:LN:30:ILE:H | 14:LN:30:ILE:HG12 | 1.55 | 0.41 |
| 19:LS:62:ARG:HH22 | 44:Lt:2485:C:H5 | 1.68 | 0.41 |
| 19:LS:72:LEU:HD22 | 19:LS:72:LEU:HA | 1.85 | 0.41 |
| 19:LS:164:LYS:HB3 | 19:LS:164:LYS:HE3 | 1.40 | 0.41 |
| 24:LX:54:LYS:HE3 | 24:LX:54:LYS:HB3 | 1.51 | 0.41 |
| 25:LY:46:PRO:HD2 | 35:Li:109:PRO:HG3 | 2.01 | 0.41 |
| 25:LY:105:LYS:HB3 | 25:LY:105:LYS:HE2 | 1.81 | 0.41 |
| 28:Lb:118:LEU:HD22 | 28:Lb:118:LEU:HA | 1.87 | 0.41 |
| 46:SB:132:PRO:HB2 | 46:SB:216:TYR:HE2 | 1.84 | 0.41 |
| 46:SB:225:LYS:H | 67:SY:23:LYS:HD3 | 1.83 | 0.41 |
| 48:SD:211:MET:HE2 | 48:SD:211:MET:HB3 | 1.70 | 0.41 |
| 50:SF:98:LEU:HD12 | 50:SF:98:LEU:HA | 1.85 | 0.41 |
| 52:SH:153:ARG:H | 52:SH:153:ARG:HG2 | 1.72 | 0.41 |
| 54:SJ:9:ASP:O | 54:SJ:13:SER:HB2 | 2.20 | 0.41 |
| 55:SK:60:LEU:HB3 | 55:SK:94:LEU:HD21 | 2.02 | 0.41 |
| 56:SL:65:VAL:HG13 | 56:SL:83:GLY:CA | 2.50 | 0.41 |
| 65:SW:114:ILE:HD13 | 65:SW:114:ILE:HA | 1.93 | 0.41 |
| 75:St:1072:G:H3' | 75:St:1073:A:H8 | 1.84 | 0.41 |
| 1:LA:119:LYS:HB2 | 1:LA:119:LYS:HE2 | 1.53 | 0.41 |
| 3:LC:110:ARG:HE | 3:LC:110:ARG:HB3 | 1.69 | 0.41 |
| 6:LF:108:ARG:CZ | 6:LF:259:ALA:HB2 | 2.50 | 0.41 |
| 9:LI:182:THR:HB | 9:LI:183:ASP:H | 1.54 | 0.41 |
| 11:LK:153:ARG:HA | 11:LK:156:LYS:HB2 | 2.02 | 0.41 |
| 16:LP:173:LYS:HE2 | 16:LP:173:LYS:HB2 | 1.65 | 0.41 |
| 19:LS:170:CYS:SG | 59:SP:77:ALA:HB3 | 2.61 | 0.41 |
| 20:LT:57:LEU:HD12 | 20:LT:57:LEU:HA | 1.77 | 0.41 |
| 22:LV:82:LEU:HD12 | 22:LV:82:LEU:HA | 1.77 | 0.41 |
| 25:LY:62:LEU:HD11 | 25:LY:97:ALA:HB1 | 2.01 | 0.41 |
| 31:Le:18:LYS:HD3 | 31:Le:18:LYS:HA | 1.90 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:Ln:170:GLY:HA3 | 39:Ln:182:ASN:HB3 | 2.02 | 0.41 |
| 44:Lt:1710:C:H2' | 44:Lt:1711:G:C8 | 2.55 | 0.41 |
| 44:Lt:2150:C:H2' | 44:Lt:2152:G:C8 | 2.55 | 0.41 |
| 49:SE:48:LEU:HD21 | 49:SE:64:ILE:HD11 | 2.02 | 0.41 |
| 50:SF:48:ARG:HB2 | 50:SF:51:LYS:HB2 | 2.02 | 0.41 |
| 50:SF:108:ARG:HG3 | 50:SF:109:GLU:N | 2.35 | 0.41 |
| 53:SI:46:LYS:HD2 | 53:SI:46:LYS:HA | 1.89 | 0.41 |
| 56:SL:51:LEU:HD13 | 75:St:960:G:C6 | 2.55 | 0.41 |
| 61:SR:31:THR:O | 61:SR:35:PRO:HD3 | 2.20 | 0.41 |
| 68:Sb:18:GLN:HE21 | 68:Sb:81:ALA:HB2 | 1.83 | 0.41 |
| 75:St:35:C:H2' | 75:St:36:C:C6 | 2.55 | 0.41 |
| 75:St:917:U:H3 | 75:St:1172:G:H1 | 1.68 | 0.41 |
| 3:LC:134:ILE:H | 3:LC:134:ILE:HG13 | 1.63 | 0.41 |
| 10:LJ:27:LYS:HB2 | 10:LJ:27:LYS:HE2 | 1.82 | 0.41 |
| 10:LJ:44:ILE:H | 10:LJ:44:ILE:HG12 | 1.46 | 0.41 |
| 11:LK:97:ILE:H | 11:LK:97:ILE:HG13 | 1.56 | 0.41 |
| 11:LK:139:ARG:HD2 | 11:LK:173:PHE:HB2 | 2.02 | 0.41 |
| 12:LL:39:GLN:H | 12:LL:39:GLN:HG3 | 1.56 | 0.41 |
| 17:LQ:102:LYS:HE2 | 17:LQ:102:LYS:HB3 | 1.61 | 0.41 |
| 20:LT:145:ARG:HH12 | 20:LT:147:PRO:HD3 | 1.86 | 0.41 |
| 30:Ld:23:LYS:HB3 | 30:Ld:23:LYS:HE2 | 1.82 | 0.41 |
| 30:Ld:55:LEU:HD13 | 30:Ld:55:LEU:HA | 1.91 | 0.41 |
| 32:Lf:55:ARG:H | 32:Lf:55:ARG:HG3 | 1.60 | 0.41 |
| 32:Lf:91:PHE:O | 32:Lf:93:ASN:N | 2.53 | 0.41 |
| 34:Lh:63:LEU:HB3 | 34:Lh:68:ARG:HG3 | 2.02 | 0.41 |
| 41:Lp:85:ARG:H | 41:Lp:85:ARG:HG2 | 1.54 | 0.41 |
| 44:Lt:15:G:H2' | 44:Lt:16:G:C8 | 2.56 | 0.41 |
| 44:Lt:630:A:C2 | 44:Lt:1623:G:H2' | 2.56 | 0.41 |
| 45:SA:204:PRO:HB2 | 63:SU:94:PHE:HD2 | 1.85 | 0.41 |
| 48:SD:88:THR:HA | 48:SD:98:THR:HA | 2.02 | 0.41 |
| 51:SG:8:LYS:HA | 51:SG:23:MET:HA | 2.02 | 0.41 |
| 51:SG:244:LYS:HD2 | 51:SG:244:LYS:HA | 1.47 | 0.41 |
| 59:SP:76:LYS:HB3 | 59:SP:76:LYS:HE3 | 1.28 | 0.41 |
| 61:SR:62:ARG:HH12 | 61:SR:89:MET:HG2 | 1.86 | 0.41 |
| 64:SV:31:LEU:HB3 | 64:SV:39:ARG:HG3 | 2.02 | 0.41 |
| 64:SV:137:THR:O | 75:St:1165:C:H3' | 2.20 | 0.41 |
| 67:SY:34:LYS:HB3 | 67:SY:34:LYS:HE2 | 1.29 | 0.41 |
| 69:Sc:14:LYS:HD2 | 69:Sc:14:LYS:HA | 1.50 | 0.41 |
| 72:Sg:47:LYS:HE3 | 72:Sg:47:LYS:HB2 | 1.78 | 0.41 |
| 1:LA:95:THR:HG23 | 1:LA:97:HIS:H | 1.86 | 0.41 |
| 3:LC:22:LYS:HD3 | 3:LC:22:LYS:HA | 1.62 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:LO:47:LYS:HG2 | 15:LO:119:TYR:HB2 | 2.02 | 0.41 |
| 16:LP:163:LYS:H | 16:LP:163:LYS:HG2 | 1.68 | 0.41 |
| 25:LY:112:LEU:HD21 | 25:LY:122:PHE:HE1 | 1.84 | 0.41 |
| 44:Lt:59:A:H2' | 44:Lt:60:G:C8 | 2.55 | 0.41 |
| 44:Lt:1911:C:H2' | 44:Lt:1912:A:C8 | 2.55 | 0.41 |
| 44:Lt:2499:C:H2' | 44:Lt:2500:G:C8 | 2.54 | 0.41 |
| 46:SB:132:PRO:HB2 | 46:SB:216:TYR:CE2 | 2.54 | 0.41 |
| 49:SE:114:ILE:HD12 | 49:SE:114:ILE:HA | 1.83 | 0.41 |
| 50:SF:57:ARG:HD3 | 50:SF:57:ARG:HA | 1.77 | 0.41 |
| 51:SG:195:VAL:HG11 | 75:St:124:G:H1' | 2.03 | 0.41 |
| 53:SI:26:LYS:HB3 | 53:SI:26:LYS:HE3 | 1.44 | 0.41 |
| 61:SR:77:ARG:HA | 61:SR:95:SER:CB | 2.50 | 0.41 |
| 67:SY:41:LEU:HD23 | 67:SY:41:LEU:HA | 1.84 | 0.41 |
| 68:Sb:43:VAL:HG11 | 68:Sb:57:LEU:HD11 | 2.02 | 0.41 |
| 69:Sc:87:LYS:H | 69:Sc:87:LYS:HG3 | 1.61 | 0.41 |
| 70:Sd:59:ILE:HG13 | 70:Sd:62:PHE:HB2 | 2.02 | 0.41 |
| 75:St:827:G:H1' | 75:St:838:G:H4' | 2.01 | 0.41 |
| 75:St:940:G:O2' | 75:St:1290:C:H4' | 2.20 | 0.41 |
| 75:St:1000:C:H2' | 75:St:1001:G:C8 | 2.55 | 0.41 |
| 1:LA:154:GLN:HE21 | 1:LA:154:GLN:HB3 | 1.51 | 0.41 |
| 1:LA:165:MET:HE2 | 1:LA:165:MET:HB2 | 1.60 | 0.41 |
| 1:LA:180:LEU:HB3 | 1:LA:181:LYS:H | 1.64 | 0.41 |
| 3:LC:24:PHE:HE1 | 3:LC:141:PRO:HG3 | 1.84 | 0.41 |
| 9:LI:105:PRO:C | 9:LI:107:LYS:N | 2.78 | 0.41 |
| 13:LM:130:ARG:HA | 44:Lt:75:G:C5 | 2.55 | 0.41 |
| 20:LT:100:MET:HB3 | 20:LT:100:MET:HE3 | 1.47 | 0.41 |
| 20:LT:135:LYS:HB2 | 20:LT:135:LYS:HE2 | 1.35 | 0.41 |
| 29:Lc:15:LYS:HB3 | 29:Lc:15:LYS:HE2 | 1.92 | 0.41 |
| 31:Le:101:SER:O | 31:Le:102:GLU:C | 2.62 | 0.41 |
| 33:Lg:10:LEU:HD12 | 33:Lg:11:PRO:HD2 | 2.01 | 0.41 |
| 41:Lp:61:LYS:HE3 | 41:Lp:61:LYS:HB2 | 1.83 | 0.41 |
| 44:Lt:684:A:H2' | 44:Lt:685:G:C8 | 2.55 | 0.41 |
| 44:Lt:1986:G:H2' | 44:Lt:1987:C:C6 | 2.56 | 0.41 |
| 44:Lt:2170:A:H2' | 44:Lt:2171:A:O4' | 2.20 | 0.41 |
| 45:SA:29:HIS:HA | 63:SU:108:MET:HE1 | 2.02 | 0.41 |
| 46:SB:70:LEU:H | 46:SB:70:LEU:HG | 1.60 | 0.41 |
| 46:SB:91:ARG:HE | 46:SB:91:ARG:HB2 | 1.59 | 0.41 |
| 47:SC:129:ILE:HG13 | 47:SC:142:VAL:CG2 | 2.51 | 0.41 |
| 49:SE:196:GLN:OE1 | 49:SE:211:LYS:HB2 | 2.19 | 0.41 |
| 49:SE:200:LYS:H | 49:SE:200:LYS:HG3 | 1.48 | 0.41 |
| 50:SF:126:ASP:HB2 | 72:Sg:51:LEU:HD21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:SG:142:LYS:HE2 | 75:St:63:C:H5 | 1.86 | 0.41 |
| 53:SI:5:HIS:HB2 | 75:St:251:C:H1' | 2.02 | 0.41 |
| 53:SI:85:ALA:HB2 | 53:SI:117:PRO:HD3 | 2.01 | 0.41 |
| 54:SJ:117:GLN:H | 54:SJ:117:GLN:HG3 | 1.56 | 0.41 |
| 59:SP:22:PRO:HA | 59:SP:65:ASN:HB3 | 2.02 | 0.41 |
| 61:SR:88:GLU:C | 61:SR:90:ILE:H | 2.28 | 0.41 |
| 69:Sc:45:ILE:HG13 | 69:Sc:45:ILE:H | 1.55 | 0.41 |
| 71:Se:48:LEU:HD23 | 71:Se:48:LEU:HA | 1.84 | 0.41 |
| 71:Se:90:HIS:CD2 | 75:St:712:C:H5" | 2.56 | 0.41 |
| 75:St:527:C:H2' | 75:St:528:A:H8 | 1.85 | 0.41 |
| 75:St:809:G:H2' | 75:St:811:C:H5' | 2.03 | 0.41 |
| 75:St:893:G:H1 | 75:St:1316:U:H3 | 1.67 | 0.41 |
| 75:St:935:U:H2' | 75:St:936:C:C6 | 2.55 | 0.41 |
| 75:St:1296:C:H2' | 75:St:1297:C:C6 | 2.56 | 0.41 |
| 1:LA:249:LYS:HD3 | 1:LA:249:LYS:HA | 1.86 | 0.41 |
| 2:LB:71:GLN:HE21 | 2:LB:71:GLN:HB2 | 1.52 | 0.41 |
| 2:LB:126:GLU:H | 2:LB:126:GLU:HG3 | 1.36 | 0.41 |
| 2:LB:366:ILE:H | 2:LB:366:ILE:HG12 | 1.53 | 0.41 |
| 13:LM:83:LEU:HD13 | 13:LM:175:MET:HB2 | 2.01 | 0.41 |
| 13:LM:124:ILE:HD13 | 13:LM:124:ILE:HA | 1.90 | 0.41 |
| 14:LN:56:MET:HE2 | 14:LN:56:MET:HB3 | 1.72 | 0.41 |
| 14:LN:87:MET:HA | 14:LN:92:GLY:HA3 | 2.03 | 0.41 |
| 16:LP:174:LYS:HE2 | 16:LP:174:LYS:HB3 | 1.32 | 0.41 |
| 21:LU:101:CYS:HB3 | 21:LU:102:ARG:H | 1.66 | 0.41 |
| 25:LY:77:LYS:HA | 25:LY:77:LYS:HD3 | 1.78 | 0.41 |
| 27:La:44:ILE:H | 27:La:44:ILE:HG12 | 1.59 | 0.41 |
| 38:Ll:10:LEU:HD22 | 38:Ll:10:LEU:HA | 1.65 | 0.41 |
| 38:Ll:12:LYS:HD2 | 38:Ll:12:LYS:HA | 1.41 | 0.41 |
| 39:Ln:12:HIS:O | 39:Ln:15:GLU:HB3 | 2.21 | 0.41 |
| 39:Ln:19:ARG:HA | 39:Ln:19:ARG:HD2 | 1.47 | 0.41 |
| 44:Lt:451:C:H2' | 44:Lt:452:G:C8 | 2.56 | 0.41 |
| 44:Lt:983:C:H2' | 44:Lt:984:C:O4' | 2.20 | 0.41 |
| 45:SA:161:PHE:HA | 67:SY:67:ARG:HB3 | 2.01 | 0.41 |
| 46:SB:153:SER:HA | 46:SB:161:VAL:O | 2.20 | 0.41 |
| 49:SE:66:GLN:CD | 75:St:366:G:H1' | 2.46 | 0.41 |
| 49:SE:92:ILE:HB | 49:SE:95:VAL:CG1 | 2.51 | 0.41 |
| 50:SF:10:LYS:O | 50:SF:11:TRP:C | 2.63 | 0.41 |
| 50:SF:178:GLN:HE21 | 50:SF:178:GLN:HB3 | 1.74 | 0.41 |
| 51:SG:119:LEU:HG | 51:SG:122:ALA:HB2 | 2.02 | 0.41 |
| 65:SW:46:ARG:H | 65:SW:46:ARG:HD3 | 1.85 | 0.41 |
| 66:SX:64:LEU:HD22 | 66:SX:64:LEU:HA | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 73:Sh:120:CYS:HB2 | 73:Sh:123:CYS:HB2 | 1.14 | 0.41 |
| 75:St:539:G:H3' | 75:St:540:G:H8 | 1.86 | 0.41 |
| 75:St:1195:C:H42 | 75:St:1208:G:H1 | 1.68 | 0.41 |
| 1:LA:14:SER:O | 1:LA:15:VAL:HB | 2.20 | 0.41 |
| 2:LB:292:ARG:HA | 2:LB:302:ASP:O | 2.21 | 0.41 |
| 16:LP:15:ARG:HH22 | 44:Lt:1017:G:H4' | 1.84 | 0.41 |
| 17:LQ:115:ILE:HB | 17:LQ:151:GLY:HA3 | 2.02 | 0.41 |
| 19:LS:98:ARG:HH22 | 19:LS:130:ASN:HA | 1.86 | 0.41 |
| 20:LT:4:LYS:HG3 | 20:LT:28:TYR:CE1 | 2.55 | 0.41 |
| 33:Lg:9:PHE:CG | 33:Lg:93:ARG:HB3 | 2.56 | 0.41 |
| 39:Ln:62:ASN:HD22 | 39:Ln:62:ASN:HA | 1.51 | 0.41 |
| 44:Lt:593:A:H5" | 44:Lt:1522:C:H5" | 2.03 | 0.41 |
| 45:SA:97:LYS:HA | 45:SA:97:LYS:HD3 | 1.72 | 0.41 |
| 47:SC:6:ARG:HA | 47:SC:6:ARG:HD3 | 1.52 | 0.41 |
| 49:SE:181:VAL:HA | 49:SE:227:VAL:HG22 | 2.01 | 0.41 |
| 51:SG:151:PHE:HD2 | 51:SG:151:PHE:HA | 1.70 | 0.41 |
| 70:Sd:89:ARG:H | 70:Sd:89:ARG:HG2 | 1.43 | 0.41 |
| 71:Se:61:LYS:HB2 | 71:Se:61:LYS:HE2 | 1.49 | 0.41 |
| 75:St:116:C:H42 | 75:St:118:C:H41 | 1.68 | 0.41 |
| 75:St:128:G:H1' | 75:St:129:A:H5' | 2.03 | 0.41 |
| 75:St:276:G:H3' | 75:St:290:G:H22 | 1.85 | 0.41 |
| 75:St:376:C:H2' | 75:St:377:A:C8 | 2.56 | 0.41 |
| 75:St:953:C:H2' | 75:St:954:A:H8 | 1.84 | 0.41 |
| 3:LC:40:LEU:O | 3:LC:43:CYS:HB2 | 2.20 | 0.41 |
| 6:LF:129:LEU:HA | 6:LF:129:LEU:HD23 | 1.77 | 0.41 |
| 6:LF:185:MET:HA | 6:LF:188:PHE:HD1 | 1.86 | 0.41 |
| 7:LG:21:LYS:H | 7:LG:21:LYS:HG2 | 1.74 | 0.41 |
| 13:LM:95:ASN:ND2 | 44:Lt:72:C:H2' | 2.34 | 0.41 |
| 16:LP:52:LEU:HD23 | 16:LP:52:LEU:HA | 1.88 | 0.41 |
| 27:La:79:MET:HE3 | 27:La:79:MET:HB3 | 1.83 | 0.41 |
| 33:Lg:59:LYS:HA | 33:Lg:59:LYS:HD2 | 1.48 | 0.41 |
| 39:Ln:202:LYS:HB2 | 39:Ln:202:LYS:HE3 | 1.73 | 0.41 |
| 41:Lp:68:ILE:H | 41:Lp:68:ILE:HG13 | 1.63 | 0.41 |
| 43:Ls:122:LYS:HA | 43:Ls:122:LYS:HD3 | 1.79 | 0.41 |
| 45:SA:185:ARG:O | 45:SA:189:ARG:HG2 | 2.21 | 0.41 |
| 46:SB:42:ILE:HA | 46:SB:42:ILE:HD13 | 1.69 | 0.41 |
| 48:SD:164:MET:O | 48:SD:168:ILE:HG13 | 2.21 | 0.41 |
| 49:SE:165:LYS:HE2 | 49:SE:165:LYS:HB3 | 1.41 | 0.41 |
| 53:SI:27:TYR:CZ | 75:St:216:G:H5" | 2.55 | 0.41 |
| 55:SK:43:ILE:HG12 | 55:SK:44:TYR:N | 2.36 | 0.41 |
| 64:SV:75:PRO:HB2 | 64:SV:85:LEU:HD21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 64:SV:115:LEU:HD12 | 64:SV:115:LEU:HA | 1.85 | 0.41 |
| 68:Sb:27:LEU:HD12 | 68:Sb:27:LEU:HA | 1.77 | 0.41 |
| 71:Se:96:PHE:HA | 71:Se:104:ILE:H | 1.86 | 0.41 |
| 75:St:1108:A:C5 | 75:St:1109:G:H1' | 2.56 | 0.41 |
| 2:LB:88:ALA:HB3 | 2:LB:160:VAL:HB | 2.03 | 0.41 |
| 2:LB:151:LYS:HE2 | 2:LB:151:LYS:HB2 | 1.79 | 0.41 |
| 2:LB:245:GLY:HA3 | 44:Lt:1521:G:H5' | 2.03 | 0.41 |
| 3:LC:6:LYS:HE3 | 3:LC:6:LYS:HB3 | 1.65 | 0.41 |
| 3:LC:210:ASN:HB2 | 44:Lt:178:A:P | 2.61 | 0.41 |
| 4:LD:4:C:H4' | 17:LQ:63:TYR:CE1 | 2.53 | 0.41 |
| 6:LF:187:ARG:HD2 | 6:LF:187:ARG:HA | 1.59 | 0.41 |
| 10:LJ:169:ARG:HE | 10:LJ:169:ARG:HB3 | 1.22 | 0.41 |
| 12:LL:13:ARG:HH22 | 12:LL:134:PRO:HA | 1.86 | 0.41 |
| 13:LM:89:ARG:HG2 | 13:LM:99:ARG:HB2 | 2.02 | 0.41 |
| 13:LM:118:LYS:HD3 | 13:LM:118:LYS:HA | 1.74 | 0.41 |
| 15:LO:110:LEU:HD23 | 15:LO:110:LEU:HA | 1.84 | 0.41 |
| 18:LR:172:GLY:CA | 18:LR:179:TRP:HB3 | 2.50 | 0.41 |
| 19:LS:10:LEU:HD21 | 44:Lt:1275:G:H4' | 2.02 | 0.41 |
| 21:LU:106:LEU:HD23 | 21:LU:106:LEU:HA | 1.89 | 0.41 |
| 22:LV:30:LEU:HD13 | 22:LV:30:LEU:HA | 1.77 | 0.41 |
| 24:LX:62:LYS:HB3 | 24:LX:62:LYS:HE3 | 1.43 | 0.41 |
| 26:LZ:111:MET:H | 26:LZ:111:MET:HG3 | 1.43 | 0.41 |
| 33:Lg:57:SER:HB3 | 33:Lg:59:LYS:HB2 | 2.03 | 0.41 |
| 34:Lh:38:LYS:HZ2 | 34:Lh:38:LYS:HG3 | 1.74 | 0.41 |
| 38:Ll:37:LYS:HG3 | 38:Ll:50:THR:HG23 | 2.03 | 0.41 |
| 39:Ln:66:CYS:HA | 39:Ln:82:LEU:HD12 | 2.02 | 0.41 |
| 40:Lo:3:ALA:HB3 | 75:St:1428:C:OP1 | 2.21 | 0.41 |
| 44:Lt:603:C:H2' | 44:Lt:604:G:C8 | 2.56 | 0.41 |
| 44:Lt:728:G:H1' | 44:Lt:729:A:N7 | 2.36 | 0.41 |
| 44:Lt:791:G:H2' | 44:Lt:792:C:C6 | 2.55 | 0.41 |
| 44:Lt:1564:A:H3' | 44:Lt:1565:A:H8 | 1.85 | 0.41 |
| 44:Lt:1637:C:H2' | 44:Lt:1638:A:C5 | 2.55 | 0.41 |
| 44:Lt:1737:G:H2' | 44:Lt:1738:G:O4' | 2.21 | 0.41 |
| 44:Lt:2306:U:H3 | 44:Lt:2361:G:H1 | 1.68 | 0.41 |
| 44:Lt:2462:G:H2' | 44:Lt:2463:G:C8 | 2.56 | 0.41 |
| 45:SA:44:PHE:HB3 | 45:SA:53:VAL:O | 2.21 | 0.41 |
| 46:SB:74:VAL:HG22 | 46:SB:96:VAL:HG22 | 2.02 | 0.41 |
| 47:SC:74:LYS:HA | 47:SC:77:TYR:HB2 | 2.03 | 0.41 |
| 48:SD:219:LYS:HE3 | 48:SD:219:LYS:HB3 | 1.43 | 0.41 |
| 49:SE:64:ILE:HG21 | 68:Sb:17:LEU:HG | 2.03 | 0.41 |
| 49:SE:66:GLN:H | 49:SE:66:GLN:HG2 | 1.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:SG:70:TYR:CD2 | 51:SG:73:VAL:HG22 | 2.56 | 0.41 |
| 51:SG:185:LYS:HE2 | 51:SG:185:LYS:HB2 | 1.87 | 0.41 |
| 52:SH:59:LYS:O | 52:SH:91:HIS:HA | 2.21 | 0.41 |
| 53:SI:10:LYS:HD2 | 53:SI:10:LYS:HA | 1.84 | 0.41 |
| 53:SI:73:SER:HB2 | 53:SI:84:LYS:HG3 | 2.03 | 0.41 |
| 53:SI:158:ILE:HD13 | 53:SI:158:ILE:HA | 1.96 | 0.41 |
| 57:SM:24:LYS:HD3 | 57:SM:24:LYS:HA | 1.32 | 0.41 |
| 57:SM:129:LEU:O | 75:St:249:G:H4' | 2.21 | 0.41 |
| 59:SP:142:LYS:HZ2 | 59:SP:142:LYS:H | 1.69 | 0.41 |
| 60:SQ:37:LYS:HB3 | 60:SQ:37:LYS:HE3 | 1.72 | 0.41 |
| 62:ST:11:GLU:C | 62:ST:13:ASN:H | 2.27 | 0.41 |
| 62:ST:40:VAL:HA | 62:ST:82:ASP:O | 2.21 | 0.41 |
| 63:SU:39:ARG:HA | 63:SU:39:ARG:HD3 | 1.16 | 0.41 |
| 69:Sc:41:THR:HG22 | 69:Sc:78:MET:HE2 | 2.03 | 0.41 |
| 69:Sc:52:SER:HB2 | 75:St:1224:G:H5" | 2.01 | 0.41 |
| 75:St:177:C:N4 | 75:St:598:C:H42 | 2.16 | 0.41 |
| 75:St:534:A:H2' | 75:St:535:A:O4' | 2.21 | 0.41 |
| 75:St:556:C:H6 | 75:St:556:C:H2' | 1.63 | 0.41 |
| 75:St:1135:G:H2' | 75:St:1136:U:C6 | 2.56 | 0.41 |
| 75:St:1254:G:H2' | 75:St:1254:G:N3 | 2.36 | 0.41 |
| 77:v:26:C:H2' | 77:v:27:U:C6 | 2.56 | 0.41 |
| 2:LB:5:LYS:HB3 | 2:LB:6:PHE:H | 1.62 | 0.41 |
| 12:LL:111:ASP:C | 12:LL:113:GLY:H | 2.29 | 0.41 |
| 19:LS:44:LEU:HD12 | 19:LS:44:LEU:HA | 1.74 | 0.41 |
| 26:LZ:1:MET:HE3 | 26:LZ:1:MET:HB3 | 1.97 | 0.41 |
| 28:Lb:115:ARG:HE | 28:Lb:115:ARG:HB3 | 1.49 | 0.41 |
| 37:Lk:52:LYS:HA | 37:Lk:55:ARG:HD2 | 2.03 | 0.41 |
| 38:Ll:6:THR:HB | 38:Ll:10:LEU:HB2 | 2.03 | 0.41 |
| 38:Ll:15:ALA:HA | 38:Ll:20:LYS:HG3 | 2.03 | 0.41 |
| 39:Ln:76:ARG:HD2 | 39:Ln:76:ARG:HA | 1.40 | 0.41 |
| 44:Lt:425:A:H8 | 44:Lt:502:G:C2 | 2.39 | 0.41 |
| 44:Lt:1282:C:H2' | 44:Lt:1283:G:C8 | 2.56 | 0.41 |
| 44:Lt:1860:A:H5" | 44:Lt:1860:A:C8 | 2.56 | 0.41 |
| 44:Lt:1873:C:H3' | 44:Lt:1874:G:C8 | 2.52 | 0.41 |
| 44:Lt:2382:C:H2' | 44:Lt:2383:G:C8 | 2.56 | 0.41 |
| 44:Lt:2410:C:H2' | 44:Lt:2411:U:C6 | 2.56 | 0.41 |
| 44:Lt:2512:C:H2' | 44:Lt:2513:C:C6 | 2.55 | 0.41 |
| 54:SJ:6:VAL:HG12 | 54:SJ:29:PRO:HG2 | 2.02 | 0.41 |
| 59:SP:73:ARG:HE | 59:SP:73:ARG:HB3 | 1.47 | 0.41 |
| 62:ST:45:GLY:N | 62:ST:81:LEU:H | 2.11 | 0.41 |
| 75:St:1013:G:H1 | 75:St:1145:C:H42 | 1.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 75:St:1155:C:H2' | 75:St:1156:C:C6 | 2.56 | 0.41 |
| 6:LF:240:LEU:H | 6:LF:240:LEU:HG | 1.35 | 0.40 |
| 8:LH:155:ARG:H | 44:Lt:1049:G:H4' | 1.86 | 0.40 |
| 9:LI:168:GLY:HA2 | 9:LI:176:THR:HG23 | 2.03 | 0.40 |
| 18:LR:51:ARG:HG3 | 18:LR:137:LEU:HD21 | 2.03 | 0.40 |
| 19:LS:123:LEU:HD13 | 19:LS:123:LEU:HA | 1.67 | 0.40 |
| 23:LW:47:LYS:HB3 | 23:LW:47:LYS:HE2 | 1.94 | 0.40 |
| 24:LX:49:LYS:HD2 | 24:LX:49:LYS:HA | 1.46 | 0.40 |
| 44:Lt:918:U:H3' | 44:Lt:919:C:H5" | 2.03 | 0.40 |
| 44:Lt:1420:C:H2' | 44:Lt:1421:G:C8 | 2.56 | 0.40 |
| 45:SA:183:LEU:HD12 | 45:SA:183:LEU:HA | 1.89 | 0.40 |
| 46:SB:48:ILE:H | 46:SB:48:ILE:HG12 | 1.43 | 0.40 |
| 48:SD:37:LYS:HD3 | 48:SD:73:PRO:HD2 | 2.02 | 0.40 |
| 49:SE:233:PRO:C | 49:SE:235:VAL:N | 2.78 | 0.40 |
| 55:SK:81:LEU:HD22 | 55:SK:81:LEU:HA | 1.92 | 0.40 |
| 66:SX:58:ARG:HA | 66:SX:90:ARG:HD3 | 2.02 | 0.40 |
| 68:Sb:59:GLY:HA2 | 75:St:407:C:H5" | 2.03 | 0.40 |
| 68:Sb:90:ARG:HE | 68:Sb:90:ARG:HB3 | 1.25 | 0.40 |
| 70:Sd:103:ARG:HA | 70:Sd:103:ARG:HD2 | 1.67 | 0.40 |
| 72:Sg:9:VAL:HG13 | 72:Sg:25:VAL:HG11 | 2.02 | 0.40 |
| 74:Sj:24:LYS:HE3 | 74:Sj:24:LYS:HB2 | 1.50 | 0.40 |
| 75:St:123:A:N6 | 75:St:158:G:H1' | 2.35 | 0.40 |
| 75:St:910:C:H2' | 75:St:911:G:O4' | 2.22 | 0.40 |
| 75:St:930:C:H1' | 75:St:951:A:H2' | 2.03 | 0.40 |
| 2:LB:19:ARG:HB2 | 2:LB:232:ARG:NH2 | 2.37 | 0.40 |
| 2:LB:86:CYS:SG | 2:LB:199:MET:HA | 2.62 | 0.40 |
| 11:LK:12:GLN:HG3 | 11:LK:57:LYS:HE3 | 2.03 | 0.40 |
| 11:LK:202:ARG:HE | 11:LK:202:ARG:HB3 | 1.54 | 0.40 |
| 12:LL:12:ILE:HD12 | 12:LL:162:TRP:HB2 | 2.03 | 0.40 |
| 13:LM:195:GLU:HB3 | 28:Lb:146:LEU:HD21 | 2.03 | 0.40 |
| 14:LN:13:VAL:HG12 | 14:LN:57:LEU:HA | 2.04 | 0.40 |
| 19:LS:184:PHE:O | 52:SH:39:MET:HG3 | 2.21 | 0.40 |
| 26:LZ:44:ILE:HD13 | 26:LZ:44:ILE:HA | 1.93 | 0.40 |
| 33:Lg:46:LEU:HD23 | 33:Lg:46:LEU:HA | 1.85 | 0.40 |
| 37:Lk:46:ARG:HD3 | 37:Lk:46:ARG:HA | 1.36 | 0.40 |
| 40:Lo:8:LYS:HB3 | 40:Lo:8:LYS:HE2 | 1.41 | 0.40 |
| 44:Lt:891:C:H2' | 44:Lt:892:G:C8 | 2.56 | 0.40 |
| 44:Lt:1877:C:H2' | 44:Lt:1878:A:H8 | 1.85 | 0.40 |
| 49:SE:26:ILE:HG13 | 49:SE:27:TRP:N | 2.36 | 0.40 |
| 51:SG:138:ARG:HH12 | 75:St:148:G:N2 | 2.18 | 0.40 |
| 51:SG:209:GLU:H | 51:SG:209:GLU:HG3 | 1.63 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 68:Sb:10:LYS:HB3 | 68:Sb:10:LYS:HE3 | 1.27 | 0.40 |
| 68:Sb:21:GLN:HB2 | 68:Sb:72:PHE:CE2 | 2.56 | 0.40 |
| 69:Sc:40:ILE:HG13 | 69:Sc:45:ILE:HG12 | 2.03 | 0.40 |
| 75:St:850:U:H2' | 75:St:851:G:C8 | 2.55 | 0.40 |
| 77:v:14:A:H5' | 77:v:16:C:H5 | 1.86 | 0.40 |
| 1:LA:204:MET:HE2 | 1:LA:209:HIS:CD2 | 2.57 | 0.40 |
| 4:LD:2:C:H2' | 4:LD:3:A:O4' | 2.20 | 0.40 |
| 5:LE:95:C:H2' | 5:LE:96:G:H8 | 1.85 | 0.40 |
| 7:LG:44:TRP:CH2 | 44:Lt:1474:A:H1' | 2.57 | 0.40 |
| 12:LL:40:LEU:HG | 12:LL:79:ILE:HD12 | 2.04 | 0.40 |
| 16:LP:48:LYS:HE3 | 16:LP:48:LYS:HB3 | 1.66 | 0.40 |
| 19:LS:173:ARG:C | 59:SP:31:GLU:HB3 | 2.47 | 0.40 |
| 26:LZ:109:LEU:HD12 | 26:LZ:109:LEU:HA | 1.85 | 0.40 |
| 27:La:119:ILE:HD13 | 27:La:119:ILE:HA | 1.70 | 0.40 |
| 28:Lb:75:ILE:HG22 | 28:Lb:114:GLY:HA2 | 2.02 | 0.40 |
| 32:Lf:27:SER:HA | 32:Lf:33:VAL:HB | 2.02 | 0.40 |
| 37:Lk:39:TYR:CD1 | 37:Lk:40:PRO:HA | 2.56 | 0.40 |
| 38:Ll:64:CYS:HB2 | 38:Ll:68:VAL:HG21 | 2.02 | 0.40 |
| 41:Lp:14:ARG:HB2 | 41:Lp:77:CYS:SG | 2.61 | 0.40 |
| 41:Lp:67:VAL:HG13 | 41:Lp:80:PHE:HB3 | 2.04 | 0.40 |
| 41:Lp:93:ARG:O | 41:Lp:94:LEU:C | 2.64 | 0.40 |
| 43:Ls:109:ASN:HB3 | 43:Ls:115:GLY:H | 1.86 | 0.40 |
| 44:Lt:873:C:H2' | 44:Lt:874:G:C8 | 2.57 | 0.40 |
| 44:Lt:1522:C:H2' | 44:Lt:1523:G:H8 | 1.84 | 0.40 |
| 47:SC:70:TYR:HA | 56:SL:101:PRO:O | 2.21 | 0.40 |
| 47:SC:91:ASN:HD21 | 47:SC:93:TRP:CD1 | 2.39 | 0.40 |
| 50:SF:73:LEU:HA | 50:SF:76:MET:SD | 2.62 | 0.40 |
| 50:SF:176:ILE:HG13 | 50:SF:179:ARG:HE | 1.86 | 0.40 |
| 52:SH:9:ILE:HG12 | 52:SH:16:LEU:HD21 | 2.03 | 0.40 |
| 52:SH:111:LYS:HB2 | 75:St:585:A:N6 | 2.36 | 0.40 |
| 53:SI:161:GLY:C | 53:SI:163:GLU:N | 2.78 | 0.40 |
| 55:SK:156:ARG:HE | 55:SK:156:ARG:HB3 | 1.62 | 0.40 |
| 55:SK:171:PRO:HD2 | 55:SK:175:LYS:CB | 2.44 | 0.40 |
| 62:ST:123:LYS:HB2 | 62:ST:123:LYS:HE2 | 1.84 | 0.40 |
| 63:SU:109:ILE:HG21 | 63:SU:116:CYS:HB2 | 2.04 | 0.40 |
| 71:Se:104:ILE:HD12 | 71:Se:104:ILE:HA | 1.71 | 0.40 |
| 75:St:1179:U:H5" | 75:St:1180:G:C8 | 2.57 | 0.40 |
| 75:St:1323:A:H5' | 75:St:1326:G:H4' | 2.02 | 0.40 |
| 1:LA:52:ARG:HG2 | 44:Lt:1438:U:H5' | 2.02 | 0.40 |
| 6:LF:288:LYS:HE3 | 6:LF:288:LYS:HB3 | 1.54 | 0.40 |
| 11:LK:39:ARG:H | 11:LK:39:ARG:HG3 | 1.63 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:LM:30:GLY:O | 13:LM:31:ARG:C | 2.65 | 0.40 |
| 14:LN:16:GLY:O | 14:LN:21:LYS:HG3 | 2.20 | 0.40 |
| 17:LQ:116:SER:HB3 | 17:LQ:149:ILE:HG13 | 2.04 | 0.40 |
| 17:LQ:119:VAL:HA | 17:LQ:145:HIS:O | 2.21 | 0.40 |
| 18:LR:26:ILE:HD12 | 18:LR:26:ILE:HA | 1.70 | 0.40 |
| 25:LY:47:ARG:H | 25:LY:47:ARG:HG2 | 1.69 | 0.40 |
| 32:Lf:133:LYS:HB2 | 32:Lf:133:LYS:HE3 | 1.61 | 0.40 |
| 34:Lh:19:LYS:HA | 34:Lh:19:LYS:HD3 | 1.91 | 0.40 |
| 34:Lh:21:VAL:HG21 | 34:Lh:33:SER:HB3 | 2.03 | 0.40 |
| 39:Ln:151:CYS:HA | 39:Ln:156:LYS:HG2 | 2.03 | 0.40 |
| 40:Lo:12:LYS:HA | 40:Lo:12:LYS:HD3 | 1.71 | 0.40 |
| 41:Lp:83:LEU:HD23 | 41:Lp:83:LEU:HA | 1.83 | 0.40 |
| 44:Lt:1100:C:H2' | 44:Lt:1101:G:H8 | 1.86 | 0.40 |
| 44:Lt:1620:A:H2' | 44:Lt:1621:C:O4' | 2.21 | 0.40 |
| 47:SC:32:SER:HA | 47:SC:36:VAL:HB | 2.04 | 0.40 |
| 49:SE:10:LYS:HA | 49:SE:27:TRP:CD1 | 2.55 | 0.40 |
| 50:SF:13:LEU:HD13 | 50:SF:13:LEU:HA | 1.84 | 0.40 |
| 52:SH:157:VAL:HA | 52:SH:188:ILE:O | 2.22 | 0.40 |
| 53:SI:113:ILE:HG13 | 53:SI:142:ALA:HB3 | 2.04 | 0.40 |
| 54:SJ:73:GLY:HA3 | 54:SJ:128:TYR:CE2 | 2.56 | 0.40 |
| 55:SK:165:LEU:O | 55:SK:166:ALA:C | 2.64 | 0.40 |
| 60:SQ:108:TYR:HE2 | 70:Sd:44:ILE:HG23 | 1.86 | 0.40 |
| 61:SR:97:TYR:HA | 61:SR:102:PHE:HA | 2.04 | 0.40 |
| 64:SV:80:ILE:HG21 | 64:SV:84:MET:HG2 | 2.03 | 0.40 |
| 75:St:175:C:H6 | 75:St:175:C:H2' | 1.76 | 0.40 |
| 75:St:945:C:H6 | 75:St:945:C:H2' | 1.70 | 0.40 |
| 77:v:74:C:H6 | 77:v:74:C:H2' | 1.62 | 0.40 |
| 2:LB:43:LEU:HD23 | 2:LB:43:LEU:HA | 1.88 | 0.40 |
| 2:LB:209:PHE:CE2 | 2:LB:338:MET:HB2 | 2.56 | 0.40 |
| 5:LE:16:A:H2' | 5:LE:17:C:C6 | 2.56 | 0.40 |
| 6:LF:217:LEU:HD12 | 6:LF:217:LEU:HA | 1.71 | 0.40 |
| 6:LF:227:LYS:HA | 6:LF:227:LYS:HD2 | 1.92 | 0.40 |
| 6:LF:289:LEU:HD13 | 6:LF:289:LEU:HA | 1.69 | 0.40 |
| 9:LI:66:ARG:H | 9:LI:66:ARG:HG2 | 1.71 | 0.40 |
| 12:LL:49:LYS:HD2 | 12:LL:62:GLY:HA2 | 2.03 | 0.40 |
| 15:LO:145:ASP:HA | 15:LO:146:PRO:HD3 | 1.97 | 0.40 |
| 16:LP:105:ILE:HG13 | 16:LP:157:ARG:HD3 | 2.03 | 0.40 |
| 19:LS:74:ARG:HA | 19:LS:74:ARG:HD3 | 1.89 | 0.40 |
| 22:LV:88:TYR:HA | 22:LV:92:GLN:HB3 | 2.02 | 0.40 |
| 22:LV:91:TYR:HB2 | 22:LV:95:PHE:CE2 | 2.57 | 0.40 |
| 24:LX:9:PHE:HB3 | 24:LX:37:CYS:SG | 2.62 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:Le:55:TRP:CZ3 | 31:Le:59:ILE:HG13 | 2.56 | 0.40 |
| 34:Lh:77:LYS:H | 34:Lh:77:LYS:HG3 | 1.74 | 0.40 |
| 39:Ln:103:PHE:HD2 | 39:Ln:103:PHE:HA | 1.80 | 0.40 |
| 44:Lt:1149:G:H2' | 44:Lt:1151:G:N7 | 2.36 | 0.40 |
| 44:Lt:1894:C:H2' | 44:Lt:1895:C:C6 | 2.56 | 0.40 |
| 49:SE:209:ARG:HA | 49:SE:219:LEU:HA | 2.03 | 0.40 |
| 55:SK:127:ARG:HB3 | 74:Sj:31:ARG:HH22 | 1.87 | 0.40 |
| 56:SL:53:VAL:HG13 | 56:SL:57:MET:HE2 | 2.03 | 0.40 |
| 56:SL:72:TRP:CD1 | 73:Sh:105:CYS:HA | 2.56 | 0.40 |
| 58:SO:24:ASP:HB3 | 58:SO:27:TYR:H | 1.85 | 0.40 |
| 62:ST:83:MET:HE2 | 62:ST:103:ILE:HG23 | 2.03 | 0.40 |
| 64:SV:100:LEU:HD23 | 64:SV:100:LEU:HA | 1.95 | 0.40 |
| 68:Sb:117:LYS:H | 68:Sb:117:LYS:HG2 | 1.31 | 0.40 |
| 70:Sd:25:ASN:HD22 | 70:Sd:77:CYS:HB3 | 1.86 | 0.40 |
| 70:Sd:89:ARG:HA | 70:Sd:92:ARG:HD2 | 2.04 | 0.40 |
| 73:Sh:113:ARG:H | 73:Sh:113:ARG:HG2 | 1.58 | 0.40 |
| 75:St:196:C:H3' | 75:St:197:G:H8 | 1.87 | 0.40 |
| 75:St:810:U:H6 | 75:St:810:U:H2' | 1.67 | 0.40 |
| 75:St:996:C:H2' | 75:St:997:G:C8 | 2.56 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | LA | 248/251 (99%) | 228 (92%) | 19 (8%) | 1 (0%) | 30 | 67 |
| 2 | LB | 376/379 (99%) | 359 (96%) | 15 (4%) | 2 (0%) | 24 | 63 |
| 3 | LC | 313/316 (99%) | 294 (94%) | 17 (5%) | 2 (1%) | 21 | 58 |
| 6 | LF | 291/297 (98%) | 272 (94%) | 19 (6%) | 0 | 100 | 100 |
| 7 | LG | 48/51 (94%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 8 | LH | 214/235 (91%) | 202 (94%) | 12 (6%) | 0 | 100 | 100 |
| 9 | LI | 193/225 (86%) | 172 (89%) | 17 (9%) | 4 (2%) | 5 | 29 |
| 10 | LJ | 182/185 (98%) | 167 (92%) | 14 (8%) | 1 (0%) | 24 | 63 |
| 11 | LK | 204/210 (97%) | 188 (92%) | 13 (6%) | 3 (2%) | 8 | 38 |
| 12 | LL | 166/173 (96%) | 153 (92%) | 10 (6%) | 3 (2%) | 6 | 33 |
| 13 | LM | 199/234 (85%) | 186 (94%) | 12 (6%) | 1 (0%) | 24 | 63 |
| 14 | LN | 128/131 (98%) | 125 (98%) | 3 (2%) | 0 | 100 | 100 |
| 15 | LO | 201/204 (98%) | 190 (94%) | 10 (5%) | 1 (0%) | 24 | 63 |
| 16 | LP | 192/197 (98%) | 180 (94%) | 9 (5%) | 3 (2%) | 7 | 37 |
| 17 | LQ | 154/164 (94%) | 146 (95%) | 8 (5%) | 0 | 100 | 100 |
| 18 | LR | 176/179 (98%) | 164 (93%) | 11 (6%) | 1 (1%) | 21 | 58 |
| 19 | LS | 190/196 (97%) | 183 (96%) | 6 (3%) | 1 (0%) | 24 | 63 |
| 20 | LT | 168/173 (97%) | 163 (97%) | 5 (3%) | 0 | 100 | 100 |
| 21 | LU | 155/159 (98%) | 134 (86%) | 17 (11%) | 4 (3%) | 4 | 25 |
| 22 | LV | 113/124 (91%) | 96 (85%) | 14 (12%) | 3 (3%) | 4 | 25 |
| 23 | LW | 133/142 (94%) | 131 (98%) | 2 (2%) | 0 | 100 | 100 |
| 24 | LX | 61/189 (32%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 25 | LY | 117/141 (83%) | 102 (87%) | 12 (10%) | 3 (3%) | 4 | 25 |
| 26 | LZ | 131/135 (97%) | 128 (98%) | 2 (2%) | 1 (1%) | 16 | 52 |
| 27 | La | 130/135 (96%) | 117 (90%) | 13 (10%) | 0 | 100 | 100 |
| 28 | Lb | 146/149 (98%) | 136 (93%) | 8 (6%) | 2 (1%) | 9 | 39 |
| 29 | Lc | 53/62 (86%) | 46 (87%) | 5 (9%) | 2 (4%) | 2 | 19 |
| 30 | Ld | 95/109 (87%) | 90 (95%) | 4 (4%) | 1 (1%) | 11 | 45 |
| 31 | Le | 98/106 (92%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 32 | Lf | 128/136 (94%) | 121 (94%) | 7 (6%) | 0 | 100 | 100 |
| 33 | Lg | 96/123 (78%) | 91 (95%) | 5 (5%) | 0 | 100 | 100 |
| 34 | Lh | 114/120 (95%) | 105 (92%) | 8 (7%) | 1 (1%) | 14 | 49 |
| 35 | Li | 120/124 (97%) | 114 (95%) | 5 (4%) | 1 (1%) | 16 | 52 |
| 36 | Lj | 87/90 (97%) | 78 (90%) | 9 (10%) | 0 | 100 | 100 |
| 37 | Lk | 86/89 (97%) | 80 (93%) | 6 (7%) | 0 | 100 | 100 |
| 38 | Ll | 70/77 (91%) | 64 (91%) | 6 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 39 | Ln | 194/217 (89%) | 145 (75%) | 37 (19%) | 12 (6%) | 1 13 |
| 40 | Lo | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 100 |
| 41 | Lp | 91/106 (86%) | 90 (99%) | 0 | 1 (1%) | 11 45 |
| 42 | Lq | 89/94 (95%) | 85 (96%) | 4 (4%) | 0 | 100 100 |
| 43 | Ls | 45/127 (35%) | 39 (87%) | 3 (7%) | 3 (7%) | 1 12 |
| 45 | SA | 195/245 (80%) | 186 (95%) | 8 (4%) | 1 (0%) | 24 63 |
| 46 | SB | 214/242 (88%) | 197 (92%) | 14 (6%) | 3 (1%) | 9 39 |
| 47 | SC | 208/217 (96%) | 190 (91%) | 13 (6%) | 5 (2%) | 4 27 |
| 48 | SD | 229/248 (92%) | 217 (95%) | 11 (5%) | 1 (0%) | 30 67 |
| 49 | SE | 258/268 (96%) | 222 (86%) | 29 (11%) | 7 (3%) | 4 25 |
| 50 | SF | 184/190 (97%) | 170 (92%) | 12 (6%) | 2 (1%) | 11 45 |
| 51 | SG | 236/248 (95%) | 213 (90%) | 20 (8%) | 3 (1%) | 9 41 |
| 52 | SH | 182/190 (96%) | 163 (90%) | 13 (7%) | 6 (3%) | 3 20 |
| 53 | SI | 171/174 (98%) | 154 (90%) | 14 (8%) | 3 (2%) | 6 33 |
| 54 | SJ | 127/130 (98%) | 120 (94%) | 5 (4%) | 2 (2%) | 7 37 |
| 55 | SK | 174/189 (92%) | 161 (92%) | 11 (6%) | 2 (1%) | 11 45 |
| 56 | SL | 105/134 (78%) | 98 (93%) | 6 (6%) | 1 (1%) | 12 47 |
| 57 | SM | 151/154 (98%) | 132 (87%) | 18 (12%) | 1 (1%) | 18 55 |
| 58 | SO | 138/144 (96%) | 127 (92%) | 8 (6%) | 3 (2%) | 5 28 |
| 59 | SP | 148/154 (96%) | 144 (97%) | 4 (3%) | 0 | 100 100 |
| 60 | SQ | 125/145 (86%) | 110 (88%) | 14 (11%) | 1 (1%) | 16 52 |
| 61 | SR | 114/145 (79%) | 100 (88%) | 11 (10%) | 3 (3%) | 4 25 |
| 62 | ST | 149/158 (94%) | 140 (94%) | 6 (4%) | 3 (2%) | 6 31 |
| 63 | SU | 119/137 (87%) | 101 (85%) | 15 (13%) | 3 (2%) | 4 26 |
| 64 | SV | 144/154 (94%) | 122 (85%) | 16 (11%) | 6 (4%) | 2 17 |
| 65 | SW | 136/139 (98%) | 125 (92%) | 9 (7%) | 2 (2%) | 8 38 |
| 66 | SX | 99/126 (79%) | 95 (96%) | 4 (4%) | 0 | 100 100 |
| 67 | SY | 84/89 (94%) | 78 (93%) | 5 (6%) | 1 (1%) | 10 42 |
| 68 | Sb | 118/132 (89%) | 103 (87%) | 11 (9%) | 4 (3%) | 3 20 |
| 69 | Sc | 73/88 (83%) | 68 (93%) | 5 (7%) | 0 | 100 100 |
| 70 | Sd | 106/109 (97%) | 100 (94%) | 5 (5%) | 1 (1%) | 14 49 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 71 | Se | 78/81 (96%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 72 | Sg | 61/64 (95%) | 52 (85%) | 9 (15%) | 0 | 100 | 100 |
| 73 | Sh | 48/51 (94%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 74 | Sj | 65/69 (94%) | 58 (89%) | 6 (9%) | 1 (2%) | 8 | 38 |
| All | All | 10257/11193 (92%) | 9455 (92%) | 680 (7%) | 122 (1%) | 13 | 42 |

All (122) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | LB | 55 | HIS |
| 9 | LI | 102 | LYS |
| 12 | LL | 24 | GLY |
| 16 | LP | 107 | PRO |
| 19 | LS | 130 | ASN |
| 29 | Lc | 50 | ASP |
| 34 | Lh | 6 | VAL |
| 39 | Ln | 17 | ILE |
| 39 | Ln | 47 | PRO |
| 39 | Ln | 72 | ARG |
| 39 | Ln | 160 | LYS |
| 39 | Ln | 197 | GLY |
| 43 | Ls | 80 | PRO |
| 47 | SC | 68 | ASN |
| 47 | SC | 152 | ARG |
| 47 | SC | 210 | ILE |
| 49 | SE | 76 | PRO |
| 51 | SG | 149 | ARG |
| 51 | SG | 173 | LEU |
| 52 | SH | 182 | GLU |
| 56 | SL | 104 | LYS |
| 58 | SO | 86 | PRO |
| 61 | SR | 70 | SER |
| 61 | SR | 100 | ARG |
| 61 | SR | 126 | VAL |
| 64 | SV | 151 | ARG |
| 9 | LI | 184 | VAL |
| 10 | LJ | 44 | ILE |
| 15 | LO | 186 | PRO |
| 22 | LV | 119 | ALA |
| 29 | Lc | 25 | LYS |
| 35 | Li | 72 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | Ln | 27 | LYS |
| 41 | Lp | 85 | ARG |
| 46 | SB | 69 | GLU |
| 46 | SB | 227 | GLU |
| 52 | SH | 9 | ILE |
| 52 | SH | 46 | ILE |
| 52 | SH | 107 | VAL |
| 54 | SJ | 29 | PRO |
| 58 | SO | 3 | LYS |
| 58 | SO | 109 | GLY |
| 62 | ST | 92 | HIS |
| 63 | SU | 89 | PRO |
| 63 | SU | 96 | VAL |
| 64 | SV | 13 | LEU |
| 64 | SV | 90 | ASP |
| 70 | Sd | 100 | ARG |
| 2 | LB | 303 | LYS |
| 3 | LC | 174 | SER |
| 11 | LK | 28 | ASP |
| 12 | LL | 25 | GLY |
| 16 | LP | 29 | GLU |
| 21 | LU | 18 | LYS |
| 21 | LU | 137 | ARG |
| 21 | LU | 157 | GLY |
| 22 | LV | 63 | ASP |
| 25 | LY | 43 | PRO |
| 25 | LY | 49 | PRO |
| 30 | Ld | 77 | SER |
| 39 | Ln | 32 | VAL |
| 39 | Ln | 134 | THR |
| 43 | Ls | 93 | MET |
| 45 | SA | 45 | ASP |
| 47 | SC | 118 | ALA |
| 49 | SE | 205 | TYR |
| 49 | SE | 234 | ALA |
| 50 | SF | 91 | GLY |
| 51 | SG | 133 | VAL |
| 55 | SK | 148 | MET |
| 55 | SK | 167 | PRO |
| 57 | SM | 96 | LYS |
| 62 | ST | 112 | LYS |
| 64 | SV | 126 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | SY | 35 | ASP |
| 68 | Sb | 51 | ASP |
| 68 | Sb | 102 | PRO |
| 74 | Sj | 43 | VAL |
| 9 | LI | 163 | THR |
| 11 | LK | 108 | ALA |
| 22 | LV | 94 | VAL |
| 28 | Lb | 95 | SER |
| 43 | Ls | 120 | LYS |
| 50 | SF | 149 | PHE |
| 60 | SQ | 138 | ASP |
| 63 | SU | 99 | ILE |
| 64 | SV | 143 | ARG |
| 65 | SW | 69 | SER |
| 68 | Sb | 100 | PRO |
| 1 | LA | 14 | SER |
| 11 | LK | 27 | PRO |
| 13 | LM | 158 | GLN |
| 18 | LR | 11 | LYS |
| 21 | LU | 121 | GLU |
| 25 | LY | 54 | SER |
| 39 | Ln | 113 | SER |
| 39 | Ln | 171 | ASN |
| 47 | SC | 11 | ASN |
| 48 | SD | 18 | ASN |
| 49 | SE | 177 | ILE |
| 12 | LL | 108 | GLU |
| 39 | Ln | 21 | THR |
| 49 | SE | 244 | ARG |
| 52 | SH | 34 | PRO |
| 53 | SI | 3 | ILE |
| 54 | SJ | 59 | ASN |
| 64 | SV | 150 | GLN |
| 65 | SW | 119 | GLY |
| 53 | SI | 173 | PRO |
| 9 | LI | 63 | PRO |
| 16 | LP | 143 | GLY |
| 53 | SI | 144 | ILE |
| 68 | Sb | 120 | GLY |
| 3 | LC | 234 | GLY |
| 28 | Lb | 75 | ILE |
| 39 | Ln | 163 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | SB | 66 | PRO |
| 62 | ST | 59 | PRO |
| 26 | LZ | 113 | GLY |
| 49 | SE | 180 | ILE |
| 49 | SE | 232 | SER |
| 52 | SH | 12 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | LA | 191/192 (100%) | 100 (52%) | 91 (48%) | 0 0 |
| 2 | LB | 312/313 (100%) | 187 (60%) | 125 (40%) | 0 1 |
| 3 | LC | 262/263 (100%) | 156 (60%) | 106 (40%) | 0 1 |
| 6 | LF | 238/242 (98%) | 133 (56%) | 105 (44%) | 0 0 |
| 7 | LG | 47/48 (98%) | 27 (57%) | 20 (43%) | 0 0 |
| 8 | LH | 185/204 (91%) | 111 (60%) | 74 (40%) | 0 1 |
| 9 | LI | 172/198 (87%) | 100 (58%) | 72 (42%) | 0 0 |
| 10 | LJ | 163/164 (99%) | 92 (56%) | 71 (44%) | 0 0 |
| 11 | LK | 173/177 (98%) | 102 (59%) | 71 (41%) | 0 0 |
| 12 | LL | 144/149 (97%) | 87 (60%) | 57 (40%) | 0 1 |
| 13 | LM | 169/197 (86%) | 92 (54%) | 77 (46%) | 0 0 |
| 14 | LN | 110/111 (99%) | 58 (53%) | 52 (47%) | 0 0 |
| 15 | LO | 174/175 (99%) | 88 (51%) | 86 (49%) | 0 0 |
| 16 | LP | 162/165 (98%) | 95 (59%) | 67 (41%) | 0 0 |
| 17 | LQ | 133/139 (96%) | 73 (55%) | 60 (45%) | 0 0 |
| 18 | LR | 154/155 (99%) | 88 (57%) | 66 (43%) | 0 0 |
| 19 | LS | 163/167 (98%) | 86 (53%) | 77 (47%) | 0 0 |
| 20 | LT | 151/154 (98%) | 93 (62%) | 58 (38%) | 0 1 |
| 21 | LU | 131/133 (98%) | 80 (61%) | 51 (39%) | 0 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 22 | LV | 101/110 (92%) | 53 (52%) | 48 (48%) | 0 | 0 |
| 23 | LW | 109/114 (96%) | 68 (62%) | 41 (38%) | 0 | 1 |
| 24 | LX | 61/174 (35%) | 37 (61%) | 24 (39%) | 0 | 1 |
| 25 | LY | 107/123 (87%) | 53 (50%) | 54 (50%) | 0 | 0 |
| 26 | LZ | 114/115 (99%) | 63 (55%) | 51 (45%) | 0 | 0 |
| 27 | La | 116/119 (98%) | 73 (63%) | 43 (37%) | 0 | 1 |
| 28 | Lb | 126/127 (99%) | 74 (59%) | 52 (41%) | 0 | 0 |
| 29 | Lc | 50/57 (88%) | 27 (54%) | 23 (46%) | 0 | 0 |
| 30 | Ld | 83/92 (90%) | 51 (61%) | 32 (39%) | 0 | 1 |
| 31 | Le | 88/92 (96%) | 48 (54%) | 40 (46%) | 0 | 0 |
| 32 | Lf | 116/120 (97%) | 61 (53%) | 55 (47%) | 0 | 0 |
| 33 | Lg | 82/103 (80%) | 39 (48%) | 43 (52%) | 0 | 0 |
| 34 | Lh | 97/100 (97%) | 51 (53%) | 46 (47%) | 0 | 0 |
| 35 | Li | 105/107 (98%) | 65 (62%) | 40 (38%) | 0 | 1 |
| 36 | Lj | 77/78 (99%) | 45 (58%) | 32 (42%) | 0 | 0 |
| 37 | Lk | 73/74 (99%) | 47 (64%) | 26 (36%) | 0 | 1 |
| 38 | Ll | 63/68 (93%) | 25 (40%) | 38 (60%) | 0 | 0 |
| 39 | Ln | 173/189 (92%) | 73 (42%) | 100 (58%) | 0 | 0 |
| 40 | Lo | 22/22 (100%) | 11 (50%) | 11 (50%) | 0 | 0 |
| 41 | Lp | 83/93 (89%) | 45 (54%) | 38 (46%) | 0 | 0 |
| 42 | Lq | 71/73 (97%) | 34 (48%) | 37 (52%) | 0 | 0 |
| 43 | Ls | 43/110 (39%) | 23 (54%) | 20 (46%) | 0 | 0 |
| 45 | SA | 172/217 (79%) | 101 (59%) | 71 (41%) | 0 | 0 |
| 46 | SB | 179/201 (89%) | 96 (54%) | 83 (46%) | 0 | 0 |
| 47 | SC | 175/182 (96%) | 88 (50%) | 87 (50%) | 0 | 0 |
| 48 | SD | 208/220 (94%) | 112 (54%) | 96 (46%) | 0 | 0 |
| 49 | SE | 228/232 (98%) | 106 (46%) | 122 (54%) | 0 | 0 |
| 50 | SF | 153/157 (98%) | 79 (52%) | 74 (48%) | 0 | 0 |
| 51 | SG | 204/213 (96%) | 102 (50%) | 102 (50%) | 0 | 0 |
| 52 | SH | 165/170 (97%) | 82 (50%) | 83 (50%) | 0 | 0 |
| 53 | SI | 147/148 (99%) | 74 (50%) | 73 (50%) | 0 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 54 | SJ | 114/115 (99%) | 53 (46%) | 61 (54%) | 0 | 0 |
| 55 | SK | 155/164 (94%) | 78 (50%) | 77 (50%) | 0 | 0 |
| 56 | SL | 96/119 (81%) | 57 (59%) | 39 (41%) | 0 | 1 |
| 57 | SM | 135/136 (99%) | 65 (48%) | 70 (52%) | 0 | 0 |
| 58 | SO | 111/114 (97%) | 57 (51%) | 54 (49%) | 0 | 0 |
| 59 | SP | 124/129 (96%) | 69 (56%) | 55 (44%) | 0 | 0 |
| 60 | SQ | 87/112 (78%) | 47 (54%) | 40 (46%) | 0 | 0 |
| 61 | SR | 104/128 (81%) | 54 (52%) | 50 (48%) | 0 | 0 |
| 62 | ST | 125/130 (96%) | 66 (53%) | 59 (47%) | 0 | 0 |
| 63 | SU | 109/124 (88%) | 54 (50%) | 55 (50%) | 0 | 0 |
| 64 | SV | 123/131 (94%) | 61 (50%) | 62 (50%) | 0 | 0 |
| 65 | SW | 114/115 (99%) | 57 (50%) | 57 (50%) | 0 | 0 |
| 66 | SX | 90/110 (82%) | 55 (61%) | 35 (39%) | 0 | 1 |
| 67 | SY | 69/72 (96%) | 41 (59%) | 28 (41%) | 0 | 1 |
| 68 | Sb | 104/113 (92%) | 57 (55%) | 47 (45%) | 0 | 0 |
| 69 | Sc | 67/79 (85%) | 27 (40%) | 40 (60%) | 0 | 0 |
| 70 | Sd | 102/103 (99%) | 52 (51%) | 50 (49%) | 0 | 0 |
| 71 | Se | 72/73 (99%) | 33 (46%) | 39 (54%) | 0 | 0 |
| 72 | Sg | 56/57 (98%) | 15 (27%) | 41 (73%) | 0 | 0 |
| 73 | Sh | 44/45 (98%) | 19 (43%) | 25 (57%) | 0 | 0 |
| 74 | Sj | 57/58 (98%) | 25 (44%) | 32 (56%) | 0 | 0 |
| All | All | 8883/9573 (93%) | 4796 (54%) | 4087 (46%) | 0 | 0 |

All (4087) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | LA | 4 | ARG |
| 1 | LA | 5 | ILE |
| 1 | LA | 6 | ARG |
| 1 | LA | 10 | LYS |
| 1 | LA | 14 | SER |
| 1 | LA | 22 | ARG |
| 1 | LA | 29 | LEU |
| 1 | LA | 30 | ARG |
| 1 | LA | 36 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | LA | 41 | VAL |
| 1 | LA | 42 | ARG |
| 1 | LA | 44 | VAL |
| 1 | LA | 48 | ILE |
| 1 | LA | 49 | LEU |
| 1 | LA | 52 | ARG |
| 1 | LA | 58 | LEU |
| 1 | LA | 61 | VAL |
| 1 | LA | 62 | GLN |
| 1 | LA | 66 | MET |
| 1 | LA | 67 | ARG |
| 1 | LA | 69 | GLU |
| 1 | LA | 71 | ARG |
| 1 | LA | 72 | VAL |
| 1 | LA | 74 | GLU |
| 1 | LA | 77 | ILE |
| 1 | LA | 82 | MET |
| 1 | LA | 84 | THR |
| 1 | LA | 87 | GLU |
| 1 | LA | 88 | VAL |
| 1 | LA | 89 | PHE |
| 1 | LA | 90 | SER |
| 1 | LA | 93 | LYS |
| 1 | LA | 96 | LEU |
| 1 | LA | 97 | HIS |
| 1 | LA | 98 | ILE |
| 1 | LA | 102 | LEU |
| 1 | LA | 104 | VAL |
| 1 | LA | 107 | ILE |
| 1 | LA | 109 | GLU |
| 1 | LA | 111 | THR |
| 1 | LA | 112 | TYR |
| 1 | LA | 113 | VAL |
| 1 | LA | 116 | VAL |
| 1 | LA | 118 | GLU |
| 1 | LA | 119 | LYS |
| 1 | LA | 121 | MET |
| 1 | LA | 122 | ASP |
| 1 | LA | 123 | ARG |
| 1 | LA | 125 | CYS |
| 1 | LA | 126 | LEU |
| 1 | LA | 134 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | LA | 141 | MET |
| 1 | LA | 142 | GLU |
| 1 | LA | 143 | THR |
| 1 | LA | 145 | LYS |
| 1 | LA | 147 | ARG |
| 1 | LA | 154 | GLN |
| 1 | LA | 155 | LYS |
| 1 | LA | 156 | LYS |
| 1 | LA | 157 | LEU |
| 1 | LA | 160 | SER |
| 1 | LA | 165 | MET |
| 1 | LA | 166 | ILE |
| 1 | LA | 168 | LEU |
| 1 | LA | 174 | ARG |
| 1 | LA | 176 | ASP |
| 1 | LA | 179 | LEU |
| 1 | LA | 180 | LEU |
| 1 | LA | 181 | LYS |
| 1 | LA | 188 | LYS |
| 1 | LA | 192 | LYS |
| 1 | LA | 193 | ARG |
| 1 | LA | 198 | VAL |
| 1 | LA | 199 | VAL |
| 1 | LA | 204 | MET |
| 1 | LA | 215 | ASN |
| 1 | LA | 217 | GLN |
| 1 | LA | 219 | ILE |
| 1 | LA | 221 | VAL |
| 1 | LA | 222 | SER |
| 1 | LA | 231 | PRO |
| 1 | LA | 234 | LYS |
| 1 | LA | 235 | VAL |
| 1 | LA | 237 | LEU |
| 1 | LA | 241 | ARG |
| 1 | LA | 242 | ARG |
| 1 | LA | 243 | THR |
| 1 | LA | 246 | SER |
| 1 | LA | 249 | LYS |
| 1 | LA | 250 | ARG |
| 1 | LA | 251 | ARG |
| 2 | LB | 10 | ARG |
| 2 | LB | 14 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | LB | 20 | LYS |
| 2 | LB | 24 | ARG |
| 2 | LB | 26 | ARG |
| 2 | LB | 28 | ARG |
| 2 | LB | 29 | CYS |
| 2 | LB | 33 | PRO |
| 2 | LB | 35 | ASP |
| 2 | LB | 36 | VAL |
| 2 | LB | 37 | GLN |
| 2 | LB | 41 | ILE |
| 2 | LB | 42 | HIS |
| 2 | LB | 54 | THR |
| 2 | LB | 55 | HIS |
| 2 | LB | 56 | VAL |
| 2 | LB | 58 | ARG |
| 2 | LB | 60 | ILE |
| 2 | LB | 62 | HIS |
| 2 | LB | 63 | ARG |
| 2 | LB | 65 | SER |
| 2 | LB | 67 | LEU |
| 2 | LB | 71 | GLN |
| 2 | LB | 74 | ASP |
| 2 | LB | 75 | GLN |
| 2 | LB | 78 | ILE |
| 2 | LB | 79 | ILE |
| 2 | LB | 84 | MET |
| 2 | LB | 85 | ILE |
| 2 | LB | 87 | THR |
| 2 | LB | 90 | ILE |
| 2 | LB | 95 | THR |
| 2 | LB | 97 | LYS |
| 2 | LB | 102 | VAL |
| 2 | LB | 110 | ILE |
| 2 | LB | 112 | GLU |
| 2 | LB | 117 | ARG |
| 2 | LB | 121 | ASN |
| 2 | LB | 126 | GLU |
| 2 | LB | 132 | THR |
| 2 | LB | 134 | MET |
| 2 | LB | 136 | LYS |
| 2 | LB | 139 | ASP |
| 2 | LB | 141 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | LB | 144 | LYS |
| 2 | LB | 146 | GLN |
| 2 | LB | 147 | LEU |
| 2 | LB | 152 | GLN |
| 2 | LB | 155 | ASP |
| 2 | LB | 160 | VAL |
| 2 | LB | 162 | HIS |
| 2 | LB | 163 | THR |
| 2 | LB | 168 | THR |
| 2 | LB | 170 | LEU |
| 2 | LB | 171 | LYS |
| 2 | LB | 174 | LYS |
| 2 | LB | 176 | ASP |
| 2 | LB | 182 | VAL |
| 2 | LB | 183 | ASN |
| 2 | LB | 187 | ASN |
| 2 | LB | 188 | VAL |
| 2 | LB | 190 | GLU |
| 2 | LB | 192 | VAL |
| 2 | LB | 198 | LEU |
| 2 | LB | 199 | MET |
| 2 | LB | 203 | ILE |
| 2 | LB | 206 | LYS |
| 2 | LB | 207 | ASP |
| 2 | LB | 210 | SER |
| 2 | LB | 211 | VAL |
| 2 | LB | 215 | ILE |
| 2 | LB | 219 | SER |
| 2 | LB | 220 | ILE |
| 2 | LB | 227 | GLU |
| 2 | LB | 229 | VAL |
| 2 | LB | 231 | THR |
| 2 | LB | 232 | ARG |
| 2 | LB | 235 | VAL |
| 2 | LB | 237 | ARG |
| 2 | LB | 240 | ARG |
| 2 | LB | 241 | LYS |
| 2 | LB | 242 | THR |
| 2 | LB | 248 | LYS |
| 2 | LB | 249 | VAL |
| 2 | LB | 251 | CYS |
| 2 | LB | 256 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | LB | 261 | GLN |
| 2 | LB | 266 | ARG |
| 2 | LB | 269 | GLN |
| 2 | LB | 270 | MET |
| 2 | LB | 272 | TYR |
| 2 | LB | 273 | PHE |
| 2 | LB | 276 | THR |
| 2 | LB | 280 | LYS |
| 2 | LB | 282 | VAL |
| 2 | LB | 287 | THR |
| 2 | LB | 289 | GLU |
| 2 | LB | 292 | ARG |
| 2 | LB | 294 | CYS |
| 2 | LB | 295 | THR |
| 2 | LB | 297 | GLU |
| 2 | LB | 302 | ASP |
| 2 | LB | 303 | LYS |
| 2 | LB | 304 | SER |
| 2 | LB | 316 | ARG |
| 2 | LB | 318 | GLN |
| 2 | LB | 320 | ASP |
| 2 | LB | 323 | MET |
| 2 | LB | 324 | ILE |
| 2 | LB | 325 | LYS |
| 2 | LB | 332 | LYS |
| 2 | LB | 337 | VAL |
| 2 | LB | 338 | MET |
| 2 | LB | 342 | LEU |
| 2 | LB | 343 | LEU |
| 2 | LB | 351 | VAL |
| 2 | LB | 353 | LEU |
| 2 | LB | 354 | GLN |
| 2 | LB | 357 | SER |
| 2 | LB | 360 | SER |
| 2 | LB | 366 | ILE |
| 2 | LB | 368 | GLU |
| 2 | LB | 370 | VAL |
| 2 | LB | 373 | ARG |
| 2 | LB | 379 | LYS |
| 3 | LC | 2 | ASN |
| 3 | LC | 6 | LYS |
| 3 | LC | 11 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | LC | 13 | THR |
| 3 | LC | 15 | VAL |
| 3 | LC | 20 | ARG |
| 3 | LC | 22 | LYS |
| 3 | LC | 23 | VAL |
| 3 | LC | 28 | LEU |
| 3 | LC | 32 | ILE |
| 3 | LC | 33 | ILE |
| 3 | LC | 40 | LEU |
| 3 | LC | 46 | THR |
| 3 | LC | 50 | VAL |
| 3 | LC | 52 | ARG |
| 3 | LC | 56 | VAL |
| 3 | LC | 57 | GLN |
| 3 | LC | 58 | CYS |
| 3 | LC | 63 | TRP |
| 3 | LC | 69 | VAL |
| 3 | LC | 71 | ARG |
| 3 | LC | 72 | LEU |
| 3 | LC | 75 | LYS |
| 3 | LC | 76 | HIS |
| 3 | LC | 91 | MET |
| 3 | LC | 98 | ILE |
| 3 | LC | 104 | LYS |
| 3 | LC | 105 | VAL |
| 3 | LC | 106 | ASN |
| 3 | LC | 107 | LEU |
| 3 | LC | 110 | ARG |
| 3 | LC | 116 | SER |
| 3 | LC | 121 | SER |
| 3 | LC | 126 | LEU |
| 3 | LC | 130 | ARG |
| 3 | LC | 134 | ILE |
| 3 | LC | 139 | SER |
| 3 | LC | 144 | VAL |
| 3 | LC | 146 | THR |
| 3 | LC | 149 | VAL |
| 3 | LC | 150 | THR |
| 3 | LC | 151 | LYS |
| 3 | LC | 153 | LYS |
| 3 | LC | 156 | LEU |
| 3 | LC | 158 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | LC | 159 | ILE |
| 3 | LC | 160 | LYS |
| 3 | LC | 164 | VAL |
| 3 | LC | 165 | LEU |
| 3 | LC | 170 | ARG |
| 3 | LC | 174 | SER |
| 3 | LC | 175 | ARG |
| 3 | LC | 177 | ILE |
| 3 | LC | 178 | ARG |
| 3 | LC | 184 | MET |
| 3 | LC | 185 | ARG |
| 3 | LC | 187 | ARG |
| 3 | LC | 188 | ARG |
| 3 | LC | 190 | ILE |
| 3 | LC | 192 | ARG |
| 3 | LC | 193 | LYS |
| 3 | LC | 197 | VAL |
| 3 | LC | 198 | ILE |
| 3 | LC | 201 | THR |
| 3 | LC | 202 | GLU |
| 3 | LC | 214 | VAL |
| 3 | LC | 215 | ASP |
| 3 | LC | 216 | LEU |
| 3 | LC | 219 | VAL |
| 3 | LC | 220 | SER |
| 3 | LC | 222 | ILE |
| 3 | LC | 224 | LEU |
| 3 | LC | 225 | LEU |
| 3 | LC | 231 | SER |
| 3 | LC | 235 | ARG |
| 3 | LC | 237 | ILE |
| 3 | LC | 239 | TRP |
| 3 | LC | 241 | LYS |
| 3 | LC | 248 | ASP |
| 3 | LC | 254 | LYS |
| 3 | LC | 255 | GLN |
| 3 | LC | 256 | ASN |
| 3 | LC | 258 | THR |
| 3 | LC | 262 | SER |
| 3 | LC | 264 | ILE |
| 3 | LC | 268 | ASP |
| 3 | LC | 269 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | LC | 271 | ARG |
| 3 | LC | 274 | GLN |
| 3 | LC | 276 | ASP |
| 3 | LC | 278 | VAL |
| 3 | LC | 280 | LYS |
| 3 | LC | 283 | VAL |
| 3 | LC | 285 | LYS |
| 3 | LC | 286 | ARG |
| 3 | LC | 289 | LEU |
| 3 | LC | 290 | VAL |
| 3 | LC | 291 | ILE |
| 3 | LC | 295 | VAL |
| 3 | LC | 300 | SER |
| 3 | LC | 301 | LYS |
| 3 | LC | 302 | GLU |
| 3 | LC | 304 | LEU |
| 3 | LC | 307 | LEU |
| 3 | LC | 310 | SER |
| 3 | LC | 312 | THR |
| 6 | LF | 6 | VAL |
| 6 | LF | 7 | GLN |
| 6 | LF | 8 | LYS |
| 6 | LF | 9 | THR |
| 6 | LF | 10 | ARG |
| 6 | LF | 11 | SER |
| 6 | LF | 14 | LYS |
| 6 | LF | 15 | ARG |
| 6 | LF | 16 | PHE |
| 6 | LF | 19 | GLN |
| 6 | LF | 21 | ARG |
| 6 | LF | 27 | LYS |
| 6 | LF | 33 | ARG |
| 6 | LF | 34 | LYS |
| 6 | LF | 37 | ILE |
| 6 | LF | 39 | GLN |
| 6 | LF | 41 | LYS |
| 6 | LF | 43 | LYS |
| 6 | LF | 50 | ARG |
| 6 | LF | 52 | VAL |
| 6 | LF | 54 | ARG |
| 6 | LF | 56 | THR |
| 6 | LF | 57 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | LF | 58 | LYS |
| 6 | LF | 60 | ILE |
| 6 | LF | 61 | ILE |
| 6 | LF | 63 | GLN |
| 6 | LF | 64 | VAL |
| 6 | LF | 68 | GLU |
| 6 | LF | 69 | LEU |
| 6 | LF | 70 | THR |
| 6 | LF | 71 | LYS |
| 6 | LF | 72 | ASP |
| 6 | LF | 76 | CYS |
| 6 | LF | 80 | SER |
| 6 | LF | 88 | ILE |
| 6 | LF | 93 | THR |
| 6 | LF | 101 | THR |
| 6 | LF | 105 | CYS |
| 6 | LF | 112 | LYS |
| 6 | LF | 113 | LEU |
| 6 | LF | 117 | ILE |
| 6 | LF | 118 | LYS |
| 6 | LF | 119 | GLU |
| 6 | LF | 122 | LEU |
| 6 | LF | 124 | GLN |
| 6 | LF | 130 | ASP |
| 6 | LF | 131 | LYS |
| 6 | LF | 133 | THR |
| 6 | LF | 135 | GLU |
| 6 | LF | 140 | ASP |
| 6 | LF | 141 | GLU |
| 6 | LF | 142 | ASN |
| 6 | LF | 144 | ASN |
| 6 | LF | 145 | GLU |
| 6 | LF | 146 | GLU |
| 6 | LF | 151 | LYS |
| 6 | LF | 158 | LEU |
| 6 | LF | 166 | ARG |
| 6 | LF | 167 | VAL |
| 6 | LF | 171 | MET |
| 6 | LF | 172 | LYS |
| 6 | LF | 175 | VAL |
| 6 | LF | 179 | LEU |
| 6 | LF | 181 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | LF | 184 | SER |
| 6 | LF | 186 | LYS |
| 6 | LF | 187 | ARG |
| 6 | LF | 193 | LYS |
| 6 | LF | 194 | ASP |
| 6 | LF | 198 | SER |
| 6 | LF | 199 | SER |
| 6 | LF | 201 | LEU |
| 6 | LF | 202 | ARG |
| 6 | LF | 203 | ASP |
| 6 | LF | 205 | ILE |
| 6 | LF | 206 | MET |
| 6 | LF | 208 | LYS |
| 6 | LF | 216 | GLU |
| 6 | LF | 217 | LEU |
| 6 | LF | 221 | ASP |
| 6 | LF | 223 | GLU |
| 6 | LF | 231 | LYS |
| 6 | LF | 237 | VAL |
| 6 | LF | 240 | LEU |
| 6 | LF | 241 | ARG |
| 6 | LF | 242 | LEU |
| 6 | LF | 254 | ARG |
| 6 | LF | 256 | ASN |
| 6 | LF | 261 | LYS |
| 6 | LF | 263 | LYS |
| 6 | LF | 265 | GLU |
| 6 | LF | 266 | ILE |
| 6 | LF | 267 | LYS |
| 6 | LF | 268 | LYS |
| 6 | LF | 274 | ARG |
| 6 | LF | 276 | THR |
| 6 | LF | 279 | GLU |
| 6 | LF | 282 | GLU |
| 6 | LF | 283 | ARG |
| 6 | LF | 284 | ILE |
| 6 | LF | 287 | LYS |
| 6 | LF | 288 | LYS |
| 6 | LF | 289 | LEU |
| 6 | LF | 290 | GLU |
| 7 | LG | 5 | LYS |
| 7 | LG | 8 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | LG | 9 | ARG |
| 7 | LG | 11 | LEU |
| 7 | LG | 18 | LYS |
| 7 | LG | 21 | LYS |
| 7 | LG | 23 | ILE |
| 7 | LG | 25 | ARG |
| 7 | LG | 28 | ILE |
| 7 | LG | 30 | LYS |
| 7 | LG | 33 | LEU |
| 7 | LG | 34 | LYS |
| 7 | LG | 36 | THR |
| 7 | LG | 37 | TRP |
| 7 | LG | 39 | TYR |
| 7 | LG | 40 | LYS |
| 7 | LG | 41 | ARG |
| 7 | LG | 46 | ARG |
| 7 | LG | 49 | LEU |
| 7 | LG | 51 | LEU |
| 8 | LH | 20 | SER |
| 8 | LH | 23 | GLU |
| 8 | LH | 24 | ARG |
| 8 | LH | 28 | LYS |
| 8 | LH | 29 | GLU |
| 8 | LH | 31 | ARG |
| 8 | LH | 34 | LEU |
| 8 | LH | 36 | LYS |
| 8 | LH | 38 | HIS |
| 8 | LH | 41 | LYS |
| 8 | LH | 48 | ARG |
| 8 | LH | 51 | ILE |
| 8 | LH | 54 | VAL |
| 8 | LH | 57 | GLU |
| 8 | LH | 59 | LYS |
| 8 | LH | 61 | ARG |
| 8 | LH | 62 | GLU |
| 8 | LH | 63 | ASN |
| 8 | LH | 65 | LEU |
| 8 | LH | 66 | LYS |
| 8 | LH | 70 | LEU |
| 8 | LH | 72 | VAL |
| 8 | LH | 74 | ASP |
| 8 | LH | 75 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | LH | 77 | LYS |
| 8 | LH | 79 | TYR |
| 8 | LH | 80 | LEU |
| 8 | LH | 81 | VAL |
| 8 | LH | 83 | ARG |
| 8 | LH | 84 | ILE |
| 8 | LH | 87 | ILE |
| 8 | LH | 88 | VAL |
| 8 | LH | 93 | LYS |
| 8 | LH | 94 | VAL |
| 8 | LH | 96 | THR |
| 8 | LH | 101 | LEU |
| 8 | LH | 102 | ARG |
| 8 | LH | 103 | LEU |
| 8 | LH | 106 | ILE |
| 8 | LH | 116 | LYS |
| 8 | LH | 119 | LEU |
| 8 | LH | 120 | ASN |
| 8 | LH | 122 | LEU |
| 8 | LH | 130 | THR |
| 8 | LH | 136 | VAL |
| 8 | LH | 139 | ILE |
| 8 | LH | 143 | ILE |
| 8 | LH | 146 | ARG |
| 8 | LH | 150 | LYS |
| 8 | LH | 151 | VAL |
| 8 | LH | 152 | ASN |
| 8 | LH | 158 | ILE |
| 8 | LH | 163 | LEU |
| 8 | LH | 164 | ILE |
| 8 | LH | 170 | LYS |
| 8 | LH | 173 | ILE |
| 8 | LH | 174 | LEU |
| 8 | LH | 177 | GLU |
| 8 | LH | 178 | ASP |
| 8 | LH | 183 | ILE |
| 8 | LH | 186 | CYS |
| 8 | LH | 188 | SER |
| 8 | LH | 189 | SER |
| 8 | LH | 196 | PHE |
| 8 | LH | 197 | LEU |
| 8 | LH | 207 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | LH | 208 | LYS |
| 8 | LH | 210 | LYS |
| 8 | LH | 211 | ARG |
| 8 | LH | 227 | ILE |
| 8 | LH | 230 | PHE |
| 8 | LH | 233 | ARG |
| 8 | LH | 234 | MET |
| 8 | LH | 235 | ILE |
| 9 | LI | 28 | LEU |
| 9 | LI | 29 | THR |
| 9 | LI | 31 | PHE |
| 9 | LI | 47 | LEU |
| 9 | LI | 48 | GLN |
| 9 | LI | 50 | ARG |
| 9 | LI | 51 | LEU |
| 9 | LI | 52 | LYS |
| 9 | LI | 56 | THR |
| 9 | LI | 57 | VAL |
| 9 | LI | 59 | GLN |
| 9 | LI | 61 | MET |
| 9 | LI | 64 | ILE |
| 9 | LI | 65 | SER |
| 9 | LI | 66 | ARG |
| 9 | LI | 69 | THR |
| 9 | LI | 71 | GLU |
| 9 | LI | 72 | ILE |
| 9 | LI | 75 | LEU |
| 9 | LI | 80 | SER |
| 9 | LI | 85 | GLU |
| 9 | LI | 86 | GLU |
| 9 | LI | 88 | LYS |
| 9 | LI | 92 | LEU |
| 9 | LI | 94 | ILE |
| 9 | LI | 98 | LYS |
| 9 | LI | 104 | LEU |
| 9 | LI | 106 | GLU |
| 9 | LI | 107 | LYS |
| 9 | LI | 111 | LEU |
| 9 | LI | 112 | VAL |
| 9 | LI | 113 | ILE |
| 9 | LI | 117 | ILE |
| 9 | LI | 118 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | LI | 120 | ILE |
| 9 | LI | 122 | SER |
| 9 | LI | 123 | LEU |
| 9 | LI | 126 | SER |
| 9 | LI | 128 | ARG |
| 9 | LI | 130 | LYS |
| 9 | LI | 132 | VAL |
| 9 | LI | 133 | LEU |
| 9 | LI | 134 | ILE |
| 9 | LI | 138 | VAL |
| 9 | LI | 141 | LEU |
| 9 | LI | 142 | GLU |
| 9 | LI | 143 | LEU |
| 9 | LI | 145 | LEU |
| 9 | LI | 149 | THR |
| 9 | LI | 153 | LYS |
| 9 | LI | 154 | MET |
| 9 | LI | 156 | VAL |
| 9 | LI | 160 | ILE |
| 9 | LI | 163 | THR |
| 9 | LI | 164 | LYS |
| 9 | LI | 169 | LYS |
| 9 | LI | 171 | VAL |
| 9 | LI | 173 | LEU |
| 9 | LI | 175 | LYS |
| 9 | LI | 179 | VAL |
| 9 | LI | 182 | THR |
| 9 | LI | 183 | ASP |
| 9 | LI | 184 | VAL |
| 9 | LI | 187 | GLU |
| 9 | LI | 196 | LEU |
| 9 | LI | 201 | HIS |
| 9 | LI | 207 | LYS |
| 9 | LI | 210 | LYS |
| 9 | LI | 212 | TYR |
| 9 | LI | 216 | VAL |
| 9 | LI | 219 | GLU |
| 9 | LI | 221 | GLU |
| 10 | LJ | 7 | MET |
| 10 | LJ | 8 | THR |
| 10 | LJ | 9 | ILE |
| 10 | LJ | 13 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | LJ | 16 | GLU |
| 10 | LJ | 17 | CYS |
| 10 | LJ | 18 | THR |
| 10 | LJ | 19 | ILE |
| 10 | LJ | 20 | ASN |
| 10 | LJ | 23 | VAL |
| 10 | LJ | 25 | THR |
| 10 | LJ | 29 | LYS |
| 10 | LJ | 30 | LYS |
| 10 | LJ | 32 | THR |
| 10 | LJ | 33 | LEU |
| 10 | LJ | 39 | HIS |
| 10 | LJ | 42 | LEU |
| 10 | LJ | 43 | ASP |
| 10 | LJ | 44 | ILE |
| 10 | LJ | 45 | THR |
| 10 | LJ | 49 | ASP |
| 10 | LJ | 51 | ILE |
| 10 | LJ | 52 | SER |
| 10 | LJ | 53 | VAL |
| 10 | LJ | 61 | LYS |
| 10 | LJ | 65 | LEU |
| 10 | LJ | 67 | ARG |
| 10 | LJ | 69 | ILE |
| 10 | LJ | 70 | CYS |
| 10 | LJ | 73 | ILE |
| 10 | LJ | 74 | GLU |
| 10 | LJ | 76 | MET |
| 10 | LJ | 78 | LYS |
| 10 | LJ | 81 | THR |
| 10 | LJ | 85 | GLU |
| 10 | LJ | 87 | LYS |
| 10 | LJ | 89 | ARG |
| 10 | LJ | 90 | LEU |
| 10 | LJ | 97 | ILE |
| 10 | LJ | 100 | THR |
| 10 | LJ | 101 | VAL |
| 10 | LJ | 102 | VAL |
| 10 | LJ | 106 | LYS |
| 10 | LJ | 108 | ILE |
| 10 | LJ | 110 | ILE |
| 10 | LJ | 111 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | LJ | 115 | HIS |
| 10 | LJ | 119 | THR |
| 10 | LJ | 120 | ARG |
| 10 | LJ | 121 | ARG |
| 10 | LJ | 128 | VAL |
| 10 | LJ | 129 | THR |
| 10 | LJ | 132 | MET |
| 10 | LJ | 133 | SER |
| 10 | LJ | 134 | THR |
| 10 | LJ | 136 | VAL |
| 10 | LJ | 137 | LYS |
| 10 | LJ | 143 | ARG |
| 10 | LJ | 145 | ILE |
| 10 | LJ | 146 | SER |
| 10 | LJ | 156 | ARG |
| 10 | LJ | 157 | ILE |
| 10 | LJ | 159 | GLU |
| 10 | LJ | 161 | LEU |
| 10 | LJ | 163 | VAL |
| 10 | LJ | 168 | LEU |
| 10 | LJ | 169 | ARG |
| 10 | LJ | 177 | VAL |
| 10 | LJ | 179 | SER |
| 10 | LJ | 182 | LEU |
| 10 | LJ | 185 | GLN |
| 11 | LK | 3 | ARG |
| 11 | LK | 7 | ARG |
| 11 | LK | 12 | GLN |
| 11 | LK | 14 | ASN |
| 11 | LK | 15 | LYS |
| 11 | LK | 19 | LYS |
| 11 | LK | 20 | SER |
| 11 | LK | 21 | ARG |
| 11 | LK | 22 | PHE |
| 11 | LK | 24 | ARG |
| 11 | LK | 26 | VAL |
| 11 | LK | 31 | ILE |
| 11 | LK | 42 | LYS |
| 11 | LK | 43 | VAL |
| 11 | LK | 48 | TYR |
| 11 | LK | 53 | LEU |
| 11 | LK | 57 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | LK | 58 | GLU |
| 11 | LK | 61 | SER |
| 11 | LK | 62 | SER |
| 11 | LK | 66 | GLU |
| 11 | LK | 72 | CYS |
| 11 | LK | 73 | ASN |
| 11 | LK | 74 | LYS |
| 11 | LK | 76 | ILE |
| 11 | LK | 78 | LYS |
| 11 | LK | 82 | LYS |
| 11 | LK | 89 | ILE |
| 11 | LK | 90 | ARG |
| 11 | LK | 96 | VAL |
| 11 | LK | 97 | ILE |
| 11 | LK | 98 | ARG |
| 11 | LK | 101 | LYS |
| 11 | LK | 102 | MET |
| 11 | LK | 103 | LEU |
| 11 | LK | 104 | SER |
| 11 | LK | 105 | CYS |
| 11 | LK | 110 | ARG |
| 11 | LK | 111 | LEU |
| 11 | LK | 112 | GLN |
| 11 | LK | 115 | MET |
| 11 | LK | 116 | ARG |
| 11 | LK | 121 | LYS |
| 11 | LK | 122 | PRO |
| 11 | LK | 123 | GLN |
| 11 | LK | 125 | THR |
| 11 | LK | 129 | VAL |
| 11 | LK | 130 | SER |
| 11 | LK | 131 | ILE |
| 11 | LK | 135 | LEU |
| 11 | LK | 136 | LEU |
| 11 | LK | 139 | ARG |
| 11 | LK | 141 | ARG |
| 11 | LK | 145 | LYS |
| 11 | LK | 149 | LYS |
| 11 | LK | 153 | ARG |
| 11 | LK | 156 | LYS |
| 11 | LK | 158 | LYS |
| 11 | LK | 159 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | LK | 163 | GLN |
| 11 | LK | 165 | ILE |
| 11 | LK | 167 | GLU |
| 11 | LK | 169 | ARG |
| 11 | LK | 173 | PHE |
| 11 | LK | 174 | THR |
| 11 | LK | 178 | LYS |
| 11 | LK | 179 | GLU |
| 11 | LK | 185 | ARG |
| 11 | LK | 201 | SER |
| 11 | LK | 202 | ARG |
| 11 | LK | 206 | LEU |
| 12 | LL | 4 | GLU |
| 12 | LL | 5 | SER |
| 12 | LL | 6 | GLU |
| 12 | LL | 7 | ASN |
| 12 | LL | 9 | MET |
| 12 | LL | 14 | ILE |
| 12 | LL | 18 | VAL |
| 12 | LL | 19 | LEU |
| 12 | LL | 21 | ILE |
| 12 | LL | 23 | ILE |
| 12 | LL | 28 | ASP |
| 12 | LL | 30 | LEU |
| 12 | LL | 31 | THR |
| 12 | LL | 32 | LYS |
| 12 | LL | 36 | VAL |
| 12 | LL | 37 | LEU |
| 12 | LL | 39 | GLN |
| 12 | LL | 42 | ASP |
| 12 | LL | 46 | THR |
| 12 | LL | 49 | LYS |
| 12 | LL | 52 | LEU |
| 12 | LL | 53 | THR |
| 12 | LL | 54 | ILE |
| 12 | LL | 55 | ARG |
| 12 | LL | 57 | PHE |
| 12 | LL | 59 | ILE |
| 12 | LL | 60 | ARG |
| 12 | LL | 61 | ARG |
| 12 | LL | 64 | LYS |
| 12 | LL | 65 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | LL | 66 | SER |
| 12 | LL | 69 | VAL |
| 12 | LL | 70 | THR |
| 12 | LL | 75 | LYS |
| 12 | LL | 77 | ARG |
| 12 | LL | 84 | LEU |
| 12 | LL | 88 | ASN |
| 12 | LL | 90 | GLU |
| 12 | LL | 94 | SER |
| 12 | LL | 98 | THR |
| 12 | LL | 106 | ILE |
| 12 | LL | 110 | ILE |
| 12 | LL | 112 | LEU |
| 12 | LL | 117 | ASP |
| 12 | LL | 122 | ILE |
| 12 | LL | 129 | VAL |
| 12 | LL | 131 | LEU |
| 12 | LL | 133 | ARG |
| 12 | LL | 140 | LYS |
| 12 | LL | 151 | SER |
| 12 | LL | 152 | HIS |
| 12 | LL | 153 | LYS |
| 12 | LL | 154 | ILE |
| 12 | LL | 155 | THR |
| 12 | LL | 160 | ARG |
| 12 | LL | 165 | ARG |
| 12 | LL | 170 | VAL |
| 13 | LM | 33 | VAL |
| 13 | LM | 38 | MET |
| 13 | LM | 39 | ARG |
| 13 | LM | 44 | THR |
| 13 | LM | 49 | ASN |
| 13 | LM | 50 | LEU |
| 13 | LM | 51 | ILE |
| 13 | LM | 52 | LYS |
| 13 | LM | 53 | ASN |
| 13 | LM | 57 | GLN |
| 13 | LM | 60 | ARG |
| 13 | LM | 62 | ILE |
| 13 | LM | 63 | ARG |
| 13 | LM | 68 | ARG |
| 13 | LM | 69 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | LM | 73 | LYS |
| 13 | LM | 75 | ILE |
| 13 | LM | 78 | CYS |
| 13 | LM | 80 | LEU |
| 13 | LM | 81 | GLN |
| 13 | LM | 82 | LYS |
| 13 | LM | 86 | SER |
| 13 | LM | 87 | VAL |
| 13 | LM | 88 | THR |
| 13 | LM | 89 | ARG |
| 13 | LM | 90 | CYS |
| 13 | LM | 93 | LYS |
| 13 | LM | 96 | LEU |
| 13 | LM | 97 | THR |
| 13 | LM | 98 | GLN |
| 13 | LM | 99 | ARG |
| 13 | LM | 102 | ARG |
| 13 | LM | 106 | LEU |
| 13 | LM | 108 | GLU |
| 13 | LM | 112 | VAL |
| 13 | LM | 115 | SER |
| 13 | LM | 126 | VAL |
| 13 | LM | 129 | ARG |
| 13 | LM | 131 | LYS |
| 13 | LM | 134 | SER |
| 13 | LM | 137 | SER |
| 13 | LM | 145 | LEU |
| 13 | LM | 146 | LYS |
| 13 | LM | 149 | LEU |
| 13 | LM | 151 | LYS |
| 13 | LM | 152 | VAL |
| 13 | LM | 153 | THR |
| 13 | LM | 154 | ILE |
| 13 | LM | 157 | LYS |
| 13 | LM | 160 | LYS |
| 13 | LM | 162 | GLU |
| 13 | LM | 163 | GLU |
| 13 | LM | 166 | GLN |
| 13 | LM | 168 | ILE |
| 13 | LM | 173 | VAL |
| 13 | LM | 175 | MET |
| 13 | LM | 177 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | LM | 178 | VAL |
| 13 | LM | 179 | ASN |
| 13 | LM | 184 | ILE |
| 13 | LM | 186 | THR |
| 13 | LM | 189 | ILE |
| 13 | LM | 191 | GLU |
| 13 | LM | 195 | GLU |
| 13 | LM | 196 | VAL |
| 13 | LM | 198 | GLU |
| 13 | LM | 199 | ASN |
| 13 | LM | 200 | LEU |
| 13 | LM | 204 | LEU |
| 13 | LM | 206 | ASN |
| 13 | LM | 208 | ARG |
| 13 | LM | 218 | LYS |
| 13 | LM | 219 | ARG |
| 13 | LM | 222 | GLU |
| 13 | LM | 223 | ARG |
| 13 | LM | 224 | GLU |
| 13 | LM | 228 | LYS |
| 14 | LN | 2 | SER |
| 14 | LN | 4 | HIS |
| 14 | LN | 5 | ARG |
| 14 | LN | 6 | PHE |
| 14 | LN | 15 | LEU |
| 14 | LN | 21 | LYS |
| 14 | LN | 23 | LYS |
| 14 | LN | 24 | LEU |
| 14 | LN | 27 | ILE |
| 14 | LN | 28 | VAL |
| 14 | LN | 30 | ILE |
| 14 | LN | 38 | ILE |
| 14 | LN | 42 | THR |
| 14 | LN | 43 | THR |
| 14 | LN | 46 | LYS |
| 14 | LN | 47 | ARG |
| 14 | LN | 49 | VAL |
| 14 | LN | 52 | LEU |
| 14 | LN | 56 | MET |
| 14 | LN | 58 | THR |
| 14 | LN | 59 | ASP |
| 14 | LN | 61 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | LN | 62 | ILE |
| 14 | LN | 63 | ASN |
| 14 | LN | 65 | SER |
| 14 | LN | 67 | LYS |
| 14 | LN | 70 | THR |
| 14 | LN | 72 | GLN |
| 14 | LN | 77 | ILE |
| 14 | LN | 78 | GLU |
| 14 | LN | 80 | SER |
| 14 | LN | 83 | ILE |
| 14 | LN | 89 | SER |
| 14 | LN | 90 | VAL |
| 14 | LN | 93 | LYS |
| 14 | LN | 94 | LYS |
| 14 | LN | 95 | ILE |
| 14 | LN | 96 | GLN |
| 14 | LN | 100 | LEU |
| 14 | LN | 103 | LYS |
| 14 | LN | 105 | THR |
| 14 | LN | 107 | GLU |
| 14 | LN | 111 | LYS |
| 14 | LN | 114 | LYS |
| 14 | LN | 116 | ARG |
| 14 | LN | 118 | GLU |
| 14 | LN | 119 | ARG |
| 14 | LN | 120 | LYS |
| 14 | LN | 121 | MET |
| 14 | LN | 123 | MET |
| 14 | LN | 130 | ILE |
| 14 | LN | 131 | LYS |
| 15 | LO | 7 | VAL |
| 15 | LO | 9 | GLU |
| 15 | LO | 12 | ARG |
| 15 | LO | 13 | LYS |
| 15 | LO | 14 | LYS |
| 15 | LO | 15 | GLN |
| 15 | LO | 16 | SER |
| 15 | LO | 17 | GLU |
| 15 | LO | 19 | LEU |
| 15 | LO | 20 | HIS |
| 15 | LO | 23 | PHE |
| 15 | LO | 24 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | LO | 26 | ARG |
| 15 | LO | 32 | GLN |
| 15 | LO | 33 | LEU |
| 15 | LO | 36 | ILE |
| 15 | LO | 37 | LYS |
| 15 | LO | 39 | CYS |
| 15 | LO | 40 | SER |
| 15 | LO | 41 | HIS |
| 15 | LO | 44 | ARG |
| 15 | LO | 47 | LYS |
| 15 | LO | 49 | ARG |
| 15 | LO | 50 | ARG |
| 15 | LO | 51 | LEU |
| 15 | LO | 54 | LYS |
| 15 | LO | 56 | LYS |
| 15 | LO | 57 | ARG |
| 15 | LO | 60 | VAL |
| 15 | LO | 61 | VAL |
| 15 | LO | 62 | TYR |
| 15 | LO | 63 | ARG |
| 15 | LO | 64 | VAL |
| 15 | LO | 66 | VAL |
| 15 | LO | 67 | ARG |
| 15 | LO | 72 | LYS |
| 15 | LO | 73 | ARG |
| 15 | LO | 74 | GLN |
| 15 | LO | 76 | VAL |
| 15 | LO | 83 | LYS |
| 15 | LO | 85 | ARG |
| 15 | LO | 89 | ILE |
| 15 | LO | 90 | VAL |
| 15 | LO | 92 | LEU |
| 15 | LO | 96 | ARG |
| 15 | LO | 97 | SER |
| 15 | LO | 98 | LEU |
| 15 | LO | 101 | LEU |
| 15 | LO | 109 | ARG |
| 15 | LO | 112 | SER |
| 15 | LO | 114 | ARG |
| 15 | LO | 115 | VAL |
| 15 | LO | 118 | SER |
| 15 | LO | 121 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | LO | 124 | ASP |
| 15 | LO | 126 | SER |
| 15 | LO | 134 | LEU |
| 15 | LO | 135 | ILE |
| 15 | LO | 143 | ARG |
| 15 | LO | 147 | LYS |
| 15 | LO | 149 | ASN |
| 15 | LO | 151 | ILE |
| 15 | LO | 153 | ASN |
| 15 | LO | 157 | LYS |
| 15 | LO | 158 | ARG |
| 15 | LO | 159 | ARG |
| 15 | LO | 160 | GLU |
| 15 | LO | 162 | ARG |
| 15 | LO | 164 | LEU |
| 15 | LO | 165 | THR |
| 15 | LO | 170 | LYS |
| 15 | LO | 172 | ARG |
| 15 | LO | 174 | LEU |
| 15 | LO | 179 | ILE |
| 15 | LO | 183 | LYS |
| 15 | LO | 184 | LEU |
| 15 | LO | 185 | ARG |
| 15 | LO | 187 | SER |
| 15 | LO | 188 | LYS |
| 15 | LO | 193 | LYS |
| 15 | LO | 197 | THR |
| 15 | LO | 198 | ARG |
| 15 | LO | 200 | LEU |
| 15 | LO | 201 | ARG |
| 15 | LO | 202 | ARG |
| 15 | LO | 204 | ARG |
| 16 | LP | 4 | ILE |
| 16 | LP | 5 | VAL |
| 16 | LP | 12 | ILE |
| 16 | LP | 13 | LEU |
| 16 | LP | 16 | LEU |
| 16 | LP | 19 | ILE |
| 16 | LP | 23 | GLU |
| 16 | LP | 24 | LEU |
| 16 | LP | 25 | LEU |
| 16 | LP | 28 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | LP | 29 | GLU |
| 16 | LP | 33 | VAL |
| 16 | LP | 34 | ARG |
| 16 | LP | 35 | CYS |
| 16 | LP | 36 | GLU |
| 16 | LP | 37 | LYS |
| 16 | LP | 39 | ILE |
| 16 | LP | 40 | ILE |
| 16 | LP | 45 | ARG |
| 16 | LP | 48 | LYS |
| 16 | LP | 50 | HIS |
| 16 | LP | 53 | LYS |
| 16 | LP | 54 | LYS |
| 16 | LP | 55 | MET |
| 16 | LP | 58 | ARG |
| 16 | LP | 59 | THR |
| 16 | LP | 64 | LEU |
| 16 | LP | 65 | ARG |
| 16 | LP | 75 | GLU |
| 16 | LP | 81 | ILE |
| 16 | LP | 90 | VAL |
| 16 | LP | 93 | SER |
| 16 | LP | 96 | MET |
| 16 | LP | 99 | LEU |
| 16 | LP | 105 | ILE |
| 16 | LP | 108 | CYS |
| 16 | LP | 109 | CYS |
| 16 | LP | 114 | ARG |
| 16 | LP | 115 | VAL |
| 16 | LP | 116 | VAL |
| 16 | LP | 117 | CYS |
| 16 | LP | 119 | SER |
| 16 | LP | 121 | MET |
| 16 | LP | 123 | TYR |
| 16 | LP | 126 | LEU |
| 16 | LP | 127 | ARG |
| 16 | LP | 129 | GLU |
| 16 | LP | 130 | ARG |
| 16 | LP | 132 | ARG |
| 16 | LP | 135 | VAL |
| 16 | LP | 137 | ARG |
| 16 | LP | 138 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | LP | 142 | ILE |
| 16 | LP | 145 | GLN |
| 16 | LP | 150 | VAL |
| 16 | LP | 152 | ARG |
| 16 | LP | 155 | LYS |
| 16 | LP | 157 | ARG |
| 16 | LP | 158 | LEU |
| 16 | LP | 161 | CYS |
| 16 | LP | 171 | ILE |
| 16 | LP | 173 | LYS |
| 16 | LP | 174 | LYS |
| 16 | LP | 175 | ILE |
| 16 | LP | 187 | ARG |
| 16 | LP | 192 | LEU |
| 16 | LP | 194 | LYS |
| 17 | LQ | 2 | VAL |
| 17 | LQ | 3 | LYS |
| 17 | LQ | 7 | LYS |
| 17 | LQ | 11 | LEU |
| 17 | LQ | 13 | VAL |
| 17 | LQ | 15 | LYS |
| 17 | LQ | 17 | ARG |
| 17 | LQ | 18 | ARG |
| 17 | LQ | 19 | ASP |
| 17 | LQ | 22 | LYS |
| 17 | LQ | 26 | LYS |
| 17 | LQ | 35 | ILE |
| 17 | LQ | 36 | LYS |
| 17 | LQ | 40 | VAL |
| 17 | LQ | 41 | LYS |
| 17 | LQ | 42 | ARG |
| 17 | LQ | 47 | LEU |
| 17 | LQ | 51 | LEU |
| 17 | LQ | 55 | GLU |
| 17 | LQ | 63 | TYR |
| 17 | LQ | 64 | LYS |
| 17 | LQ | 66 | VAL |
| 17 | LQ | 68 | ARG |
| 17 | LQ | 70 | SER |
| 17 | LQ | 71 | GLN |
| 17 | LQ | 75 | SER |
| 17 | LQ | 78 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | LQ | 79 | LYS |
| 17 | LQ | 84 | GLU |
| 17 | LQ | 87 | VAL |
| 17 | LQ | 88 | VAL |
| 17 | LQ | 89 | VAL |
| 17 | LQ | 91 | LYS |
| 17 | LQ | 94 | LEU |
| 17 | LQ | 95 | LYS |
| 17 | LQ | 99 | SER |
| 17 | LQ | 102 | LYS |
| 17 | LQ | 105 | HIS |
| 17 | LQ | 106 | LYS |
| 17 | LQ | 107 | LYS |
| 17 | LQ | 109 | GLU |
| 17 | LQ | 110 | ASP |
| 17 | LQ | 112 | LEU |
| 17 | LQ | 115 | ILE |
| 17 | LQ | 121 | ARG |
| 17 | LQ | 125 | ARG |
| 17 | LQ | 127 | ARG |
| 17 | LQ | 128 | ARG |
| 17 | LQ | 129 | THR |
| 17 | LQ | 131 | ARG |
| 17 | LQ | 133 | HIS |
| 17 | LQ | 135 | ARG |
| 17 | LQ | 138 | LYS |
| 17 | LQ | 140 | GLU |
| 17 | LQ | 146 | VAL |
| 17 | LQ | 147 | GLU |
| 17 | LQ | 149 | ILE |
| 17 | LQ | 150 | VAL |
| 17 | LQ | 155 | LEU |
| 17 | LQ | 157 | VAL |
| 18 | LR | 3 | ILE |
| 18 | LR | 4 | ASP |
| 18 | LR | 5 | LEU |
| 18 | LR | 6 | LYS |
| 18 | LR | 7 | THR |
| 18 | LR | 10 | LYS |
| 18 | LR | 13 | LYS |
| 18 | LR | 18 | GLU |
| 18 | LR | 20 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | LR | 26 | ILE |
| 18 | LR | 34 | LYS |
| 18 | LR | 40 | THR |
| 18 | LR | 42 | GLU |
| 18 | LR | 52 | LEU |
| 18 | LR | 56 | LYS |
| 18 | LR | 57 | THR |
| 18 | LR | 63 | SER |
| 18 | LR | 66 | ARG |
| 18 | LR | 70 | LEU |
| 18 | LR | 73 | LYS |
| 18 | LR | 74 | ARG |
| 18 | LR | 76 | ASP |
| 18 | LR | 78 | ILE |
| 18 | LR | 80 | VAL |
| 18 | LR | 83 | SER |
| 18 | LR | 86 | THR |
| 18 | LR | 92 | VAL |
| 18 | LR | 94 | ILE |
| 18 | LR | 96 | ARG |
| 18 | LR | 97 | MET |
| 18 | LR | 98 | THR |
| 18 | LR | 99 | ILE |
| 18 | LR | 100 | CYS |
| 18 | LR | 103 | LYS |
| 18 | LR | 105 | SER |
| 18 | LR | 107 | THR |
| 18 | LR | 109 | ARG |
| 18 | LR | 110 | SER |
| 18 | LR | 111 | ARG |
| 18 | LR | 112 | ILE |
| 18 | LR | 113 | GLU |
| 18 | LR | 114 | LYS |
| 18 | LR | 119 | CYS |
| 18 | LR | 120 | MET |
| 18 | LR | 121 | SER |
| 18 | LR | 123 | ASP |
| 18 | LR | 125 | LEU |
| 18 | LR | 129 | LYS |
| 18 | LR | 131 | THR |
| 18 | LR | 136 | VAL |
| 18 | LR | 139 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | LR | 141 | ARG |
| 18 | LR | 145 | ARG |
| 18 | LR | 147 | VAL |
| 18 | LR | 148 | CYS |
| 18 | LR | 151 | PHE |
| 18 | LR | 156 | ARG |
| 18 | LR | 158 | ASN |
| 18 | LR | 159 | SER |
| 18 | LR | 164 | LYS |
| 18 | LR | 166 | GLU |
| 18 | LR | 168 | LYS |
| 18 | LR | 170 | ARG |
| 18 | LR | 174 | ARG |
| 18 | LR | 176 | ARG |
| 18 | LR | 179 | TRP |
| 19 | LS | 4 | LEU |
| 19 | LS | 5 | ARG |
| 19 | LS | 6 | LEU |
| 19 | LS | 7 | GLN |
| 19 | LS | 8 | LYS |
| 19 | LS | 10 | LEU |
| 19 | LS | 14 | VAL |
| 19 | LS | 15 | LEU |
| 19 | LS | 19 | LYS |
| 19 | LS | 23 | ARG |
| 19 | LS | 25 | ASN |
| 19 | LS | 30 | LYS |
| 19 | LS | 32 | ILE |
| 19 | LS | 34 | GLN |
| 19 | LS | 37 | SER |
| 19 | LS | 41 | ILE |
| 19 | LS | 43 | SER |
| 19 | LS | 44 | LEU |
| 19 | LS | 49 | ILE |
| 19 | LS | 52 | LYS |
| 19 | LS | 53 | LEU |
| 19 | LS | 55 | ILE |
| 19 | LS | 56 | LYS |
| 19 | LS | 58 | SER |
| 19 | LS | 59 | SER |
| 19 | LS | 62 | ARG |
| 19 | LS | 64 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | LS | 66 | ARG |
| 19 | LS | 71 | ARG |
| 19 | LS | 72 | LEU |
| 19 | LS | 74 | ARG |
| 19 | LS | 80 | LYS |
| 19 | LS | 81 | ARG |
| 19 | LS | 82 | ARG |
| 19 | LS | 84 | THR |
| 19 | LS | 85 | ARG |
| 19 | LS | 86 | GLU |
| 19 | LS | 88 | ARG |
| 19 | LS | 92 | LYS |
| 19 | LS | 93 | THR |
| 19 | LS | 94 | LEU |
| 19 | LS | 97 | GLN |
| 19 | LS | 103 | ARG |
| 19 | LS | 104 | ARG |
| 19 | LS | 113 | GLU |
| 19 | LS | 118 | HIS |
| 19 | LS | 119 | LEU |
| 19 | LS | 123 | LEU |
| 19 | LS | 131 | MET |
| 19 | LS | 133 | LYS |
| 19 | LS | 136 | ARG |
| 19 | LS | 137 | VAL |
| 19 | LS | 138 | LEU |
| 19 | LS | 139 | LEU |
| 19 | LS | 147 | LYS |
| 19 | LS | 150 | GLU |
| 19 | LS | 152 | GLU |
| 19 | LS | 154 | LYS |
| 19 | LS | 155 | LYS |
| 19 | LS | 156 | LYS |
| 19 | LS | 158 | GLU |
| 19 | LS | 162 | ARG |
| 19 | LS | 163 | ARG |
| 19 | LS | 164 | LYS |
| 19 | LS | 165 | LYS |
| 19 | LS | 168 | GLN |
| 19 | LS | 170 | CYS |
| 19 | LS | 171 | LYS |
| 19 | LS | 176 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | LS | 177 | VAL |
| 19 | LS | 181 | ARG |
| 19 | LS | 182 | LEU |
| 19 | LS | 187 | THR |
| 19 | LS | 189 | ILE |
| 19 | LS | 190 | PHE |
| 19 | LS | 191 | THR |
| 19 | LS | 192 | GLU |
| 20 | LT | 7 | VAL |
| 20 | LT | 11 | ARG |
| 20 | LT | 15 | GLU |
| 20 | LT | 21 | GLU |
| 20 | LT | 24 | ARG |
| 20 | LT | 25 | MET |
| 20 | LT | 26 | THR |
| 20 | LT | 32 | GLU |
| 20 | LT | 36 | LYS |
| 20 | LT | 43 | LEU |
| 20 | LT | 44 | LYS |
| 20 | LT | 47 | LYS |
| 20 | LT | 50 | LYS |
| 20 | LT | 55 | GLU |
| 20 | LT | 56 | ILE |
| 20 | LT | 57 | LEU |
| 20 | LT | 59 | CYS |
| 20 | LT | 62 | ILE |
| 20 | LT | 63 | GLU |
| 20 | LT | 65 | ASN |
| 20 | LT | 67 | ASP |
| 20 | LT | 68 | PHE |
| 20 | LT | 70 | LYS |
| 20 | LT | 71 | ASN |
| 20 | LT | 75 | LEU |
| 20 | LT | 81 | ARG |
| 20 | LT | 82 | VAL |
| 20 | LT | 87 | MET |
| 20 | LT | 89 | ARG |
| 20 | LT | 91 | VAL |
| 20 | LT | 92 | ARG |
| 20 | LT | 95 | THR |
| 20 | LT | 98 | ARG |
| 20 | LT | 100 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | LT | 102 | LYS |
| 20 | LT | 103 | VAL |
| 20 | LT | 106 | GLU |
| 20 | LT | 107 | MET |
| 20 | LT | 112 | ARG |
| 20 | LT | 124 | LYS |
| 20 | LT | 126 | VAL |
| 20 | LT | 130 | ASP |
| 20 | LT | 135 | LYS |
| 20 | LT | 136 | VAL |
| 20 | LT | 138 | MET |
| 20 | LT | 139 | PHE |
| 20 | LT | 140 | THR |
| 20 | LT | 142 | LYS |
| 20 | LT | 144 | VAL |
| 20 | LT | 150 | CYS |
| 20 | LT | 152 | TYR |
| 20 | LT | 153 | VAL |
| 20 | LT | 156 | LYS |
| 20 | LT | 157 | ARG |
| 20 | LT | 163 | ARG |
| 20 | LT | 165 | GLN |
| 20 | LT | 167 | ARG |
| 20 | LT | 171 | VAL |
| 21 | LU | 2 | THR |
| 21 | LU | 4 | SER |
| 21 | LU | 5 | GLN |
| 21 | LU | 8 | ARG |
| 21 | LU | 17 | ARG |
| 21 | LU | 18 | LYS |
| 21 | LU | 21 | ARG |
| 21 | LU | 26 | ASN |
| 21 | LU | 27 | LEU |
| 21 | LU | 32 | ARG |
| 21 | LU | 33 | VAL |
| 21 | LU | 35 | LYS |
| 21 | LU | 40 | VAL |
| 21 | LU | 42 | ILE |
| 21 | LU | 43 | LYS |
| 21 | LU | 50 | LYS |
| 21 | LU | 52 | MET |
| 21 | LU | 55 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | LU | 63 | THR |
| 21 | LU | 67 | ILE |
| 21 | LU | 75 | GLN |
| 21 | LU | 76 | ILE |
| 21 | LU | 77 | GLN |
| 21 | LU | 79 | ARG |
| 21 | LU | 80 | VAL |
| 21 | LU | 81 | ARG |
| 21 | LU | 83 | ARG |
| 21 | LU | 84 | ILE |
| 21 | LU | 86 | LEU |
| 21 | LU | 87 | LYS |
| 21 | LU | 89 | ILE |
| 21 | LU | 93 | LEU |
| 21 | LU | 94 | GLU |
| 21 | LU | 96 | VAL |
| 21 | LU | 102 | ARG |
| 21 | LU | 103 | LYS |
| 21 | LU | 109 | VAL |
| 21 | LU | 117 | ARG |
| 21 | LU | 118 | LEU |
| 21 | LU | 120 | LYS |
| 21 | LU | 121 | GLU |
| 21 | LU | 126 | VAL |
| 21 | LU | 137 | ARG |
| 21 | LU | 141 | VAL |
| 21 | LU | 142 | VAL |
| 21 | LU | 144 | ILE |
| 21 | LU | 146 | SER |
| 21 | LU | 150 | ILE |
| 21 | LU | 151 | THR |
| 21 | LU | 153 | LEU |
| 21 | LU | 158 | VAL |
| 22 | LV | 9 | VAL |
| 22 | LV | 10 | LYS |
| 22 | LV | 11 | LYS |
| 22 | LV | 12 | GLU |
| 22 | LV | 16 | ILE |
| 22 | LV | 20 | VAL |
| 22 | LV | 21 | ASP |
| 22 | LV | 26 | LYS |
| 22 | LV | 27 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | LV | 28 | LEU |
| 22 | LV | 29 | GLU |
| 22 | LV | 30 | LEU |
| 22 | LV | 40 | ARG |
| 22 | LV | 41 | THR |
| 22 | LV | 45 | ILE |
| 22 | LV | 46 | ASN |
| 22 | LV | 49 | LYS |
| 22 | LV | 50 | HIS |
| 22 | LV | 55 | LYS |
| 22 | LV | 56 | VAL |
| 22 | LV | 58 | CYS |
| 22 | LV | 59 | SER |
| 22 | LV | 63 | ASP |
| 22 | LV | 66 | VAL |
| 22 | LV | 68 | GLN |
| 22 | LV | 70 | THR |
| 22 | LV | 73 | GLU |
| 22 | LV | 79 | VAL |
| 22 | LV | 80 | LYS |
| 22 | LV | 82 | LEU |
| 22 | LV | 84 | LYS |
| 22 | LV | 89 | GLN |
| 22 | LV | 90 | ASP |
| 22 | LV | 91 | TYR |
| 22 | LV | 92 | GLN |
| 22 | LV | 96 | ARG |
| 22 | LV | 97 | VAL |
| 22 | LV | 98 | LEU |
| 22 | LV | 100 | THR |
| 22 | LV | 102 | LYS |
| 22 | LV | 104 | THR |
| 22 | LV | 106 | THR |
| 22 | LV | 108 | LYS |
| 22 | LV | 110 | TYR |
| 22 | LV | 112 | ILE |
| 22 | LV | 114 | ASP |
| 22 | LV | 117 | ASP |
| 22 | LV | 121 | THR |
| 23 | LW | 8 | SER |
| 23 | LW | 14 | LYS |
| 23 | LW | 18 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | LW | 19 | CYS |
| 23 | LW | 26 | VAL |
| 23 | LW | 27 | ILE |
| 23 | LW | 33 | SER |
| 23 | LW | 36 | LYS |
| 23 | LW | 39 | ASN |
| 23 | LW | 40 | MET |
| 23 | LW | 55 | LYS |
| 23 | LW | 61 | MET |
| 23 | LW | 64 | ILE |
| 23 | LW | 65 | THR |
| 23 | LW | 69 | ASP |
| 23 | LW | 71 | LYS |
| 23 | LW | 73 | GLU |
| 23 | LW | 74 | LEU |
| 23 | LW | 76 | ARG |
| 23 | LW | 77 | LYS |
| 23 | LW | 78 | VAL |
| 23 | LW | 79 | THR |
| 23 | LW | 84 | VAL |
| 23 | LW | 92 | ARG |
| 23 | LW | 93 | LYS |
| 23 | LW | 96 | VAL |
| 23 | LW | 98 | ILE |
| 23 | LW | 99 | TYR |
| 23 | LW | 103 | ASN |
| 23 | LW | 108 | ILE |
| 23 | LW | 111 | LYS |
| 23 | LW | 114 | LEU |
| 23 | LW | 115 | LYS |
| 23 | LW | 118 | SER |
| 23 | LW | 125 | LYS |
| 23 | LW | 129 | ASP |
| 23 | LW | 133 | LYS |
| 23 | LW | 134 | ILE |
| 23 | LW | 137 | THR |
| 23 | LW | 139 | GLU |
| 23 | LW | 141 | VAL |
| 24 | LX | 4 | ILE |
| 24 | LX | 6 | HIS |
| 24 | LX | 7 | CYS |
| 24 | LX | 8 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | LX | 12 | LYS |
| 24 | LX | 14 | VAL |
| 24 | LX | 18 | LYS |
| 24 | LX | 20 | ILE |
| 24 | LX | 22 | PHE |
| 24 | LX | 28 | ARG |
| 24 | LX | 29 | VAL |
| 24 | LX | 36 | LYS |
| 24 | LX | 37 | CYS |
| 24 | LX | 39 | ARG |
| 24 | LX | 42 | LYS |
| 24 | LX | 43 | MET |
| 24 | LX | 44 | LYS |
| 24 | LX | 49 | LYS |
| 24 | LX | 50 | VAL |
| 24 | LX | 51 | ARG |
| 24 | LX | 54 | LYS |
| 24 | LX | 60 | HIS |
| 24 | LX | 62 | LYS |
| 24 | LX | 64 | MET |
| 25 | LY | 23 | LYS |
| 25 | LY | 24 | LYS |
| 25 | LY | 25 | ILE |
| 25 | LY | 28 | ASN |
| 25 | LY | 29 | VAL |
| 25 | LY | 37 | LEU |
| 25 | LY | 39 | HIS |
| 25 | LY | 40 | LYS |
| 25 | LY | 41 | LYS |
| 25 | LY | 44 | LEU |
| 25 | LY | 45 | TYR |
| 25 | LY | 50 | ILE |
| 25 | LY | 51 | LYS |
| 25 | LY | 52 | LYS |
| 25 | LY | 54 | SER |
| 25 | LY | 56 | ASP |
| 25 | LY | 66 | ILE |
| 25 | LY | 67 | LYS |
| 25 | LY | 68 | THR |
| 25 | LY | 69 | ASP |
| 25 | LY | 70 | GLU |
| 25 | LY | 73 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | LY | 74 | GLN |
| 25 | LY | 75 | ILE |
| 25 | LY | 76 | GLU |
| 25 | LY | 78 | ASN |
| 25 | LY | 81 | ILE |
| 25 | LY | 83 | PHE |
| 25 | LY | 84 | ILE |
| 25 | LY | 87 | ARG |
| 25 | LY | 91 | LYS |
| 25 | LY | 94 | ILE |
| 25 | LY | 96 | LYS |
| 25 | LY | 98 | PHE |
| 25 | LY | 99 | GLU |
| 25 | LY | 105 | LYS |
| 25 | LY | 106 | VAL |
| 25 | LY | 109 | VAL |
| 25 | LY | 110 | ASN |
| 25 | LY | 111 | THR |
| 25 | LY | 112 | LEU |
| 25 | LY | 113 | ILE |
| 25 | LY | 114 | THR |
| 25 | LY | 118 | LEU |
| 25 | LY | 119 | LYS |
| 25 | LY | 120 | LYS |
| 25 | LY | 123 | ILE |
| 25 | LY | 128 | ASP |
| 25 | LY | 129 | VAL |
| 25 | LY | 130 | GLN |
| 25 | LY | 133 | ASP |
| 25 | LY | 137 | LYS |
| 25 | LY | 138 | MET |
| 25 | LY | 140 | LEU |
| 26 | LZ | 1 | MET |
| 26 | LZ | 2 | LYS |
| 26 | LZ | 3 | LEU |
| 26 | LZ | 5 | SER |
| 26 | LZ | 8 | THR |
| 26 | LZ | 10 | SER |
| 26 | LZ | 13 | LYS |
| 26 | LZ | 14 | CYS |
| 26 | LZ | 20 | THR |
| 26 | LZ | 22 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | LZ | 28 | LYS |
| 26 | LZ | 30 | MET |
| 26 | LZ | 34 | LEU |
| 26 | LZ | 36 | LYS |
| 26 | LZ | 37 | GLU |
| 26 | LZ | 38 | LEU |
| 26 | LZ | 39 | ARG |
| 26 | LZ | 41 | GLU |
| 26 | LZ | 43 | LYS |
| 26 | LZ | 47 | MET |
| 26 | LZ | 54 | ILE |
| 26 | LZ | 55 | VAL |
| 26 | LZ | 57 | ILE |
| 26 | LZ | 59 | THR |
| 26 | LZ | 63 | LYS |
| 26 | LZ | 67 | LYS |
| 26 | LZ | 69 | VAL |
| 26 | LZ | 70 | GLU |
| 26 | LZ | 71 | VAL |
| 26 | LZ | 72 | ARG |
| 26 | LZ | 74 | ARG |
| 26 | LZ | 77 | LYS |
| 26 | LZ | 78 | ILE |
| 26 | LZ | 79 | CYS |
| 26 | LZ | 80 | VAL |
| 26 | LZ | 85 | GLN |
| 26 | LZ | 86 | LYS |
| 26 | LZ | 88 | ARG |
| 26 | LZ | 91 | GLU |
| 26 | LZ | 95 | VAL |
| 26 | LZ | 99 | ILE |
| 26 | LZ | 102 | SER |
| 26 | LZ | 105 | ILE |
| 26 | LZ | 106 | ILE |
| 26 | LZ | 107 | LYS |
| 26 | LZ | 111 | MET |
| 26 | LZ | 114 | SER |
| 26 | LZ | 116 | TYR |
| 26 | LZ | 119 | ILE |
| 26 | LZ | 128 | GLU |
| 26 | LZ | 133 | ILE |
| 27 | La | 5 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | La | 7 | LYS |
| 27 | La | 13 | ILE |
| 27 | La | 14 | VAL |
| 27 | La | 18 | ARG |
| 27 | La | 25 | VAL |
| 27 | La | 27 | VAL |
| 27 | La | 30 | LEU |
| 27 | La | 33 | ASN |
| 27 | La | 35 | ARG |
| 27 | La | 40 | ILE |
| 27 | La | 44 | ILE |
| 27 | La | 50 | ARG |
| 27 | La | 52 | THR |
| 27 | La | 53 | ASN |
| 27 | La | 54 | SER |
| 27 | La | 56 | SER |
| 27 | La | 58 | GLU |
| 27 | La | 61 | VAL |
| 27 | La | 63 | ARG |
| 27 | La | 65 | ARG |
| 27 | La | 66 | VAL |
| 27 | La | 71 | LYS |
| 27 | La | 73 | MET |
| 27 | La | 76 | ASN |
| 27 | La | 78 | LEU |
| 27 | La | 79 | MET |
| 27 | La | 82 | SER |
| 27 | La | 86 | GLU |
| 27 | La | 90 | LYS |
| 27 | La | 93 | ILE |
| 27 | La | 94 | SER |
| 27 | La | 97 | THR |
| 27 | La | 105 | ARG |
| 27 | La | 106 | GLU |
| 27 | La | 107 | ILE |
| 27 | La | 117 | ARG |
| 27 | La | 119 | ILE |
| 27 | La | 120 | LEU |
| 27 | La | 129 | THR |
| 27 | La | 130 | LYS |
| 27 | La | 131 | LEU |
| 27 | La | 133 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | Lb | 3 | THR |
| 28 | Lb | 4 | ARG |
| 28 | Lb | 7 | LYS |
| 28 | Lb | 9 | ARG |
| 28 | Lb | 15 | ARG |
| 28 | Lb | 16 | GLN |
| 28 | Lb | 17 | MET |
| 28 | Lb | 21 | ARG |
| 28 | Lb | 26 | ARG |
| 28 | Lb | 27 | LYS |
| 28 | Lb | 32 | ARG |
| 28 | Lb | 34 | LYS |
| 28 | Lb | 40 | HIS |
| 28 | Lb | 41 | LYS |
| 28 | Lb | 53 | PHE |
| 28 | Lb | 55 | LYS |
| 28 | Lb | 56 | LEU |
| 28 | Lb | 64 | ARG |
| 28 | Lb | 68 | GLU |
| 28 | Lb | 69 | TYR |
| 28 | Lb | 72 | THR |
| 28 | Lb | 73 | ILE |
| 28 | Lb | 75 | ILE |
| 28 | Lb | 76 | ASP |
| 28 | Lb | 78 | ILE |
| 28 | Lb | 85 | GLU |
| 28 | Lb | 86 | GLN |
| 28 | Lb | 87 | ARG |
| 28 | Lb | 88 | ASP |
| 28 | Lb | 91 | LEU |
| 28 | Lb | 94 | LYS |
| 28 | Lb | 95 | SER |
| 28 | Lb | 97 | THR |
| 28 | Lb | 101 | VAL |
| 28 | Lb | 104 | VAL |
| 28 | Lb | 105 | THR |
| 28 | Lb | 106 | ARG |
| 28 | Lb | 115 | ARG |
| 28 | Lb | 118 | LEU |
| 28 | Lb | 120 | GLN |
| 28 | Lb | 123 | ILE |
| 28 | Lb | 125 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | Lb | 131 | SER |
| 28 | Lb | 133 | ASP |
| 28 | Lb | 135 | GLU |
| 28 | Lb | 136 | LYS |
| 28 | Lb | 140 | GLU |
| 28 | Lb | 141 | VAL |
| 28 | Lb | 144 | VAL |
| 28 | Lb | 146 | LEU |
| 28 | Lb | 147 | LEU |
| 28 | Lb | 148 | VAL |
| 29 | Lc | 3 | LYS |
| 29 | Lc | 5 | LYS |
| 29 | Lc | 8 | THR |
| 29 | Lc | 10 | LYS |
| 29 | Lc | 14 | ARG |
| 29 | Lc | 17 | HIS |
| 29 | Lc | 22 | LYS |
| 29 | Lc | 23 | LYS |
| 29 | Lc | 25 | LYS |
| 29 | Lc | 27 | SER |
| 29 | Lc | 30 | THR |
| 29 | Lc | 31 | SER |
| 29 | Lc | 33 | LYS |
| 29 | Lc | 38 | LYS |
| 29 | Lc | 40 | LEU |
| 29 | Lc | 41 | ARG |
| 29 | Lc | 43 | LEU |
| 29 | Lc | 44 | ARG |
| 29 | Lc | 45 | ARG |
| 29 | Lc | 46 | SER |
| 29 | Lc | 52 | ARG |
| 29 | Lc | 53 | GLN |
| 29 | Lc | 56 | ARG |
| 30 | Ld | 14 | ILE |
| 30 | Ld | 16 | LEU |
| 30 | Ld | 18 | LEU |
| 30 | Ld | 23 | LYS |
| 30 | Ld | 26 | LYS |
| 30 | Ld | 27 | TYR |
| 30 | Ld | 28 | THR |
| 30 | Ld | 29 | LEU |
| 30 | Ld | 32 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | Ld | 38 | ILE |
| 30 | Ld | 40 | ASP |
| 30 | Ld | 42 | LYS |
| 30 | Ld | 44 | GLN |
| 30 | Ld | 47 | PHE |
| 30 | Ld | 48 | MET |
| 30 | Ld | 52 | CYS |
| 30 | Ld | 55 | LEU |
| 30 | Ld | 57 | LYS |
| 30 | Ld | 60 | VAL |
| 30 | Ld | 61 | ASP |
| 30 | Ld | 63 | LEU |
| 30 | Ld | 66 | LEU |
| 30 | Ld | 68 | LYS |
| 30 | Ld | 71 | VAL |
| 30 | Ld | 80 | GLU |
| 30 | Ld | 93 | ILE |
| 30 | Ld | 94 | MET |
| 30 | Ld | 95 | THR |
| 30 | Ld | 96 | ILE |
| 30 | Ld | 104 | LEU |
| 30 | Ld | 105 | THR |
| 30 | Ld | 108 | LEU |
| 31 | Le | 3 | ILE |
| 31 | Le | 4 | VAL |
| 31 | Le | 6 | GLU |
| 31 | Le | 8 | THR |
| 31 | Le | 9 | ILE |
| 31 | Le | 11 | LEU |
| 31 | Le | 13 | LYS |
| 31 | Le | 16 | ARG |
| 31 | Le | 26 | ILE |
| 31 | Le | 31 | ILE |
| 31 | Le | 32 | ARG |
| 31 | Le | 35 | VAL |
| 31 | Le | 36 | GLU |
| 31 | Le | 42 | GLU |
| 31 | Le | 43 | ASP |
| 31 | Le | 46 | LEU |
| 31 | Le | 51 | ASN |
| 31 | Le | 54 | VAL |
| 31 | Le | 56 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | Le | 59 | ILE |
| 31 | Le | 61 | HIS |
| 31 | Le | 65 | ARG |
| 31 | Le | 69 | GLU |
| 31 | Le | 71 | ARG |
| 31 | Le | 73 | GLU |
| 31 | Le | 75 | ASP |
| 31 | Le | 77 | GLU |
| 31 | Le | 79 | LYS |
| 31 | Le | 83 | VAL |
| 31 | Le | 84 | ILE |
| 31 | Le | 86 | LYS |
| 31 | Le | 89 | GLU |
| 31 | Le | 91 | PHE |
| 31 | Le | 92 | LYS |
| 31 | Le | 93 | HIS |
| 31 | Le | 96 | THR |
| 31 | Le | 98 | LYS |
| 31 | Le | 99 | LYS |
| 31 | Le | 101 | SER |
| 31 | Le | 102 | GLU |
| 32 | Lf | 6 | ILE |
| 32 | Lf | 11 | HIS |
| 32 | Lf | 12 | LYS |
| 32 | Lf | 13 | ILE |
| 32 | Lf | 15 | ILE |
| 32 | Lf | 16 | LYS |
| 32 | Lf | 17 | LYS |
| 32 | Lf | 18 | ARG |
| 32 | Lf | 19 | LYS |
| 32 | Lf | 21 | LYS |
| 32 | Lf | 23 | ILE |
| 32 | Lf | 24 | ARG |
| 32 | Lf | 28 | GLU |
| 32 | Lf | 33 | VAL |
| 32 | Lf | 34 | LYS |
| 32 | Lf | 36 | SER |
| 32 | Lf | 38 | ARG |
| 32 | Lf | 41 | ARG |
| 32 | Lf | 43 | ILE |
| 32 | Lf | 47 | MET |
| 32 | Lf | 52 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | Lf | 55 | ARG |
| 32 | Lf | 57 | MET |
| 32 | Lf | 60 | ILE |
| 32 | Lf | 65 | ASP |
| 32 | Lf | 69 | ARG |
| 32 | Lf | 79 | HIS |
| 32 | Lf | 81 | ILE |
| 32 | Lf | 84 | VAL |
| 32 | Lf | 87 | LEU |
| 32 | Lf | 90 | LEU |
| 32 | Lf | 91 | PHE |
| 32 | Lf | 92 | MET |
| 32 | Lf | 95 | LYS |
| 32 | Lf | 100 | GLN |
| 32 | Lf | 101 | ILE |
| 32 | Lf | 103 | HIS |
| 32 | Lf | 105 | VAL |
| 32 | Lf | 106 | SER |
| 32 | Lf | 108 | ARG |
| 32 | Lf | 109 | SER |
| 32 | Lf | 110 | ARG |
| 32 | Lf | 111 | LYS |
| 32 | Lf | 112 | GLN |
| 32 | Lf | 113 | ILE |
| 32 | Lf | 114 | LEU |
| 32 | Lf | 118 | LYS |
| 32 | Lf | 120 | MET |
| 32 | Lf | 123 | ARG |
| 32 | Lf | 124 | VAL |
| 32 | Lf | 126 | ASN |
| 32 | Lf | 128 | ASP |
| 32 | Lf | 133 | LYS |
| 32 | Lf | 134 | GLU |
| 32 | Lf | 135 | GLU |
| 33 | Lg | 2 | GLU |
| 33 | Lg | 3 | GLU |
| 33 | Lg | 4 | ILE |
| 33 | Lg | 7 | LYS |
| 33 | Lg | 8 | THR |
| 33 | Lg | 9 | PHE |
| 33 | Lg | 10 | LEU |
| 33 | Lg | 13 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | Lg | 15 | VAL |
| 33 | Lg | 19 | ARG |
| 33 | Lg | 20 | SER |
| 33 | Lg | 21 | ARG |
| 33 | Lg | 23 | LYS |
| 33 | Lg | 25 | ARG |
| 33 | Lg | 27 | ASN |
| 33 | Lg | 28 | VAL |
| 33 | Lg | 30 | LEU |
| 33 | Lg | 33 | VAL |
| 33 | Lg | 34 | SER |
| 33 | Lg | 38 | THR |
| 33 | Lg | 41 | GLU |
| 33 | Lg | 42 | THR |
| 33 | Lg | 43 | ASP |
| 33 | Lg | 44 | LYS |
| 33 | Lg | 46 | LEU |
| 33 | Lg | 48 | ARG |
| 33 | Lg | 50 | ILE |
| 33 | Lg | 52 | ILE |
| 33 | Lg | 53 | ILE |
| 33 | Lg | 59 | LYS |
| 33 | Lg | 64 | LYS |
| 33 | Lg | 67 | ARG |
| 33 | Lg | 74 | MET |
| 33 | Lg | 75 | VAL |
| 33 | Lg | 81 | THR |
| 33 | Lg | 83 | LEU |
| 33 | Lg | 87 | LEU |
| 33 | Lg | 91 | LYS |
| 33 | Lg | 92 | VAL |
| 33 | Lg | 93 | ARG |
| 33 | Lg | 94 | VAL |
| 33 | Lg | 96 | TYR |
| 33 | Lg | 99 | ILE |
| 34 | Lh | 5 | ARG |
| 34 | Lh | 6 | VAL |
| 34 | Lh | 7 | THR |
| 34 | Lh | 9 | ARG |
| 34 | Lh | 10 | PHE |
| 34 | Lh | 11 | HIS |
| 34 | Lh | 13 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | Lh | 16 | THR |
| 34 | Lh | 19 | LYS |
| 34 | Lh | 20 | ILE |
| 34 | Lh | 21 | VAL |
| 34 | Lh | 22 | ARG |
| 34 | Lh | 24 | LYS |
| 34 | Lh | 30 | ARG |
| 34 | Lh | 31 | LEU |
| 34 | Lh | 32 | THR |
| 34 | Lh | 33 | SER |
| 34 | Lh | 34 | LEU |
| 34 | Lh | 35 | ARG |
| 34 | Lh | 36 | VAL |
| 34 | Lh | 37 | LYS |
| 34 | Lh | 38 | LYS |
| 34 | Lh | 39 | LEU |
| 34 | Lh | 45 | CYS |
| 34 | Lh | 50 | LYS |
| 34 | Lh | 51 | GLN |
| 34 | Lh | 52 | ILE |
| 34 | Lh | 55 | ILE |
| 34 | Lh | 57 | ARG |
| 34 | Lh | 58 | VAL |
| 34 | Lh | 59 | ILE |
| 34 | Lh | 63 | LEU |
| 34 | Lh | 69 | LYS |
| 34 | Lh | 70 | VAL |
| 34 | Lh | 72 | ARG |
| 34 | Lh | 77 | LYS |
| 34 | Lh | 78 | LEU |
| 34 | Lh | 86 | HIS |
| 34 | Lh | 87 | ILE |
| 34 | Lh | 95 | GLU |
| 34 | Lh | 99 | LEU |
| 34 | Lh | 101 | GLU |
| 34 | Lh | 105 | GLN |
| 34 | Lh | 106 | THR |
| 34 | Lh | 108 | LYS |
| 34 | Lh | 109 | THR |
| 35 | Li | 33 | LYS |
| 35 | Li | 35 | LYS |
| 35 | Li | 36 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | Li | 38 | VAL |
| 35 | Li | 42 | GLN |
| 35 | Li | 44 | ASP |
| 35 | Li | 47 | ARG |
| 35 | Li | 48 | LYS |
| 35 | Li | 51 | ASP |
| 35 | Li | 52 | LEU |
| 35 | Li | 53 | LYS |
| 35 | Li | 55 | GLU |
| 35 | Li | 57 | LEU |
| 35 | Li | 63 | LYS |
| 35 | Li | 69 | VAL |
| 35 | Li | 77 | ARG |
| 35 | Li | 78 | VAL |
| 35 | Li | 81 | LYS |
| 35 | Li | 82 | ASP |
| 35 | Li | 85 | ARG |
| 35 | Li | 87 | LEU |
| 35 | Li | 90 | ILE |
| 35 | Li | 97 | GLU |
| 35 | Li | 108 | ILE |
| 35 | Li | 110 | LYS |
| 35 | Li | 111 | THR |
| 35 | Li | 121 | ARG |
| 35 | Li | 127 | LYS |
| 35 | Li | 130 | ARG |
| 35 | Li | 131 | LEU |
| 35 | Li | 132 | LEU |
| 35 | Li | 134 | SER |
| 35 | Li | 135 | LYS |
| 35 | Li | 139 | ARG |
| 35 | Li | 141 | LEU |
| 35 | Li | 142 | GLN |
| 35 | Li | 145 | LYS |
| 35 | Li | 147 | LYS |
| 35 | Li | 150 | VAL |
| 35 | Li | 151 | LYS |
| 36 | Lj | 9 | LYS |
| 36 | Lj | 10 | LYS |
| 36 | Lj | 14 | VAL |
| 36 | Lj | 15 | VAL |
| 36 | Lj | 16 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | Lj | 17 | ILE |
| 36 | Lj | 18 | VAL |
| 36 | Lj | 21 | LYS |
| 36 | Lj | 23 | GLU |
| 36 | Lj | 25 | LYS |
| 36 | Lj | 27 | LYS |
| 36 | Lj | 30 | GLN |
| 36 | Lj | 31 | GLU |
| 36 | Lj | 34 | LYS |
| 36 | Lj | 37 | ILE |
| 36 | Lj | 40 | CYS |
| 36 | Lj | 41 | THR |
| 36 | Lj | 53 | LEU |
| 36 | Lj | 55 | ARG |
| 36 | Lj | 56 | MET |
| 36 | Lj | 67 | LYS |
| 36 | Lj | 68 | LYS |
| 36 | Lj | 70 | LEU |
| 36 | Lj | 73 | ILE |
| 36 | Lj | 74 | LYS |
| 36 | Lj | 75 | ARG |
| 36 | Lj | 77 | LYS |
| 36 | Lj | 79 | LYS |
| 36 | Lj | 80 | ARG |
| 36 | Lj | 83 | LEU |
| 36 | Lj | 88 | ARG |
| 36 | Lj | 90 | ILE |
| 37 | Lk | 3 | LYS |
| 37 | Lk | 7 | SER |
| 37 | Lk | 10 | LYS |
| 37 | Lk | 11 | ARG |
| 37 | Lk | 14 | ARG |
| 37 | Lk | 18 | SER |
| 37 | Lk | 26 | SER |
| 37 | Lk | 31 | LYS |
| 37 | Lk | 36 | SER |
| 37 | Lk | 43 | LYS |
| 37 | Lk | 44 | MET |
| 37 | Lk | 46 | ARG |
| 37 | Lk | 48 | ASN |
| 37 | Lk | 49 | TRP |
| 37 | Lk | 52 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | Lk | 54 | LEU |
| 37 | Lk | 57 | ARG |
| 37 | Lk | 58 | THR |
| 37 | Lk | 69 | LYS |
| 37 | Lk | 78 | THR |
| 37 | Lk | 80 | LYS |
| 37 | Lk | 82 | ASN |
| 37 | Lk | 84 | ARG |
| 37 | Lk | 85 | LYS |
| 37 | Lk | 86 | TYR |
| 37 | Lk | 89 | LYS |
| 38 | Ll | 4 | THR |
| 38 | Ll | 5 | ILE |
| 38 | Ll | 6 | THR |
| 38 | Ll | 7 | GLU |
| 38 | Ll | 10 | LEU |
| 38 | Ll | 11 | MET |
| 38 | Ll | 12 | LYS |
| 38 | Ll | 13 | MET |
| 38 | Ll | 14 | ILE |
| 38 | Ll | 18 | ARG |
| 38 | Ll | 20 | LYS |
| 38 | Ll | 22 | LEU |
| 38 | Ll | 23 | VAL |
| 38 | Ll | 24 | VAL |
| 38 | Ll | 25 | LYS |
| 38 | Ll | 26 | SER |
| 38 | Ll | 27 | CYS |
| 38 | Ll | 31 | ARG |
| 38 | Ll | 32 | LEU |
| 38 | Ll | 36 | VAL |
| 38 | Ll | 38 | LEU |
| 38 | Ll | 39 | LYS |
| 38 | Ll | 41 | ARG |
| 38 | Ll | 44 | LYS |
| 38 | Ll | 46 | LEU |
| 38 | Ll | 49 | LEU |
| 38 | Ll | 50 | THR |
| 38 | Ll | 51 | VAL |
| 38 | Ll | 55 | ASP |
| 38 | Ll | 56 | ASP |
| 38 | Ll | 58 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | Ll | 60 | ILE |
| 38 | Ll | 62 | LYS |
| 38 | Ll | 67 | LYS |
| 38 | Ll | 68 | VAL |
| 38 | Ll | 70 | VAL |
| 38 | Ll | 71 | GLN |
| 38 | Ll | 73 | VAL |
| 39 | Ln | 4 | ILE |
| 39 | Ln | 7 | GLU |
| 39 | Ln | 9 | LEU |
| 39 | Ln | 12 | HIS |
| 39 | Ln | 13 | ILE |
| 39 | Ln | 15 | GLU |
| 39 | Ln | 17 | ILE |
| 39 | Ln | 19 | ARG |
| 39 | Ln | 23 | GLU |
| 39 | Ln | 24 | LYS |
| 39 | Ln | 26 | ARG |
| 39 | Ln | 27 | LYS |
| 39 | Ln | 30 | GLU |
| 39 | Ln | 31 | THR |
| 39 | Ln | 32 | VAL |
| 39 | Ln | 34 | LEU |
| 39 | Ln | 35 | GLN |
| 39 | Ln | 36 | VAL |
| 39 | Ln | 42 | ASP |
| 39 | Ln | 44 | LYS |
| 39 | Ln | 45 | LYS |
| 39 | Ln | 46 | ASP |
| 39 | Ln | 48 | ARG |
| 39 | Ln | 51 | LEU |
| 39 | Ln | 62 | ASN |
| 39 | Ln | 64 | LYS |
| 39 | Ln | 65 | LEU |
| 39 | Ln | 66 | CYS |
| 39 | Ln | 67 | VAL |
| 39 | Ln | 68 | ILE |
| 39 | Ln | 72 | ARG |
| 39 | Ln | 73 | ASP |
| 39 | Ln | 76 | ARG |
| 39 | Ln | 78 | LYS |
| 39 | Ln | 80 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | Ln | 82 | LEU |
| 39 | Ln | 83 | ASN |
| 39 | Ln | 84 | TYR |
| 39 | Ln | 85 | VAL |
| 39 | Ln | 86 | GLU |
| 39 | Ln | 87 | ILE |
| 39 | Ln | 89 | HIS |
| 39 | Ln | 92 | GLN |
| 39 | Ln | 99 | GLN |
| 39 | Ln | 101 | LYS |
| 39 | Ln | 102 | LYS |
| 39 | Ln | 103 | PHE |
| 39 | Ln | 105 | LYS |
| 39 | Ln | 106 | SER |
| 39 | Ln | 107 | TYR |
| 39 | Ln | 109 | VAL |
| 39 | Ln | 110 | PHE |
| 39 | Ln | 111 | LEU |
| 39 | Ln | 114 | LYS |
| 39 | Ln | 115 | SER |
| 39 | Ln | 116 | LEU |
| 39 | Ln | 117 | ILE |
| 39 | Ln | 118 | ARG |
| 39 | Ln | 119 | GLN |
| 39 | Ln | 120 | ILE |
| 39 | Ln | 122 | VAL |
| 39 | Ln | 123 | TYR |
| 39 | Ln | 130 | LYS |
| 39 | Ln | 133 | ARG |
| 39 | Ln | 134 | THR |
| 39 | Ln | 136 | LEU |
| 39 | Ln | 141 | ASP |
| 39 | Ln | 144 | LEU |
| 39 | Ln | 147 | LYS |
| 39 | Ln | 148 | VAL |
| 39 | Ln | 149 | LEU |
| 39 | Ln | 150 | GLU |
| 39 | Ln | 151 | CYS |
| 39 | Ln | 156 | LYS |
| 39 | Ln | 157 | VAL |
| 39 | Ln | 158 | GLN |
| 39 | Ln | 159 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | Ln | 160 | LYS |
| 39 | Ln | 163 | VAL |
| 39 | Ln | 165 | LEU |
| 39 | Ln | 167 | TRP |
| 39 | Ln | 173 | LYS |
| 39 | Ln | 183 | ILE |
| 39 | Ln | 187 | LEU |
| 39 | Ln | 188 | ASN |
| 39 | Ln | 189 | PHE |
| 39 | Ln | 190 | LEU |
| 39 | Ln | 193 | GLN |
| 39 | Ln | 194 | LEU |
| 39 | Ln | 195 | LYS |
| 39 | Ln | 196 | LYS |
| 39 | Ln | 199 | GLN |
| 39 | Ln | 201 | ILE |
| 39 | Ln | 202 | LYS |
| 39 | Ln | 204 | VAL |
| 39 | Ln | 207 | LYS |
| 39 | Ln | 210 | MET |
| 39 | Ln | 213 | SER |
| 39 | Ln | 215 | ARG |
| 39 | Ln | 216 | ILE |
| 40 | Lo | 1 | MET |
| 40 | Lo | 4 | LYS |
| 40 | Lo | 8 | LYS |
| 40 | Lo | 9 | ARG |
| 40 | Lo | 12 | LYS |
| 40 | Lo | 16 | LYS |
| 40 | Lo | 17 | ARG |
| 40 | Lo | 20 | MET |
| 40 | Lo | 21 | LYS |
| 40 | Lo | 24 | SER |
| 40 | Lo | 25 | LYS |
| 41 | Lp | 2 | VAL |
| 41 | Lp | 3 | THR |
| 41 | Lp | 8 | ARG |
| 41 | Lp | 12 | CYS |
| 41 | Lp | 13 | LYS |
| 41 | Lp | 15 | GLU |
| 41 | Lp | 17 | LYS |
| 41 | Lp | 20 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | Lp | 24 | SER |
| 41 | Lp | 25 | LEU |
| 41 | Lp | 27 | LYS |
| 41 | Lp | 31 | ASP |
| 41 | Lp | 33 | LEU |
| 41 | Lp | 34 | LEU |
| 41 | Lp | 43 | ARG |
| 41 | Lp | 45 | GLN |
| 41 | Lp | 46 | ARG |
| 41 | Lp | 57 | ARG |
| 41 | Lp | 58 | ARG |
| 41 | Lp | 61 | LYS |
| 41 | Lp | 62 | THR |
| 41 | Lp | 64 | LYS |
| 41 | Lp | 66 | GLN |
| 41 | Lp | 67 | VAL |
| 41 | Lp | 68 | ILE |
| 41 | Lp | 71 | THR |
| 41 | Lp | 76 | LYS |
| 41 | Lp | 78 | GLN |
| 41 | Lp | 79 | THR |
| 41 | Lp | 81 | GLN |
| 41 | Lp | 82 | VAL |
| 41 | Lp | 83 | LEU |
| 41 | Lp | 85 | ARG |
| 41 | Lp | 86 | CYS |
| 41 | Lp | 88 | ARG |
| 41 | Lp | 89 | LEU |
| 41 | Lp | 91 | ILE |
| 41 | Lp | 93 | ARG |
| 42 | Lq | 1 | MET |
| 42 | Lq | 4 | ARG |
| 42 | Lq | 5 | THR |
| 42 | Lq | 6 | LYS |
| 42 | Lq | 7 | LYS |
| 42 | Lq | 11 | THR |
| 42 | Lq | 13 | LYS |
| 42 | Lq | 16 | THR |
| 42 | Lq | 20 | ARG |
| 42 | Lq | 24 | LYS |
| 42 | Lq | 25 | GLN |
| 42 | Lq | 26 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 42 | Lq | 28 | LYS |
| 42 | Lq | 29 | ILE |
| 42 | Lq | 38 | THR |
| 42 | Lq | 39 | CYS |
| 42 | Lq | 41 | PHE |
| 42 | Lq | 46 | LYS |
| 42 | Lq | 47 | VAL |
| 42 | Lq | 48 | ARG |
| 42 | Lq | 50 | THR |
| 42 | Lq | 52 | CYS |
| 42 | Lq | 54 | ILE |
| 42 | Lq | 56 | THR |
| 42 | Lq | 57 | CYS |
| 42 | Lq | 62 | LYS |
| 42 | Lq | 63 | THR |
| 42 | Lq | 71 | LEU |
| 42 | Lq | 73 | THR |
| 42 | Lq | 74 | GLU |
| 42 | Lq | 80 | ARG |
| 42 | Lq | 83 | ILE |
| 42 | Lq | 84 | ARG |
| 42 | Lq | 86 | LEU |
| 42 | Lq | 88 | LEU |
| 42 | Lq | 90 | ARG |
| 42 | Lq | 91 | GLU |
| 43 | Ls | 78 | MET |
| 43 | Ls | 81 | THR |
| 43 | Ls | 82 | LEU |
| 43 | Ls | 83 | ILE |
| 43 | Ls | 85 | LEU |
| 43 | Ls | 93 | MET |
| 43 | Ls | 94 | MET |
| 43 | Ls | 96 | CYS |
| 43 | Ls | 97 | ARG |
| 43 | Ls | 102 | ARG |
| 43 | Ls | 106 | ARG |
| 43 | Ls | 110 | CYS |
| 43 | Ls | 111 | ARG |
| 43 | Ls | 114 | ARG |
| 43 | Ls | 117 | ASN |
| 43 | Ls | 119 | ARG |
| 43 | Ls | 120 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 43 | Ls | 121 | LYS |
| 43 | Ls | 122 | LYS |
| 43 | Ls | 123 | LEU |
| 45 | SA | 20 | VAL |
| 45 | SA | 21 | LYS |
| 45 | SA | 23 | MET |
| 45 | SA | 28 | THR |
| 45 | SA | 30 | LEU |
| 45 | SA | 32 | VAL |
| 45 | SA | 33 | ARG |
| 45 | SA | 37 | ARG |
| 45 | SA | 38 | ARG |
| 45 | SA | 43 | ILE |
| 45 | SA | 45 | ASP |
| 45 | SA | 46 | ARG |
| 45 | SA | 49 | ASP |
| 45 | SA | 51 | THR |
| 45 | SA | 53 | VAL |
| 45 | SA | 55 | ASN |
| 45 | SA | 56 | LEU |
| 45 | SA | 58 | LYS |
| 45 | SA | 62 | LYS |
| 45 | SA | 63 | ILE |
| 45 | SA | 69 | ILE |
| 45 | SA | 71 | VAL |
| 45 | SA | 78 | GLU |
| 45 | SA | 79 | ILE |
| 45 | SA | 82 | VAL |
| 45 | SA | 85 | ARG |
| 45 | SA | 87 | ASP |
| 45 | SA | 89 | GLN |
| 45 | SA | 92 | ILE |
| 45 | SA | 94 | LYS |
| 45 | SA | 95 | PHE |
| 45 | SA | 97 | LYS |
| 45 | SA | 98 | TYR |
| 45 | SA | 114 | THR |
| 45 | SA | 116 | ARG |
| 45 | SA | 117 | MET |
| 45 | SA | 118 | ASN |
| 45 | SA | 127 | LEU |
| 45 | SA | 128 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | SA | 129 | VAL |
| 45 | SA | 133 | VAL |
| 45 | SA | 134 | VAL |
| 45 | SA | 139 | ILE |
| 45 | SA | 140 | LEU |
| 45 | SA | 143 | SER |
| 45 | SA | 147 | ILE |
| 45 | SA | 149 | THR |
| 45 | SA | 152 | LEU |
| 45 | SA | 155 | SER |
| 45 | SA | 159 | LEU |
| 45 | SA | 160 | LYS |
| 45 | SA | 164 | VAL |
| 45 | SA | 170 | ASN |
| 45 | SA | 171 | LYS |
| 45 | SA | 172 | THR |
| 45 | SA | 174 | MET |
| 45 | SA | 176 | ILE |
| 45 | SA | 178 | LEU |
| 45 | SA | 181 | TRP |
| 45 | SA | 182 | LEU |
| 45 | SA | 185 | ARG |
| 45 | SA | 186 | GLU |
| 45 | SA | 190 | LEU |
| 45 | SA | 193 | SER |
| 45 | SA | 194 | ILE |
| 45 | SA | 195 | SER |
| 45 | SA | 196 | ARG |
| 45 | SA | 198 | GLU |
| 45 | SA | 206 | LEU |
| 45 | SA | 208 | VAL |
| 45 | SA | 210 | LEU |
| 46 | SB | 28 | HIS |
| 46 | SB | 30 | SER |
| 46 | SB | 31 | THR |
| 46 | SB | 32 | LYS |
| 46 | SB | 33 | LEU |
| 46 | SB | 36 | LEU |
| 46 | SB | 37 | VAL |
| 46 | SB | 41 | LYS |
| 46 | SB | 42 | ILE |
| 46 | SB | 43 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | SB | 48 | ILE |
| 46 | SB | 50 | LYS |
| 46 | SB | 52 | SER |
| 46 | SB | 53 | LEU |
| 46 | SB | 55 | ILE |
| 46 | SB | 56 | LYS |
| 46 | SB | 57 | GLU |
| 46 | SB | 58 | THR |
| 46 | SB | 59 | GLU |
| 46 | SB | 61 | ILE |
| 46 | SB | 67 | LYS |
| 46 | SB | 69 | GLU |
| 46 | SB | 70 | LEU |
| 46 | SB | 72 | GLU |
| 46 | SB | 73 | GLU |
| 46 | SB | 81 | GLN |
| 46 | SB | 82 | LYS |
| 46 | SB | 85 | THR |
| 46 | SB | 88 | GLN |
| 46 | SB | 89 | ARG |
| 46 | SB | 90 | THR |
| 46 | SB | 91 | ARG |
| 46 | SB | 96 | VAL |
| 46 | SB | 97 | ILE |
| 46 | SB | 98 | VAL |
| 46 | SB | 101 | ARG |
| 46 | SB | 102 | ASP |
| 46 | SB | 105 | ILE |
| 46 | SB | 111 | VAL |
| 46 | SB | 113 | LYS |
| 46 | SB | 114 | GLU |
| 46 | SB | 115 | VAL |
| 46 | SB | 119 | ILE |
| 46 | SB | 120 | LYS |
| 46 | SB | 121 | LYS |
| 46 | SB | 124 | LYS |
| 46 | SB | 128 | LEU |
| 46 | SB | 131 | VAL |
| 46 | SB | 141 | LYS |
| 46 | SB | 142 | LEU |
| 46 | SB | 148 | VAL |
| 46 | SB | 151 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | SB | 153 | SER |
| 46 | SB | 160 | ARG |
| 46 | SB | 163 | LEU |
| 46 | SB | 164 | ILE |
| 46 | SB | 175 | SER |
| 46 | SB | 178 | VAL |
| 46 | SB | 180 | LYS |
| 46 | SB | 182 | LEU |
| 46 | SB | 183 | GLU |
| 46 | SB | 184 | PHE |
| 46 | SB | 187 | VAL |
| 46 | SB | 190 | VAL |
| 46 | SB | 192 | THR |
| 46 | SB | 195 | SER |
| 46 | SB | 199 | ARG |
| 46 | SB | 200 | THR |
| 46 | SB | 201 | LEU |
| 46 | SB | 202 | MET |
| 46 | SB | 213 | LYS |
| 46 | SB | 218 | ILE |
| 46 | SB | 223 | LEU |
| 46 | SB | 225 | LYS |
| 46 | SB | 226 | LYS |
| 46 | SB | 227 | GLU |
| 46 | SB | 229 | LEU |
| 46 | SB | 231 | HIS |
| 46 | SB | 232 | VAL |
| 46 | SB | 233 | GLN |
| 46 | SB | 235 | ILE |
| 46 | SB | 236 | ARG |
| 46 | SB | 240 | LEU |
| 47 | SC | 5 | VAL |
| 47 | SC | 6 | ARG |
| 47 | SC | 7 | ARG |
| 47 | SC | 10 | GLU |
| 47 | SC | 12 | VAL |
| 47 | SC | 14 | TYR |
| 47 | SC | 18 | LEU |
| 47 | SC | 22 | ILE |
| 47 | SC | 23 | MET |
| 47 | SC | 24 | GLU |
| 47 | SC | 26 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | SC | 28 | HIS |
| 47 | SC | 33 | ARG |
| 47 | SC | 34 | GLU |
| 47 | SC | 36 | VAL |
| 47 | SC | 42 | SER |
| 47 | SC | 45 | LEU |
| 47 | SC | 48 | THR |
| 47 | SC | 52 | ILE |
| 47 | SC | 55 | ILE |
| 47 | SC | 58 | CYS |
| 47 | SC | 62 | GLU |
| 47 | SC | 67 | ASP |
| 47 | SC | 73 | HIS |
| 47 | SC | 74 | LYS |
| 47 | SC | 75 | ILE |
| 47 | SC | 77 | TYR |
| 47 | SC | 79 | LEU |
| 47 | SC | 82 | ARG |
| 47 | SC | 84 | MET |
| 47 | SC | 86 | ASP |
| 47 | SC | 91 | ASN |
| 47 | SC | 92 | ILE |
| 47 | SC | 95 | ASP |
| 47 | SC | 97 | ILE |
| 47 | SC | 98 | ILE |
| 47 | SC | 99 | LYS |
| 47 | SC | 100 | ARG |
| 47 | SC | 102 | LEU |
| 47 | SC | 103 | SER |
| 47 | SC | 107 | MET |
| 47 | SC | 111 | LEU |
| 47 | SC | 112 | ARG |
| 47 | SC | 114 | LYS |
| 47 | SC | 115 | LEU |
| 47 | SC | 119 | MET |
| 47 | SC | 122 | ARG |
| 47 | SC | 123 | ARG |
| 47 | SC | 126 | TYR |
| 47 | SC | 129 | ILE |
| 47 | SC | 130 | ARG |
| 47 | SC | 134 | ARG |
| 47 | SC | 140 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | SC | 142 | VAL |
| 47 | SC | 143 | ILE |
| 47 | SC | 144 | VAL |
| 47 | SC | 147 | LYS |
| 47 | SC | 148 | LEU |
| 47 | SC | 152 | ARG |
| 47 | SC | 154 | ARG |
| 47 | SC | 156 | ASN |
| 47 | SC | 159 | LYS |
| 47 | SC | 160 | GLU |
| 47 | SC | 162 | CYS |
| 47 | SC | 165 | SER |
| 47 | SC | 166 | THR |
| 47 | SC | 170 | LYS |
| 47 | SC | 171 | ARG |
| 47 | SC | 173 | PHE |
| 47 | SC | 178 | THR |
| 47 | SC | 179 | ARG |
| 47 | SC | 181 | ILE |
| 47 | SC | 182 | LYS |
| 47 | SC | 183 | MET |
| 47 | SC | 184 | ARG |
| 47 | SC | 187 | VAL |
| 47 | SC | 188 | ILE |
| 47 | SC | 190 | VAL |
| 47 | SC | 191 | LYS |
| 47 | SC | 192 | VAL |
| 47 | SC | 193 | ARG |
| 47 | SC | 194 | ILE |
| 47 | SC | 200 | ARG |
| 47 | SC | 203 | VAL |
| 47 | SC | 207 | LYS |
| 47 | SC | 208 | ILE |
| 47 | SC | 210 | ILE |
| 48 | SD | 10 | LYS |
| 48 | SD | 11 | LYS |
| 48 | SD | 12 | LYS |
| 48 | SD | 15 | GLN |
| 48 | SD | 16 | ARG |
| 48 | SD | 17 | LYS |
| 48 | SD | 23 | LEU |
| 48 | SD | 24 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | SD | 25 | LYS |
| 48 | SD | 26 | GLU |
| 48 | SD | 30 | VAL |
| 48 | SD | 37 | LYS |
| 48 | SD | 44 | THR |
| 48 | SD | 46 | VAL |
| 48 | SD | 47 | THR |
| 48 | SD | 48 | LYS |
| 48 | SD | 49 | THR |
| 48 | SD | 54 | VAL |
| 48 | SD | 56 | THR |
| 48 | SD | 58 | VAL |
| 48 | SD | 61 | HIS |
| 48 | SD | 62 | ARG |
| 48 | SD | 63 | VAL |
| 48 | SD | 66 | VAL |
| 48 | SD | 67 | ASN |
| 48 | SD | 68 | LEU |
| 48 | SD | 71 | LEU |
| 48 | SD | 76 | GLU |
| 48 | SD | 77 | ASP |
| 48 | SD | 78 | LEU |
| 48 | SD | 81 | ASN |
| 48 | SD | 88 | THR |
| 48 | SD | 89 | GLN |
| 48 | SD | 90 | LEU |
| 48 | SD | 92 | SER |
| 48 | SD | 95 | LYS |
| 48 | SD | 96 | CYS |
| 48 | SD | 98 | THR |
| 48 | SD | 103 | MET |
| 48 | SD | 105 | ILE |
| 48 | SD | 106 | THR |
| 48 | SD | 107 | ARG |
| 48 | SD | 113 | LEU |
| 48 | SD | 115 | ARG |
| 48 | SD | 118 | CYS |
| 48 | SD | 119 | ASP |
| 48 | SD | 121 | ILE |
| 48 | SD | 123 | VAL |
| 48 | SD | 125 | MET |
| 48 | SD | 126 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | SD | 127 | ILE |
| 48 | SD | 133 | TYR |
| 48 | SD | 134 | LEU |
| 48 | SD | 137 | VAL |
| 48 | SD | 139 | VAL |
| 48 | SD | 142 | PHE |
| 48 | SD | 143 | THR |
| 48 | SD | 145 | ARG |
| 48 | SD | 146 | PHE |
| 48 | SD | 147 | ARG |
| 48 | SD | 152 | LYS |
| 48 | SD | 156 | VAL |
| 48 | SD | 157 | LYS |
| 48 | SD | 159 | ARG |
| 48 | SD | 160 | VAL |
| 48 | SD | 161 | ILE |
| 48 | SD | 162 | ARG |
| 48 | SD | 168 | ILE |
| 48 | SD | 172 | LEU |
| 48 | SD | 178 | LYS |
| 48 | SD | 181 | ILE |
| 48 | SD | 184 | LEU |
| 48 | SD | 185 | VAL |
| 48 | SD | 186 | THR |
| 48 | SD | 188 | LEU |
| 48 | SD | 192 | GLU |
| 48 | SD | 196 | LYS |
| 48 | SD | 201 | LEU |
| 48 | SD | 202 | GLN |
| 48 | SD | 203 | LYS |
| 48 | SD | 204 | ILE |
| 48 | SD | 206 | MET |
| 48 | SD | 209 | ASP |
| 48 | SD | 212 | ILE |
| 48 | SD | 213 | ARG |
| 48 | SD | 214 | ARG |
| 48 | SD | 216 | LYS |
| 48 | SD | 218 | VAL |
| 48 | SD | 219 | LYS |
| 48 | SD | 220 | ARG |
| 48 | SD | 222 | ARG |
| 48 | SD | 227 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | SD | 228 | LEU |
| 48 | SD | 233 | ASP |
| 48 | SD | 237 | VAL |
| 48 | SD | 238 | ARG |
| 49 | SE | 5 | VAL |
| 49 | SE | 6 | ARG |
| 49 | SE | 7 | LYS |
| 49 | SE | 8 | HIS |
| 49 | SE | 9 | LEU |
| 49 | SE | 10 | LYS |
| 49 | SE | 16 | LYS |
| 49 | SE | 19 | LEU |
| 49 | SE | 20 | LEU |
| 49 | SE | 22 | LYS |
| 49 | SE | 23 | MET |
| 49 | SE | 26 | ILE |
| 49 | SE | 30 | ARG |
| 49 | SE | 33 | ASN |
| 49 | SE | 40 | GLU |
| 49 | SE | 41 | CYS |
| 49 | SE | 42 | ILE |
| 49 | SE | 44 | LEU |
| 49 | SE | 45 | ILE |
| 49 | SE | 46 | LEU |
| 49 | SE | 48 | LEU |
| 49 | SE | 53 | HIS |
| 49 | SE | 58 | TYR |
| 49 | SE | 61 | THR |
| 49 | SE | 62 | SER |
| 49 | SE | 64 | ILE |
| 49 | SE | 65 | LEU |
| 49 | SE | 66 | GLN |
| 49 | SE | 67 | ASP |
| 49 | SE | 70 | VAL |
| 49 | SE | 71 | LEU |
| 49 | SE | 72 | ILE |
| 49 | SE | 75 | LYS |
| 49 | SE | 78 | THR |
| 49 | SE | 82 | PHE |
| 49 | SE | 84 | VAL |
| 49 | SE | 87 | MET |
| 49 | SE | 88 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | SE | 89 | VAL |
| 49 | SE | 94 | LYS |
| 49 | SE | 95 | VAL |
| 49 | SE | 97 | LYS |
| 49 | SE | 98 | THR |
| 49 | SE | 99 | PHE |
| 49 | SE | 101 | VAL |
| 49 | SE | 102 | LEU |
| 49 | SE | 103 | TYR |
| 49 | SE | 104 | ASP |
| 49 | SE | 105 | VAL |
| 49 | SE | 106 | LYS |
| 49 | SE | 108 | ARG |
| 49 | SE | 111 | LEU |
| 49 | SE | 112 | VAL |
| 49 | SE | 114 | ILE |
| 49 | SE | 116 | SER |
| 49 | SE | 118 | GLU |
| 49 | SE | 122 | LYS |
| 49 | SE | 123 | LEU |
| 49 | SE | 124 | CYS |
| 49 | SE | 125 | ARG |
| 49 | SE | 126 | VAL |
| 49 | SE | 128 | LYS |
| 49 | SE | 129 | ILE |
| 49 | SE | 134 | LYS |
| 49 | SE | 136 | MET |
| 49 | SE | 139 | LEU |
| 49 | SE | 142 | HIS |
| 49 | SE | 146 | THR |
| 49 | SE | 147 | ILE |
| 49 | SE | 153 | ASP |
| 49 | SE | 155 | LYS |
| 49 | SE | 156 | THR |
| 49 | SE | 158 | ASP |
| 49 | SE | 161 | LYS |
| 49 | SE | 164 | LEU |
| 49 | SE | 165 | LYS |
| 49 | SE | 166 | THR |
| 49 | SE | 168 | LYS |
| 49 | SE | 169 | ILE |
| 49 | SE | 174 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | SE | 176 | ASP |
| 49 | SE | 179 | LYS |
| 49 | SE | 182 | MET |
| 49 | SE | 183 | VAL |
| 49 | SE | 184 | THR |
| 49 | SE | 187 | ARG |
| 49 | SE | 194 | THR |
| 49 | SE | 195 | ILE |
| 49 | SE | 196 | GLN |
| 49 | SE | 198 | ILE |
| 49 | SE | 200 | LYS |
| 49 | SE | 201 | HIS |
| 49 | SE | 202 | MET |
| 49 | SE | 207 | MET |
| 49 | SE | 208 | ILE |
| 49 | SE | 210 | MET |
| 49 | SE | 211 | LYS |
| 49 | SE | 213 | THR |
| 49 | SE | 217 | GLU |
| 49 | SE | 218 | PHE |
| 49 | SE | 219 | LEU |
| 49 | SE | 220 | THR |
| 49 | SE | 224 | ASN |
| 49 | SE | 226 | PHE |
| 49 | SE | 227 | VAL |
| 49 | SE | 228 | ILE |
| 49 | SE | 232 | SER |
| 49 | SE | 235 | VAL |
| 49 | SE | 237 | ILE |
| 49 | SE | 240 | THR |
| 49 | SE | 243 | ILE |
| 49 | SE | 244 | ARG |
| 49 | SE | 246 | ASP |
| 49 | SE | 247 | ILE |
| 49 | SE | 248 | ILE |
| 49 | SE | 249 | LYS |
| 49 | SE | 252 | GLU |
| 49 | SE | 254 | ARG |
| 49 | SE | 255 | LEU |
| 49 | SE | 257 | SER |
| 49 | SE | 258 | ILE |
| 49 | SE | 260 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | SF | 5 | VAL |
| 50 | SF | 7 | LEU |
| 50 | SF | 9 | ASN |
| 50 | SF | 10 | LYS |
| 50 | SF | 13 | LEU |
| 50 | SF | 14 | THR |
| 50 | SF | 17 | LYS |
| 50 | SF | 18 | CYS |
| 50 | SF | 21 | GLU |
| 50 | SF | 23 | LEU |
| 50 | SF | 24 | GLU |
| 50 | SF | 29 | ILE |
| 50 | SF | 33 | SER |
| 50 | SF | 38 | SER |
| 50 | SF | 41 | ARG |
| 50 | SF | 42 | TRP |
| 50 | SF | 48 | ARG |
| 50 | SF | 49 | LYS |
| 50 | SF | 51 | LYS |
| 50 | SF | 52 | CYS |
| 50 | SF | 54 | VAL |
| 50 | SF | 56 | GLU |
| 50 | SF | 57 | ARG |
| 50 | SF | 59 | THR |
| 50 | SF | 63 | MET |
| 50 | SF | 64 | MET |
| 50 | SF | 65 | HIS |
| 50 | SF | 67 | ARG |
| 50 | SF | 68 | ASN |
| 50 | SF | 69 | SER |
| 50 | SF | 72 | LYS |
| 50 | SF | 73 | LEU |
| 50 | SF | 74 | MET |
| 50 | SF | 76 | MET |
| 50 | SF | 77 | LYS |
| 50 | SF | 85 | LEU |
| 50 | SF | 87 | ASN |
| 50 | SF | 90 | THR |
| 50 | SF | 95 | VAL |
| 50 | SF | 108 | ARG |
| 50 | SF | 109 | GLU |
| 50 | SF | 110 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | SF | 112 | CYS |
| 50 | SF | 113 | ARG |
| 50 | SF | 114 | ILE |
| 50 | SF | 116 | LYS |
| 50 | SF | 119 | GLN |
| 50 | SF | 120 | VAL |
| 50 | SF | 121 | ARG |
| 50 | SF | 122 | ARG |
| 50 | SF | 123 | GLN |
| 50 | SF | 125 | VAL |
| 50 | SF | 126 | ASP |
| 50 | SF | 128 | SER |
| 50 | SF | 130 | LEU |
| 50 | SF | 131 | ARG |
| 50 | SF | 133 | VAL |
| 50 | SF | 135 | ILE |
| 50 | SF | 137 | ILE |
| 50 | SF | 139 | ASN |
| 50 | SF | 145 | ARG |
| 50 | SF | 146 | LYS |
| 50 | SF | 150 | ARG |
| 50 | SF | 151 | LYS |
| 50 | SF | 152 | VAL |
| 50 | SF | 161 | GLU |
| 50 | SF | 164 | MET |
| 50 | SF | 171 | ASP |
| 50 | SF | 172 | LYS |
| 50 | SF | 173 | SER |
| 50 | SF | 184 | ARG |
| 50 | SF | 185 | ILE |
| 50 | SF | 188 | SER |
| 50 | SF | 190 | ARG |
| 51 | SG | 9 | VAL |
| 51 | SG | 11 | ILE |
| 51 | SG | 12 | SER |
| 51 | SG | 20 | LYS |
| 51 | SG | 22 | LEU |
| 51 | SG | 23 | MET |
| 51 | SG | 24 | ILE |
| 51 | SG | 28 | ARG |
| 51 | SG | 33 | ILE |
| 51 | SG | 36 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | SG | 38 | MET |
| 51 | SG | 41 | GLU |
| 51 | SG | 49 | GLU |
| 51 | SG | 50 | GLU |
| 51 | SG | 55 | THR |
| 51 | SG | 56 | PHE |
| 51 | SG | 57 | ARG |
| 51 | SG | 58 | ILE |
| 51 | SG | 59 | THR |
| 51 | SG | 63 | ASP |
| 51 | SG | 65 | GLN |
| 51 | SG | 69 | MET |
| 51 | SG | 70 | TYR |
| 51 | SG | 73 | VAL |
| 51 | SG | 74 | LEU |
| 51 | SG | 75 | LYS |
| 51 | SG | 77 | GLN |
| 51 | SG | 78 | ARG |
| 51 | SG | 80 | ARG |
| 51 | SG | 81 | LEU |
| 51 | SG | 82 | LEU |
| 51 | SG | 83 | LEU |
| 51 | SG | 84 | ARG |
| 51 | SG | 88 | LYS |
| 51 | SG | 95 | ASN |
| 51 | SG | 97 | GLU |
| 51 | SG | 99 | LYS |
| 51 | SG | 107 | ILE |
| 51 | SG | 108 | VAL |
| 51 | SG | 111 | ASP |
| 51 | SG | 115 | LEU |
| 51 | SG | 118 | VAL |
| 51 | SG | 119 | LEU |
| 51 | SG | 120 | VAL |
| 51 | SG | 126 | THR |
| 51 | SG | 130 | LEU |
| 51 | SG | 131 | THR |
| 51 | SG | 135 | VAL |
| 51 | SG | 137 | LYS |
| 51 | SG | 138 | ARG |
| 51 | SG | 139 | LEU |
| 51 | SG | 140 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | SG | 141 | PRO |
| 51 | SG | 142 | LYS |
| 51 | SG | 145 | SER |
| 51 | SG | 150 | LEU |
| 51 | SG | 151 | PHE |
| 51 | SG | 153 | LEU |
| 51 | SG | 155 | THR |
| 51 | SG | 156 | THR |
| 51 | SG | 158 | VAL |
| 51 | SG | 161 | LYS |
| 51 | SG | 163 | GLN |
| 51 | SG | 165 | LEU |
| 51 | SG | 169 | LEU |
| 51 | SG | 170 | ILE |
| 51 | SG | 171 | LYS |
| 51 | SG | 172 | GLU |
| 51 | SG | 183 | GLU |
| 51 | SG | 184 | LYS |
| 51 | SG | 185 | LYS |
| 51 | SG | 187 | LYS |
| 51 | SG | 190 | LYS |
| 51 | SG | 191 | VAL |
| 51 | SG | 193 | ARG |
| 51 | SG | 194 | VAL |
| 51 | SG | 195 | VAL |
| 51 | SG | 197 | ASP |
| 51 | SG | 199 | LYS |
| 51 | SG | 200 | TYR |
| 51 | SG | 202 | ARG |
| 51 | SG | 203 | LYS |
| 51 | SG | 209 | GLU |
| 51 | SG | 211 | LYS |
| 51 | SG | 214 | MET |
| 51 | SG | 215 | ARG |
| 51 | SG | 216 | LYS |
| 51 | SG | 217 | SER |
| 51 | SG | 218 | LEU |
| 51 | SG | 225 | LYS |
| 51 | SG | 227 | LEU |
| 51 | SG | 228 | LEU |
| 51 | SG | 231 | MET |
| 51 | SG | 233 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | SG | 234 | GLN |
| 51 | SG | 235 | HIS |
| 51 | SG | 238 | ARG |
| 51 | SG | 239 | ILE |
| 51 | SG | 240 | TYR |
| 51 | SG | 241 | LYS |
| 51 | SG | 244 | LYS |
| 51 | SG | 245 | ARG |
| 52 | SH | 9 | ILE |
| 52 | SH | 11 | LYS |
| 52 | SH | 14 | GLU |
| 52 | SH | 15 | LYS |
| 52 | SH | 16 | LEU |
| 52 | SH | 18 | GLU |
| 52 | SH | 19 | LEU |
| 52 | SH | 21 | LYS |
| 52 | SH | 22 | GLN |
| 52 | SH | 23 | VAL |
| 52 | SH | 26 | THR |
| 52 | SH | 27 | LEU |
| 52 | SH | 28 | LEU |
| 52 | SH | 30 | LEU |
| 52 | SH | 32 | ASP |
| 52 | SH | 35 | ASP |
| 52 | SH | 36 | LEU |
| 52 | SH | 37 | ARG |
| 52 | SH | 41 | LEU |
| 52 | SH | 43 | THR |
| 52 | SH | 44 | LEU |
| 52 | SH | 47 | SER |
| 52 | SH | 50 | LYS |
| 52 | SH | 52 | ILE |
| 52 | SH | 55 | ASP |
| 52 | SH | 57 | ASP |
| 52 | SH | 59 | LYS |
| 52 | SH | 62 | VAL |
| 52 | SH | 63 | VAL |
| 52 | SH | 72 | SER |
| 52 | SH | 73 | PHE |
| 52 | SH | 76 | ASN |
| 52 | SH | 80 | LEU |
| 52 | SH | 81 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | SH | 83 | LYS |
| 52 | SH | 84 | LEU |
| 52 | SH | 85 | GLU |
| 52 | SH | 89 | SER |
| 52 | SH | 92 | ARG |
| 52 | SH | 95 | ILE |
| 52 | SH | 98 | ASN |
| 52 | SH | 99 | ARG |
| 52 | SH | 100 | THR |
| 52 | SH | 102 | MET |
| 52 | SH | 103 | LYS |
| 52 | SH | 107 | VAL |
| 52 | SH | 108 | PHE |
| 52 | SH | 111 | LYS |
| 52 | SH | 112 | LYS |
| 52 | SH | 113 | SER |
| 52 | SH | 114 | ILE |
| 52 | SH | 115 | ARG |
| 52 | SH | 116 | ARG |
| 52 | SH | 118 | ARG |
| 52 | SH | 121 | THR |
| 52 | SH | 125 | VAL |
| 52 | SH | 129 | ILE |
| 52 | SH | 133 | ILE |
| 52 | SH | 134 | CYS |
| 52 | SH | 137 | ILE |
| 52 | SH | 138 | HIS |
| 52 | SH | 142 | LYS |
| 52 | SH | 143 | ARG |
| 52 | SH | 145 | LEU |
| 52 | SH | 153 | ARG |
| 52 | SH | 154 | LEU |
| 52 | SH | 155 | GLN |
| 52 | SH | 156 | VAL |
| 52 | SH | 157 | VAL |
| 52 | SH | 158 | LEU |
| 52 | SH | 160 | LYS |
| 52 | SH | 162 | VAL |
| 52 | SH | 163 | TYR |
| 52 | SH | 165 | GLU |
| 52 | SH | 169 | ARG |
| 52 | SH | 171 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | SH | 178 | LYS |
| 52 | SH | 180 | LEU |
| 52 | SH | 182 | GLU |
| 52 | SH | 183 | ARG |
| 52 | SH | 185 | THR |
| 52 | SH | 186 | GLU |
| 52 | SH | 188 | ILE |
| 53 | SI | 4 | THR |
| 53 | SI | 8 | MET |
| 53 | SI | 10 | LYS |
| 53 | SI | 11 | ARG |
| 53 | SI | 13 | LYS |
| 53 | SI | 17 | VAL |
| 53 | SI | 18 | GLN |
| 53 | SI | 20 | LYS |
| 53 | SI | 21 | TRP |
| 53 | SI | 22 | HIS |
| 53 | SI | 23 | LYS |
| 53 | SI | 24 | LYS |
| 53 | SI | 26 | LYS |
| 53 | SI | 29 | LEU |
| 53 | SI | 31 | ARG |
| 53 | SI | 36 | THR |
| 53 | SI | 37 | LYS |
| 53 | SI | 38 | LEU |
| 53 | SI | 39 | ILE |
| 53 | SI | 40 | VAL |
| 53 | SI | 41 | LYS |
| 53 | SI | 42 | VAL |
| 53 | SI | 43 | THR |
| 53 | SI | 44 | SER |
| 53 | SI | 45 | LYS |
| 53 | SI | 46 | LYS |
| 53 | SI | 48 | GLU |
| 53 | SI | 50 | GLN |
| 53 | SI | 51 | LYS |
| 53 | SI | 53 | SER |
| 53 | SI | 54 | THR |
| 53 | SI | 55 | ILE |
| 53 | SI | 56 | ARG |
| 53 | SI | 62 | ILE |
| 53 | SI | 64 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 53 | SI | 70 | SER |
| 53 | SI | 71 | HIS |
| 53 | SI | 74 | PHE |
| 53 | SI | 89 | GLN |
| 53 | SI | 91 | VAL |
| 53 | SI | 92 | TYR |
| 53 | SI | 94 | SER |
| 53 | SI | 96 | SER |
| 53 | SI | 97 | ASN |
| 53 | SI | 100 | VAL |
| 53 | SI | 102 | THR |
| 53 | SI | 105 | LEU |
| 53 | SI | 106 | VAL |
| 53 | SI | 107 | LYS |
| 53 | SI | 110 | VAL |
| 53 | SI | 112 | GLN |
| 53 | SI | 118 | PHE |
| 53 | SI | 119 | LYS |
| 53 | SI | 129 | LYS |
| 53 | SI | 131 | ILE |
| 53 | SI | 132 | LEU |
| 53 | SI | 135 | ILE |
| 53 | SI | 136 | ARG |
| 53 | SI | 138 | ASP |
| 53 | SI | 141 | LEU |
| 53 | SI | 145 | SER |
| 53 | SI | 146 | SER |
| 53 | SI | 147 | ARG |
| 53 | SI | 151 | VAL |
| 53 | SI | 153 | THR |
| 53 | SI | 157 | TYR |
| 53 | SI | 158 | ILE |
| 53 | SI | 159 | LEU |
| 53 | SI | 160 | GLU |
| 53 | SI | 164 | LEU |
| 53 | SI | 170 | LYS |
| 53 | SI | 171 | LEU |
| 53 | SI | 174 | LYS |
| 54 | SJ | 2 | VAL |
| 54 | SJ | 4 | ILE |
| 54 | SJ | 8 | ARG |
| 54 | SJ | 11 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | SJ | 12 | LYS |
| 54 | SJ | 14 | ILE |
| 54 | SJ | 15 | CYS |
| 54 | SJ | 16 | ASN |
| 54 | SJ | 18 | GLN |
| 54 | SJ | 19 | ARG |
| 54 | SJ | 20 | ILE |
| 54 | SJ | 22 | LYS |
| 54 | SJ | 23 | LYS |
| 54 | SJ | 24 | GLN |
| 54 | SJ | 28 | ARG |
| 54 | SJ | 31 | SER |
| 54 | SJ | 32 | LYS |
| 54 | SJ | 33 | VAL |
| 54 | SJ | 35 | ILE |
| 54 | SJ | 38 | LEU |
| 54 | SJ | 39 | GLN |
| 54 | SJ | 40 | LEU |
| 54 | SJ | 43 | LYS |
| 54 | SJ | 47 | ILE |
| 54 | SJ | 49 | ASP |
| 54 | SJ | 52 | VAL |
| 54 | SJ | 53 | VAL |
| 54 | SJ | 54 | ASP |
| 54 | SJ | 58 | SER |
| 54 | SJ | 60 | ARG |
| 54 | SJ | 61 | ILE |
| 54 | SJ | 62 | VAL |
| 54 | SJ | 65 | LEU |
| 54 | SJ | 66 | ILE |
| 54 | SJ | 69 | LEU |
| 54 | SJ | 70 | ASN |
| 54 | SJ | 74 | VAL |
| 54 | SJ | 78 | ARG |
| 54 | SJ | 81 | ILE |
| 54 | SJ | 84 | ASN |
| 54 | SJ | 85 | ASP |
| 54 | SJ | 87 | GLU |
| 54 | SJ | 88 | LYS |
| 54 | SJ | 90 | VAL |
| 54 | SJ | 92 | ASN |
| 54 | SJ | 93 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | SJ | 94 | LEU |
| 54 | SJ | 97 | ARG |
| 54 | SJ | 98 | LEU |
| 54 | SJ | 99 | PHE |
| 54 | SJ | 102 | ILE |
| 54 | SJ | 106 | THR |
| 54 | SJ | 108 | GLN |
| 54 | SJ | 111 | MET |
| 54 | SJ | 112 | ASP |
| 54 | SJ | 113 | HIS |
| 54 | SJ | 117 | GLN |
| 54 | SJ | 118 | HIS |
| 54 | SJ | 119 | ARG |
| 54 | SJ | 120 | GLN |
| 54 | SJ | 121 | ILE |
| 55 | SK | 2 | ARG |
| 55 | SK | 3 | ILE |
| 55 | SK | 5 | ARG |
| 55 | SK | 9 | SER |
| 55 | SK | 10 | SER |
| 55 | SK | 11 | LYS |
| 55 | SK | 14 | SER |
| 55 | SK | 15 | THR |
| 55 | SK | 17 | LYS |
| 55 | SK | 18 | LYS |
| 55 | SK | 21 | THR |
| 55 | SK | 22 | LYS |
| 55 | SK | 24 | ARG |
| 55 | SK | 32 | CYS |
| 55 | SK | 38 | LYS |
| 55 | SK | 40 | LYS |
| 55 | SK | 41 | ARG |
| 55 | SK | 43 | ILE |
| 55 | SK | 45 | ARG |
| 55 | SK | 47 | ARG |
| 55 | SK | 50 | LEU |
| 55 | SK | 52 | LYS |
| 55 | SK | 53 | ILE |
| 55 | SK | 54 | ARG |
| 55 | SK | 55 | ARG |
| 55 | SK | 58 | ARG |
| 55 | SK | 61 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | SK | 63 | LEU |
| 55 | SK | 68 | ILE |
| 55 | SK | 69 | LYS |
| 55 | SK | 71 | ARG |
| 55 | SK | 77 | LEU |
| 55 | SK | 78 | LEU |
| 55 | SK | 79 | ARG |
| 55 | SK | 81 | LEU |
| 55 | SK | 84 | LEU |
| 55 | SK | 86 | ILE |
| 55 | SK | 87 | LEU |
| 55 | SK | 90 | GLU |
| 55 | SK | 93 | GLN |
| 55 | SK | 95 | ASP |
| 55 | SK | 96 | TYR |
| 55 | SK | 100 | LEU |
| 55 | SK | 101 | ARG |
| 55 | SK | 102 | ILE |
| 55 | SK | 103 | GLU |
| 55 | SK | 105 | ILE |
| 55 | SK | 107 | LYS |
| 55 | SK | 108 | ARG |
| 55 | SK | 110 | LEU |
| 55 | SK | 112 | SER |
| 55 | SK | 118 | LYS |
| 55 | SK | 121 | LYS |
| 55 | SK | 122 | SER |
| 55 | SK | 123 | VAL |
| 55 | SK | 129 | MET |
| 55 | SK | 131 | LYS |
| 55 | SK | 133 | ARG |
| 55 | SK | 136 | SER |
| 55 | SK | 137 | VAL |
| 55 | SK | 143 | ASN |
| 55 | SK | 144 | ILE |
| 55 | SK | 147 | TYR |
| 55 | SK | 151 | ILE |
| 55 | SK | 152 | SER |
| 55 | SK | 153 | ASN |
| 55 | SK | 154 | THR |
| 55 | SK | 156 | ARG |
| 55 | SK | 159 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | SK | 163 | SER |
| 55 | SK | 167 | PRO |
| 55 | SK | 168 | ASN |
| 55 | SK | 170 | LYS |
| 55 | SK | 173 | ARG |
| 55 | SK | 174 | THR |
| 55 | SK | 175 | LYS |
| 55 | SK | 176 | ARG |
| 56 | SL | 2 | VAL |
| 56 | SL | 4 | ILE |
| 56 | SL | 6 | LYS |
| 56 | SL | 12 | VAL |
| 56 | SL | 16 | LEU |
| 56 | SL | 18 | GLU |
| 56 | SL | 19 | ASN |
| 56 | SL | 24 | LEU |
| 56 | SL | 26 | GLU |
| 56 | SL | 27 | TYR |
| 56 | SL | 29 | ARG |
| 56 | SL | 30 | VAL |
| 56 | SL | 33 | VAL |
| 56 | SL | 36 | ILE |
| 56 | SL | 37 | THR |
| 56 | SL | 49 | THR |
| 56 | SL | 53 | VAL |
| 56 | SL | 54 | ASN |
| 56 | SL | 56 | ILE |
| 56 | SL | 57 | MET |
| 56 | SL | 58 | GLN |
| 56 | SL | 60 | LEU |
| 56 | SL | 61 | GLU |
| 56 | SL | 63 | ARG |
| 56 | SL | 67 | LYS |
| 56 | SL | 69 | THR |
| 56 | SL | 72 | TRP |
| 56 | SL | 74 | HIS |
| 56 | SL | 79 | LEU |
| 56 | SL | 81 | GLU |
| 56 | SL | 82 | LYS |
| 56 | SL | 84 | GLU |
| 56 | SL | 87 | ILE |
| 56 | SL | 89 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 56 | SL | 94 | THR |
| 56 | SL | 104 | LYS |
| 56 | SL | 106 | SER |
| 56 | SL | 107 | ILE |
| 56 | SL | 108 | LYS |
| 57 | SM | 3 | GLU |
| 57 | SM | 4 | ASN |
| 57 | SM | 5 | GLN |
| 57 | SM | 8 | ARG |
| 57 | SM | 11 | HIS |
| 57 | SM | 12 | LYS |
| 57 | SM | 20 | ARG |
| 57 | SM | 21 | PHE |
| 57 | SM | 22 | LEU |
| 57 | SM | 23 | ARG |
| 57 | SM | 24 | LYS |
| 57 | SM | 28 | ARG |
| 57 | SM | 29 | CYS |
| 57 | SM | 30 | LEU |
| 57 | SM | 33 | TYR |
| 57 | SM | 34 | LYS |
| 57 | SM | 35 | SER |
| 57 | SM | 38 | MET |
| 57 | SM | 40 | TYR |
| 57 | SM | 42 | THR |
| 57 | SM | 44 | ILE |
| 57 | SM | 47 | ILE |
| 57 | SM | 51 | TYR |
| 57 | SM | 54 | LYS |
| 57 | SM | 55 | LYS |
| 57 | SM | 59 | THR |
| 57 | SM | 61 | ASN |
| 57 | SM | 62 | VAL |
| 57 | SM | 63 | SER |
| 57 | SM | 64 | ILE |
| 57 | SM | 65 | ARG |
| 57 | SM | 68 | ILE |
| 57 | SM | 72 | VAL |
| 57 | SM | 73 | VAL |
| 57 | SM | 75 | SER |
| 57 | SM | 77 | LYS |
| 57 | SM | 78 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | SM | 83 | ILE |
| 57 | SM | 84 | VAL |
| 57 | SM | 89 | LEU |
| 57 | SM | 92 | VAL |
| 57 | SM | 93 | GLN |
| 57 | SM | 95 | TYR |
| 57 | SM | 96 | LYS |
| 57 | SM | 99 | GLU |
| 57 | SM | 100 | ARG |
| 57 | SM | 101 | ARG |
| 57 | SM | 104 | HIS |
| 57 | SM | 105 | VAL |
| 57 | SM | 110 | SER |
| 57 | SM | 113 | PHE |
| 57 | SM | 114 | ARG |
| 57 | SM | 115 | VAL |
| 57 | SM | 116 | LYS |
| 57 | SM | 117 | GLU |
| 57 | SM | 120 | ILE |
| 57 | SM | 121 | VAL |
| 57 | SM | 126 | CYS |
| 57 | SM | 127 | ARG |
| 57 | SM | 129 | LEU |
| 57 | SM | 130 | SER |
| 57 | SM | 131 | LYS |
| 57 | SM | 133 | ILE |
| 57 | SM | 134 | ARG |
| 57 | SM | 136 | ASN |
| 57 | SM | 139 | LYS |
| 57 | SM | 140 | VAL |
| 57 | SM | 148 | LYS |
| 57 | SM | 149 | LYS |
| 57 | SM | 154 | PHE |
| 58 | SO | 11 | ARG |
| 58 | SO | 14 | ARG |
| 58 | SO | 16 | ILE |
| 58 | SO | 17 | ARG |
| 58 | SO | 20 | GLN |
| 58 | SO | 21 | ARG |
| 58 | SO | 22 | TRP |
| 58 | SO | 24 | ASP |
| 58 | SO | 26 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 58 | SO | 28 | ARG |
| 58 | SO | 29 | LYS |
| 58 | SO | 32 | LEU |
| 58 | SO | 37 | LYS |
| 58 | SO | 41 | LEU |
| 58 | SO | 42 | GLU |
| 58 | SO | 45 | CYS |
| 58 | SO | 46 | MET |
| 58 | SO | 48 | ARG |
| 58 | SO | 50 | ILE |
| 58 | SO | 51 | VAL |
| 58 | SO | 52 | THR |
| 58 | SO | 54 | LYS |
| 58 | SO | 55 | ILE |
| 58 | SO | 57 | ILE |
| 58 | SO | 61 | GLN |
| 58 | SO | 63 | ASN |
| 58 | SO | 64 | SER |
| 58 | SO | 66 | VAL |
| 58 | SO | 68 | LYS |
| 58 | SO | 72 | VAL |
| 58 | SO | 76 | LYS |
| 58 | SO | 81 | ILE |
| 58 | SO | 85 | VAL |
| 58 | SO | 91 | LEU |
| 58 | SO | 92 | THR |
| 58 | SO | 95 | ASP |
| 58 | SO | 98 | ASP |
| 58 | SO | 100 | VAL |
| 58 | SO | 105 | PHE |
| 58 | SO | 110 | ARG |
| 58 | SO | 112 | VAL |
| 58 | SO | 115 | ILE |
| 58 | SO | 118 | CYS |
| 58 | SO | 119 | ARG |
| 58 | SO | 123 | ILE |
| 58 | SO | 124 | LYS |
| 58 | SO | 128 | ILE |
| 58 | SO | 130 | LEU |
| 58 | SO | 131 | LEU |
| 58 | SO | 133 | LEU |
| 58 | SO | 135 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 58 | SO | 136 | ARG |
| 58 | SO | 138 | ARG |
| 58 | SO | 140 | LYS |
| 59 | SP | 3 | ARG |
| 59 | SP | 4 | MET |
| 59 | SP | 9 | LYS |
| 59 | SP | 11 | ILE |
| 59 | SP | 13 | ARG |
| 59 | SP | 14 | SER |
| 59 | SP | 16 | ILE |
| 59 | SP | 25 | TRP |
| 59 | SP | 26 | ASN |
| 59 | SP | 27 | LYS |
| 59 | SP | 29 | THR |
| 59 | SP | 31 | GLU |
| 59 | SP | 34 | CYS |
| 59 | SP | 35 | GLU |
| 59 | SP | 37 | ILE |
| 59 | SP | 39 | LYS |
| 59 | SP | 43 | LYS |
| 59 | SP | 45 | THR |
| 59 | SP | 48 | SER |
| 59 | SP | 49 | GLN |
| 59 | SP | 50 | ILE |
| 59 | SP | 52 | LEU |
| 59 | SP | 60 | ILE |
| 59 | SP | 63 | VAL |
| 59 | SP | 64 | LYS |
| 59 | SP | 67 | THR |
| 59 | SP | 69 | SER |
| 59 | SP | 70 | LYS |
| 59 | SP | 72 | VAL |
| 59 | SP | 73 | ARG |
| 59 | SP | 74 | ILE |
| 59 | SP | 76 | LYS |
| 59 | SP | 78 | LYS |
| 59 | SP | 80 | LEU |
| 59 | SP | 84 | ILE |
| 59 | SP | 91 | MET |
| 59 | SP | 94 | LYS |
| 59 | SP | 98 | ILE |
| 59 | SP | 99 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 59 | SP | 100 | LYS |
| 59 | SP | 102 | LEU |
| 59 | SP | 104 | ARG |
| 59 | SP | 112 | LYS |
| 59 | SP | 114 | ARG |
| 59 | SP | 120 | SER |
| 59 | SP | 121 | ARG |
| 59 | SP | 125 | LEU |
| 59 | SP | 131 | GLN |
| 59 | SP | 134 | ARG |
| 59 | SP | 135 | LEU |
| 59 | SP | 138 | THR |
| 59 | SP | 142 | LYS |
| 59 | SP | 143 | SER |
| 59 | SP | 144 | ASP |
| 59 | SP | 145 | GLN |
| 60 | SQ | 26 | GLU |
| 60 | SQ | 28 | PHE |
| 60 | SQ | 30 | VAL |
| 60 | SQ | 33 | ILE |
| 60 | SQ | 37 | LYS |
| 60 | SQ | 40 | THR |
| 60 | SQ | 42 | ILE |
| 60 | SQ | 44 | VAL |
| 60 | SQ | 47 | LEU |
| 60 | SQ | 50 | ARG |
| 60 | SQ | 57 | SER |
| 60 | SQ | 60 | MET |
| 60 | SQ | 61 | LYS |
| 60 | SQ | 64 | ARG |
| 60 | SQ | 66 | CYS |
| 60 | SQ | 68 | GLU |
| 60 | SQ | 79 | GLN |
| 60 | SQ | 81 | LEU |
| 60 | SQ | 82 | ILE |
| 60 | SQ | 83 | GLU |
| 60 | SQ | 84 | ILE |
| 60 | SQ | 85 | ILE |
| 60 | SQ | 93 | VAL |
| 60 | SQ | 96 | LYS |
| 60 | SQ | 97 | ILE |
| 60 | SQ | 105 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 60 | SQ | 116 | ILE |
| 60 | SQ | 120 | VAL |
| 60 | SQ | 124 | ILE |
| 60 | SQ | 126 | ILE |
| 60 | SQ | 131 | ASP |
| 60 | SQ | 133 | THR |
| 60 | SQ | 139 | ARG |
| 60 | SQ | 140 | THR |
| 60 | SQ | 143 | LYS |
| 60 | SQ | 146 | ARG |
| 60 | SQ | 147 | ARG |
| 60 | SQ | 149 | ARG |
| 60 | SQ | 150 | ARG |
| 60 | SQ | 151 | LEU |
| 61 | SR | 18 | ARG |
| 61 | SR | 20 | VAL |
| 61 | SR | 21 | GLU |
| 61 | SR | 22 | VAL |
| 61 | SR | 24 | LYS |
| 61 | SR | 25 | LEU |
| 61 | SR | 28 | MET |
| 61 | SR | 29 | LYS |
| 61 | SR | 31 | THR |
| 61 | SR | 33 | ILE |
| 61 | SR | 34 | LEU |
| 61 | SR | 36 | LYS |
| 61 | SR | 40 | ARG |
| 61 | SR | 41 | CYS |
| 61 | SR | 42 | ARG |
| 61 | SR | 45 | ILE |
| 61 | SR | 47 | LYS |
| 61 | SR | 50 | LEU |
| 61 | SR | 51 | SER |
| 61 | SR | 56 | ARG |
| 61 | SR | 60 | LYS |
| 61 | SR | 61 | LEU |
| 61 | SR | 63 | LEU |
| 61 | SR | 64 | ARG |
| 61 | SR | 65 | ARG |
| 61 | SR | 72 | LYS |
| 61 | SR | 75 | ILE |
| 61 | SR | 76 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 61 | SR | 77 | ARG |
| 61 | SR | 78 | THR |
| 61 | SR | 82 | ASP |
| 61 | SR | 83 | MET |
| 61 | SR | 84 | ILE |
| 61 | SR | 88 | GLU |
| 61 | SR | 92 | MET |
| 61 | SR | 93 | THR |
| 61 | SR | 96 | VAL |
| 61 | SR | 98 | ASN |
| 61 | SR | 100 | ARG |
| 61 | SR | 101 | GLN |
| 61 | SR | 103 | ILE |
| 61 | SR | 107 | ILE |
| 61 | SR | 111 | MET |
| 61 | SR | 114 | ARG |
| 61 | SR | 117 | ARG |
| 61 | SR | 118 | GLU |
| 61 | SR | 123 | TYR |
| 61 | SR | 125 | ILE |
| 61 | SR | 126 | VAL |
| 61 | SR | 128 | HIS |
| 62 | ST | 10 | LEU |
| 62 | ST | 12 | ARG |
| 62 | ST | 14 | ASP |
| 62 | ST | 15 | ILE |
| 62 | ST | 17 | VAL |
| 62 | ST | 20 | ARG |
| 62 | ST | 22 | LYS |
| 62 | ST | 24 | THR |
| 62 | ST | 26 | HIS |
| 62 | ST | 27 | THR |
| 62 | ST | 28 | LEU |
| 62 | ST | 30 | LYS |
| 62 | ST | 32 | LYS |
| 62 | ST | 37 | VAL |
| 62 | ST | 41 | LYS |
| 62 | ST | 47 | ILE |
| 62 | ST | 48 | LEU |
| 62 | ST | 49 | VAL |
| 62 | ST | 50 | ASN |
| 62 | ST | 52 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 62 | ST | 54 | LEU |
| 62 | ST | 56 | LEU |
| 62 | ST | 57 | VAL |
| 62 | ST | 61 | ILE |
| 62 | ST | 63 | ARG |
| 62 | ST | 64 | THR |
| 62 | ST | 65 | LYS |
| 62 | ST | 66 | VAL |
| 62 | ST | 67 | SER |
| 62 | ST | 70 | ILE |
| 62 | ST | 71 | MET |
| 62 | ST | 77 | LEU |
| 62 | ST | 83 | MET |
| 62 | ST | 86 | LYS |
| 62 | ST | 92 | HIS |
| 62 | ST | 93 | VAL |
| 62 | ST | 94 | SER |
| 62 | ST | 96 | ILE |
| 62 | ST | 100 | ARG |
| 62 | ST | 103 | ILE |
| 62 | ST | 107 | VAL |
| 62 | ST | 108 | LEU |
| 62 | ST | 112 | LYS |
| 62 | ST | 113 | ASP |
| 62 | ST | 114 | GLU |
| 62 | ST | 117 | ARG |
| 62 | ST | 124 | LEU |
| 62 | ST | 127 | TYR |
| 62 | ST | 130 | GLN |
| 62 | ST | 133 | VAL |
| 62 | ST | 134 | SER |
| 62 | ST | 140 | GLU |
| 62 | ST | 142 | LYS |
| 62 | ST | 143 | LYS |
| 62 | ST | 144 | PHE |
| 62 | ST | 147 | ARG |
| 62 | ST | 153 | ARG |
| 62 | ST | 154 | GLN |
| 62 | ST | 156 | SER |
| 63 | SU | 3 | LYS |
| 63 | SU | 4 | VAL |
| 63 | SU | 5 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 63 | SU | 6 | THR |
| 63 | SU | 7 | LYS |
| 63 | SU | 8 | THR |
| 63 | SU | 11 | ARG |
| 63 | SU | 19 | ASN |
| 63 | SU | 22 | GLU |
| 63 | SU | 25 | LYS |
| 63 | SU | 27 | LYS |
| 63 | SU | 33 | LYS |
| 63 | SU | 35 | ILE |
| 63 | SU | 37 | SER |
| 63 | SU | 38 | LYS |
| 63 | SU | 39 | ARG |
| 63 | SU | 43 | ILE |
| 63 | SU | 44 | ILE |
| 63 | SU | 46 | SER |
| 63 | SU | 47 | LYS |
| 63 | SU | 50 | ARG |
| 63 | SU | 52 | LYS |
| 63 | SU | 59 | THR |
| 63 | SU | 61 | MET |
| 63 | SU | 63 | ARG |
| 63 | SU | 64 | VAL |
| 63 | SU | 65 | VAL |
| 63 | SU | 66 | LYS |
| 63 | SU | 72 | ILE |
| 63 | SU | 73 | SER |
| 63 | SU | 74 | LEU |
| 63 | SU | 75 | ARG |
| 63 | SU | 76 | LEU |
| 63 | SU | 81 | ARG |
| 63 | SU | 83 | ARG |
| 63 | SU | 84 | ARG |
| 63 | SU | 87 | TYR |
| 63 | SU | 90 | LYS |
| 63 | SU | 91 | LYS |
| 63 | SU | 93 | GLU |
| 63 | SU | 96 | VAL |
| 63 | SU | 97 | GLU |
| 63 | SU | 99 | ILE |
| 63 | SU | 100 | THR |
| 63 | SU | 101 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 63 | SU | 104 | THR |
| 63 | SU | 105 | THR |
| 63 | SU | 107 | GLN |
| 63 | SU | 108 | MET |
| 63 | SU | 109 | ILE |
| 63 | SU | 112 | ILE |
| 63 | SU | 114 | PHE |
| 63 | SU | 117 | MET |
| 63 | SU | 121 | LEU |
| 63 | SU | 122 | LYS |
| 64 | SV | 11 | ARG |
| 64 | SV | 14 | LEU |
| 64 | SV | 15 | ARG |
| 64 | SV | 16 | MET |
| 64 | SV | 20 | ASN |
| 64 | SV | 21 | ILE |
| 64 | SV | 24 | LYS |
| 64 | SV | 26 | VAL |
| 64 | SV | 27 | LEU |
| 64 | SV | 28 | GLU |
| 64 | SV | 31 | LEU |
| 64 | SV | 32 | VAL |
| 64 | SV | 35 | LYS |
| 64 | SV | 39 | ARG |
| 64 | SV | 40 | ARG |
| 64 | SV | 44 | VAL |
| 64 | SV | 46 | LEU |
| 64 | SV | 47 | LYS |
| 64 | SV | 48 | LYS |
| 64 | SV | 50 | ASN |
| 64 | SV | 52 | ASP |
| 64 | SV | 55 | LYS |
| 64 | SV | 59 | GLU |
| 64 | SV | 60 | LEU |
| 64 | SV | 61 | THR |
| 64 | SV | 65 | GLU |
| 64 | SV | 71 | VAL |
| 64 | SV | 76 | LEU |
| 64 | SV | 77 | SER |
| 64 | SV | 84 | MET |
| 64 | SV | 85 | LEU |
| 64 | SV | 86 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 64 | SV | 88 | ASN |
| 64 | SV | 91 | PHE |
| 64 | SV | 92 | GLU |
| 64 | SV | 95 | LYS |
| 64 | SV | 97 | MET |
| 64 | SV | 99 | ILE |
| 64 | SV | 101 | VAL |
| 64 | SV | 103 | THR |
| 64 | SV | 104 | ILE |
| 64 | SV | 107 | THR |
| 64 | SV | 109 | ARG |
| 64 | SV | 112 | LEU |
| 64 | SV | 113 | GLU |
| 64 | SV | 114 | ARG |
| 64 | SV | 117 | LYS |
| 64 | SV | 119 | ARG |
| 64 | SV | 124 | VAL |
| 64 | SV | 126 | HIS |
| 64 | SV | 127 | HIS |
| 64 | SV | 131 | LYS |
| 64 | SV | 133 | ARG |
| 64 | SV | 137 | THR |
| 64 | SV | 138 | LYS |
| 64 | SV | 143 | ARG |
| 64 | SV | 145 | HIS |
| 64 | SV | 147 | VAL |
| 64 | SV | 149 | VAL |
| 64 | SV | 150 | GLN |
| 64 | SV | 151 | ARG |
| 64 | SV | 152 | LYS |
| 65 | SW | 4 | VAL |
| 65 | SW | 13 | ILE |
| 65 | SW | 20 | LEU |
| 65 | SW | 21 | LYS |
| 65 | SW | 25 | ILE |
| 65 | SW | 26 | ILE |
| 65 | SW | 27 | LYS |
| 65 | SW | 28 | CYS |
| 65 | SW | 31 | PHE |
| 65 | SW | 34 | TYR |
| 65 | SW | 36 | LYS |
| 65 | SW | 39 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 65 | SW | 41 | ARG |
| 65 | SW | 46 | ARG |
| 65 | SW | 47 | ASP |
| 65 | SW | 49 | ASP |
| 65 | SW | 50 | TRP |
| 65 | SW | 52 | TYR |
| 65 | SW | 54 | LYS |
| 65 | SW | 61 | HIS |
| 65 | SW | 62 | PHE |
| 65 | SW | 63 | TYR |
| 65 | SW | 64 | ILE |
| 65 | SW | 67 | SER |
| 65 | SW | 70 | ILE |
| 65 | SW | 75 | LEU |
| 65 | SW | 77 | ARG |
| 65 | SW | 78 | LYS |
| 65 | SW | 81 | SER |
| 65 | SW | 82 | LEU |
| 65 | SW | 86 | LYS |
| 65 | SW | 87 | THR |
| 65 | SW | 88 | THR |
| 65 | SW | 90 | HIS |
| 65 | SW | 91 | HIS |
| 65 | SW | 93 | LYS |
| 65 | SW | 94 | ARG |
| 65 | SW | 96 | SER |
| 65 | SW | 98 | LYS |
| 65 | SW | 100 | ILE |
| 65 | SW | 102 | SER |
| 65 | SW | 104 | VAL |
| 65 | SW | 106 | GLN |
| 65 | SW | 107 | PHE |
| 65 | SW | 108 | LEU |
| 65 | SW | 112 | LEU |
| 65 | SW | 113 | LEU |
| 65 | SW | 114 | ILE |
| 65 | SW | 117 | GLU |
| 65 | SW | 118 | ARG |
| 65 | SW | 120 | ARG |
| 65 | SW | 121 | HIS |
| 65 | SW | 122 | ILE |
| 65 | SW | 129 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 65 | SW | 131 | GLU |
| 65 | SW | 135 | GLU |
| 65 | SW | 137 | LEU |
| 66 | SX | 28 | ILE |
| 66 | SX | 30 | VAL |
| 66 | SX | 32 | LYS |
| 66 | SX | 33 | ASP |
| 66 | SX | 34 | LEU |
| 66 | SX | 37 | VAL |
| 66 | SX | 38 | GLU |
| 66 | SX | 44 | ILE |
| 66 | SX | 46 | LYS |
| 66 | SX | 53 | ILE |
| 66 | SX | 58 | ARG |
| 66 | SX | 63 | ARG |
| 66 | SX | 64 | LEU |
| 66 | SX | 67 | THR |
| 66 | SX | 69 | ARG |
| 66 | SX | 71 | SER |
| 66 | SX | 75 | GLU |
| 66 | SX | 77 | THR |
| 66 | SX | 79 | THR |
| 66 | SX | 84 | GLU |
| 66 | SX | 88 | TYR |
| 66 | SX | 89 | LYS |
| 66 | SX | 101 | ILE |
| 66 | SX | 103 | THR |
| 66 | SX | 104 | ILE |
| 66 | SX | 105 | LEU |
| 66 | SX | 106 | SER |
| 66 | SX | 107 | LYS |
| 66 | SX | 109 | VAL |
| 66 | SX | 110 | VAL |
| 66 | SX | 114 | ILE |
| 66 | SX | 115 | GLN |
| 66 | SX | 117 | THR |
| 66 | SX | 118 | VAL |
| 66 | SX | 119 | GLU |
| 67 | SY | 8 | MET |
| 67 | SY | 12 | SER |
| 67 | SY | 14 | VAL |
| 67 | SY | 15 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | SY | 17 | ASP |
| 67 | SY | 22 | ARG |
| 67 | SY | 23 | LYS |
| 67 | SY | 24 | CYS |
| 67 | SY | 27 | THR |
| 67 | SY | 30 | LEU |
| 67 | SY | 31 | ILE |
| 67 | SY | 34 | LYS |
| 67 | SY | 39 | VAL |
| 67 | SY | 45 | ARG |
| 67 | SY | 49 | LYS |
| 67 | SY | 51 | LYS |
| 67 | SY | 53 | ILE |
| 67 | SY | 56 | ASN |
| 67 | SY | 57 | TYR |
| 67 | SY | 58 | VAL |
| 67 | SY | 63 | CYS |
| 67 | SY | 66 | ILE |
| 67 | SY | 69 | ARG |
| 67 | SY | 72 | VAL |
| 67 | SY | 74 | SER |
| 67 | SY | 85 | LEU |
| 67 | SY | 86 | MET |
| 67 | SY | 88 | ARG |
| 68 | Sb | 2 | PRO |
| 68 | Sb | 3 | GLU |
| 68 | Sb | 4 | ILE |
| 68 | Sb | 7 | LYS |
| 68 | Sb | 9 | ARG |
| 68 | Sb | 10 | LYS |
| 68 | Sb | 12 | LEU |
| 68 | Sb | 13 | ASN |
| 68 | Sb | 14 | ASN |
| 68 | Sb | 17 | LEU |
| 68 | Sb | 19 | ARG |
| 68 | Sb | 22 | CYS |
| 68 | Sb | 23 | VAL |
| 68 | Sb | 24 | VAL |
| 68 | Sb | 27 | LEU |
| 68 | Sb | 34 | GLU |
| 68 | Sb | 40 | LYS |
| 68 | Sb | 42 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 68 | Sb | 45 | GLN |
| 68 | Sb | 47 | LEU |
| 68 | Sb | 52 | GLN |
| 68 | Sb | 53 | LYS |
| 68 | Sb | 54 | ASN |
| 68 | Sb | 55 | ILE |
| 68 | Sb | 56 | VAL |
| 68 | Sb | 57 | LEU |
| 68 | Sb | 62 | THR |
| 68 | Sb | 72 | PHE |
| 68 | Sb | 79 | MET |
| 68 | Sb | 80 | ASP |
| 68 | Sb | 82 | LEU |
| 68 | Sb | 83 | MET |
| 68 | Sb | 90 | ARG |
| 68 | Sb | 91 | LYS |
| 68 | Sb | 96 | LEU |
| 68 | Sb | 97 | ILE |
| 68 | Sb | 98 | GLU |
| 68 | Sb | 101 | LYS |
| 68 | Sb | 105 | ARG |
| 68 | Sb | 106 | LYS |
| 68 | Sb | 108 | LEU |
| 68 | Sb | 111 | LEU |
| 68 | Sb | 112 | LYS |
| 68 | Sb | 115 | ARG |
| 68 | Sb | 117 | LYS |
| 68 | Sb | 118 | LYS |
| 68 | Sb | 119 | ARG |
| 69 | Sc | 14 | LYS |
| 69 | Sc | 15 | VAL |
| 69 | Sc | 24 | GLU |
| 69 | Sc | 29 | GLU |
| 69 | Sc | 31 | LEU |
| 69 | Sc | 34 | ILE |
| 69 | Sc | 35 | LYS |
| 69 | Sc | 37 | SER |
| 69 | Sc | 38 | LYS |
| 69 | Sc | 40 | ILE |
| 69 | Sc | 41 | THR |
| 69 | Sc | 43 | THR |
| 69 | Sc | 44 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 69 | Sc | 45 | ILE |
| 69 | Sc | 46 | CYS |
| 69 | Sc | 47 | GLU |
| 69 | Sc | 48 | ARG |
| 69 | Sc | 49 | LEU |
| 69 | Sc | 50 | ARG |
| 69 | Sc | 52 | SER |
| 69 | Sc | 53 | VAL |
| 69 | Sc | 55 | LEU |
| 69 | Sc | 57 | LYS |
| 69 | Sc | 59 | VAL |
| 69 | Sc | 60 | MET |
| 69 | Sc | 63 | LEU |
| 69 | Sc | 65 | LYS |
| 69 | Sc | 66 | SER |
| 69 | Sc | 69 | PHE |
| 69 | Sc | 71 | ILE |
| 69 | Sc | 72 | VAL |
| 69 | Sc | 73 | SER |
| 69 | Sc | 75 | SER |
| 69 | Sc | 76 | SER |
| 69 | Sc | 78 | MET |
| 69 | Sc | 79 | THR |
| 69 | Sc | 81 | PHE |
| 69 | Sc | 82 | LYS |
| 69 | Sc | 86 | LYS |
| 69 | Sc | 87 | LYS |
| 70 | Sd | 3 | VAL |
| 70 | Sd | 4 | LYS |
| 70 | Sd | 5 | ARG |
| 70 | Sd | 12 | LYS |
| 70 | Sd | 18 | THR |
| 70 | Sd | 19 | ASN |
| 70 | Sd | 20 | ILE |
| 70 | Sd | 22 | ARG |
| 70 | Sd | 28 | ARG |
| 70 | Sd | 30 | VAL |
| 70 | Sd | 33 | ASP |
| 70 | Sd | 34 | LYS |
| 70 | Sd | 35 | VAL |
| 70 | Sd | 36 | ILE |
| 70 | Sd | 37 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 70 | Sd | 38 | ARG |
| 70 | Sd | 42 | ARG |
| 70 | Sd | 43 | ASN |
| 70 | Sd | 44 | ILE |
| 70 | Sd | 45 | VAL |
| 70 | Sd | 49 | ILE |
| 70 | Sd | 51 | ASP |
| 70 | Sd | 52 | ASP |
| 70 | Sd | 54 | LEU |
| 70 | Sd | 57 | CYS |
| 70 | Sd | 59 | ILE |
| 70 | Sd | 60 | GLN |
| 70 | Sd | 64 | ILE |
| 70 | Sd | 66 | LYS |
| 70 | Sd | 67 | LEU |
| 70 | Sd | 77 | CYS |
| 70 | Sd | 81 | ASN |
| 70 | Sd | 83 | ILE |
| 70 | Sd | 84 | VAL |
| 70 | Sd | 87 | ARG |
| 70 | Sd | 89 | ARG |
| 70 | Sd | 90 | GLU |
| 70 | Sd | 91 | ASP |
| 70 | Sd | 92 | ARG |
| 70 | Sd | 93 | LYS |
| 70 | Sd | 95 | ARG |
| 70 | Sd | 96 | THR |
| 70 | Sd | 99 | LYS |
| 70 | Sd | 100 | ARG |
| 70 | Sd | 103 | ARG |
| 70 | Sd | 105 | SER |
| 70 | Sd | 106 | SER |
| 70 | Sd | 107 | GLN |
| 70 | Sd | 108 | LYS |
| 70 | Sd | 109 | LYS |
| 71 | Se | 45 | ASN |
| 71 | Se | 46 | VAL |
| 71 | Se | 49 | LEU |
| 71 | Se | 50 | TYR |
| 71 | Se | 52 | ASP |
| 71 | Se | 54 | VAL |
| 71 | Se | 56 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 71 | Se | 58 | ARG |
| 71 | Se | 59 | LYS |
| 71 | Se | 61 | LYS |
| 71 | Se | 63 | LYS |
| 71 | Se | 65 | LEU |
| 71 | Se | 66 | VAL |
| 71 | Se | 67 | GLN |
| 71 | Se | 71 | SER |
| 71 | Se | 76 | ILE |
| 71 | Se | 77 | LYS |
| 71 | Se | 78 | CYS |
| 71 | Se | 81 | CYS |
| 71 | Se | 82 | GLN |
| 71 | Se | 83 | ASP |
| 71 | Se | 84 | ILE |
| 71 | Se | 85 | VAL |
| 71 | Se | 86 | VAL |
| 71 | Se | 87 | VAL |
| 71 | Se | 93 | THR |
| 71 | Se | 95 | VAL |
| 71 | Se | 101 | THR |
| 71 | Se | 102 | SER |
| 71 | Se | 103 | GLN |
| 71 | Se | 104 | ILE |
| 71 | Se | 105 | SER |
| 71 | Se | 106 | ILE |
| 71 | Se | 115 | THR |
| 71 | Se | 118 | VAL |
| 71 | Se | 119 | GLU |
| 71 | Se | 120 | ARG |
| 71 | Se | 121 | TYR |
| 71 | Se | 123 | GLN |
| 72 | Sg | 3 | GLU |
| 72 | Sg | 5 | ILE |
| 72 | Sg | 6 | ASN |
| 72 | Sg | 8 | ARG |
| 72 | Sg | 11 | GLU |
| 72 | Sg | 13 | LEU |
| 72 | Sg | 15 | ARG |
| 72 | Sg | 16 | THR |
| 72 | Sg | 19 | ARG |
| 72 | Sg | 22 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 72 | Sg | 23 | THR |
| 72 | Sg | 24 | GLN |
| 72 | Sg | 25 | VAL |
| 72 | Sg | 26 | LYS |
| 72 | Sg | 27 | VAL |
| 72 | Sg | 28 | GLU |
| 72 | Sg | 29 | PHE |
| 72 | Sg | 30 | MET |
| 72 | Sg | 33 | GLU |
| 72 | Sg | 34 | LYS |
| 72 | Sg | 35 | ARG |
| 72 | Sg | 36 | GLN |
| 72 | Sg | 37 | ILE |
| 72 | Sg | 41 | VAL |
| 72 | Sg | 42 | ILE |
| 72 | Sg | 45 | VAL |
| 72 | Sg | 46 | ARG |
| 72 | Sg | 47 | LYS |
| 72 | Sg | 48 | ASP |
| 72 | Sg | 49 | ASP |
| 72 | Sg | 50 | ILE |
| 72 | Sg | 53 | LEU |
| 72 | Sg | 54 | MET |
| 72 | Sg | 55 | GLU |
| 72 | Sg | 56 | SER |
| 72 | Sg | 58 | ARG |
| 72 | Sg | 59 | GLU |
| 72 | Sg | 61 | ARG |
| 72 | Sg | 62 | ARG |
| 72 | Sg | 63 | LEU |
| 72 | Sg | 64 | ARG |
| 73 | Sh | 87 | MET |
| 73 | Sh | 88 | ARG |
| 73 | Sh | 91 | GLU |
| 73 | Sh | 92 | PHE |
| 73 | Sh | 94 | THR |
| 73 | Sh | 96 | ILE |
| 73 | Sh | 99 | LYS |
| 73 | Sh | 101 | GLU |
| 73 | Sh | 102 | CYS |
| 73 | Sh | 103 | ARG |
| 73 | Sh | 104 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 73 | Sh | 105 | CYS |
| 73 | Sh | 110 | SER |
| 73 | Sh | 112 | TYR |
| 73 | Sh | 113 | ARG |
| 73 | Sh | 117 | LEU |
| 73 | Sh | 119 | ILE |
| 73 | Sh | 120 | CYS |
| 73 | Sh | 122 | ARG |
| 73 | Sh | 123 | CYS |
| 73 | Sh | 126 | GLU |
| 73 | Sh | 130 | LYS |
| 73 | Sh | 131 | ILE |
| 73 | Sh | 135 | LYS |
| 73 | Sh | 136 | LEU |
| 74 | Sj | 1 | ARG |
| 74 | Sj | 3 | HIS |
| 74 | Sj | 7 | THR |
| 74 | Sj | 8 | SER |
| 74 | Sj | 11 | LYS |
| 74 | Sj | 13 | ARG |
| 74 | Sj | 16 | THR |
| 74 | Sj | 18 | LYS |
| 74 | Sj | 19 | LYS |
| 74 | Sj | 20 | GLU |
| 74 | Sj | 22 | LYS |
| 74 | Sj | 23 | GLU |
| 74 | Sj | 24 | LYS |
| 74 | Sj | 26 | ARG |
| 74 | Sj | 29 | ARG |
| 74 | Sj | 31 | ARG |
| 74 | Sj | 35 | ARG |
| 74 | Sj | 36 | LEU |
| 74 | Sj | 40 | LYS |
| 74 | Sj | 43 | VAL |
| 74 | Sj | 45 | ASP |
| 74 | Sj | 48 | ILE |
| 74 | Sj | 52 | ARG |
| 74 | Sj | 53 | ARG |
| 74 | Sj | 54 | LEU |
| 74 | Sj | 57 | ASN |
| 74 | Sj | 59 | LEU |
| 74 | Sj | 60 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 74 | Sj | 61 | ILE |
| 74 | Sj | 63 | GLN |
| 74 | Sj | 64 | LYS |
| 74 | Sj | 65 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (259) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | LA | 62 | GLN |
| 1 | LA | 92 | ASN |
| 1 | LA | 97 | HIS |
| 1 | LA | 140 | ASN |
| 1 | LA | 154 | GLN |
| 1 | LA | 209 | HIS |
| 1 | LA | 216 | HIS |
| 2 | LB | 62 | HIS |
| 2 | LB | 68 | HIS |
| 2 | LB | 69 | ASN |
| 2 | LB | 71 | GLN |
| 2 | LB | 75 | GLN |
| 2 | LB | 121 | ASN |
| 2 | LB | 269 | GLN |
| 2 | LB | 281 | GLN |
| 2 | LB | 340 | ASN |
| 2 | LB | 364 | HIS |
| 3 | LC | 34 | ASN |
| 3 | LC | 123 | ASN |
| 3 | LC | 218 | HIS |
| 3 | LC | 232 | HIS |
| 3 | LC | 279 | GLN |
| 6 | LF | 39 | GLN |
| 6 | LF | 138 | HIS |
| 6 | LF | 144 | ASN |
| 6 | LF | 148 | HIS |
| 6 | LF | 183 | HIS |
| 6 | LF | 209 | HIS |
| 6 | LF | 250 | HIS |
| 8 | LH | 38 | HIS |
| 8 | LH | 69 | GLN |
| 8 | LH | 120 | ASN |
| 8 | LH | 162 | ASN |
| 8 | LH | 171 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | LH | 181 | HIS |
| 8 | LH | 203 | ASN |
| 9 | LI | 67 | ASN |
| 9 | LI | 74 | ASN |
| 9 | LI | 185 | ASN |
| 10 | LJ | 94 | HIS |
| 10 | LJ | 116 | GLN |
| 10 | LJ | 152 | HIS |
| 10 | LJ | 183 | GLN |
| 10 | LJ | 185 | GLN |
| 11 | LK | 14 | ASN |
| 11 | LK | 59 | GLN |
| 11 | LK | 86 | HIS |
| 11 | LK | 163 | GLN |
| 11 | LK | 195 | ASN |
| 12 | LL | 7 | ASN |
| 12 | LL | 38 | GLN |
| 13 | LM | 66 | GLN |
| 13 | LM | 70 | GLN |
| 13 | LM | 165 | GLN |
| 14 | LN | 48 | GLN |
| 14 | LN | 97 | GLN |
| 15 | LO | 8 | GLN |
| 15 | LO | 41 | HIS |
| 15 | LO | 74 | GLN |
| 15 | LO | 117 | ASN |
| 15 | LO | 139 | HIS |
| 15 | LO | 149 | ASN |
| 15 | LO | 153 | ASN |
| 16 | LP | 26 | HIS |
| 16 | LP | 28 | HIS |
| 16 | LP | 50 | HIS |
| 17 | LQ | 27 | ASN |
| 17 | LQ | 96 | GLN |
| 17 | LQ | 100 | ASN |
| 17 | LQ | 142 | GLN |
| 18 | LR | 58 | ASN |
| 18 | LR | 134 | ASN |
| 18 | LR | 139 | GLN |
| 18 | LR | 167 | HIS |
| 19 | LS | 75 | HIS |
| 19 | LS | 146 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | LS | 168 | GLN |
| 19 | LS | 186 | GLN |
| 20 | LT | 42 | HIS |
| 20 | LT | 65 | ASN |
| 20 | LT | 86 | ASN |
| 21 | LU | 5 | GLN |
| 21 | LU | 31 | ASN |
| 21 | LU | 54 | HIS |
| 21 | LU | 58 | ASN |
| 21 | LU | 66 | ASN |
| 21 | LU | 77 | GLN |
| 21 | LU | 90 | ASN |
| 21 | LU | 95 | HIS |
| 22 | LV | 13 | GLN |
| 22 | LV | 50 | HIS |
| 22 | LV | 68 | GLN |
| 22 | LV | 89 | GLN |
| 23 | LW | 103 | ASN |
| 23 | LW | 142 | HIS |
| 24 | LX | 25 | ASN |
| 24 | LX | 38 | HIS |
| 25 | LY | 28 | ASN |
| 25 | LY | 30 | HIS |
| 25 | LY | 39 | HIS |
| 26 | LZ | 42 | HIS |
| 26 | LZ | 85 | GLN |
| 27 | La | 19 | HIS |
| 27 | La | 53 | ASN |
| 27 | La | 112 | ASN |
| 28 | Lb | 14 | HIS |
| 28 | Lb | 28 | HIS |
| 28 | Lb | 49 | HIS |
| 28 | Lb | 70 | ASN |
| 28 | Lb | 86 | GLN |
| 29 | Lc | 6 | ASN |
| 29 | Lc | 7 | HIS |
| 29 | Lc | 12 | GLN |
| 29 | Lc | 53 | GLN |
| 31 | Le | 12 | ASN |
| 32 | Lf | 49 | HIS |
| 32 | Lf | 100 | GLN |
| 32 | Lf | 103 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | Lf | 112 | GLN |
| 33 | Lg | 24 | GLN |
| 34 | Lh | 66 | GLN |
| 34 | Lh | 67 | GLN |
| 34 | Lh | 93 | ASN |
| 36 | Lj | 29 | HIS |
| 36 | Lj | 57 | ASN |
| 36 | Lj | 61 | HIS |
| 37 | Lk | 30 | GLN |
| 38 | Ll | 33 | GLN |
| 38 | Ll | 53 | ASN |
| 38 | Ll | 71 | GLN |
| 39 | Ln | 62 | ASN |
| 39 | Ln | 94 | ASN |
| 39 | Ln | 119 | GLN |
| 39 | Ln | 158 | GLN |
| 39 | Ln | 188 | ASN |
| 39 | Ln | 199 | GLN |
| 42 | Lq | 25 | GLN |
| 45 | SA | 47 | GLN |
| 45 | SA | 55 | ASN |
| 45 | SA | 112 | ASN |
| 45 | SA | 118 | ASN |
| 45 | SA | 137 | GLN |
| 45 | SA | 169 | ASN |
| 45 | SA | 170 | ASN |
| 46 | SB | 81 | GLN |
| 46 | SB | 83 | GLN |
| 46 | SB | 88 | GLN |
| 46 | SB | 95 | HIS |
| 46 | SB | 129 | ASN |
| 46 | SB | 194 | GLN |
| 46 | SB | 203 | ASN |
| 46 | SB | 231 | HIS |
| 47 | SC | 28 | HIS |
| 47 | SC | 73 | HIS |
| 47 | SC | 91 | ASN |
| 47 | SC | 156 | ASN |
| 48 | SD | 18 | ASN |
| 48 | SD | 81 | ASN |
| 48 | SD | 89 | GLN |
| 48 | SD | 99 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | SD | 101 | HIS |
| 48 | SD | 235 | ASN |
| 48 | SD | 239 | ASN |
| 49 | SE | 8 | HIS |
| 49 | SE | 36 | HIS |
| 49 | SE | 56 | ASN |
| 49 | SE | 151 | HIS |
| 49 | SE | 163 | ASN |
| 49 | SE | 201 | HIS |
| 49 | SE | 224 | ASN |
| 50 | SF | 9 | ASN |
| 50 | SF | 119 | GLN |
| 50 | SF | 134 | ASN |
| 50 | SF | 139 | ASN |
| 50 | SF | 165 | ASN |
| 51 | SG | 19 | ASN |
| 51 | SG | 31 | GLN |
| 51 | SG | 65 | GLN |
| 51 | SG | 92 | HIS |
| 51 | SG | 163 | GLN |
| 51 | SG | 175 | HIS |
| 52 | SH | 22 | GLN |
| 52 | SH | 71 | GLN |
| 52 | SH | 151 | ASN |
| 52 | SH | 155 | GLN |
| 53 | SI | 28 | ASN |
| 53 | SI | 93 | ASN |
| 53 | SI | 112 | GLN |
| 53 | SI | 124 | ASN |
| 54 | SJ | 39 | GLN |
| 54 | SJ | 59 | ASN |
| 54 | SJ | 120 | GLN |
| 55 | SK | 66 | ASN |
| 55 | SK | 124 | HIS |
| 55 | SK | 128 | ASN |
| 55 | SK | 134 | HIS |
| 56 | SL | 15 | HIS |
| 56 | SL | 19 | ASN |
| 56 | SL | 47 | ASN |
| 56 | SL | 54 | ASN |
| 56 | SL | 58 | GLN |
| 57 | SM | 4 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | SM | 5 | GLN |
| 57 | SM | 11 | HIS |
| 57 | SM | 13 | GLN |
| 57 | SM | 15 | GLN |
| 57 | SM | 41 | HIS |
| 57 | SM | 61 | ASN |
| 57 | SM | 74 | HIS |
| 57 | SM | 93 | GLN |
| 57 | SM | 136 | ASN |
| 58 | SO | 61 | GLN |
| 58 | SO | 73 | GLN |
| 58 | SO | 96 | ASN |
| 59 | SP | 36 | GLN |
| 59 | SP | 57 | GLN |
| 59 | SP | 62 | GLN |
| 59 | SP | 123 | HIS |
| 60 | SQ | 94 | HIS |
| 61 | SR | 48 | HIS |
| 61 | SR | 98 | ASN |
| 61 | SR | 128 | HIS |
| 62 | ST | 33 | ASN |
| 62 | ST | 50 | ASN |
| 62 | ST | 92 | HIS |
| 62 | ST | 101 | GLN |
| 62 | ST | 154 | GLN |
| 63 | SU | 62 | ASN |
| 64 | SV | 8 | ASN |
| 64 | SV | 22 | GLN |
| 64 | SV | 50 | ASN |
| 64 | SV | 88 | ASN |
| 64 | SV | 127 | HIS |
| 64 | SV | 135 | GLN |
| 64 | SV | 136 | HIS |
| 65 | SW | 106 | GLN |
| 67 | SY | 36 | HIS |
| 67 | SY | 40 | GLN |
| 67 | SY | 56 | ASN |
| 68 | Sb | 14 | ASN |
| 68 | Sb | 18 | GLN |
| 68 | Sb | 54 | ASN |
| 68 | Sb | 74 | ASN |
| 68 | Sb | 77 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 68 | Sb | 110 | ASN |
| 69 | Sc | 42 | HIS |
| 70 | Sd | 7 | ASN |
| 70 | Sd | 25 | ASN |
| 70 | Sd | 47 | ASN |
| 70 | Sd | 55 | ASN |
| 70 | Sd | 69 | ASN |
| 70 | Sd | 72 | GLN |
| 70 | Sd | 82 | HIS |
| 70 | Sd | 107 | GLN |
| 71 | Se | 45 | ASN |
| 71 | Se | 60 | HIS |
| 71 | Se | 123 | GLN |
| 72 | Sg | 24 | GLN |
| 74 | Sj | 57 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 4 | LD | 141/142 (99%) | 72 (51%) | 9 (6%) |
| 44 | Lt | 2588/2697 (95%) | 1300 (50%) | 0 |
| 5 | LE | 116/121 (95%) | 60 (51%) | 7 (6%) |
| 75 | St | 1453/1454 (99%) | 831 (57%) | 0 |
| 76 | u | 74/75 (98%) | 42 (56%) | 0 |
| 77 | v | 74/75 (98%) | 57 (77%) | 0 |
| 78 | y | 9/11 (81%) | 6 (66%) | 0 |
| All | All | 4455/4575 (97%) | 2368 (53%) | 16 (0%) |

All (2368) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | LD | 3 | A |
| 4 | LD | 6 | C |
| 4 | LD | 8 | C |
| 4 | LD | 9 | C |
| 4 | LD | 10 | G |
| 4 | LD | 11 | C |
| 4 | LD | 12 | C |
| 4 | LD | 16 | G |
| 4 | LD | 17 | G |
| 4 | LD | 20 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | LD | 21 | C |
| 4 | LD | 24 | C |
| 4 | LD | 25 | G |
| 4 | LD | 28 | C |
| 4 | LD | 30 | G |
| 4 | LD | 31 | G |
| 4 | LD | 35 | G |
| 4 | LD | 36 | C |
| 4 | LD | 39 | C |
| 4 | LD | 40 | G |
| 4 | LD | 41 | A |
| 4 | LD | 45 | G |
| 4 | LD | 47 | G |
| 4 | LD | 48 | C |
| 4 | LD | 52 | G |
| 4 | LD | 53 | G |
| 4 | LD | 54 | A |
| 4 | LD | 55 | G |
| 4 | LD | 59 | G |
| 4 | LD | 60 | A |
| 4 | LD | 63 | C |
| 4 | LD | 64 | G |
| 4 | LD | 69 | G |
| 4 | LD | 71 | G |
| 4 | LD | 72 | G |
| 4 | LD | 73 | A |
| 4 | LD | 74 | C |
| 4 | LD | 75 | C |
| 4 | LD | 76 | C |
| 4 | LD | 79 | C |
| 4 | LD | 80 | C |
| 4 | LD | 81 | G |
| 4 | LD | 83 | C |
| 4 | LD | 84 | C |
| 4 | LD | 85 | C |
| 4 | LD | 86 | G |
| 4 | LD | 87 | A |
| 4 | LD | 88 | G |
| 4 | LD | 92 | C |
| 4 | LD | 93 | A |
| 4 | LD | 100 | C |
| 4 | LD | 104 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | LD | 105 | A |
| 4 | LD | 106 | C |
| 4 | LD | 108 | C |
| 4 | LD | 109 | A |
| 4 | LD | 111 | C |
| 4 | LD | 112 | G |
| 4 | LD | 113 | C |
| 4 | LD | 115 | C |
| 4 | LD | 116 | C |
| 4 | LD | 117 | C |
| 4 | LD | 118 | C |
| 4 | LD | 119 | G |
| 4 | LD | 125 | G |
| 4 | LD | 126 | C |
| 4 | LD | 131 | U |
| 4 | LD | 133 | G |
| 4 | LD | 135 | C |
| 4 | LD | 136 | G |
| 4 | LD | 140 | G |
| 4 | LD | 142 | C |
| 5 | LE | 3 | G |
| 5 | LE | 7 | G |
| 5 | LE | 9 | C |
| 5 | LE | 11 | A |
| 5 | LE | 14 | C |
| 5 | LE | 15 | U |
| 5 | LE | 20 | C |
| 5 | LE | 22 | G |
| 5 | LE | 23 | A |
| 5 | LE | 24 | A |
| 5 | LE | 27 | U |
| 5 | LE | 29 | C |
| 5 | LE | 30 | U |
| 5 | LE | 31 | U |
| 5 | LE | 32 | A |
| 5 | LE | 33 | A |
| 5 | LE | 34 | C |
| 5 | LE | 35 | U |
| 5 | LE | 36 | C |
| 5 | LE | 38 | U |
| 5 | LE | 39 | U |
| 5 | LE | 40 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | LE | 42 | G |
| 5 | LE | 43 | A |
| 5 | LE | 44 | A |
| 5 | LE | 46 | U |
| 5 | LE | 47 | A |
| 5 | LE | 50 | A |
| 5 | LE | 52 | G |
| 5 | LE | 53 | A |
| 5 | LE | 54 | G |
| 5 | LE | 55 | A |
| 5 | LE | 61 | C |
| 5 | LE | 62 | G |
| 5 | LE | 63 | U |
| 5 | LE | 64 | C |
| 5 | LE | 65 | A |
| 5 | LE | 66 | G |
| 5 | LE | 67 | G |
| 5 | LE | 72 | G |
| 5 | LE | 75 | A |
| 5 | LE | 77 | U |
| 5 | LE | 80 | U |
| 5 | LE | 88 | G |
| 5 | LE | 92 | C |
| 5 | LE | 93 | G |
| 5 | LE | 94 | U |
| 5 | LE | 96 | G |
| 5 | LE | 98 | G |
| 5 | LE | 99 | G |
| 5 | LE | 100 | G |
| 5 | LE | 102 | A |
| 5 | LE | 106 | G |
| 5 | LE | 107 | G |
| 5 | LE | 109 | G |
| 5 | LE | 110 | U |
| 5 | LE | 111 | G |
| 5 | LE | 113 | C |
| 5 | LE | 114 | G |
| 5 | LE | 115 | A |
| 44 | Lt | 3 | C |
| 44 | Lt | 9 | U |
| 44 | Lt | 10 | G |
| 44 | Lt | 12 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 15 | G |
| 44 | Lt | 18 | G |
| 44 | Lt | 19 | G |
| 44 | Lt | 20 | G |
| 44 | Lt | 21 | G |
| 44 | Lt | 24 | G |
| 44 | Lt | 26 | C |
| 44 | Lt | 28 | G |
| 44 | Lt | 29 | G |
| 44 | Lt | 30 | C |
| 44 | Lt | 39 | A |
| 44 | Lt | 40 | G |
| 44 | Lt | 42 | A |
| 44 | Lt | 43 | U |
| 44 | Lt | 47 | A |
| 44 | Lt | 48 | G |
| 44 | Lt | 49 | U |
| 44 | Lt | 56 | C |
| 44 | Lt | 58 | G |
| 44 | Lt | 59 | A |
| 44 | Lt | 64 | A |
| 44 | Lt | 65 | A |
| 44 | Lt | 66 | A |
| 44 | Lt | 67 | C |
| 44 | Lt | 68 | C |
| 44 | Lt | 69 | A |
| 44 | Lt | 71 | C |
| 44 | Lt | 72 | C |
| 44 | Lt | 73 | G |
| 44 | Lt | 75 | G |
| 44 | Lt | 76 | A |
| 44 | Lt | 80 | C |
| 44 | Lt | 82 | C |
| 44 | Lt | 83 | G |
| 44 | Lt | 84 | C |
| 44 | Lt | 85 | U |
| 44 | Lt | 86 | A |
| 44 | Lt | 87 | G |
| 44 | Lt | 88 | C |
| 44 | Lt | 90 | G |
| 44 | Lt | 91 | C |
| 44 | Lt | 92 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 95 | C |
| 44 | Lt | 97 | A |
| 44 | Lt | 100 | C |
| 44 | Lt | 101 | G |
| 44 | Lt | 106 | G |
| 44 | Lt | 107 | A |
| 44 | Lt | 109 | C |
| 44 | Lt | 117 | G |
| 44 | Lt | 118 | A |
| 44 | Lt | 119 | A |
| 44 | Lt | 120 | G |
| 44 | Lt | 121 | G |
| 44 | Lt | 122 | C |
| 44 | Lt | 123 | G |
| 44 | Lt | 124 | C |
| 44 | Lt | 128 | G |
| 44 | Lt | 150 | C |
| 44 | Lt | 153 | C |
| 44 | Lt | 158 | G |
| 44 | Lt | 160 | G |
| 44 | Lt | 162 | C |
| 44 | Lt | 164 | G |
| 44 | Lt | 165 | A |
| 44 | Lt | 167 | G |
| 44 | Lt | 168 | G |
| 44 | Lt | 172 | C |
| 44 | Lt | 173 | G |
| 44 | Lt | 176 | C |
| 44 | Lt | 178 | A |
| 44 | Lt | 179 | G |
| 44 | Lt | 184 | U |
| 44 | Lt | 185 | G |
| 44 | Lt | 186 | C |
| 44 | Lt | 187 | A |
| 44 | Lt | 189 | G |
| 44 | Lt | 190 | C |
| 44 | Lt | 194 | G |
| 44 | Lt | 198 | G |
| 44 | Lt | 199 | G |
| 44 | Lt | 224 | U |
| 44 | Lt | 225 | A |
| 44 | Lt | 233 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 235 | G |
| 44 | Lt | 238 | C |
| 44 | Lt | 239 | G |
| 44 | Lt | 249 | A |
| 44 | Lt | 250 | A |
| 44 | Lt | 251 | G |
| 44 | Lt | 252 | G |
| 44 | Lt | 254 | A |
| 44 | Lt | 256 | G |
| 44 | Lt | 258 | G |
| 44 | Lt | 259 | C |
| 44 | Lt | 260 | G |
| 44 | Lt | 261 | G |
| 44 | Lt | 262 | C |
| 44 | Lt | 267 | C |
| 44 | Lt | 272 | G |
| 44 | Lt | 275 | A |
| 44 | Lt | 277 | A |
| 44 | Lt | 278 | U |
| 44 | Lt | 280 | C |
| 44 | Lt | 281 | G |
| 44 | Lt | 284 | C |
| 44 | Lt | 287 | G |
| 44 | Lt | 288 | G |
| 44 | Lt | 289 | A |
| 44 | Lt | 291 | C |
| 44 | Lt | 292 | G |
| 44 | Lt | 293 | A |
| 44 | Lt | 294 | U |
| 44 | Lt | 295 | A |
| 44 | Lt | 298 | G |
| 44 | Lt | 300 | A |
| 44 | Lt | 301 | C |
| 44 | Lt | 302 | C |
| 44 | Lt | 303 | A |
| 44 | Lt | 304 | A |
| 44 | Lt | 308 | G |
| 44 | Lt | 312 | G |
| 44 | Lt | 314 | G |
| 44 | Lt | 317 | A |
| 44 | Lt | 320 | G |
| 44 | Lt | 321 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 322 | U |
| 44 | Lt | 326 | A |
| 44 | Lt | 327 | A |
| 44 | Lt | 328 | G |
| 44 | Lt | 331 | C |
| 44 | Lt | 332 | G |
| 44 | Lt | 335 | C |
| 44 | Lt | 336 | U |
| 44 | Lt | 337 | G |
| 44 | Lt | 339 | G |
| 44 | Lt | 340 | G |
| 44 | Lt | 341 | C |
| 44 | Lt | 343 | G |
| 44 | Lt | 345 | U |
| 44 | Lt | 349 | A |
| 44 | Lt | 350 | A |
| 44 | Lt | 351 | G |
| 44 | Lt | 352 | A |
| 44 | Lt | 354 | C |
| 44 | Lt | 365 | C |
| 44 | Lt | 368 | C |
| 44 | Lt | 369 | C |
| 44 | Lt | 370 | G |
| 44 | Lt | 372 | C |
| 44 | Lt | 375 | C |
| 44 | Lt | 376 | C |
| 44 | Lt | 377 | C |
| 44 | Lt | 378 | G |
| 44 | Lt | 379 | C |
| 44 | Lt | 384 | C |
| 44 | Lt | 385 | C |
| 44 | Lt | 387 | G |
| 44 | Lt | 389 | C |
| 44 | Lt | 390 | U |
| 44 | Lt | 393 | A |
| 44 | Lt | 394 | A |
| 44 | Lt | 395 | A |
| 44 | Lt | 396 | C |
| 44 | Lt | 397 | A |
| 44 | Lt | 398 | C |
| 44 | Lt | 409 | G |
| 44 | Lt | 416 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 417 | C |
| 44 | Lt | 420 | C |
| 44 | Lt | 421 | G |
| 44 | Lt | 423 | C |
| 44 | Lt | 424 | G |
| 44 | Lt | 425 | A |
| 44 | Lt | 427 | C |
| 44 | Lt | 429 | C |
| 44 | Lt | 434 | G |
| 44 | Lt | 435 | A |
| 44 | Lt | 436 | G |
| 44 | Lt | 437 | C |
| 44 | Lt | 438 | C |
| 44 | Lt | 439 | C |
| 44 | Lt | 443 | C |
| 44 | Lt | 444 | G |
| 44 | Lt | 447 | G |
| 44 | Lt | 449 | A |
| 44 | Lt | 454 | G |
| 44 | Lt | 456 | G |
| 44 | Lt | 458 | G |
| 44 | Lt | 459 | A |
| 44 | Lt | 460 | G |
| 44 | Lt | 461 | A |
| 44 | Lt | 463 | G |
| 44 | Lt | 464 | C |
| 44 | Lt | 466 | C |
| 44 | Lt | 468 | G |
| 44 | Lt | 471 | C |
| 44 | Lt | 476 | C |
| 44 | Lt | 477 | A |
| 44 | Lt | 479 | G |
| 44 | Lt | 483 | C |
| 44 | Lt | 484 | U |
| 44 | Lt | 486 | C |
| 44 | Lt | 487 | G |
| 44 | Lt | 493 | G |
| 44 | Lt | 494 | C |
| 44 | Lt | 495 | G |
| 44 | Lt | 497 | G |
| 44 | Lt | 498 | G |
| 44 | Lt | 501 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 502 | G |
| 44 | Lt | 503 | A |
| 44 | Lt | 507 | G |
| 44 | Lt | 508 | C |
| 44 | Lt | 509 | G |
| 44 | Lt | 510 | G |
| 44 | Lt | 513 | C |
| 44 | Lt | 516 | G |
| 44 | Lt | 517 | G |
| 44 | Lt | 518 | G |
| 44 | Lt | 519 | C |
| 44 | Lt | 525 | A |
| 44 | Lt | 527 | G |
| 44 | Lt | 534 | U |
| 44 | Lt | 535 | C |
| 44 | Lt | 537 | A |
| 44 | Lt | 538 | U |
| 44 | Lt | 539 | G |
| 44 | Lt | 542 | C |
| 44 | Lt | 543 | G |
| 44 | Lt | 544 | G |
| 44 | Lt | 546 | G |
| 44 | Lt | 547 | A |
| 44 | Lt | 549 | G |
| 44 | Lt | 554 | G |
| 44 | Lt | 556 | C |
| 44 | Lt | 558 | G |
| 44 | Lt | 561 | C |
| 44 | Lt | 562 | G |
| 44 | Lt | 569 | U |
| 44 | Lt | 570 | G |
| 44 | Lt | 575 | A |
| 44 | Lt | 576 | G |
| 44 | Lt | 577 | G |
| 44 | Lt | 578 | C |
| 44 | Lt | 581 | G |
| 44 | Lt | 583 | C |
| 44 | Lt | 588 | U |
| 44 | Lt | 589 | G |
| 44 | Lt | 591 | U |
| 44 | Lt | 592 | G |
| 44 | Lt | 596 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 597 | G |
| 44 | Lt | 598 | C |
| 44 | Lt | 601 | A |
| 44 | Lt | 605 | C |
| 44 | Lt | 607 | C |
| 44 | Lt | 609 | U |
| 44 | Lt | 611 | G |
| 44 | Lt | 612 | G |
| 44 | Lt | 613 | A |
| 44 | Lt | 618 | G |
| 44 | Lt | 619 | G |
| 44 | Lt | 624 | G |
| 44 | Lt | 625 | G |
| 44 | Lt | 626 | G |
| 44 | Lt | 631 | A |
| 44 | Lt | 632 | A |
| 44 | Lt | 633 | G |
| 44 | Lt | 634 | A |
| 44 | Lt | 638 | A |
| 44 | Lt | 640 | C |
| 44 | Lt | 641 | G |
| 44 | Lt | 642 | A |
| 44 | Lt | 644 | C |
| 44 | Lt | 645 | C |
| 44 | Lt | 649 | U |
| 44 | Lt | 650 | G |
| 44 | Lt | 653 | A |
| 44 | Lt | 654 | G |
| 44 | Lt | 655 | C |
| 44 | Lt | 656 | U |
| 44 | Lt | 658 | G |
| 44 | Lt | 661 | G |
| 44 | Lt | 664 | U |
| 44 | Lt | 666 | C |
| 44 | Lt | 671 | U |
| 44 | Lt | 677 | C |
| 44 | Lt | 679 | A |
| 44 | Lt | 680 | G |
| 44 | Lt | 681 | G |
| 44 | Lt | 682 | A |
| 44 | Lt | 688 | G |
| 44 | Lt | 691 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 692 | C |
| 44 | Lt | 695 | C |
| 44 | Lt | 696 | G |
| 44 | Lt | 697 | C |
| 44 | Lt | 699 | G |
| 44 | Lt | 700 | U |
| 44 | Lt | 704 | G |
| 44 | Lt | 705 | G |
| 44 | Lt | 709 | G |
| 44 | Lt | 710 | U |
| 44 | Lt | 715 | C |
| 44 | Lt | 716 | G |
| 44 | Lt | 719 | G |
| 44 | Lt | 720 | G |
| 44 | Lt | 721 | C |
| 44 | Lt | 722 | C |
| 44 | Lt | 723 | G |
| 44 | Lt | 724 | G |
| 44 | Lt | 725 | C |
| 44 | Lt | 727 | G |
| 44 | Lt | 728 | G |
| 44 | Lt | 729 | A |
| 44 | Lt | 730 | G |
| 44 | Lt | 733 | G |
| 44 | Lt | 734 | G |
| 44 | Lt | 735 | G |
| 44 | Lt | 736 | G |
| 44 | Lt | 737 | G |
| 44 | Lt | 738 | C |
| 44 | Lt | 739 | C |
| 44 | Lt | 741 | G |
| 44 | Lt | 742 | C |
| 44 | Lt | 743 | C |
| 44 | Lt | 744 | C |
| 44 | Lt | 745 | C |
| 44 | Lt | 746 | U |
| 44 | Lt | 748 | G |
| 44 | Lt | 752 | G |
| 44 | Lt | 754 | C |
| 44 | Lt | 757 | C |
| 44 | Lt | 760 | A |
| 44 | Lt | 761 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 764 | C |
| 44 | Lt | 765 | C |
| 44 | Lt | 767 | A |
| 44 | Lt | 769 | G |
| 44 | Lt | 770 | G |
| 44 | Lt | 772 | C |
| 44 | Lt | 776 | G |
| 44 | Lt | 777 | C |
| 44 | Lt | 781 | C |
| 44 | Lt | 784 | G |
| 44 | Lt | 787 | G |
| 44 | Lt | 788 | C |
| 44 | Lt | 789 | U |
| 44 | Lt | 790 | G |
| 44 | Lt | 791 | G |
| 44 | Lt | 792 | C |
| 44 | Lt | 794 | U |
| 44 | Lt | 795 | G |
| 44 | Lt | 796 | G |
| 44 | Lt | 797 | G |
| 44 | Lt | 799 | G |
| 44 | Lt | 800 | G |
| 44 | Lt | 802 | G |
| 44 | Lt | 803 | C |
| 44 | Lt | 805 | G |
| 44 | Lt | 806 | G |
| 44 | Lt | 807 | C |
| 44 | Lt | 808 | G |
| 44 | Lt | 809 | A |
| 44 | Lt | 814 | G |
| 44 | Lt | 816 | G |
| 44 | Lt | 818 | G |
| 44 | Lt | 819 | G |
| 44 | Lt | 820 | C |
| 44 | Lt | 821 | G |
| 44 | Lt | 827 | G |
| 44 | Lt | 829 | C |
| 44 | Lt | 832 | U |
| 44 | Lt | 834 | C |
| 44 | Lt | 836 | G |
| 44 | Lt | 837 | G |
| 44 | Lt | 838 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 839 | A |
| 44 | Lt | 841 | G |
| 44 | Lt | 844 | G |
| 44 | Lt | 846 | A |
| 44 | Lt | 848 | G |
| 44 | Lt | 853 | A |
| 44 | Lt | 854 | G |
| 44 | Lt | 855 | G |
| 44 | Lt | 858 | G |
| 44 | Lt | 860 | A |
| 44 | Lt | 861 | C |
| 44 | Lt | 865 | C |
| 44 | Lt | 869 | A |
| 44 | Lt | 870 | C |
| 44 | Lt | 874 | G |
| 44 | Lt | 876 | G |
| 44 | Lt | 882 | G |
| 44 | Lt | 883 | U |
| 44 | Lt | 888 | C |
| 44 | Lt | 889 | G |
| 44 | Lt | 890 | C |
| 44 | Lt | 891 | C |
| 44 | Lt | 895 | G |
| 44 | Lt | 898 | C |
| 44 | Lt | 900 | C |
| 44 | Lt | 901 | G |
| 44 | Lt | 902 | G |
| 44 | Lt | 903 | A |
| 44 | Lt | 906 | G |
| 44 | Lt | 907 | G |
| 44 | Lt | 908 | C |
| 44 | Lt | 913 | G |
| 44 | Lt | 916 | G |
| 44 | Lt | 917 | G |
| 44 | Lt | 918 | U |
| 44 | Lt | 919 | C |
| 44 | Lt | 920 | C |
| 44 | Lt | 921 | C |
| 44 | Lt | 922 | G |
| 44 | Lt | 923 | A |
| 44 | Lt | 981 | A |
| 44 | Lt | 983 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 986 | A |
| 44 | Lt | 987 | A |
| 44 | Lt | 989 | C |
| 44 | Lt | 990 | G |
| 44 | Lt | 993 | C |
| 44 | Lt | 997 | C |
| 44 | Lt | 998 | C |
| 44 | Lt | 1001 | A |
| 44 | Lt | 1005 | U |
| 44 | Lt | 1006 | G |
| 44 | Lt | 1007 | G |
| 44 | Lt | 1008 | A |
| 44 | Lt | 1009 | G |
| 44 | Lt | 1010 | C |
| 44 | Lt | 1013 | G |
| 44 | Lt | 1015 | C |
| 44 | Lt | 1016 | G |
| 44 | Lt | 1017 | G |
| 44 | Lt | 1018 | A |
| 44 | Lt | 1019 | G |
| 44 | Lt | 1024 | G |
| 44 | Lt | 1025 | G |
| 44 | Lt | 1026 | A |
| 44 | Lt | 1027 | C |
| 44 | Lt | 1030 | G |
| 44 | Lt | 1031 | C |
| 44 | Lt | 1032 | G |
| 44 | Lt | 1033 | C |
| 44 | Lt | 1036 | G |
| 44 | Lt | 1037 | G |
| 44 | Lt | 1038 | C |
| 44 | Lt | 1046 | C |
| 44 | Lt | 1047 | G |
| 44 | Lt | 1052 | G |
| 44 | Lt | 1053 | G |
| 44 | Lt | 1054 | G |
| 44 | Lt | 1055 | U |
| 44 | Lt | 1061 | G |
| 44 | Lt | 1064 | G |
| 44 | Lt | 1065 | C |
| 44 | Lt | 1066 | A |
| 44 | Lt | 1067 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1070 | G |
| 44 | Lt | 1072 | C |
| 44 | Lt | 1073 | C |
| 44 | Lt | 1074 | C |
| 44 | Lt | 1075 | G |
| 44 | Lt | 1076 | G |
| 44 | Lt | 1079 | G |
| 44 | Lt | 1080 | C |
| 44 | Lt | 1081 | G |
| 44 | Lt | 1084 | G |
| 44 | Lt | 1086 | C |
| 44 | Lt | 1087 | G |
| 44 | Lt | 1089 | C |
| 44 | Lt | 1091 | C |
| 44 | Lt | 1093 | C |
| 44 | Lt | 1095 | G |
| 44 | Lt | 1096 | G |
| 44 | Lt | 1100 | C |
| 44 | Lt | 1105 | G |
| 44 | Lt | 1106 | A |
| 44 | Lt | 1109 | G |
| 44 | Lt | 1111 | C |
| 44 | Lt | 1114 | C |
| 44 | Lt | 1115 | U |
| 44 | Lt | 1116 | G |
| 44 | Lt | 1117 | G |
| 44 | Lt | 1118 | U |
| 44 | Lt | 1119 | G |
| 44 | Lt | 1120 | C |
| 44 | Lt | 1121 | A |
| 44 | Lt | 1122 | G |
| 44 | Lt | 1125 | C |
| 44 | Lt | 1129 | G |
| 44 | Lt | 1132 | G |
| 44 | Lt | 1134 | A |
| 44 | Lt | 1135 | G |
| 44 | Lt | 1136 | U |
| 44 | Lt | 1137 | A |
| 44 | Lt | 1138 | G |
| 44 | Lt | 1140 | C |
| 44 | Lt | 1141 | G |
| 44 | Lt | 1142 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1143 | U |
| 44 | Lt | 1144 | A |
| 44 | Lt | 1150 | C |
| 44 | Lt | 1151 | G |
| 44 | Lt | 1152 | C |
| 44 | Lt | 1153 | C |
| 44 | Lt | 1154 | C |
| 44 | Lt | 1155 | C |
| 44 | Lt | 1159 | G |
| 44 | Lt | 1164 | G |
| 44 | Lt | 1165 | A |
| 44 | Lt | 1166 | G |
| 44 | Lt | 1167 | G |
| 44 | Lt | 1168 | G |
| 44 | Lt | 1169 | G |
| 44 | Lt | 1170 | G |
| 44 | Lt | 1172 | G |
| 44 | Lt | 1176 | G |
| 44 | Lt | 1177 | G |
| 44 | Lt | 1178 | U |
| 44 | Lt | 1179 | U |
| 44 | Lt | 1184 | G |
| 44 | Lt | 1187 | G |
| 44 | Lt | 1191 | G |
| 44 | Lt | 1192 | C |
| 44 | Lt | 1195 | C |
| 44 | Lt | 1198 | G |
| 44 | Lt | 1199 | C |
| 44 | Lt | 1203 | G |
| 44 | Lt | 1204 | G |
| 44 | Lt | 1206 | U |
| 44 | Lt | 1207 | G |
| 44 | Lt | 1208 | A |
| 44 | Lt | 1210 | U |
| 44 | Lt | 1216 | C |
| 44 | Lt | 1217 | U |
| 44 | Lt | 1220 | G |
| 44 | Lt | 1222 | G |
| 44 | Lt | 1226 | G |
| 44 | Lt | 1233 | A |
| 44 | Lt | 1237 | G |
| 44 | Lt | 1238 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1239 | A |
| 44 | Lt | 1240 | A |
| 44 | Lt | 1241 | G |
| 44 | Lt | 1242 | G |
| 44 | Lt | 1243 | G |
| 44 | Lt | 1244 | G |
| 44 | Lt | 1245 | C |
| 44 | Lt | 1248 | G |
| 44 | Lt | 1249 | C |
| 44 | Lt | 1250 | C |
| 44 | Lt | 1252 | G |
| 44 | Lt | 1253 | C |
| 44 | Lt | 1257 | U |
| 44 | Lt | 1258 | C |
| 44 | Lt | 1260 | A |
| 44 | Lt | 1261 | A |
| 44 | Lt | 1262 | C |
| 44 | Lt | 1263 | G |
| 44 | Lt | 1265 | G |
| 44 | Lt | 1269 | C |
| 44 | Lt | 1270 | C |
| 44 | Lt | 1272 | G |
| 44 | Lt | 1274 | G |
| 44 | Lt | 1276 | A |
| 44 | Lt | 1277 | G |
| 44 | Lt | 1278 | A |
| 44 | Lt | 1279 | C |
| 44 | Lt | 1290 | G |
| 44 | Lt | 1292 | G |
| 44 | Lt | 1295 | C |
| 44 | Lt | 1297 | C |
| 44 | Lt | 1298 | C |
| 44 | Lt | 1299 | G |
| 44 | Lt | 1303 | A |
| 44 | Lt | 1304 | G |
| 44 | Lt | 1308 | C |
| 44 | Lt | 1309 | C |
| 44 | Lt | 1310 | C |
| 44 | Lt | 1311 | G |
| 44 | Lt | 1317 | C |
| 44 | Lt | 1318 | G |
| 44 | Lt | 1323 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1324 | G |
| 44 | Lt | 1328 | A |
| 44 | Lt | 1329 | C |
| 44 | Lt | 1332 | G |
| 44 | Lt | 1339 | G |
| 44 | Lt | 1340 | G |
| 44 | Lt | 1343 | G |
| 44 | Lt | 1344 | G |
| 44 | Lt | 1347 | G |
| 44 | Lt | 1349 | G |
| 44 | Lt | 1350 | C |
| 44 | Lt | 1355 | G |
| 44 | Lt | 1359 | G |
| 44 | Lt | 1361 | G |
| 44 | Lt | 1362 | A |
| 44 | Lt | 1365 | G |
| 44 | Lt | 1366 | C |
| 44 | Lt | 1367 | C |
| 44 | Lt | 1369 | C |
| 44 | Lt | 1372 | A |
| 44 | Lt | 1373 | G |
| 44 | Lt | 1376 | C |
| 44 | Lt | 1378 | C |
| 44 | Lt | 1379 | G |
| 44 | Lt | 1380 | G |
| 44 | Lt | 1381 | A |
| 44 | Lt | 1382 | C |
| 44 | Lt | 1383 | G |
| 44 | Lt | 1386 | U |
| 44 | Lt | 1387 | U |
| 44 | Lt | 1388 | G |
| 44 | Lt | 1389 | C |
| 44 | Lt | 1391 | C |
| 44 | Lt | 1392 | G |
| 44 | Lt | 1394 | A |
| 44 | Lt | 1395 | G |
| 44 | Lt | 1399 | G |
| 44 | Lt | 1400 | G |
| 44 | Lt | 1401 | G |
| 44 | Lt | 1405 | C |
| 44 | Lt | 1406 | G |
| 44 | Lt | 1407 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1412 | G |
| 44 | Lt | 1413 | G |
| 44 | Lt | 1414 | A |
| 44 | Lt | 1419 | G |
| 44 | Lt | 1423 | G |
| 44 | Lt | 1427 | C |
| 44 | Lt | 1428 | C |
| 44 | Lt | 1431 | C |
| 44 | Lt | 1436 | C |
| 44 | Lt | 1437 | C |
| 44 | Lt | 1438 | U |
| 44 | Lt | 1440 | A |
| 44 | Lt | 1444 | G |
| 44 | Lt | 1447 | G |
| 44 | Lt | 1448 | G |
| 44 | Lt | 1449 | G |
| 44 | Lt | 1451 | G |
| 44 | Lt | 1452 | G |
| 44 | Lt | 1453 | C |
| 44 | Lt | 1454 | G |
| 44 | Lt | 1455 | C |
| 44 | Lt | 1456 | C |
| 44 | Lt | 1458 | G |
| 44 | Lt | 1461 | G |
| 44 | Lt | 1464 | C |
| 44 | Lt | 1466 | C |
| 44 | Lt | 1467 | C |
| 44 | Lt | 1469 | U |
| 44 | Lt | 1470 | A |
| 44 | Lt | 1473 | G |
| 44 | Lt | 1474 | A |
| 44 | Lt | 1478 | C |
| 44 | Lt | 1479 | A |
| 44 | Lt | 1481 | C |
| 44 | Lt | 1482 | A |
| 44 | Lt | 1483 | G |
| 44 | Lt | 1484 | G |
| 44 | Lt | 1485 | A |
| 44 | Lt | 1486 | C |
| 44 | Lt | 1487 | U |
| 44 | Lt | 1489 | C |
| 44 | Lt | 1490 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1491 | G |
| 44 | Lt | 1496 | A |
| 44 | Lt | 1497 | G |
| 44 | Lt | 1498 | C |
| 44 | Lt | 1499 | A |
| 44 | Lt | 1501 | C |
| 44 | Lt | 1504 | C |
| 44 | Lt | 1507 | G |
| 44 | Lt | 1510 | C |
| 44 | Lt | 1511 | G |
| 44 | Lt | 1512 | G |
| 44 | Lt | 1513 | G |
| 44 | Lt | 1515 | G |
| 44 | Lt | 1516 | C |
| 44 | Lt | 1517 | G |
| 44 | Lt | 1518 | A |
| 44 | Lt | 1521 | G |
| 44 | Lt | 1522 | C |
| 44 | Lt | 1524 | G |
| 44 | Lt | 1528 | A |
| 44 | Lt | 1531 | G |
| 44 | Lt | 1532 | A |
| 44 | Lt | 1533 | A |
| 44 | Lt | 1536 | C |
| 44 | Lt | 1538 | G |
| 44 | Lt | 1541 | A |
| 44 | Lt | 1550 | C |
| 44 | Lt | 1552 | U |
| 44 | Lt | 1553 | A |
| 44 | Lt | 1556 | C |
| 44 | Lt | 1558 | C |
| 44 | Lt | 1559 | G |
| 44 | Lt | 1560 | G |
| 44 | Lt | 1562 | A |
| 44 | Lt | 1564 | A |
| 44 | Lt | 1565 | A |
| 44 | Lt | 1566 | G |
| 44 | Lt | 1567 | G |
| 44 | Lt | 1573 | C |
| 44 | Lt | 1575 | C |
| 44 | Lt | 1579 | C |
| 44 | Lt | 1580 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1581 | G |
| 44 | Lt | 1582 | C |
| 44 | Lt | 1585 | G |
| 44 | Lt | 1586 | C |
| 44 | Lt | 1588 | G |
| 44 | Lt | 1589 | G |
| 44 | Lt | 1590 | G |
| 44 | Lt | 1591 | U |
| 44 | Lt | 1593 | A |
| 44 | Lt | 1594 | G |
| 44 | Lt | 1596 | A |
| 44 | Lt | 1597 | C |
| 44 | Lt | 1599 | G |
| 44 | Lt | 1600 | G |
| 44 | Lt | 1601 | A |
| 44 | Lt | 1602 | A |
| 44 | Lt | 1604 | G |
| 44 | Lt | 1605 | G |
| 44 | Lt | 1606 | A |
| 44 | Lt | 1611 | G |
| 44 | Lt | 1615 | U |
| 44 | Lt | 1618 | C |
| 44 | Lt | 1619 | G |
| 44 | Lt | 1620 | A |
| 44 | Lt | 1624 | U |
| 44 | Lt | 1626 | U |
| 44 | Lt | 1629 | U |
| 44 | Lt | 1630 | A |
| 44 | Lt | 1633 | A |
| 44 | Lt | 1640 | C |
| 44 | Lt | 1641 | G |
| 44 | Lt | 1646 | G |
| 44 | Lt | 1647 | A |
| 44 | Lt | 1648 | G |
| 44 | Lt | 1649 | G |
| 44 | Lt | 1655 | A |
| 44 | Lt | 1657 | C |
| 44 | Lt | 1658 | C |
| 44 | Lt | 1664 | U |
| 44 | Lt | 1668 | G |
| 44 | Lt | 1670 | G |
| 44 | Lt | 1671 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1672 | C |
| 44 | Lt | 1673 | G |
| 44 | Lt | 1676 | A |
| 44 | Lt | 1677 | U |
| 44 | Lt | 1683 | C |
| 44 | Lt | 1684 | C |
| 44 | Lt | 1686 | A |
| 44 | Lt | 1687 | G |
| 44 | Lt | 1688 | U |
| 44 | Lt | 1692 | A |
| 44 | Lt | 1693 | C |
| 44 | Lt | 1694 | G |
| 44 | Lt | 1696 | C |
| 44 | Lt | 1697 | C |
| 44 | Lt | 1699 | U |
| 44 | Lt | 1702 | C |
| 44 | Lt | 1703 | C |
| 44 | Lt | 1704 | G |
| 44 | Lt | 1705 | U |
| 44 | Lt | 1706 | G |
| 44 | Lt | 1707 | A |
| 44 | Lt | 1711 | G |
| 44 | Lt | 1715 | C |
| 44 | Lt | 1717 | C |
| 44 | Lt | 1718 | C |
| 44 | Lt | 1719 | G |
| 44 | Lt | 1720 | A |
| 44 | Lt | 1721 | A |
| 44 | Lt | 1727 | G |
| 44 | Lt | 1731 | A |
| 44 | Lt | 1732 | A |
| 44 | Lt | 1737 | G |
| 44 | Lt | 1740 | A |
| 44 | Lt | 1741 | G |
| 44 | Lt | 1742 | U |
| 44 | Lt | 1744 | A |
| 44 | Lt | 1745 | C |
| 44 | Lt | 1746 | U |
| 44 | Lt | 1747 | A |
| 44 | Lt | 1748 | U |
| 44 | Lt | 1749 | G |
| 44 | Lt | 1750 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1751 | C |
| 44 | Lt | 1752 | U |
| 44 | Lt | 1753 | C |
| 44 | Lt | 1754 | U |
| 44 | Lt | 1755 | C |
| 44 | Lt | 1757 | U |
| 44 | Lt | 1758 | A |
| 44 | Lt | 1759 | A |
| 44 | Lt | 1760 | G |
| 44 | Lt | 1761 | G |
| 44 | Lt | 1762 | U |
| 44 | Lt | 1764 | G |
| 44 | Lt | 1767 | A |
| 44 | Lt | 1768 | A |
| 44 | Lt | 1769 | A |
| 44 | Lt | 1772 | C |
| 44 | Lt | 1773 | C |
| 44 | Lt | 1775 | C |
| 44 | Lt | 1776 | G |
| 44 | Lt | 1778 | C |
| 44 | Lt | 1779 | G |
| 44 | Lt | 1780 | G |
| 44 | Lt | 1781 | G |
| 44 | Lt | 1782 | C |
| 44 | Lt | 1783 | A |
| 44 | Lt | 1786 | U |
| 44 | Lt | 1792 | C |
| 44 | Lt | 1793 | G |
| 44 | Lt | 1795 | G |
| 44 | Lt | 1796 | C |
| 44 | Lt | 1797 | A |
| 44 | Lt | 1798 | U |
| 44 | Lt | 1801 | A |
| 44 | Lt | 1802 | U |
| 44 | Lt | 1803 | G |
| 44 | Lt | 1805 | A |
| 44 | Lt | 1807 | C |
| 44 | Lt | 1808 | A |
| 44 | Lt | 1811 | G |
| 44 | Lt | 1812 | A |
| 44 | Lt | 1822 | U |
| 44 | Lt | 1823 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1824 | U |
| 44 | Lt | 1827 | C |
| 44 | Lt | 1829 | A |
| 44 | Lt | 1832 | C |
| 44 | Lt | 1833 | G |
| 44 | Lt | 1835 | G |
| 44 | Lt | 1839 | C |
| 44 | Lt | 1849 | C |
| 44 | Lt | 1851 | A |
| 44 | Lt | 1852 | G |
| 44 | Lt | 1853 | C |
| 44 | Lt | 1854 | C |
| 44 | Lt | 1855 | U |
| 44 | Lt | 1856 | C |
| 44 | Lt | 1860 | A |
| 44 | Lt | 1861 | A |
| 44 | Lt | 1862 | C |
| 44 | Lt | 1863 | G |
| 44 | Lt | 1864 | G |
| 44 | Lt | 1865 | G |
| 44 | Lt | 1866 | C |
| 44 | Lt | 1868 | A |
| 44 | Lt | 1873 | C |
| 44 | Lt | 1874 | G |
| 44 | Lt | 1875 | G |
| 44 | Lt | 1879 | G |
| 44 | Lt | 1880 | C |
| 44 | Lt | 1881 | G |
| 44 | Lt | 1882 | G |
| 44 | Lt | 1883 | G |
| 44 | Lt | 1885 | C |
| 44 | Lt | 1886 | A |
| 44 | Lt | 1887 | A |
| 44 | Lt | 1888 | G |
| 44 | Lt | 1889 | A |
| 44 | Lt | 1890 | A |
| 44 | Lt | 1891 | G |
| 44 | Lt | 1892 | A |
| 44 | Lt | 1896 | U |
| 44 | Lt | 1897 | U |
| 44 | Lt | 1898 | U |
| 44 | Lt | 1899 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1906 | G |
| 44 | Lt | 1907 | A |
| 44 | Lt | 1910 | C |
| 44 | Lt | 1911 | C |
| 44 | Lt | 1912 | A |
| 44 | Lt | 1914 | C |
| 44 | Lt | 1915 | C |
| 44 | Lt | 1920 | C |
| 44 | Lt | 1922 | U |
| 44 | Lt | 1923 | G |
| 44 | Lt | 1926 | G |
| 44 | Lt | 1928 | G |
| 44 | Lt | 1931 | G |
| 44 | Lt | 1932 | G |
| 44 | Lt | 1933 | G |
| 44 | Lt | 1934 | C |
| 44 | Lt | 1935 | G |
| 44 | Lt | 1939 | G |
| 44 | Lt | 1940 | G |
| 44 | Lt | 1941 | C |
| 44 | Lt | 1942 | G |
| 44 | Lt | 1943 | C |
| 44 | Lt | 1944 | A |
| 44 | Lt | 1945 | G |
| 44 | Lt | 1946 | C |
| 44 | Lt | 1947 | G |
| 44 | Lt | 1948 | C |
| 44 | Lt | 1949 | A |
| 44 | Lt | 1950 | C |
| 44 | Lt | 1953 | G |
| 44 | Lt | 1954 | G |
| 44 | Lt | 1955 | G |
| 44 | Lt | 1956 | A |
| 44 | Lt | 1957 | G |
| 44 | Lt | 1959 | C |
| 44 | Lt | 1960 | C |
| 44 | Lt | 1961 | G |
| 44 | Lt | 1962 | C |
| 44 | Lt | 1963 | G |
| 44 | Lt | 1964 | C |
| 44 | Lt | 1965 | C |
| 44 | Lt | 1966 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 1967 | C |
| 44 | Lt | 1968 | U |
| 44 | Lt | 1969 | G |
| 44 | Lt | 1971 | G |
| 44 | Lt | 1972 | A |
| 44 | Lt | 1973 | C |
| 44 | Lt | 1974 | A |
| 44 | Lt | 1975 | C |
| 44 | Lt | 1976 | C |
| 44 | Lt | 1977 | C |
| 44 | Lt | 1979 | G |
| 44 | Lt | 1980 | A |
| 44 | Lt | 1982 | G |
| 44 | Lt | 1984 | C |
| 44 | Lt | 1985 | C |
| 44 | Lt | 1986 | G |
| 44 | Lt | 1988 | C |
| 44 | Lt | 1989 | G |
| 44 | Lt | 1992 | G |
| 44 | Lt | 1993 | C |
| 44 | Lt | 1994 | C |
| 44 | Lt | 1995 | C |
| 44 | Lt | 2000 | C |
| 44 | Lt | 2003 | C |
| 44 | Lt | 2004 | C |
| 44 | Lt | 2005 | G |
| 44 | Lt | 2008 | C |
| 44 | Lt | 2009 | G |
| 44 | Lt | 2010 | C |
| 44 | Lt | 2011 | G |
| 44 | Lt | 2012 | C |
| 44 | Lt | 2013 | G |
| 44 | Lt | 2017 | A |
| 44 | Lt | 2018 | C |
| 44 | Lt | 2022 | C |
| 44 | Lt | 2023 | C |
| 44 | Lt | 2024 | C |
| 44 | Lt | 2027 | G |
| 44 | Lt | 2030 | G |
| 44 | Lt | 2031 | G |
| 44 | Lt | 2033 | A |
| 44 | Lt | 2035 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2036 | U |
| 44 | Lt | 2038 | G |
| 44 | Lt | 2041 | U |
| 44 | Lt | 2042 | G |
| 44 | Lt | 2044 | G |
| 44 | Lt | 2045 | G |
| 44 | Lt | 2046 | C |
| 44 | Lt | 2047 | G |
| 44 | Lt | 2048 | G |
| 44 | Lt | 2049 | C |
| 44 | Lt | 2050 | G |
| 44 | Lt | 2051 | C |
| 44 | Lt | 2052 | G |
| 44 | Lt | 2059 | A |
| 44 | Lt | 2060 | C |
| 44 | Lt | 2061 | A |
| 44 | Lt | 2062 | C |
| 44 | Lt | 2065 | G |
| 44 | Lt | 2066 | A |
| 44 | Lt | 2067 | C |
| 44 | Lt | 2068 | C |
| 44 | Lt | 2072 | G |
| 44 | Lt | 2073 | G |
| 44 | Lt | 2075 | G |
| 44 | Lt | 2076 | U |
| 44 | Lt | 2079 | C |
| 44 | Lt | 2080 | A |
| 44 | Lt | 2081 | C |
| 44 | Lt | 2082 | G |
| 44 | Lt | 2090 | C |
| 44 | Lt | 2091 | A |
| 44 | Lt | 2092 | G |
| 44 | Lt | 2093 | C |
| 44 | Lt | 2094 | G |
| 44 | Lt | 2095 | A |
| 44 | Lt | 2098 | A |
| 44 | Lt | 2101 | G |
| 44 | Lt | 2102 | A |
| 44 | Lt | 2103 | G |
| 44 | Lt | 2104 | A |
| 44 | Lt | 2105 | C |
| 44 | Lt | 2106 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2108 | C |
| 44 | Lt | 2111 | G |
| 44 | Lt | 2112 | C |
| 44 | Lt | 2113 | G |
| 44 | Lt | 2114 | G |
| 44 | Lt | 2115 | A |
| 44 | Lt | 2116 | G |
| 44 | Lt | 2117 | C |
| 44 | Lt | 2118 | A |
| 44 | Lt | 2119 | G |
| 44 | Lt | 2120 | A |
| 44 | Lt | 2126 | A |
| 44 | Lt | 2127 | C |
| 44 | Lt | 2128 | A |
| 44 | Lt | 2129 | A |
| 44 | Lt | 2130 | G |
| 44 | Lt | 2132 | C |
| 44 | Lt | 2136 | C |
| 44 | Lt | 2137 | C |
| 44 | Lt | 2138 | G |
| 44 | Lt | 2144 | C |
| 44 | Lt | 2145 | G |
| 44 | Lt | 2146 | C |
| 44 | Lt | 2151 | C |
| 44 | Lt | 2152 | G |
| 44 | Lt | 2153 | U |
| 44 | Lt | 2155 | C |
| 44 | Lt | 2158 | G |
| 44 | Lt | 2159 | C |
| 44 | Lt | 2161 | C |
| 44 | Lt | 2163 | G |
| 44 | Lt | 2164 | G |
| 44 | Lt | 2168 | C |
| 44 | Lt | 2171 | A |
| 44 | Lt | 2174 | C |
| 44 | Lt | 2177 | G |
| 44 | Lt | 2178 | G |
| 44 | Lt | 2179 | C |
| 44 | Lt | 2182 | A |
| 44 | Lt | 2184 | C |
| 44 | Lt | 2185 | G |
| 44 | Lt | 2186 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2196 | G |
| 44 | Lt | 2199 | C |
| 44 | Lt | 2200 | C |
| 44 | Lt | 2201 | G |
| 44 | Lt | 2202 | G |
| 44 | Lt | 2203 | C |
| 44 | Lt | 2205 | G |
| 44 | Lt | 2207 | G |
| 44 | Lt | 2208 | G |
| 44 | Lt | 2209 | G |
| 44 | Lt | 2212 | C |
| 44 | Lt | 2213 | G |
| 44 | Lt | 2214 | G |
| 44 | Lt | 2215 | A |
| 44 | Lt | 2216 | G |
| 44 | Lt | 2217 | G |
| 44 | Lt | 2218 | U |
| 44 | Lt | 2219 | G |
| 44 | Lt | 2220 | G |
| 44 | Lt | 2221 | C |
| 44 | Lt | 2222 | A |
| 44 | Lt | 2223 | G |
| 44 | Lt | 2224 | A |
| 44 | Lt | 2225 | A |
| 44 | Lt | 2226 | A |
| 44 | Lt | 2227 | A |
| 44 | Lt | 2230 | U |
| 44 | Lt | 2231 | A |
| 44 | Lt | 2232 | C |
| 44 | Lt | 2233 | C |
| 44 | Lt | 2234 | A |
| 44 | Lt | 2239 | G |
| 44 | Lt | 2240 | A |
| 44 | Lt | 2241 | U |
| 44 | Lt | 2242 | A |
| 44 | Lt | 2244 | C |
| 44 | Lt | 2249 | U |
| 44 | Lt | 2251 | G |
| 44 | Lt | 2254 | G |
| 44 | Lt | 2256 | C |
| 44 | Lt | 2260 | G |
| 44 | Lt | 2261 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2262 | G |
| 44 | Lt | 2268 | G |
| 44 | Lt | 2269 | C |
| 44 | Lt | 2270 | A |
| 44 | Lt | 2271 | G |
| 44 | Lt | 2272 | C |
| 44 | Lt | 2273 | G |
| 44 | Lt | 2274 | A |
| 44 | Lt | 2276 | G |
| 44 | Lt | 2278 | G |
| 44 | Lt | 2282 | U |
| 44 | Lt | 2283 | U |
| 44 | Lt | 2284 | U |
| 44 | Lt | 2285 | U |
| 44 | Lt | 2286 | G |
| 44 | Lt | 2290 | C |
| 44 | Lt | 2291 | U |
| 44 | Lt | 2294 | G |
| 44 | Lt | 2295 | A |
| 44 | Lt | 2296 | U |
| 44 | Lt | 2298 | U |
| 44 | Lt | 2299 | C |
| 44 | Lt | 2307 | C |
| 44 | Lt | 2309 | U |
| 44 | Lt | 2310 | A |
| 44 | Lt | 2311 | C |
| 44 | Lt | 2314 | U |
| 44 | Lt | 2315 | C |
| 44 | Lt | 2317 | G |
| 44 | Lt | 2320 | C |
| 44 | Lt | 2321 | G |
| 44 | Lt | 2322 | C |
| 44 | Lt | 2323 | A |
| 44 | Lt | 2326 | G |
| 44 | Lt | 2327 | G |
| 44 | Lt | 2329 | G |
| 44 | Lt | 2330 | C |
| 44 | Lt | 2334 | A |
| 44 | Lt | 2335 | G |
| 44 | Lt | 2339 | C |
| 44 | Lt | 2341 | G |
| 44 | Lt | 2344 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2346 | U |
| 44 | Lt | 2347 | U |
| 44 | Lt | 2348 | C |
| 44 | Lt | 2355 | U |
| 44 | Lt | 2356 | C |
| 44 | Lt | 2357 | A |
| 44 | Lt | 2358 | A |
| 44 | Lt | 2359 | G |
| 44 | Lt | 2360 | G |
| 44 | Lt | 2362 | A |
| 44 | Lt | 2363 | U |
| 44 | Lt | 2364 | C |
| 44 | Lt | 2365 | G |
| 44 | Lt | 2369 | G |
| 44 | Lt | 2370 | C |
| 44 | Lt | 2372 | G |
| 44 | Lt | 2373 | G |
| 44 | Lt | 2376 | U |
| 44 | Lt | 2377 | U |
| 44 | Lt | 2388 | G |
| 44 | Lt | 2393 | A |
| 44 | Lt | 2394 | G |
| 44 | Lt | 2400 | U |
| 44 | Lt | 2401 | U |
| 44 | Lt | 2403 | U |
| 44 | Lt | 2405 | C |
| 44 | Lt | 2411 | U |
| 44 | Lt | 2412 | G |
| 44 | Lt | 2413 | G |
| 44 | Lt | 2414 | C |
| 44 | Lt | 2416 | C |
| 44 | Lt | 2418 | G |
| 44 | Lt | 2419 | G |
| 44 | Lt | 2420 | G |
| 44 | Lt | 2421 | G |
| 44 | Lt | 2423 | C |
| 44 | Lt | 2424 | A |
| 44 | Lt | 2427 | G |
| 44 | Lt | 2429 | A |
| 44 | Lt | 2430 | C |
| 44 | Lt | 2431 | G |
| 44 | Lt | 2434 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2437 | C |
| 44 | Lt | 2439 | A |
| 44 | Lt | 2440 | G |
| 44 | Lt | 2441 | U |
| 44 | Lt | 2448 | G |
| 44 | Lt | 2450 | A |
| 44 | Lt | 2451 | A |
| 44 | Lt | 2456 | C |
| 44 | Lt | 2457 | G |
| 44 | Lt | 2458 | C |
| 44 | Lt | 2465 | C |
| 44 | Lt | 2467 | G |
| 44 | Lt | 2470 | A |
| 44 | Lt | 2471 | G |
| 44 | Lt | 2472 | C |
| 44 | Lt | 2473 | C |
| 44 | Lt | 2474 | C |
| 44 | Lt | 2475 | C |
| 44 | Lt | 2479 | G |
| 44 | Lt | 2480 | U |
| 44 | Lt | 2482 | G |
| 44 | Lt | 2483 | C |
| 44 | Lt | 2485 | C |
| 44 | Lt | 2486 | G |
| 44 | Lt | 2487 | G |
| 44 | Lt | 2491 | G |
| 44 | Lt | 2492 | G |
| 44 | Lt | 2493 | C |
| 44 | Lt | 2494 | A |
| 44 | Lt | 2495 | G |
| 44 | Lt | 2496 | C |
| 44 | Lt | 2497 | G |
| 44 | Lt | 2500 | G |
| 44 | Lt | 2506 | C |
| 44 | Lt | 2508 | G |
| 44 | Lt | 2509 | C |
| 44 | Lt | 2510 | G |
| 44 | Lt | 2511 | C |
| 44 | Lt | 2514 | G |
| 44 | Lt | 2515 | G |
| 44 | Lt | 2516 | G |
| 44 | Lt | 2523 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2525 | G |
| 44 | Lt | 2531 | C |
| 44 | Lt | 2532 | G |
| 44 | Lt | 2533 | C |
| 44 | Lt | 2534 | C |
| 44 | Lt | 2536 | C |
| 44 | Lt | 2537 | U |
| 44 | Lt | 2538 | A |
| 44 | Lt | 2539 | A |
| 44 | Lt | 2541 | C |
| 44 | Lt | 2546 | A |
| 44 | Lt | 2547 | C |
| 44 | Lt | 2553 | C |
| 44 | Lt | 2555 | C |
| 44 | Lt | 2556 | G |
| 44 | Lt | 2562 | C |
| 44 | Lt | 2563 | G |
| 44 | Lt | 2565 | C |
| 44 | Lt | 2566 | C |
| 44 | Lt | 2567 | G |
| 44 | Lt | 2572 | C |
| 44 | Lt | 2573 | G |
| 44 | Lt | 2575 | G |
| 44 | Lt | 2579 | C |
| 44 | Lt | 2580 | A |
| 44 | Lt | 2581 | G |
| 44 | Lt | 2582 | C |
| 44 | Lt | 2584 | C |
| 44 | Lt | 2585 | C |
| 44 | Lt | 2586 | G |
| 44 | Lt | 2591 | C |
| 44 | Lt | 2592 | C |
| 44 | Lt | 2593 | G |
| 44 | Lt | 2594 | U |
| 44 | Lt | 2595 | C |
| 44 | Lt | 2596 | G |
| 44 | Lt | 2597 | C |
| 44 | Lt | 2598 | C |
| 44 | Lt | 2601 | G |
| 44 | Lt | 2603 | G |
| 44 | Lt | 2604 | G |
| 44 | Lt | 2605 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | Lt | 2607 | C |
| 44 | Lt | 2608 | C |
| 44 | Lt | 2609 | C |
| 44 | Lt | 2610 | G |
| 44 | Lt | 2611 | C |
| 44 | Lt | 2614 | G |
| 44 | Lt | 2616 | G |
| 44 | Lt | 2619 | G |
| 44 | Lt | 2627 | G |
| 44 | Lt | 2628 | G |
| 44 | Lt | 2630 | G |
| 44 | Lt | 2632 | G |
| 44 | Lt | 2633 | G |
| 44 | Lt | 2634 | C |
| 44 | Lt | 2635 | G |
| 44 | Lt | 2638 | C |
| 44 | Lt | 2641 | G |
| 44 | Lt | 2642 | U |
| 44 | Lt | 2649 | C |
| 44 | Lt | 2652 | A |
| 44 | Lt | 2653 | G |
| 44 | Lt | 2654 | C |
| 44 | Lt | 2655 | C |
| 44 | Lt | 2656 | C |
| 44 | Lt | 2657 | U |
| 44 | Lt | 2658 | G |
| 44 | Lt | 2668 | G |
| 44 | Lt | 2670 | G |
| 44 | Lt | 2672 | G |
| 44 | Lt | 2674 | C |
| 44 | Lt | 2675 | G |
| 44 | Lt | 2680 | U |
| 44 | Lt | 2683 | A |
| 44 | Lt | 2687 | C |
| 44 | Lt | 2688 | G |
| 44 | Lt | 2689 | C |
| 75 | St | 2 | A |
| 75 | St | 3 | U |
| 75 | St | 8 | U |
| 75 | St | 9 | C |
| 75 | St | 11 | A |
| 75 | St | 13 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 14 | C |
| 75 | St | 18 | C |
| 75 | St | 20 | G |
| 75 | St | 22 | G |
| 75 | St | 23 | C |
| 75 | St | 24 | G |
| 75 | St | 25 | C |
| 75 | St | 26 | G |
| 75 | St | 27 | A |
| 75 | St | 31 | U |
| 75 | St | 32 | C |
| 75 | St | 33 | U |
| 75 | St | 34 | C |
| 75 | St | 35 | C |
| 75 | St | 39 | A |
| 75 | St | 40 | G |
| 75 | St | 41 | G |
| 75 | St | 42 | A |
| 75 | St | 43 | C |
| 75 | St | 44 | G |
| 75 | St | 45 | A |
| 75 | St | 46 | A |
| 75 | St | 49 | C |
| 75 | St | 52 | G |
| 75 | St | 54 | A |
| 75 | St | 55 | U |
| 75 | St | 56 | G |
| 75 | St | 57 | C |
| 75 | St | 58 | C |
| 75 | St | 59 | C |
| 75 | St | 61 | C |
| 75 | St | 62 | U |
| 75 | St | 63 | C |
| 75 | St | 64 | A |
| 75 | St | 65 | C |
| 75 | St | 66 | C |
| 75 | St | 68 | G |
| 75 | St | 69 | G |
| 75 | St | 70 | G |
| 75 | St | 71 | A |
| 75 | St | 76 | G |
| 75 | St | 79 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 81 | C |
| 75 | St | 82 | G |
| 75 | St | 84 | C |
| 75 | St | 86 | C |
| 75 | St | 87 | A |
| 75 | St | 88 | G |
| 75 | St | 91 | C |
| 75 | St | 92 | A |
| 75 | St | 96 | G |
| 75 | St | 98 | U |
| 75 | St | 101 | A |
| 75 | St | 102 | C |
| 75 | St | 103 | C |
| 75 | St | 112 | C |
| 75 | St | 114 | G |
| 75 | St | 115 | U |
| 75 | St | 116 | C |
| 75 | St | 118 | C |
| 75 | St | 119 | U |
| 75 | St | 120 | G |
| 75 | St | 121 | C |
| 75 | St | 122 | U |
| 75 | St | 123 | A |
| 75 | St | 124 | G |
| 75 | St | 125 | C |
| 75 | St | 126 | C |
| 75 | St | 127 | G |
| 75 | St | 128 | G |
| 75 | St | 129 | A |
| 75 | St | 130 | C |
| 75 | St | 133 | C |
| 75 | St | 134 | G |
| 75 | St | 136 | U |
| 75 | St | 137 | G |
| 75 | St | 138 | G |
| 75 | St | 139 | C |
| 75 | St | 140 | A |
| 75 | St | 141 | A |
| 75 | St | 144 | C |
| 75 | St | 145 | G |
| 75 | St | 146 | G |
| 75 | St | 148 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 149 | C |
| 75 | St | 151 | A |
| 75 | St | 152 | A |
| 75 | St | 153 | G |
| 75 | St | 154 | A |
| 75 | St | 157 | U |
| 75 | St | 159 | C |
| 75 | St | 160 | G |
| 75 | St | 161 | C |
| 75 | St | 162 | G |
| 75 | St | 163 | C |
| 75 | St | 164 | A |
| 75 | St | 165 | C |
| 75 | St | 166 | G |
| 75 | St | 167 | G |
| 75 | St | 168 | G |
| 75 | St | 169 | C |
| 75 | St | 170 | G |
| 75 | St | 171 | C |
| 75 | St | 172 | G |
| 75 | St | 173 | C |
| 75 | St | 174 | G |
| 75 | St | 175 | C |
| 75 | St | 176 | C |
| 75 | St | 177 | C |
| 75 | St | 178 | C |
| 75 | St | 179 | G |
| 75 | St | 180 | C |
| 75 | St | 181 | G |
| 75 | St | 182 | G |
| 75 | St | 183 | G |
| 75 | St | 184 | C |
| 75 | St | 185 | G |
| 75 | St | 187 | G |
| 75 | St | 188 | C |
| 75 | St | 189 | A |
| 75 | St | 190 | G |
| 75 | St | 194 | G |
| 75 | St | 195 | A |
| 75 | St | 196 | C |
| 75 | St | 197 | G |
| 75 | St | 198 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 199 | A |
| 75 | St | 200 | G |
| 75 | St | 201 | C |
| 75 | St | 202 | G |
| 75 | St | 203 | A |
| 75 | St | 204 | C |
| 75 | St | 205 | G |
| 75 | St | 206 | G |
| 75 | St | 207 | C |
| 75 | St | 210 | G |
| 75 | St | 211 | C |
| 75 | St | 212 | C |
| 75 | St | 216 | G |
| 75 | St | 219 | U |
| 75 | St | 220 | C |
| 75 | St | 221 | C |
| 75 | St | 222 | G |
| 75 | St | 224 | G |
| 75 | St | 228 | U |
| 75 | St | 229 | C |
| 75 | St | 231 | C |
| 75 | St | 237 | C |
| 75 | St | 238 | G |
| 75 | St | 239 | G |
| 75 | St | 240 | C |
| 75 | St | 241 | G |
| 75 | St | 248 | C |
| 75 | St | 249 | G |
| 75 | St | 250 | G |
| 75 | St | 251 | C |
| 75 | St | 258 | A |
| 75 | St | 259 | G |
| 75 | St | 261 | G |
| 75 | St | 263 | C |
| 75 | St | 264 | C |
| 75 | St | 265 | G |
| 75 | St | 272 | G |
| 75 | St | 274 | C |
| 75 | St | 281 | U |
| 75 | St | 283 | A |
| 75 | St | 286 | G |
| 75 | St | 290 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 291 | A |
| 75 | St | 294 | C |
| 75 | St | 296 | G |
| 75 | St | 298 | A |
| 75 | St | 299 | G |
| 75 | St | 300 | A |
| 75 | St | 301 | G |
| 75 | St | 303 | G |
| 75 | St | 304 | G |
| 75 | St | 308 | U |
| 75 | St | 309 | G |
| 75 | St | 310 | C |
| 75 | St | 313 | G |
| 75 | St | 314 | A |
| 75 | St | 315 | C |
| 75 | St | 316 | G |
| 75 | St | 317 | G |
| 75 | St | 319 | C |
| 75 | St | 320 | C |
| 75 | St | 323 | A |
| 75 | St | 325 | A |
| 75 | St | 329 | A |
| 75 | St | 330 | A |
| 75 | St | 331 | G |
| 75 | St | 332 | G |
| 75 | St | 333 | A |
| 75 | St | 335 | G |
| 75 | St | 336 | G |
| 75 | St | 337 | C |
| 75 | St | 338 | A |
| 75 | St | 339 | G |
| 75 | St | 340 | C |
| 75 | St | 341 | A |
| 75 | St | 342 | G |
| 75 | St | 343 | G |
| 75 | St | 344 | C |
| 75 | St | 347 | G |
| 75 | St | 348 | G |
| 75 | St | 349 | A |
| 75 | St | 350 | A |
| 75 | St | 352 | U |
| 75 | St | 353 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 354 | G |
| 75 | St | 355 | C |
| 75 | St | 357 | C |
| 75 | St | 358 | A |
| 75 | St | 360 | U |
| 75 | St | 361 | G |
| 75 | St | 362 | C |
| 75 | St | 363 | G |
| 75 | St | 365 | G |
| 75 | St | 366 | G |
| 75 | St | 367 | C |
| 75 | St | 368 | G |
| 75 | St | 369 | C |
| 75 | St | 370 | G |
| 75 | St | 371 | C |
| 75 | St | 372 | G |
| 75 | St | 374 | G |
| 75 | St | 375 | G |
| 75 | St | 376 | C |
| 75 | St | 381 | A |
| 75 | St | 382 | C |
| 75 | St | 383 | G |
| 75 | St | 384 | G |
| 75 | St | 385 | G |
| 75 | St | 386 | G |
| 75 | St | 388 | G |
| 75 | St | 390 | G |
| 75 | St | 391 | C |
| 75 | St | 392 | G |
| 75 | St | 394 | G |
| 75 | St | 395 | A |
| 75 | St | 396 | G |
| 75 | St | 397 | C |
| 75 | St | 398 | G |
| 75 | St | 399 | A |
| 75 | St | 403 | G |
| 75 | St | 407 | C |
| 75 | St | 409 | A |
| 75 | St | 410 | C |
| 75 | St | 411 | A |
| 75 | St | 416 | C |
| 75 | St | 417 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 418 | G |
| 75 | St | 420 | C |
| 75 | St | 421 | G |
| 75 | St | 422 | C |
| 75 | St | 423 | G |
| 75 | St | 424 | C |
| 75 | St | 425 | A |
| 75 | St | 426 | G |
| 75 | St | 427 | C |
| 75 | St | 429 | G |
| 75 | St | 430 | A |
| 75 | St | 431 | G |
| 75 | St | 432 | G |
| 75 | St | 434 | C |
| 75 | St | 435 | A |
| 75 | St | 436 | A |
| 75 | St | 437 | G |
| 75 | St | 438 | G |
| 75 | St | 439 | U |
| 75 | St | 441 | U |
| 75 | St | 444 | G |
| 75 | St | 445 | C |
| 75 | St | 447 | A |
| 75 | St | 448 | G |
| 75 | St | 454 | G |
| 75 | St | 456 | G |
| 75 | St | 457 | G |
| 75 | St | 458 | U |
| 75 | St | 459 | A |
| 75 | St | 460 | A |
| 75 | St | 461 | U |
| 75 | St | 462 | U |
| 75 | St | 463 | C |
| 75 | St | 464 | C |
| 75 | St | 465 | A |
| 75 | St | 466 | G |
| 75 | St | 467 | C |
| 75 | St | 468 | U |
| 75 | St | 472 | C |
| 75 | St | 474 | A |
| 75 | St | 475 | G |
| 75 | St | 476 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 477 | G |
| 75 | St | 486 | C |
| 75 | St | 487 | G |
| 75 | St | 488 | C |
| 75 | St | 489 | U |
| 75 | St | 491 | C |
| 75 | St | 494 | C |
| 75 | St | 495 | A |
| 75 | St | 496 | G |
| 75 | St | 499 | G |
| 75 | St | 500 | A |
| 75 | St | 502 | A |
| 75 | St | 503 | C |
| 75 | St | 504 | G |
| 75 | St | 509 | U |
| 75 | St | 510 | A |
| 75 | St | 515 | G |
| 75 | St | 518 | C |
| 75 | St | 519 | C |
| 75 | St | 520 | C |
| 75 | St | 521 | C |
| 75 | St | 524 | C |
| 75 | St | 525 | G |
| 75 | St | 527 | C |
| 75 | St | 530 | G |
| 75 | St | 534 | A |
| 75 | St | 535 | A |
| 75 | St | 544 | G |
| 75 | St | 545 | C |
| 75 | St | 546 | U |
| 75 | St | 547 | C |
| 75 | St | 548 | C |
| 75 | St | 550 | G |
| 75 | St | 551 | G |
| 75 | St | 553 | A |
| 75 | St | 554 | G |
| 75 | St | 555 | G |
| 75 | St | 556 | C |
| 75 | St | 557 | C |
| 75 | St | 558 | C |
| 75 | St | 559 | G |
| 75 | St | 560 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 561 | U |
| 75 | St | 564 | C |
| 75 | St | 566 | C |
| 75 | St | 567 | C |
| 75 | St | 568 | G |
| 75 | St | 569 | C |
| 75 | St | 570 | C |
| 75 | St | 571 | G |
| 75 | St | 573 | G |
| 75 | St | 574 | U |
| 75 | St | 576 | G |
| 75 | St | 577 | G |
| 75 | St | 578 | A |
| 75 | St | 579 | C |
| 75 | St | 581 | G |
| 75 | St | 584 | C |
| 75 | St | 585 | A |
| 75 | St | 586 | G |
| 75 | St | 588 | G |
| 75 | St | 589 | G |
| 75 | St | 590 | G |
| 75 | St | 592 | G |
| 75 | St | 593 | C |
| 75 | St | 594 | G |
| 75 | St | 595 | G |
| 75 | St | 596 | C |
| 75 | St | 597 | G |
| 75 | St | 598 | C |
| 75 | St | 600 | C |
| 75 | St | 602 | G |
| 75 | St | 603 | C |
| 75 | St | 605 | G |
| 75 | St | 606 | C |
| 75 | St | 607 | C |
| 75 | St | 608 | G |
| 75 | St | 609 | C |
| 75 | St | 610 | A |
| 75 | St | 611 | G |
| 75 | St | 614 | C |
| 75 | St | 615 | C |
| 75 | St | 616 | G |
| 75 | St | 617 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 618 | G |
| 75 | St | 624 | C |
| 75 | St | 626 | G |
| 75 | St | 627 | G |
| 75 | St | 630 | G |
| 75 | St | 633 | G |
| 75 | St | 634 | C |
| 75 | St | 635 | A |
| 75 | St | 638 | G |
| 75 | St | 639 | G |
| 75 | St | 640 | U |
| 75 | St | 645 | G |
| 75 | St | 647 | C |
| 75 | St | 649 | G |
| 75 | St | 650 | G |
| 75 | St | 651 | G |
| 75 | St | 652 | A |
| 75 | St | 658 | G |
| 75 | St | 659 | A |
| 75 | St | 663 | A |
| 75 | St | 667 | U |
| 75 | St | 668 | G |
| 75 | St | 669 | A |
| 75 | St | 672 | C |
| 75 | St | 673 | C |
| 75 | St | 674 | G |
| 75 | St | 675 | C |
| 75 | St | 677 | G |
| 75 | St | 678 | A |
| 75 | St | 680 | A |
| 75 | St | 682 | C |
| 75 | St | 683 | G |
| 75 | St | 684 | C |
| 75 | St | 685 | C |
| 75 | St | 686 | G |
| 75 | St | 687 | G |
| 75 | St | 689 | C |
| 75 | St | 693 | C |
| 75 | St | 694 | A |
| 75 | St | 695 | G |
| 75 | St | 696 | G |
| 75 | St | 698 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 699 | C |
| 75 | St | 700 | C |
| 75 | St | 701 | U |
| 75 | St | 702 | G |
| 75 | St | 703 | C |
| 75 | St | 704 | C |
| 75 | St | 713 | C |
| 75 | St | 714 | U |
| 75 | St | 715 | C |
| 75 | St | 718 | U |
| 75 | St | 719 | C |
| 75 | St | 720 | A |
| 75 | St | 723 | C |
| 75 | St | 727 | G |
| 75 | St | 728 | G |
| 75 | St | 729 | C |
| 75 | St | 731 | A |
| 75 | St | 732 | A |
| 75 | St | 737 | G |
| 75 | St | 738 | G |
| 75 | St | 744 | A |
| 75 | St | 746 | A |
| 75 | St | 747 | A |
| 75 | St | 750 | C |
| 75 | St | 751 | G |
| 75 | St | 752 | A |
| 75 | St | 754 | C |
| 75 | St | 758 | C |
| 75 | St | 759 | A |
| 75 | St | 761 | C |
| 75 | St | 763 | C |
| 75 | St | 770 | C |
| 75 | St | 774 | G |
| 75 | St | 777 | G |
| 75 | St | 779 | A |
| 75 | St | 780 | A |
| 75 | St | 782 | C |
| 75 | St | 783 | G |
| 75 | St | 784 | G |
| 75 | St | 785 | U |
| 75 | St | 786 | G |
| 75 | St | 789 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 790 | C |
| 75 | St | 792 | C |
| 75 | St | 793 | C |
| 75 | St | 794 | G |
| 75 | St | 797 | G |
| 75 | St | 798 | C |
| 75 | St | 801 | G |
| 75 | St | 802 | C |
| 75 | St | 803 | G |
| 75 | St | 805 | G |
| 75 | St | 807 | G |
| 75 | St | 808 | C |
| 75 | St | 809 | G |
| 75 | St | 810 | U |
| 75 | St | 811 | C |
| 75 | St | 814 | G |
| 75 | St | 815 | C |
| 75 | St | 816 | C |
| 75 | St | 817 | G |
| 75 | St | 820 | C |
| 75 | St | 821 | G |
| 75 | St | 822 | C |
| 75 | St | 823 | C |
| 75 | St | 829 | A |
| 75 | St | 832 | C |
| 75 | St | 833 | C |
| 75 | St | 834 | G |
| 75 | St | 835 | G |
| 75 | St | 836 | G |
| 75 | St | 837 | A |
| 75 | St | 838 | G |
| 75 | St | 840 | C |
| 75 | St | 841 | U |
| 75 | St | 842 | C |
| 75 | St | 843 | C |
| 75 | St | 844 | G |
| 75 | St | 845 | G |
| 75 | St | 847 | C |
| 75 | St | 848 | U |
| 75 | St | 852 | G |
| 75 | St | 853 | G |
| 75 | St | 857 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 859 | U |
| 75 | St | 862 | G |
| 75 | St | 863 | G |
| 75 | St | 868 | A |
| 75 | St | 872 | C |
| 75 | St | 880 | U |
| 75 | St | 881 | G |
| 75 | St | 887 | A |
| 75 | St | 888 | U |
| 75 | St | 896 | G |
| 75 | St | 898 | G |
| 75 | St | 899 | G |
| 75 | St | 900 | U |
| 75 | St | 902 | C |
| 75 | St | 903 | C |
| 75 | St | 904 | A |
| 75 | St | 909 | A |
| 75 | St | 911 | G |
| 75 | St | 914 | G |
| 75 | St | 917 | U |
| 75 | St | 918 | C |
| 75 | St | 919 | U |
| 75 | St | 925 | U |
| 75 | St | 929 | U |
| 75 | St | 931 | U |
| 75 | St | 932 | G |
| 75 | St | 934 | C |
| 75 | St | 938 | A |
| 75 | St | 940 | G |
| 75 | St | 941 | C |
| 75 | St | 942 | G |
| 75 | St | 943 | C |
| 75 | St | 944 | G |
| 75 | St | 945 | C |
| 75 | St | 946 | A |
| 75 | St | 947 | C |
| 75 | St | 950 | C |
| 75 | St | 952 | C |
| 75 | St | 953 | C |
| 75 | St | 955 | G |
| 75 | St | 956 | G |
| 75 | St | 958 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 959 | C |
| 75 | St | 960 | G |
| 75 | St | 961 | G |
| 75 | St | 962 | A |
| 75 | St | 963 | C |
| 75 | St | 964 | G |
| 75 | St | 965 | C |
| 75 | St | 970 | A |
| 75 | St | 971 | G |
| 75 | St | 972 | G |
| 75 | St | 973 | A |
| 75 | St | 974 | C |
| 75 | St | 975 | C |
| 75 | St | 984 | G |
| 75 | St | 985 | G |
| 75 | St | 986 | C |
| 75 | St | 987 | G |
| 75 | St | 988 | C |
| 75 | St | 989 | G |
| 75 | St | 991 | U |
| 75 | St | 993 | U |
| 75 | St | 994 | C |
| 75 | St | 995 | G |
| 75 | St | 996 | C |
| 75 | St | 997 | G |
| 75 | St | 998 | A |
| 75 | St | 999 | U |
| 75 | St | 1000 | C |
| 75 | St | 1001 | G |
| 75 | St | 1002 | C |
| 75 | St | 1003 | G |
| 75 | St | 1004 | C |
| 75 | St | 1005 | G |
| 75 | St | 1007 | G |
| 75 | St | 1012 | G |
| 75 | St | 1013 | G |
| 75 | St | 1015 | G |
| 75 | St | 1016 | C |
| 75 | St | 1017 | A |
| 75 | St | 1018 | U |
| 75 | St | 1020 | G |
| 75 | St | 1026 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 1027 | C |
| 75 | St | 1028 | C |
| 75 | St | 1029 | A |
| 75 | St | 1030 | G |
| 75 | St | 1032 | C |
| 75 | St | 1039 | G |
| 75 | St | 1043 | G |
| 75 | St | 1045 | C |
| 75 | St | 1048 | C |
| 75 | St | 1049 | U |
| 75 | St | 1050 | G |
| 75 | St | 1056 | U |
| 75 | St | 1057 | U |
| 75 | St | 1058 | G |
| 75 | St | 1059 | C |
| 75 | St | 1062 | C |
| 75 | St | 1063 | A |
| 75 | St | 1067 | A |
| 75 | St | 1068 | G |
| 75 | St | 1070 | G |
| 75 | St | 1076 | C |
| 75 | St | 1079 | G |
| 75 | St | 1080 | C |
| 75 | St | 1083 | C |
| 75 | St | 1085 | G |
| 75 | St | 1087 | C |
| 75 | St | 1088 | G |
| 75 | St | 1089 | C |
| 75 | St | 1090 | C |
| 75 | St | 1091 | G |
| 75 | St | 1092 | C |
| 75 | St | 1095 | G |
| 75 | St | 1096 | A |
| 75 | St | 1098 | G |
| 75 | St | 1099 | G |
| 75 | St | 1102 | C |
| 75 | St | 1105 | G |
| 75 | St | 1106 | G |
| 75 | St | 1107 | C |
| 75 | St | 1110 | C |
| 75 | St | 1111 | G |
| 75 | St | 1112 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 1113 | G |
| 75 | St | 1114 | A |
| 75 | St | 1115 | G |
| 75 | St | 1119 | G |
| 75 | St | 1120 | G |
| 75 | St | 1121 | C |
| 75 | St | 1123 | G |
| 75 | St | 1125 | G |
| 75 | St | 1126 | C |
| 75 | St | 1127 | G |
| 75 | St | 1128 | A |
| 75 | St | 1132 | C |
| 75 | St | 1133 | A |
| 75 | St | 1134 | G |
| 75 | St | 1137 | C |
| 75 | St | 1138 | U |
| 75 | St | 1139 | G |
| 75 | St | 1141 | G |
| 75 | St | 1142 | A |
| 75 | St | 1147 | C |
| 75 | St | 1149 | C |
| 75 | St | 1150 | A |
| 75 | St | 1151 | G |
| 75 | St | 1152 | A |
| 75 | St | 1153 | C |
| 75 | St | 1160 | G |
| 75 | St | 1161 | G |
| 75 | St | 1162 | C |
| 75 | St | 1163 | C |
| 75 | St | 1164 | G |
| 75 | St | 1165 | C |
| 75 | St | 1166 | A |
| 75 | St | 1170 | G |
| 75 | St | 1175 | A |
| 75 | St | 1177 | A |
| 75 | St | 1178 | C |
| 75 | St | 1179 | U |
| 75 | St | 1180 | G |
| 75 | St | 1181 | G |
| 75 | St | 1182 | C |
| 75 | St | 1183 | G |
| 75 | St | 1185 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 1186 | G |
| 75 | St | 1187 | C |
| 75 | St | 1188 | C |
| 75 | St | 1189 | A |
| 75 | St | 1190 | G |
| 75 | St | 1191 | C |
| 75 | St | 1192 | C |
| 75 | St | 1194 | G |
| 75 | St | 1195 | C |
| 75 | St | 1199 | C |
| 75 | St | 1200 | G |
| 75 | St | 1202 | C |
| 75 | St | 1204 | G |
| 75 | St | 1205 | G |
| 75 | St | 1208 | G |
| 75 | St | 1210 | G |
| 75 | St | 1212 | G |
| 75 | St | 1213 | G |
| 75 | St | 1214 | A |
| 75 | St | 1215 | G |
| 75 | St | 1219 | C |
| 75 | St | 1220 | C |
| 75 | St | 1223 | C |
| 75 | St | 1224 | G |
| 75 | St | 1225 | U |
| 75 | St | 1226 | G |
| 75 | St | 1227 | G |
| 75 | St | 1228 | C |
| 75 | St | 1229 | C |
| 75 | St | 1230 | G |
| 75 | St | 1231 | G |
| 75 | St | 1232 | G |
| 75 | St | 1237 | C |
| 75 | St | 1238 | G |
| 75 | St | 1240 | G |
| 75 | St | 1243 | G |
| 75 | St | 1246 | A |
| 75 | St | 1247 | C |
| 75 | St | 1248 | G |
| 75 | St | 1253 | C |
| 75 | St | 1254 | G |
| 75 | St | 1255 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 1256 | G |
| 75 | St | 1257 | C |
| 75 | St | 1261 | A |
| 75 | St | 1262 | G |
| 75 | St | 1263 | G |
| 75 | St | 1264 | A |
| 75 | St | 1265 | A |
| 75 | St | 1266 | U |
| 75 | St | 1267 | G |
| 75 | St | 1268 | U |
| 75 | St | 1271 | U |
| 75 | St | 1272 | G |
| 75 | St | 1273 | U |
| 75 | St | 1275 | G |
| 75 | St | 1278 | G |
| 75 | St | 1279 | C |
| 75 | St | 1283 | C |
| 75 | St | 1287 | C |
| 75 | St | 1288 | A |
| 75 | St | 1289 | C |
| 75 | St | 1292 | C |
| 75 | St | 1295 | G |
| 75 | St | 1296 | C |
| 75 | St | 1301 | C |
| 75 | St | 1302 | G |
| 75 | St | 1304 | G |
| 75 | St | 1306 | C |
| 75 | St | 1307 | C |
| 75 | St | 1310 | G |
| 75 | St | 1313 | C |
| 75 | St | 1319 | A |
| 75 | St | 1321 | A |
| 75 | St | 1322 | C |
| 75 | St | 1323 | A |
| 75 | St | 1325 | C |
| 75 | St | 1326 | G |
| 75 | St | 1327 | C |
| 75 | St | 1330 | G |
| 75 | St | 1331 | U |
| 75 | St | 1332 | C |
| 75 | St | 1334 | C |
| 75 | St | 1337 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 1339 | A |
| 75 | St | 1341 | C |
| 75 | St | 1345 | U |
| 75 | St | 1346 | G |
| 75 | St | 1347 | G |
| 75 | St | 1348 | G |
| 75 | St | 1350 | G |
| 75 | St | 1351 | C |
| 75 | St | 1352 | G |
| 75 | St | 1353 | G |
| 75 | St | 1355 | G |
| 75 | St | 1356 | G |
| 75 | St | 1359 | A |
| 75 | St | 1360 | G |
| 75 | St | 1361 | C |
| 75 | St | 1363 | C |
| 75 | St | 1364 | C |
| 75 | St | 1367 | G |
| 75 | St | 1368 | G |
| 75 | St | 1369 | A |
| 75 | St | 1370 | C |
| 75 | St | 1371 | G |
| 75 | St | 1372 | C |
| 75 | St | 1373 | G |
| 75 | St | 1374 | C |
| 75 | St | 1375 | G |
| 75 | St | 1376 | A |
| 75 | St | 1378 | G |
| 75 | St | 1381 | C |
| 75 | St | 1382 | C |
| 75 | St | 1383 | G |
| 75 | St | 1389 | C |
| 75 | St | 1392 | C |
| 75 | St | 1393 | G |
| 75 | St | 1395 | G |
| 75 | St | 1399 | G |
| 75 | St | 1401 | A |
| 75 | St | 1404 | A |
| 75 | St | 1410 | A |
| 75 | St | 1411 | A |
| 75 | St | 1412 | G |
| 75 | St | 1415 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 75 | St | 1417 | A |
| 75 | St | 1418 | A |
| 75 | St | 1420 | A |
| 75 | St | 1421 | A |
| 75 | St | 1422 | G |
| 75 | St | 1423 | G |
| 75 | St | 1424 | U |
| 75 | St | 1425 | A |
| 75 | St | 1426 | U |
| 75 | St | 1428 | C |
| 75 | St | 1430 | U |
| 75 | St | 1431 | A |
| 75 | St | 1433 | G |
| 75 | St | 1434 | U |
| 75 | St | 1435 | G |
| 75 | St | 1437 | A |
| 75 | St | 1438 | C |
| 75 | St | 1443 | G |
| 75 | St | 1444 | G |
| 75 | St | 1447 | G |
| 75 | St | 1448 | G |
| 75 | St | 1449 | A |
| 75 | St | 1450 | U |
| 75 | St | 1451 | C |
| 75 | St | 1452 | C |
| 75 | St | 1453 | U |
| 75 | St | 1454 | U |
| 76 | u | 2 | G |
| 76 | u | 3 | C |
| 76 | u | 4 | A |
| 76 | u | 6 | A |
| 76 | u | 7 | G |
| 76 | u | 8 | U |
| 76 | u | 9 | G |
| 76 | u | 10 | G |
| 76 | u | 11 | C |
| 76 | u | 15 | G |
| 76 | u | 16 | C |
| 76 | u | 17 | G |
| 76 | u | 18 | G |
| 76 | u | 19 | A |
| 76 | u | 20 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | u | 22 | C |
| 76 | u | 25 | G |
| 76 | u | 27 | U |
| 76 | u | 28 | G |
| 76 | u | 30 | G |
| 76 | u | 32 | C |
| 76 | u | 37 | A |
| 76 | u | 40 | C |
| 76 | u | 41 | A |
| 76 | u | 42 | G |
| 76 | u | 44 | G |
| 76 | u | 45 | G |
| 76 | u | 46 | U |
| 76 | u | 47 | C |
| 76 | u | 48 | G |
| 76 | u | 50 | U |
| 76 | u | 56 | G |
| 76 | u | 57 | A |
| 76 | u | 58 | A |
| 76 | u | 59 | A |
| 76 | u | 63 | U |
| 76 | u | 69 | G |
| 76 | u | 70 | C |
| 76 | u | 71 | U |
| 76 | u | 73 | C |
| 76 | u | 74 | C |
| 76 | u | 75 | A |
| 77 | v | 2 | G |
| 77 | v | 3 | C |
| 77 | v | 4 | A |
| 77 | v | 5 | G |
| 77 | v | 6 | A |
| 77 | v | 7 | G |
| 77 | v | 9 | G |
| 77 | v | 10 | G |
| 77 | v | 11 | C |
| 77 | v | 12 | G |
| 77 | v | 13 | C |
| 77 | v | 14 | A |
| 77 | v | 15 | G |
| 77 | v | 16 | C |
| 77 | v | 17 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 77 | v | 18 | G |
| 77 | v | 19 | A |
| 77 | v | 20 | A |
| 77 | v | 21 | G |
| 77 | v | 22 | C |
| 77 | v | 26 | C |
| 77 | v | 27 | U |
| 77 | v | 28 | G |
| 77 | v | 29 | G |
| 77 | v | 30 | G |
| 77 | v | 31 | C |
| 77 | v | 32 | C |
| 77 | v | 33 | C |
| 77 | v | 34 | U |
| 77 | v | 35 | C |
| 77 | v | 39 | C |
| 77 | v | 40 | C |
| 77 | v | 45 | G |
| 77 | v | 46 | U |
| 77 | v | 47 | C |
| 77 | v | 48 | G |
| 77 | v | 49 | A |
| 77 | v | 50 | U |
| 77 | v | 51 | G |
| 77 | v | 52 | G |
| 77 | v | 53 | A |
| 77 | v | 54 | U |
| 77 | v | 55 | C |
| 77 | v | 56 | G |
| 77 | v | 57 | A |
| 77 | v | 58 | A |
| 77 | v | 61 | C |
| 77 | v | 62 | A |
| 77 | v | 65 | C |
| 77 | v | 66 | U |
| 77 | v | 67 | C |
| 77 | v | 69 | G |
| 77 | v | 71 | U |
| 77 | v | 72 | A |
| 77 | v | 73 | C |
| 77 | v | 74 | C |
| 77 | v | 75 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 78 | y | 34 | A |
| 78 | y | 35 | U |
| 78 | y | 37 | G |
| 78 | y | 38 | A |
| 78 | y | 39 | G |
| 78 | y | 40 | A |

All (16) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | LD | 8 | C |
| 4 | LD | 24 | C |
| 4 | LD | 39 | C |
| 4 | LD | 40 | G |
| 4 | LD | 52 | G |
| 4 | LD | 73 | A |
| 4 | LD | 83 | C |
| 4 | LD | 87 | A |
| 4 | LD | 117 | C |
| 5 | LE | 13 | C |
| 5 | LE | 31 | U |
| 5 | LE | 38 | U |
| 5 | LE | 50 | A |
| 5 | LE | 62 | G |
| 5 | LE | 63 | U |
| 5 | LE | 110 | U |

## 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.

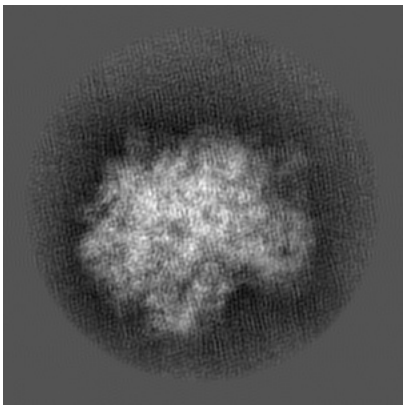
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16228. These allow visual inspection of the internal detail of the map and identification of artifacts.

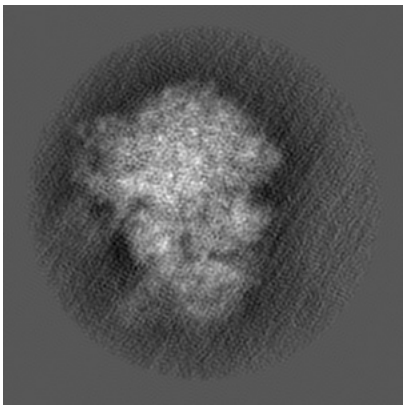
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

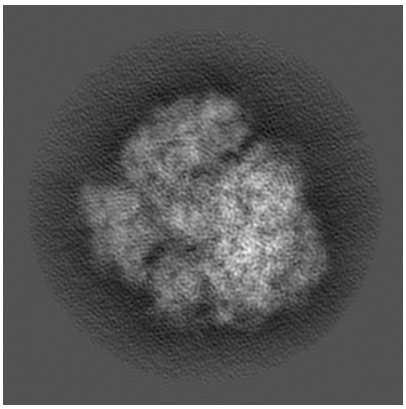
### 6.1.1 Primary map



X

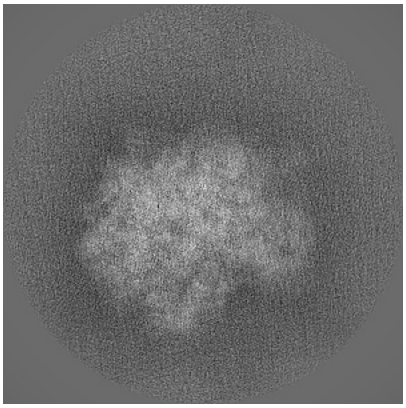


Y

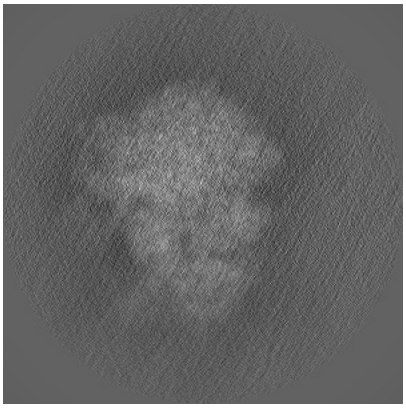


Z

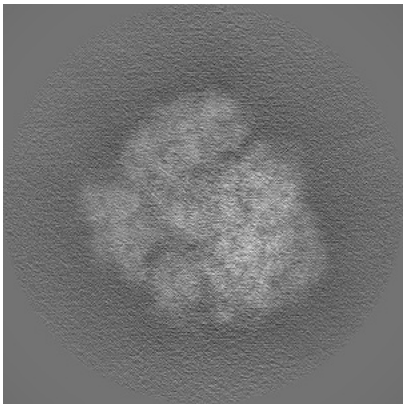
### 6.1.2 Raw map



X



Y

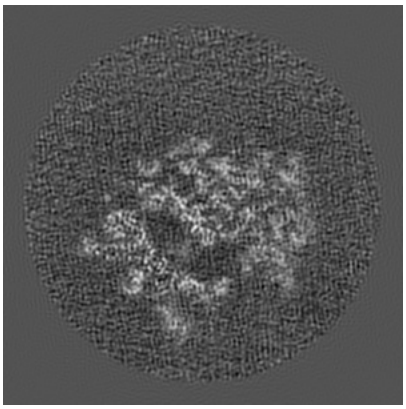


Z

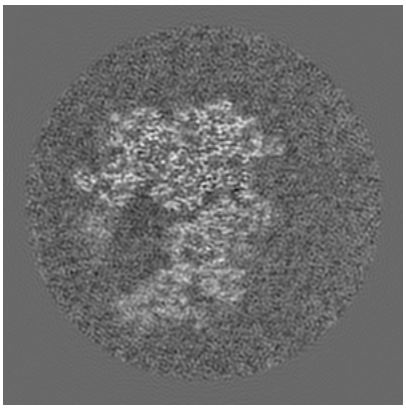
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

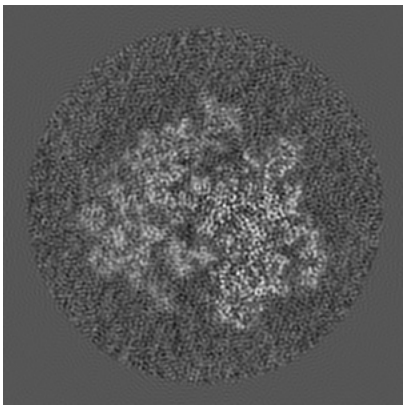
### 6.2.1 Primary map



X Index: 250

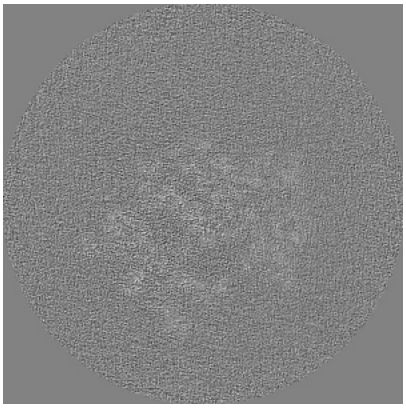


Y Index: 250

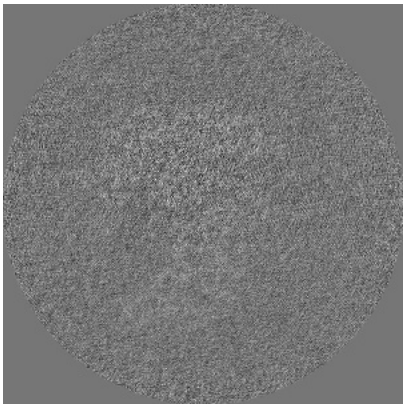


Z Index: 250

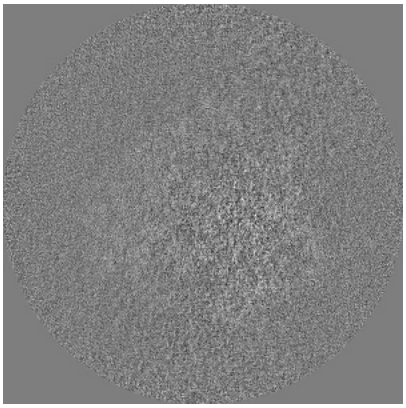
### 6.2.2 Raw map



X Index: 250



Y Index: 250

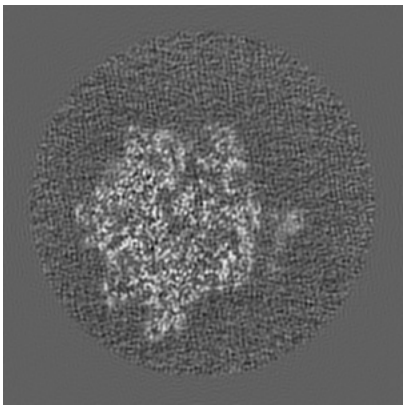


Z Index: 250

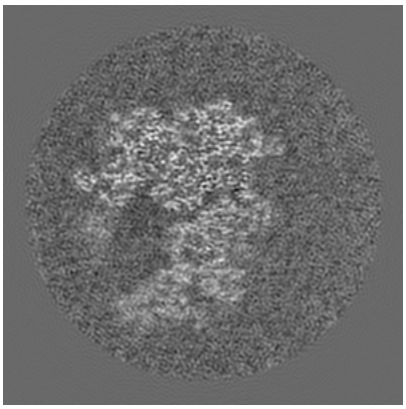
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

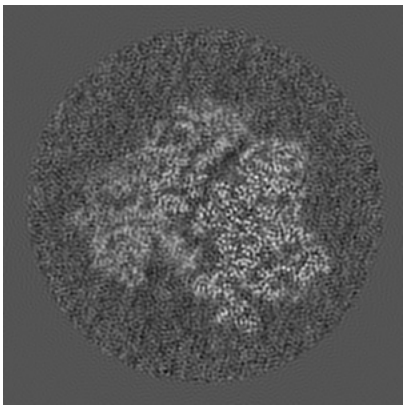
### 6.3.1 Primary map



X Index: 306

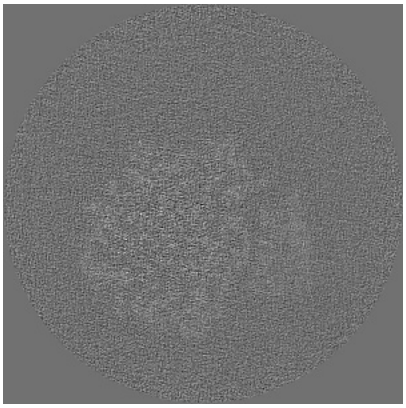


Y Index: 250

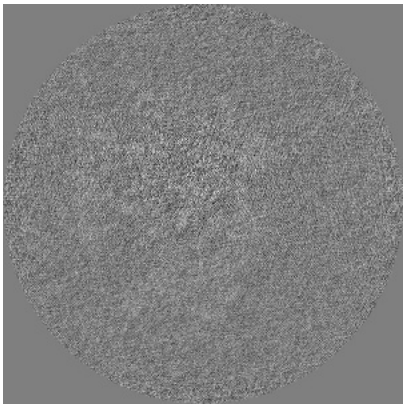


Z Index: 239

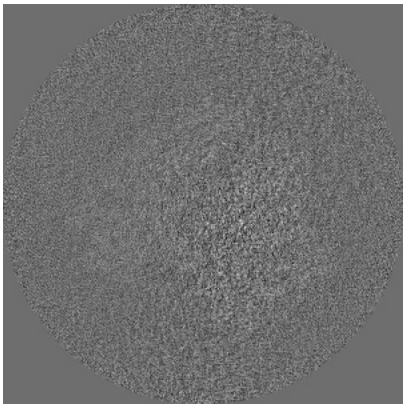
### 6.3.2 Raw map



X Index: 284



Y Index: 224

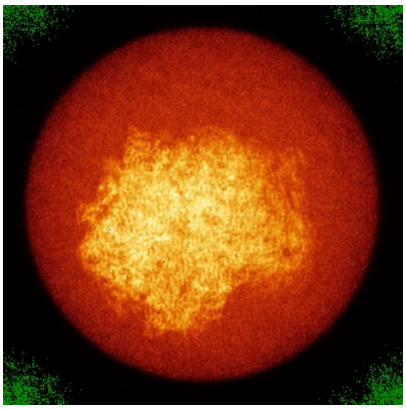


Z Index: 242

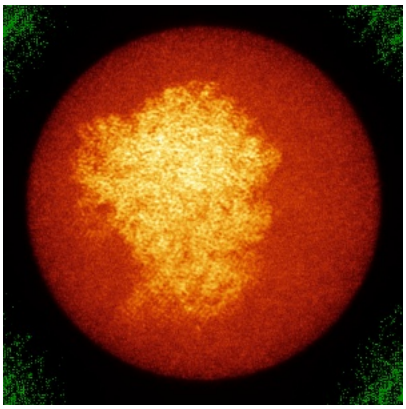
The images above show the largest variance slices of the map in three orthogonal directions.

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

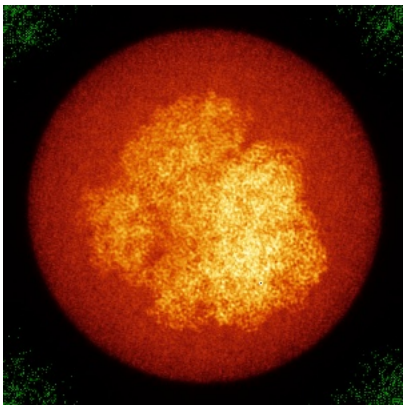
### 6.4.1 Primary map



X

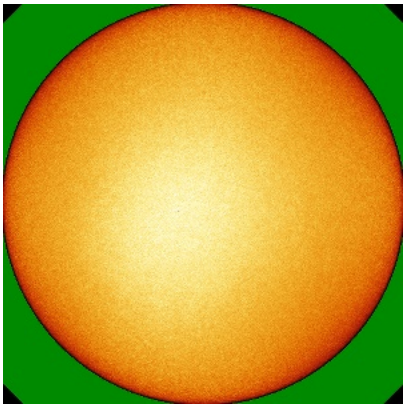


Y

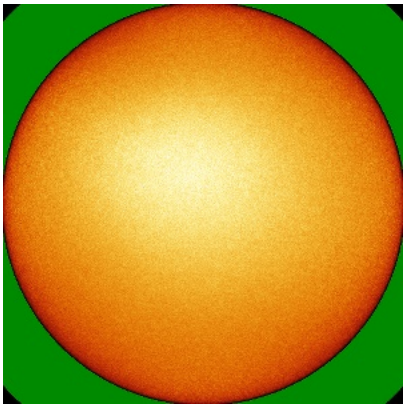


Z

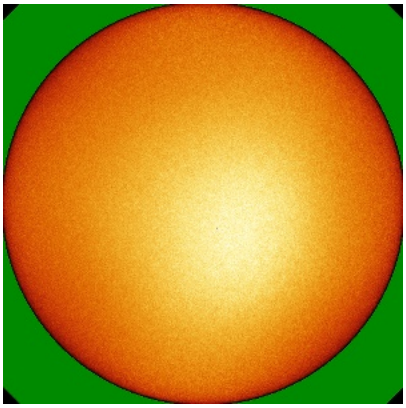
### 6.4.2 Raw map



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.

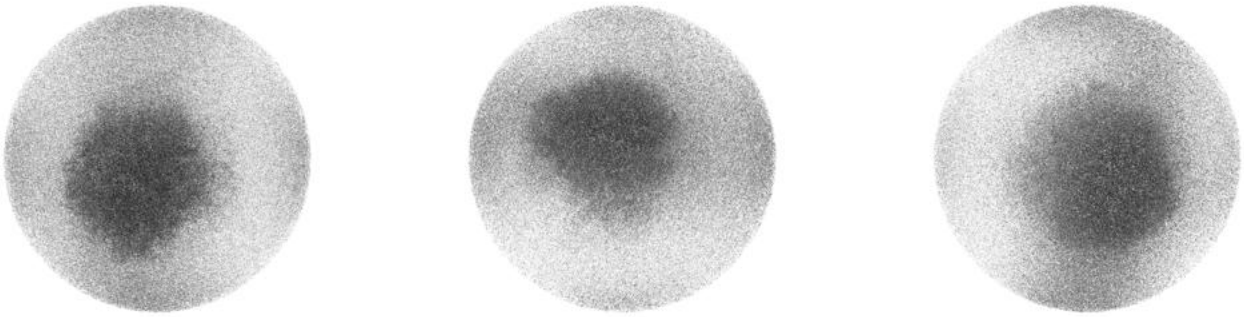
## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. 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



X Y Z

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.

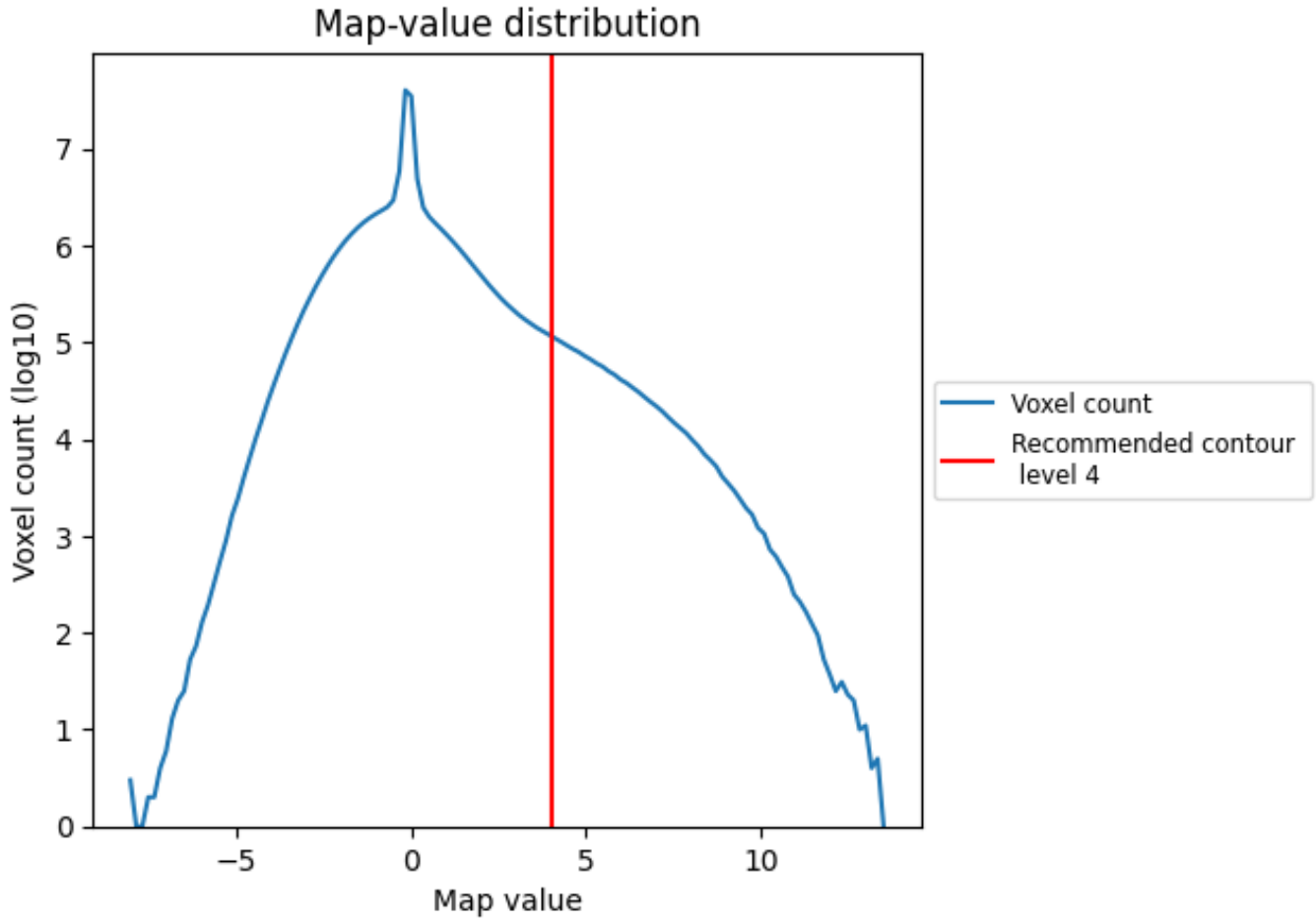
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

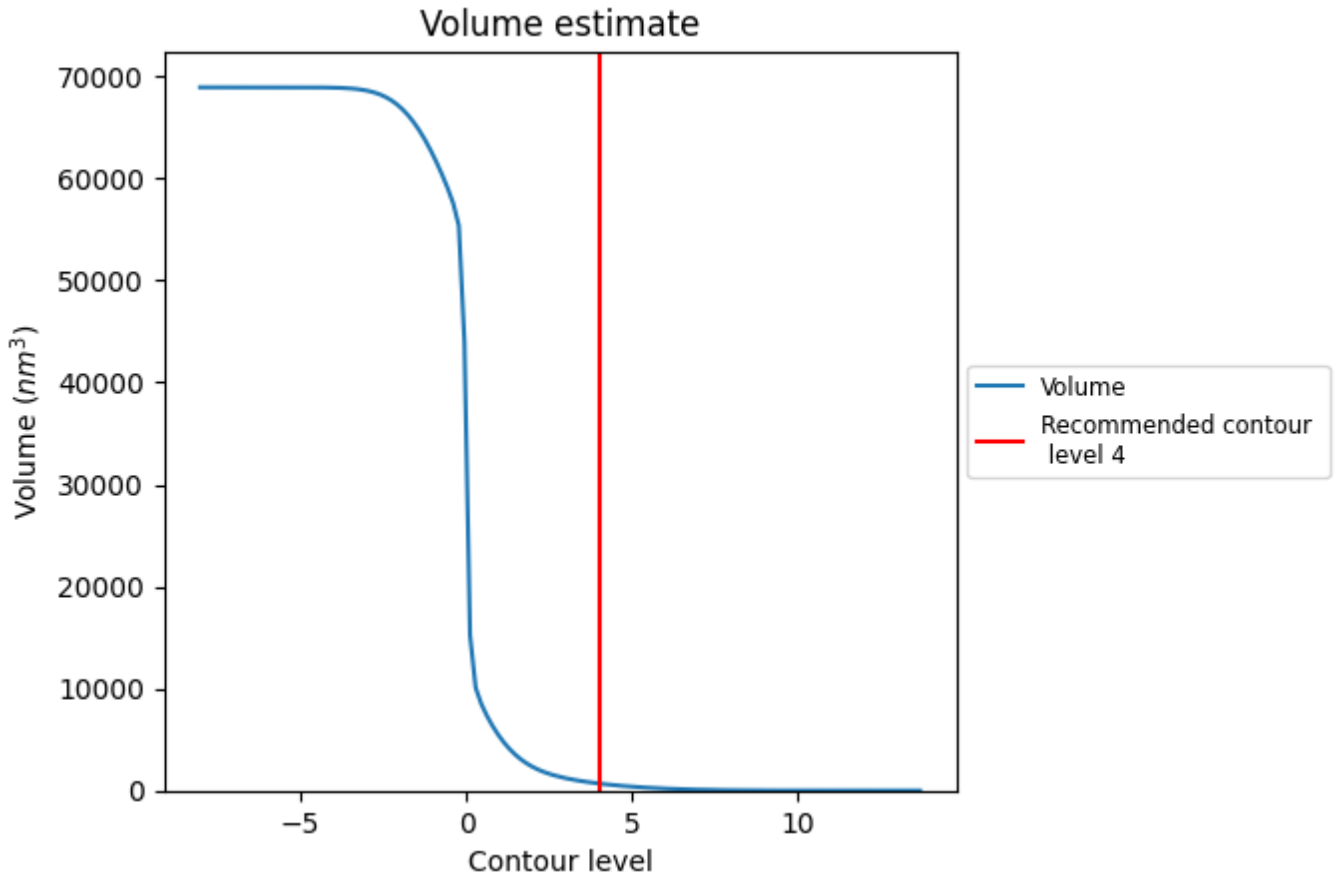
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

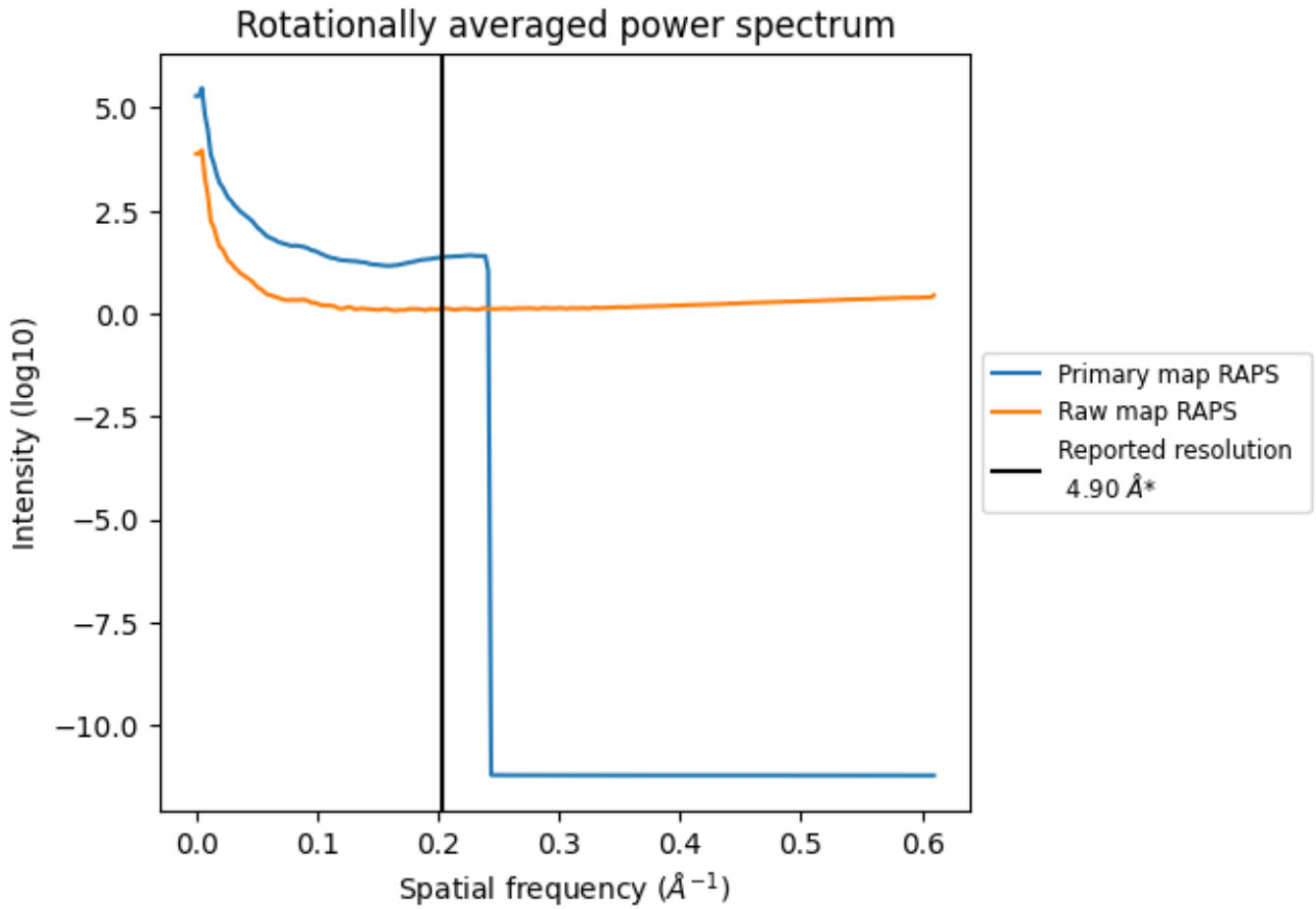
## 7.2 Volume estimate




The volume at the recommended contour level is 692 $nm^3$; this corresponds to an approximate mass of 625 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 (i)

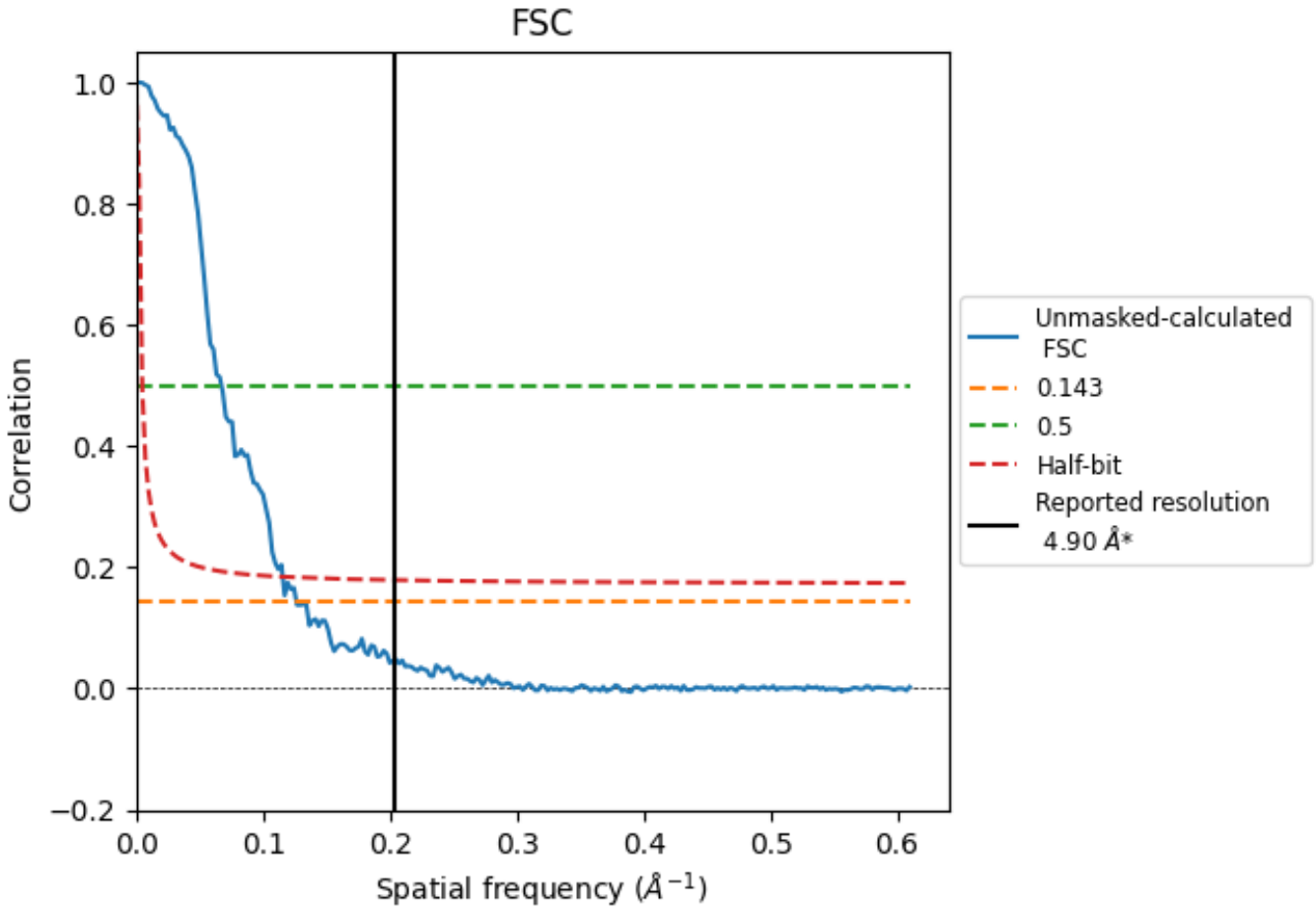



*Reported resolution corresponds to spatial frequency of 0.204 $Å^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.204 $Å^{-1}$

## 8.2 Resolution estimates (i)

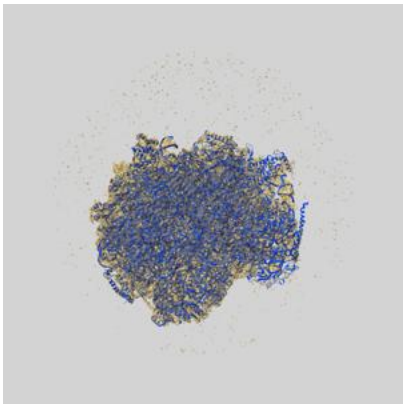
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.90 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 7.91 | 14.88 | 8.65 |

*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 7.91 differs from the reported value 4.9 by more than 10 %

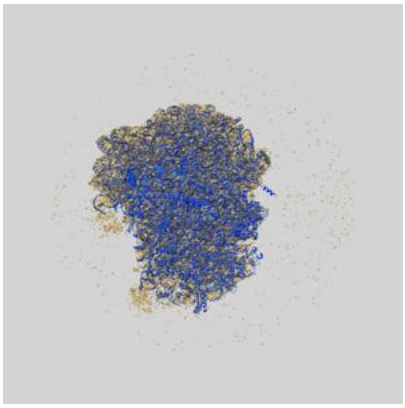
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16228 and PDB model 8BTD. Per-residue inclusion information can be found in section 3 on page 18.

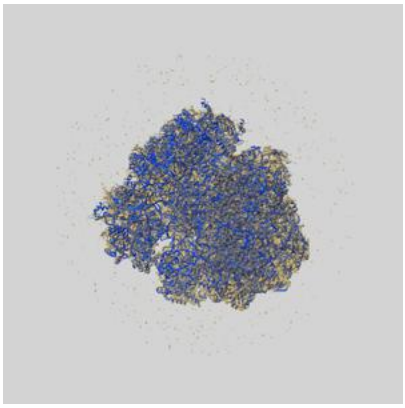
## 9.1 Map-model overlay



X



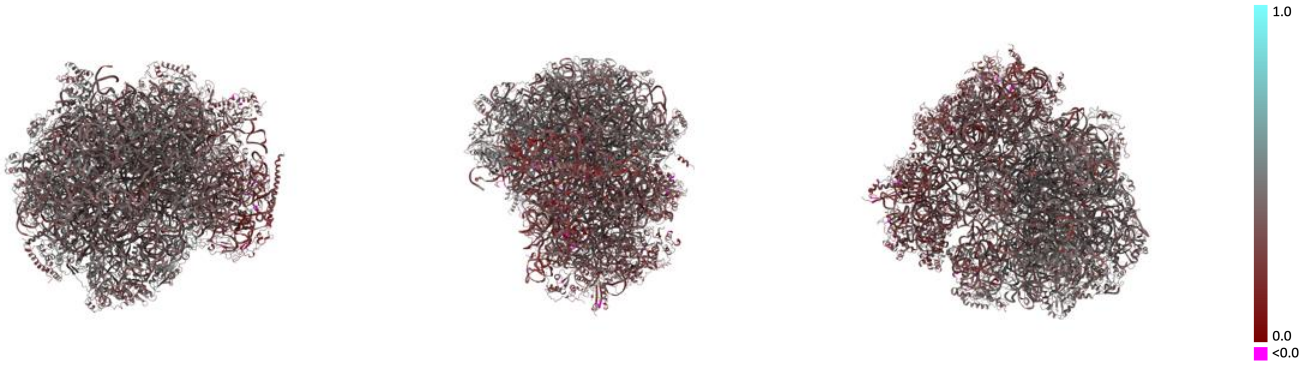
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

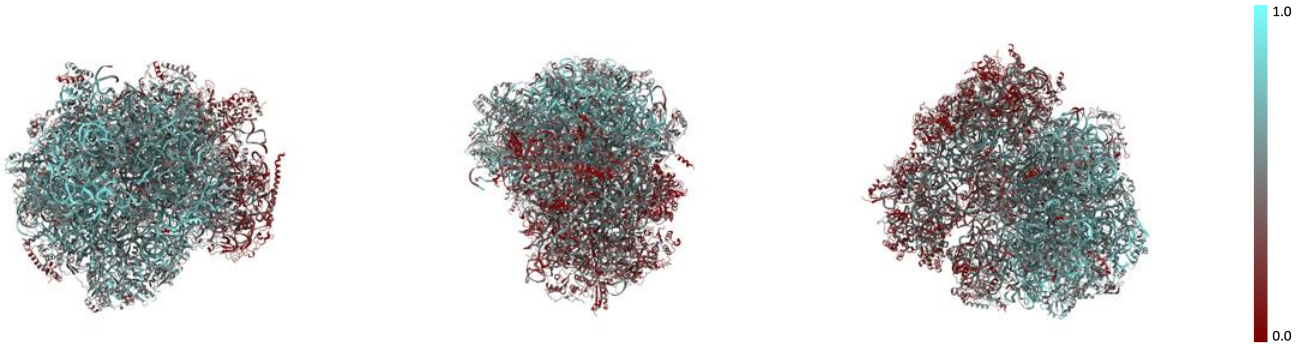
## 9.2 Q-score mapped to coordinate model




X Y Z

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

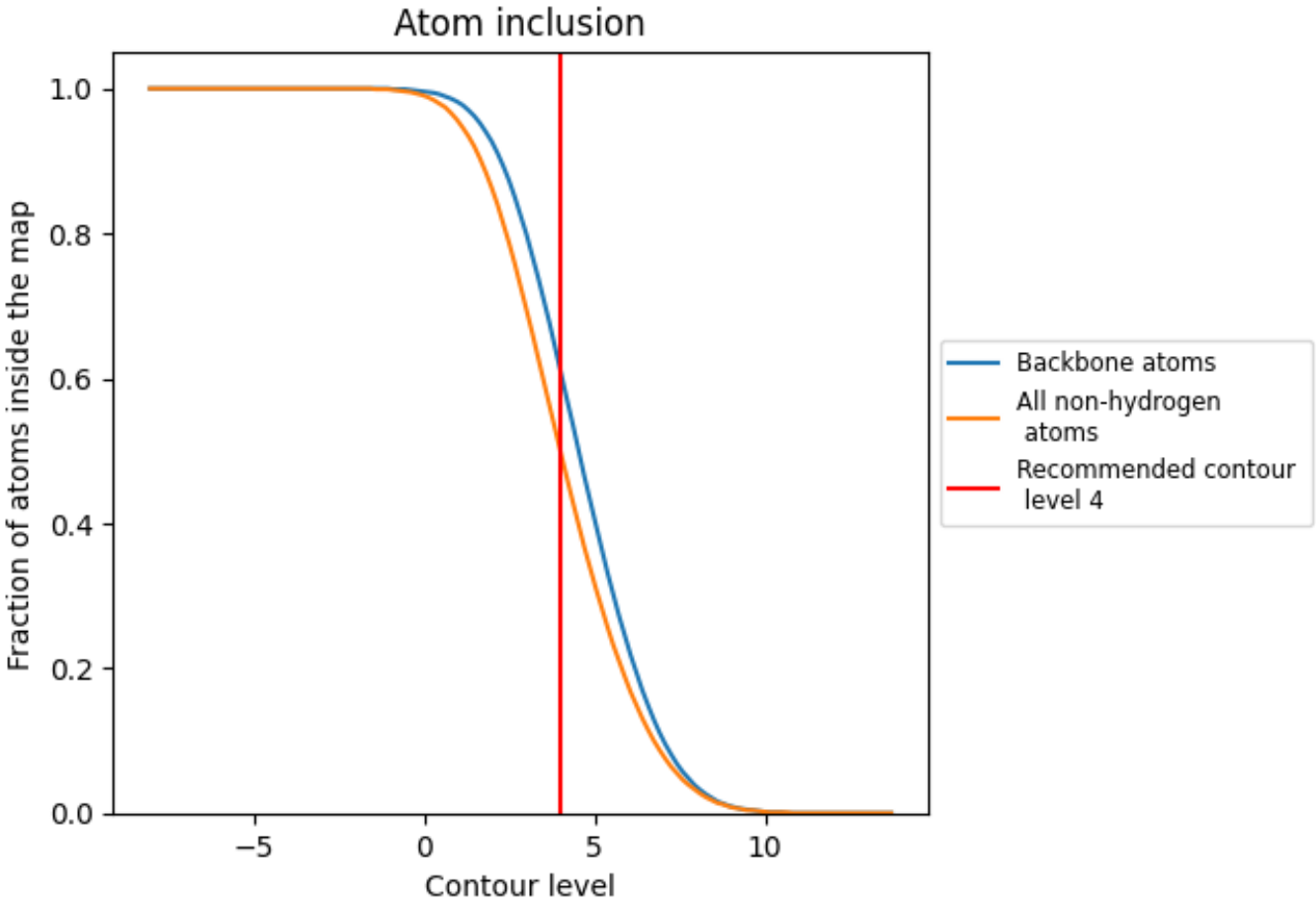
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

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 (4).

## 9.4 Atom inclusion (i)




At the recommended contour level, 61% of all backbone atoms, 50% 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 (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4980 | 0.3660 |
| LA | 0.4830 | 0.4370 |
| LB | 0.5250 | 0.4300 |
| LC | 0.5340 | 0.4260 |
| LD | 0.6830 | 0.3760 |
| LE | 0.7080 | 0.3780 |
| LF | 0.4580 | 0.4010 |
| LG | 0.4960 | 0.4190 |
| LH | 0.4510 | 0.4110 |
| LI | 0.4740 | 0.4090 |
| LJ | 0.5070 | 0.4290 |
| LK | 0.4230 | 0.4240 |
| LL | 0.4420 | 0.4070 |
| LM | 0.5320 | 0.4260 |
| LN | 0.5080 | 0.4120 |
| LO | 0.5360 | 0.4380 |
| LP | 0.5210 | 0.4090 |
| LQ | 0.5040 | 0.4300 |
| LR | 0.5080 | 0.4260 |
| LS | 0.4230 | 0.3910 |
| LT | 0.5240 | 0.4270 |
| LU | 0.4870 | 0.4280 |
| LV | 0.3960 | 0.3800 |
| LW | 0.5060 | 0.4230 |
| LX | 0.4930 | 0.4130 |
| LY | 0.5470 | 0.4390 |
| LZ | 0.5820 | 0.4300 |
| La | 0.3980 | 0.3880 |
| Lb | 0.5610 | 0.4360 |
| Lc | 0.4930 | 0.4090 |
| Ld | 0.4850 | 0.4150 |
| Le | 0.5420 | 0.4330 |
| Lf | 0.5000 | 0.4270 |
| Lg | 0.5450 | 0.4460 |
| Lh | 0.4440 | 0.4220 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| Li | 0.5070 | 0.4080 |
| Lj | 0.4450 | 0.4160 |
| Lk | 0.5780 | 0.4510 |
| Ll | 0.4010 | 0.3810 |
| Ln | 0.1070 | 0.3090 |
| Lo | 0.3400 | 0.4030 |
| Lp | 0.5150 | 0.4480 |
| Lq | 0.5150 | 0.4120 |
| Ls | 0.5050 | 0.3990 |
| Lt | 0.6680 | 0.3820 |
| SA | 0.2590 | 0.3360 |
| SB | 0.3080 | 0.3600 |
| SC | 0.2300 | 0.3100 |
| SD | 0.3280 | 0.3650 |
| SE | 0.2170 | 0.2960 |
| SF | 0.2320 | 0.3270 |
| SG | 0.1210 | 0.2870 |
| SH | 0.1900 | 0.3310 |
| SI | 0.2000 | 0.3350 |
| SJ | 0.3270 | 0.3610 |
| SK | 0.2340 | 0.3010 |
| SL | 0.2250 | 0.2630 |
| SM | 0.1970 | 0.3300 |
| SO | 0.2890 | 0.3890 |
| SP | 0.2940 | 0.3470 |
| SQ | 0.3890 | 0.3870 |
| SR | 0.2090 | 0.3480 |
| ST | 0.2050 | 0.3120 |
| SU | 0.2040 | 0.3100 |
| SV | 0.2670 | 0.3600 |
| SW | 0.2550 | 0.3070 |
| SX | 0.1840 | 0.2540 |
| SY | 0.2210 | 0.3430 |
| Sb | 0.1830 | 0.2960 |
| Sc | 0.2130 | 0.3180 |
| Sd | 0.3320 | 0.3870 |
| Se | 0.2160 | 0.3640 |
| Sg | 0.2020 | 0.3380 |
| Sh | 0.2860 | 0.3270 |
| Sj | 0.1820 | 0.3340 |
| St | 0.4870 | 0.3070 |
| u | 0.4300 | 0.3030 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| v | 0.0970 | 0.1980 |
| y | 0.2850 | 0.3110 |