# Full wwPDB EM Validation Report

Mar 28, 2026 – 06:18 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 6RXY / pdb_00006rxy |
| EMDB ID | : | EMD-10055 |
| Title | : | Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from Chaetomium thermophilum, state a |
| Authors | : | Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E. |
| Deposited on | : | 2019-06-10 |
| Resolution | : | 4.70 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 (i) 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 (i)) were used in the production of this report:

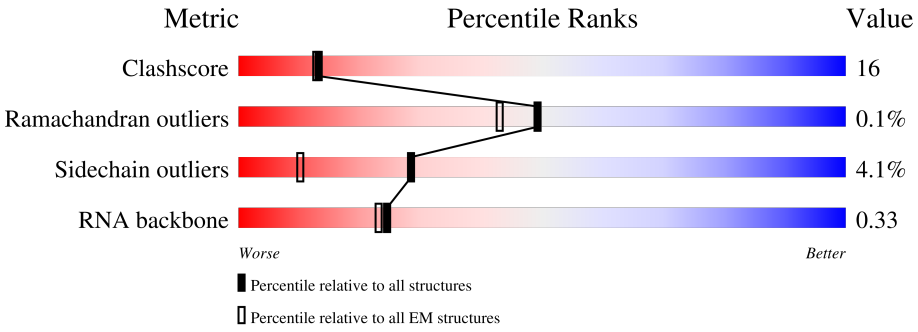
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025)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

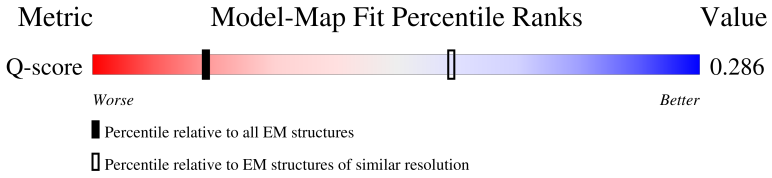
# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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 | 1989 ( 4.20 - 5.20 ) |

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 | UA | 904 | 60% 31% • 7% |
| 2 | UB | 907 | 38% 18% 44% |
| 3 | UC | 648 | 8% • 89% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | UD | 884 | 51% 36% 13% |
| 5 | UF | 414 | 56% 24% 20% |
| 6 | UG | 558 | 50% 29% 20% |
| 7 | UJ | 1802 | 20% 31% 13% 55% |
| 8 | UK | 270 | 56% 24% 20% |
| 9 | UL | 962 | 45% 36% 18% |
| 10 | UM | 912 | 25% 49% 25% 26% |
| 11 | UN | 938 | 10% 6% 84% |
| 12 | UO | 557 | 55% 35% 10% |
| 13 | UQ | 960 | 49% 32% 18% |
| 14 | UR | 618 | 44% 28% 28% |
| 15 | UU | 1049 | 54% 30% 14% |
| 16 | UX | 193 | 52% 46% |
| 17 | UZ | 391 | 35% 24% 40% |
| 18 | CA | 313 | 45% 31% 23% |
| 18 | CB | 313 | 47% 29% 24% |
| 19 | CC | 523 | 47% 27% 26% |
| 20 | CD | 582 | 46% 26% 28% |
| 21 | CE | 127 | 70% 22% 5% |
| 21 | CF | 127 | 11% 58% 36% 6% |
| 22 | CG | 630 | 15% 41% 19% 40% |
| 23 | CH | 411 | 58% 36% 5% |
| 24 | CI | 1163 | 43% 27% 29% |
| 25 | CJ | 183 | 58% 38% |
| 26 | CK | 297 | 53% 45% |

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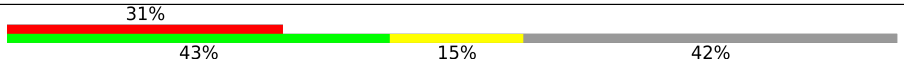
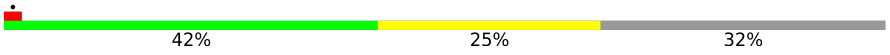
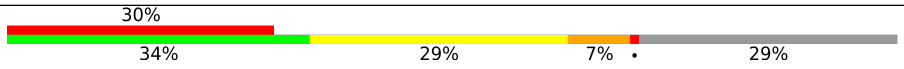
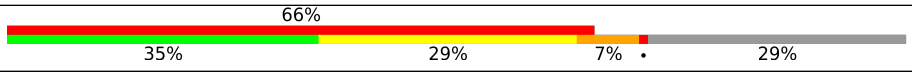
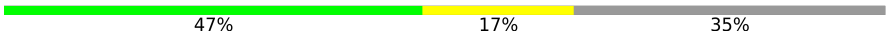
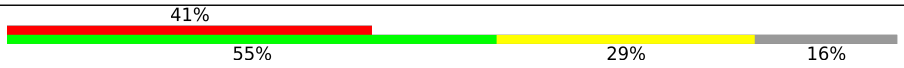
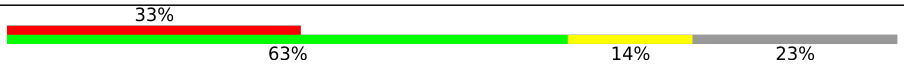
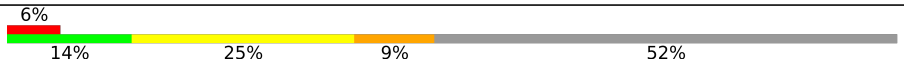
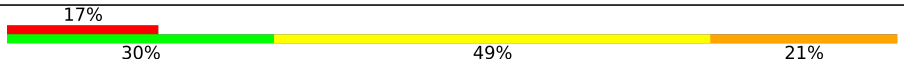
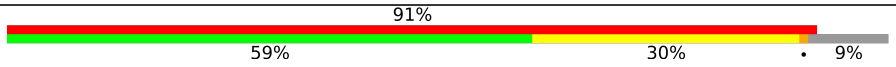
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 27 | CL | 785 | |
| 28 | CM | 446 | |
| 29 | CN | 252 | |
| 29 | CO | 252 | |
| 30 | CP | 322 |   |
| 31 | CQ | 259 |   |
| 32 | CR | 1073 |   |
| 32 | CS | 1073 |   |
| 33 | CT | 203 |   |
| 34 | Cc | 212 | |
| 35 | Ce | 203 | |
| 36 | Cg | 190 |   |
| 37 | Ch | 151 | |
| 38 | Ci | 150 |   |
| 39 | Cj | 143 | |
| 40 | Cm | 130 | |
| 41 | Cn | 145 | |
| 42 | Cp | 68 | |
| 43 | CU | 311 | |
| 44 | C1 | 2323 |   |
| 45 | C2 | 230 |   |
| 46 | UV | 1171 |   |
| 47 | CV | 322 | |
| 48 | UH | 930 | |
| 49 | UE | 410 | |

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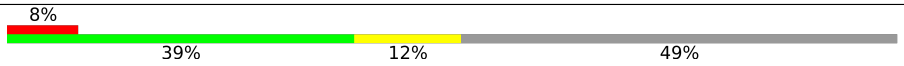
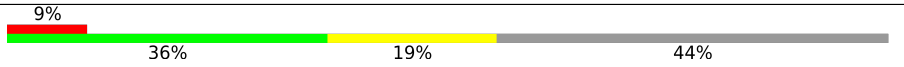
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 49 | UI | 410 | |
| 50 | US | 549 | |
| 51 | Cl | 156 |   |
| 52 | CX | 480 |   |
| 53 | UP | 364 | |
| 54 | Cz | 1796 | |

# 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 180242 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 Periodic tryptophan protein 2-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | UA | 839 | 6366 | 4101 | 1136 | 1105 | 24 | 0 | 0 |

- Molecule 2 is a protein called Utp2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | UB | 512 | 4079 | 2576 | 781 | 711 | 11 | 0 | 0 |

- Molecule 3 is a protein called Utp3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | UC | 74 | 588 | 371 | 120 | 97 | 0 | 0 |

- Molecule 4 is a protein called Utp4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | UD | 772 | 6071 | 3851 | 1093 | 1103 | 24 | 0 | 0 |

- Molecule 5 is a protein called Utp6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | UF | 331 | 2591 | 1674 | 504 | 399 | 14 | 0 | 0 |

- Molecule 6 is a protein called Utp7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | UG | 448 | 3444 | 2197 | 646 | 590 | 11 | 0 | 0 |

- Molecule 7 is a protein called Utp10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | UJ | 808 | Total | C | N | O | S | 0 | 0 |
| | | | 6180 | 3965 | 1077 | 1115 | 23 | | |

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | UK | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1687 | 1062 | 351 | 269 | 5 | | |

- Molecule 9 is a protein called Utp12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | UL | 785 | Total | C | N | O | S | 0 | 0 |
| | | | 6175 | 3940 | 1088 | 1130 | 17 | | |

- Molecule 10 is a protein called Utp13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | UM | 679 | Total | C | N | O | S | 0 | 0 |
| | | | 5273 | 3351 | 924 | 986 | 12 | | |

- Molecule 11 is a protein called Utp14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | UN | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1209 | 770 | 228 | 206 | 5 | | |

- Molecule 12 is a protein called Utp15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | UO | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 3819 | 2422 | 699 | 684 | 14 | | |

- Molecule 13 is a protein called Utp17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | UQ | 789 | Total | C | N | O | S | 0 | 0 |
| | | | 6008 | 3831 | 1037 | 1119 | 21 | | |

- Molecule 14 is a protein called Utp18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | UR | 447 | Total | C | N | O | S | 0 | 0 |
| | | | 3491 | 2209 | 656 | 616 | 10 | | |

- Molecule 15 is a protein called Utp21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | UU | 902 | Total | C | N | O | S | 0 | 0 |
| | | | 6734 | 4336 | 1236 | 1136 | 26 | | |

- Molecule 16 is a protein called Utp24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | UX | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1470 | 932 | 282 | 246 | 10 | | |

- Molecule 17 is a protein called Utp30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | UZ | 235 | Total | C | N | O | S | 0 | 0 |
| | | | 1815 | 1184 | 330 | 298 | 3 | | |

- Molecule 18 is a protein called Nop1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | CA | 242 | Total | C | N | O | S | 0 | 0 |
| | | | 1778 | 1149 | 327 | 293 | 9 | | |
| 18 | CB | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1816 | 1154 | 318 | 335 | 9 | | |

- Molecule 19 is a protein called Nop56.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | CC | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 2866 | 1836 | 527 | 492 | 11 | | |

- Molecule 20 is a protein called Nop58.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | CD | 420 | Total | C | N | O | S | 0 | 0 |
| | | | 3150 | 2023 | 560 | 557 | 10 | | |

- Molecule 21 is a protein called Snu13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | CE | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 879 | 557 | 165 | 154 | 3 | | |
| 21 | CF | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 864 | 550 | 161 | 150 | 3 | | |

- Molecule 22 is a protein called Rrp9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | CG | 378 | Total | C | N | O | S | 0 | 0 |
| | | | 2922 | 1865 | 527 | 517 | 13 | | |

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | CH | 389 | Total | C | N | O | S | 0 | 0 |
| | | | 2888 | 1827 | 526 | 525 | 10 | | |

- Molecule 24 is a protein called Bms1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | CI | 822 | Total | C | N | O | S | 0 | 0 |
| | | | 6486 | 4169 | 1213 | 1077 | 27 | | |

- Molecule 25 is a protein called Imp3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | CJ | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1434 | 918 | 283 | 226 | 7 | | |

- Molecule 26 is a protein called Imp4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | CK | 297 | Total | C | N | O | S | 0 | 0 |
| | | | 2329 | 1476 | 445 | 400 | 8 | | |

- Molecule 27 is a protein called Mpp10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | CL | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1786 | 1114 | 339 | 327 | 6 | | |

- Molecule 28 is a protein called Sof1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | CM | 445 | Total | C | N | O | S | 0 | 0 |
| | | | 3501 | 2195 | 672 | 619 | 15 | | |

- Molecule 29 is a protein called Emg1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | CN | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1762 | 1119 | 306 | 327 | 10 | | |
| 29 | CO | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1683 | 1067 | 293 | 313 | 10 | | |

- Molecule 30 is a protein called KRR1 small subunit processome component.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | CP | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1504 | 961 | 269 | 265 | 9 | | |

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | CQ | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1361 | 862 | 250 | 242 | 7 | | |

- Molecule 32 is a protein called Kre33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | CR | 760 | Total | C | N | O | S | 0 | 0 |
| | | | 5989 | 3851 | 1024 | 1087 | 27 | | |
| 32 | CS | 760 | Total | C | N | O | S | 0 | 0 |
| | | | 5989 | 3851 | 1024 | 1087 | 27 | | |

- Molecule 33 is a protein called Fcf2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | CT | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1035 | 656 | 197 | 178 | 4 | | |

- Molecule 34 is a protein called 40S ribosomal protein s5-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | Cc | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1464 | 926 | 278 | 253 | 7 | | |

- Molecule 35 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 35 | Ce | 159 | Total | C | N | O | 0 | 0 |
| | | | 1279 | 810 | 237 | 232 | | |

- Molecule 36 is a protein called 40S ribosomal protein s9-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | Cg | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1242 | 801 | 255 | 184 | 2 | | |

- Molecule 37 is a protein called 40S ribosomal protein S13-like protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 37 | Ch | 49 | Total | C | N | O | 0 | 0 |
| | | | 416 | 270 | 82 | 64 | | |

- Molecule 38 is a protein called 40S ribosomal protein S14-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | Ci | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 791 | 492 | 154 | 141 | 4 | | |

- Molecule 39 is a protein called 40S ribosomal protein S16-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | Cj | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 943 | 613 | 177 | 151 | 2 | | |

- Molecule 40 is a protein called 40S ribosomal protein S22-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | Cm | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 985 | 632 | 184 | 164 | 5 | | |

- Molecule 41 is a protein called 40S ribosomal protein s23-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | Cn | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 702 | 456 | 134 | 110 | 2 | | |

- Molecule 42 is a protein called 40S ribosomal protein S28-like protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 42 | Cp | 61 | Total | C | N | O | 0 | 0 |
| | | | 455 | 284 | 97 | 74 | | |

- Molecule 43 is a protein called Faf1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | CU | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1009 | 623 | 205 | 175 | 6 | | |

- Molecule 44 is a RNA chain called 35S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | C1 | 1106 | Total | C | N | O | P | 0 | 0 |
| | | | 23604 | 10525 | 4233 | 7740 | 1106 | | |

- Molecule 45 is a RNA chain called U3 snoRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | C2 | 230 | Total | C | N | O | P | 0 | 0 |
| | | | 4891 | 2182 | 856 | 1623 | 230 | | |

- Molecule 46 is a protein called U3 small nucleolar RNA-associated protein 22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | UV | 1061 | Total | C | N | O | S | 0 | 0 |
| | | | 8424 | 5399 | 1480 | 1523 | 22 | | |

- Molecule 47 is a protein called Rrp7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | CV | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1145 | 729 | 198 | 216 | 2 | | |

- Molecule 48 is a protein called Utp8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | UH | 359 | Total | C | N | O | S | 0 | 0 |
| | | | 2809 | 1773 | 496 | 527 | 13 | | |

- Molecule 49 is a protein called Utp5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | UE | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 972 | 608 | 183 | 175 | 6 | | |
| 49 | UI | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 972 | 608 | 183 | 175 | 6 | | |

- Molecule 50 is a protein called Noc4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | US | 451 | Total | C | N | O | S | 0 | 0 |
| | | | 3672 | 2389 | 608 | 660 | 15 | | |

- Molecule 51 is a protein called Rps18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | Cl | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 633 | 400 | 115 | 117 | 1 | | |

- Molecule 52 is a protein called Enp1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | CX | 267 | Total | C | N | O | S | 0 | 0 |
| | | | 2130 | 1384 | 374 | 362 | 10 | | |

- Molecule 53 is a protein called Utp16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 53 | UP | 54 | Total | C | N | O | 0 | 0 |
| | | | 422 | 264 | 88 | 70 | | |

- Molecule 54 is a protein called Rrp5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | Cz | 275 | Total | C | N | O | S | 0 | 0 |
| | | | 2259 | 1435 | 401 | 420 | 3 | | |

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

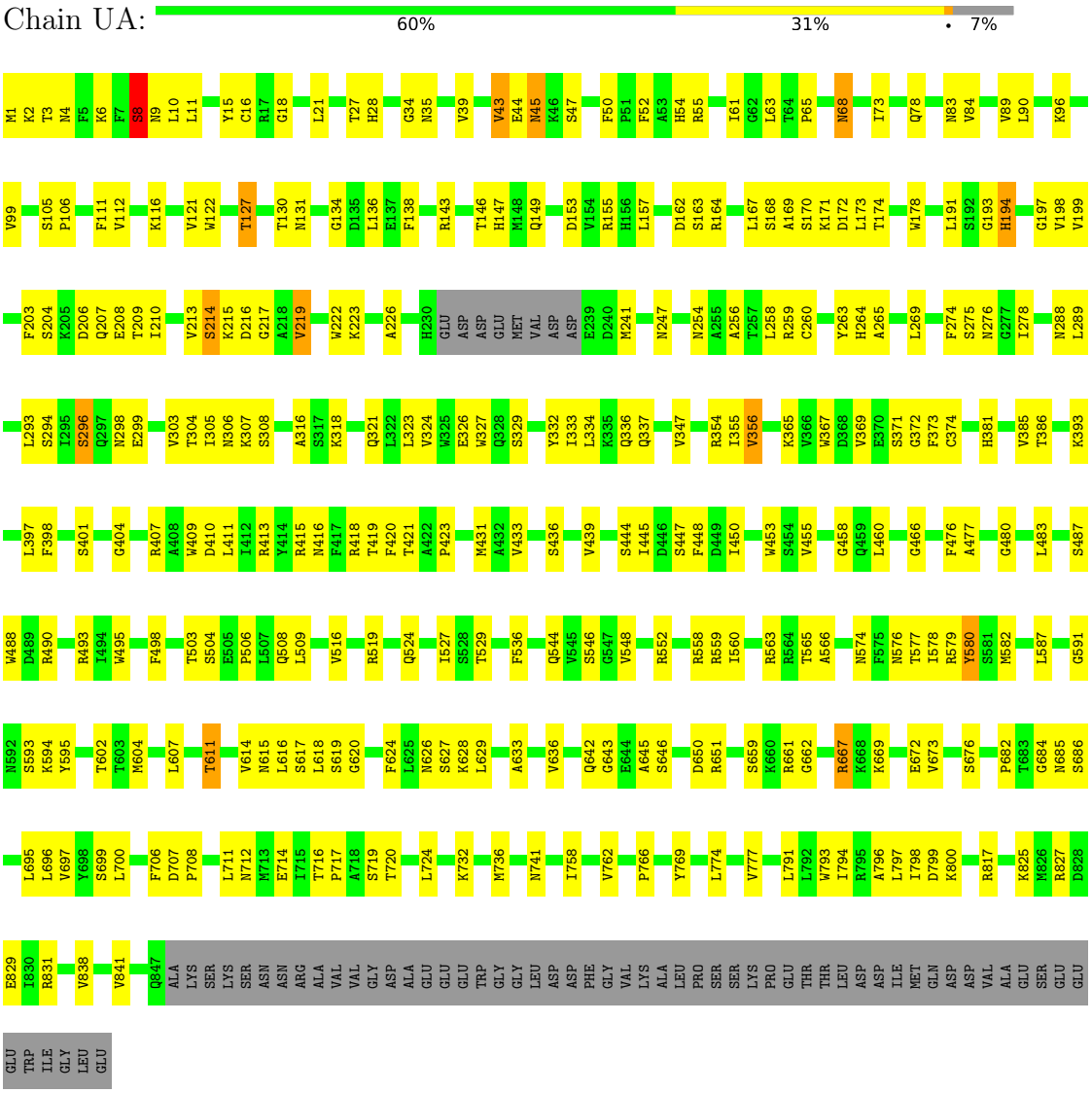
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 55 | UX | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

# 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.

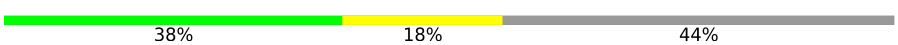
• Molecule 1: Periodic tryptophan protein 2-like protein

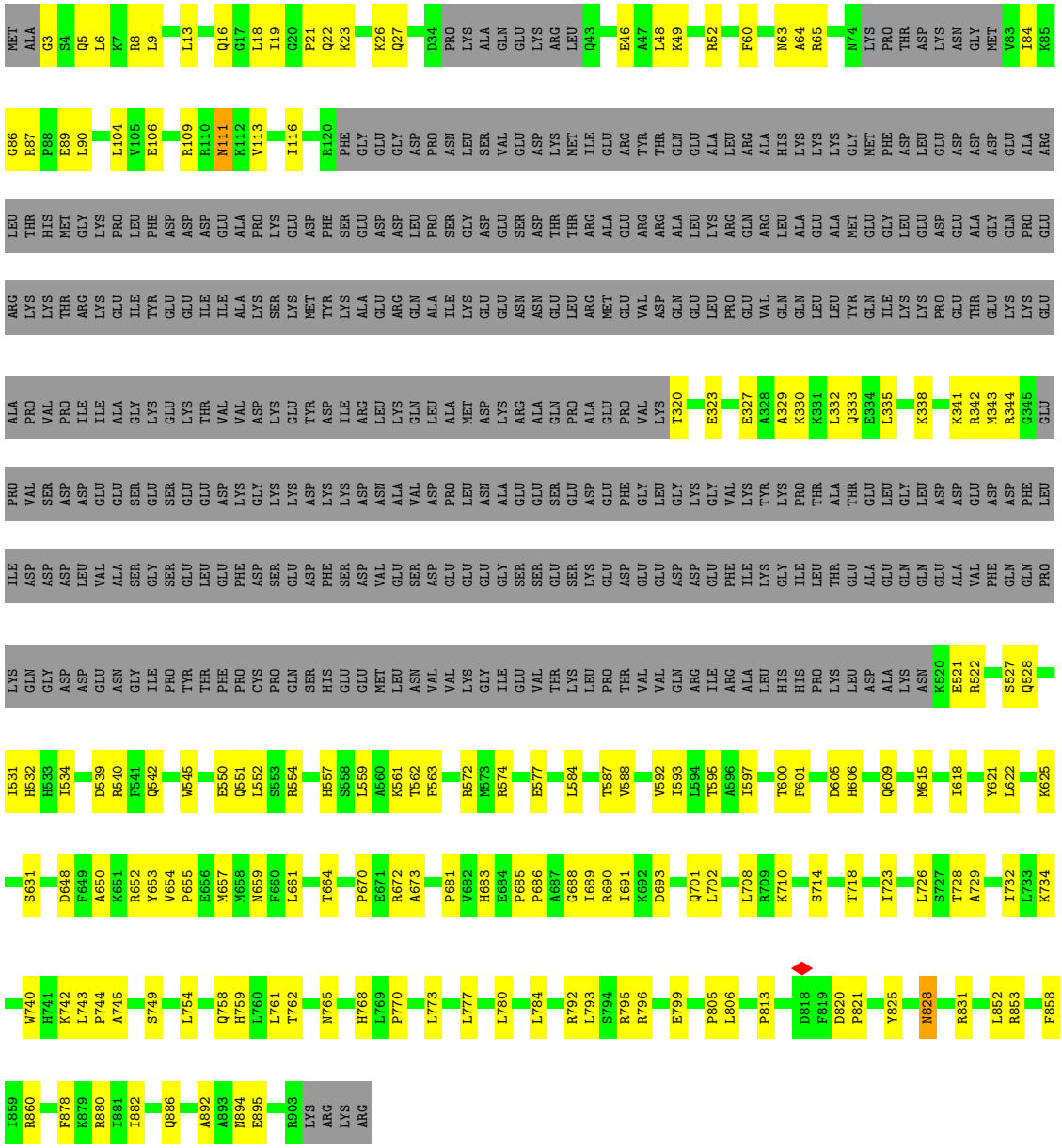
Chain UA:




• Molecule 2: Utp2

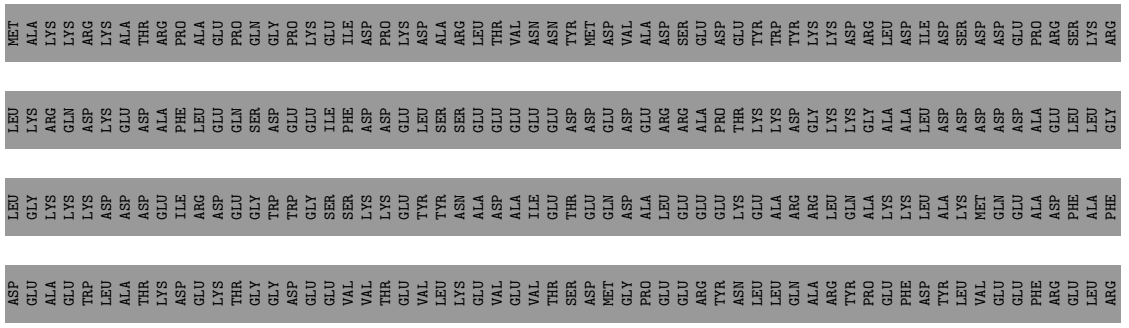
Chain UB:

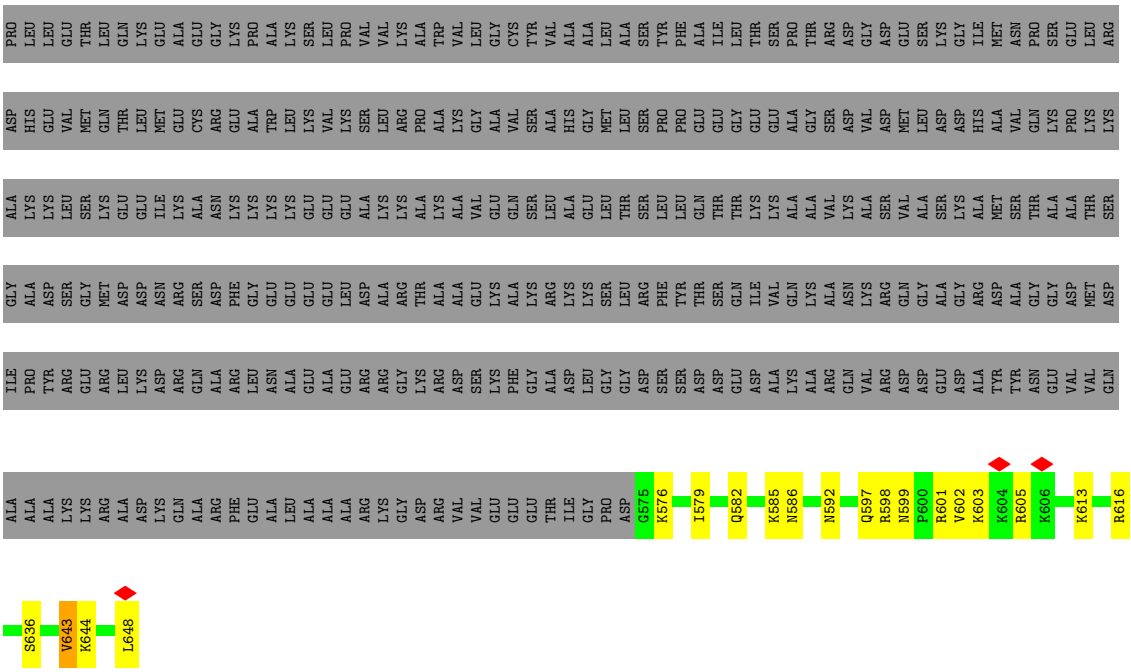




• Molecule 3: Utp3

Chain UC:

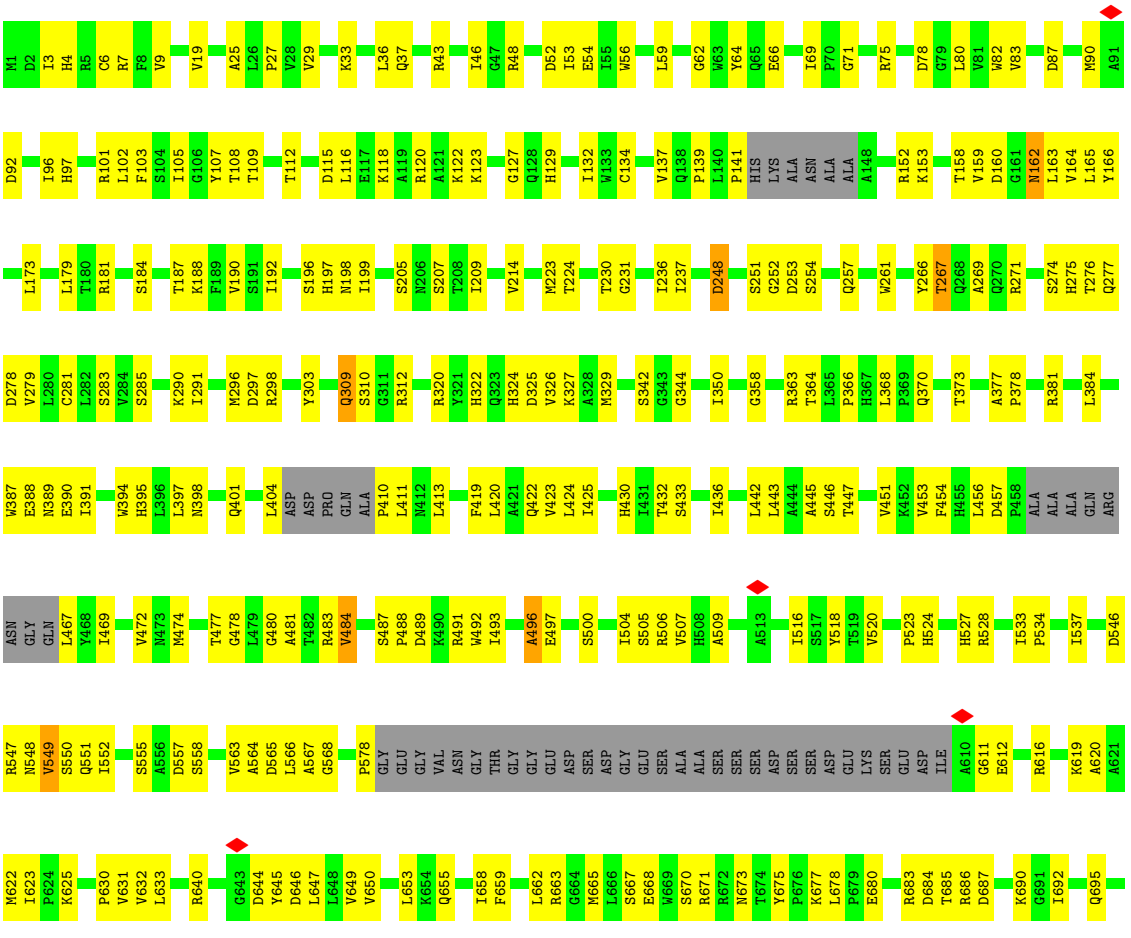


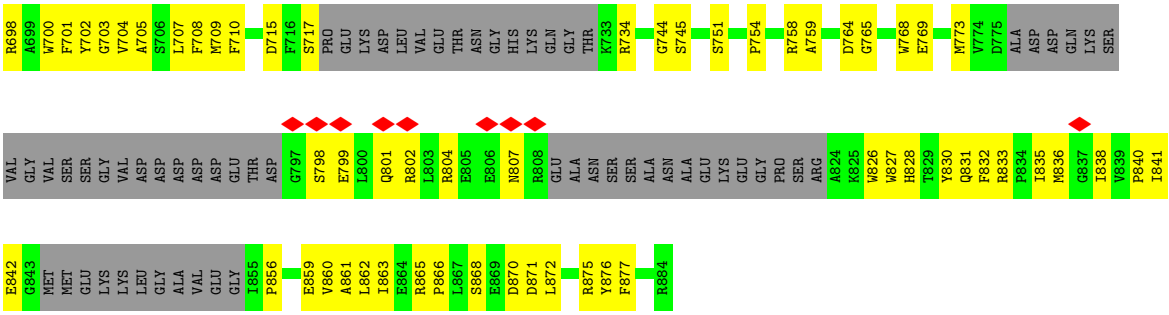




• Molecule 4: Utp4

Chain UD:



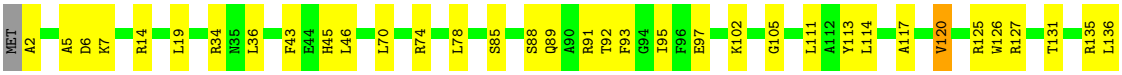


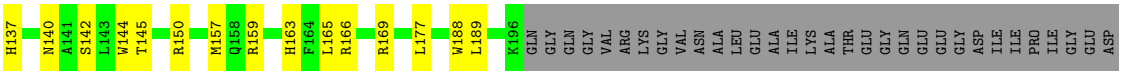


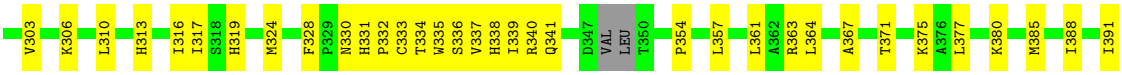


• Molecule 5: Utp6

Chain UF:

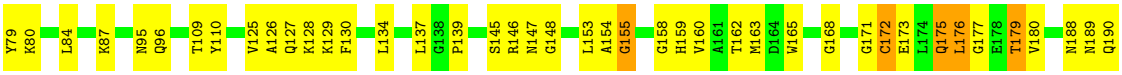


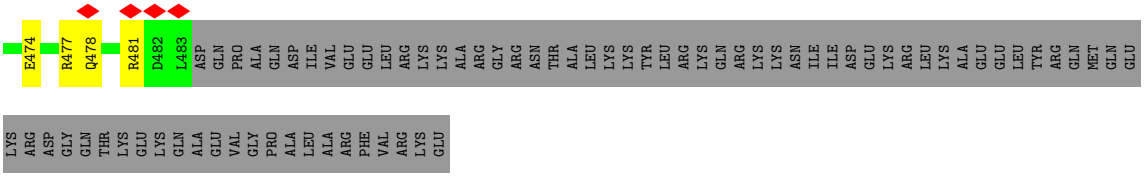




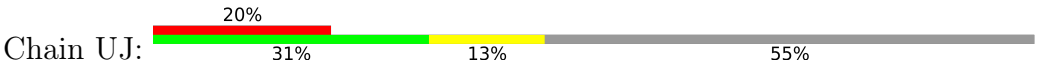
• Molecule 6: Utp7

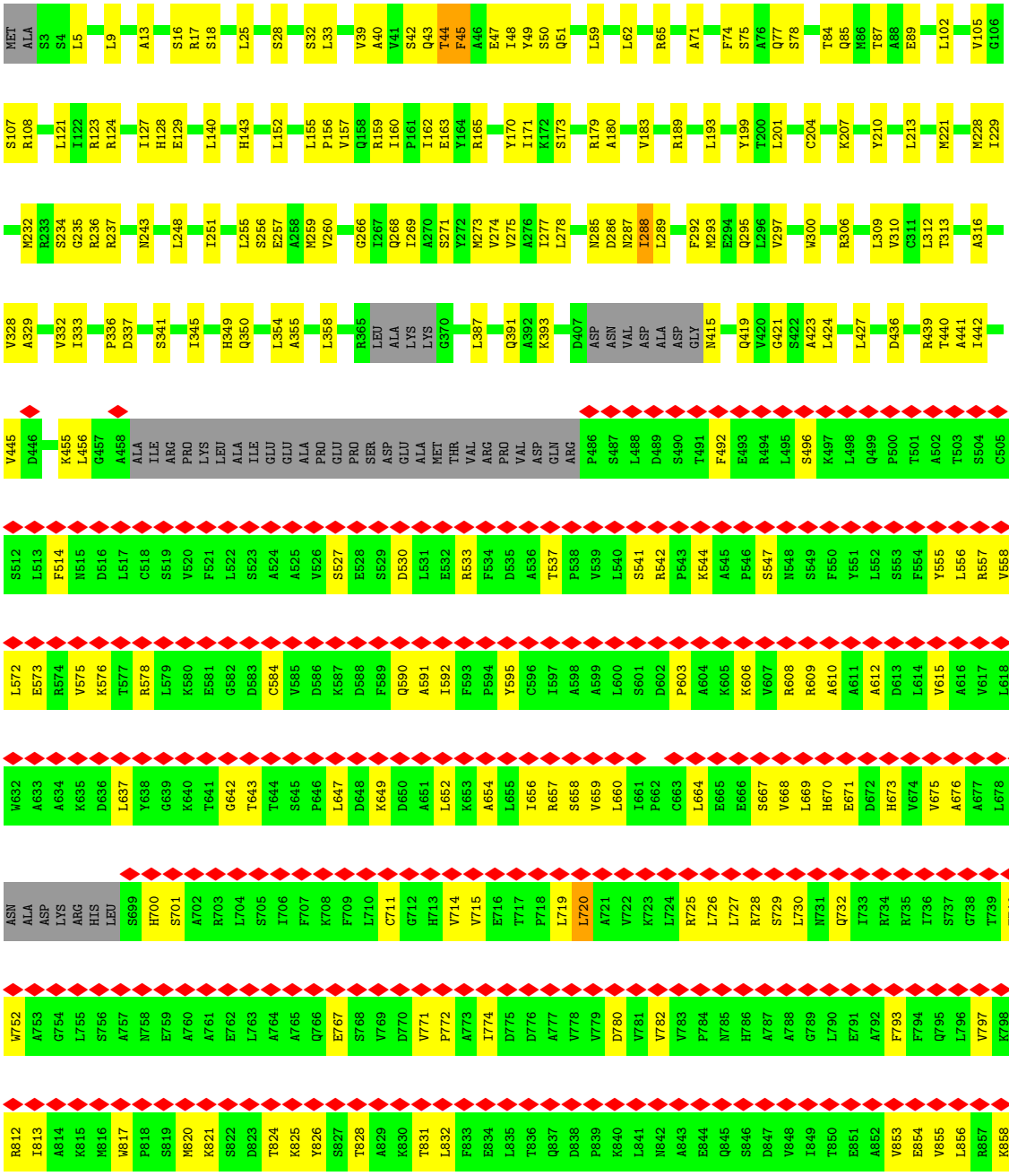
Chain UG:

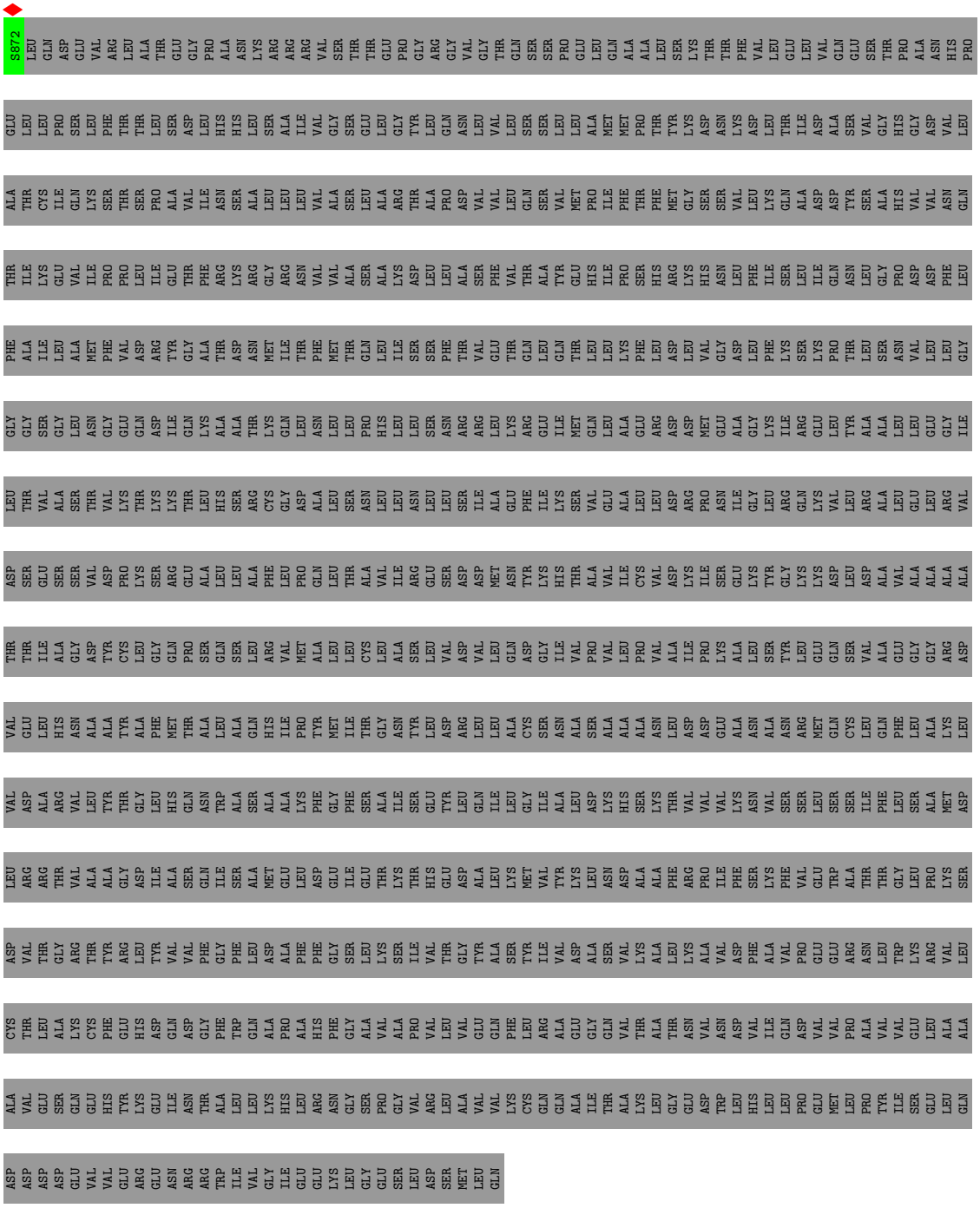





• Molecule 7: Utp10

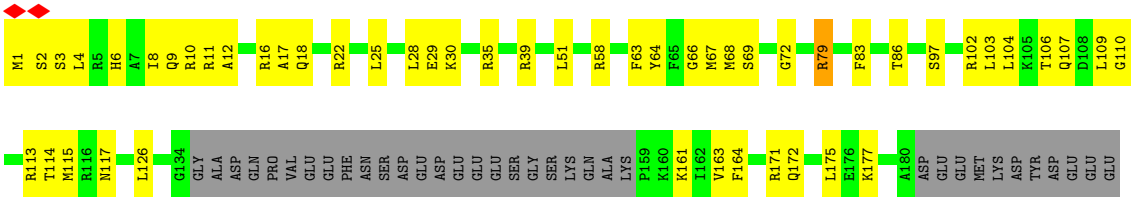


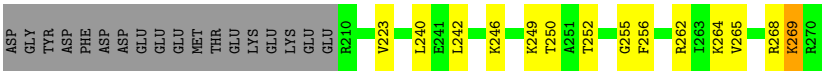






• Molecule 8: U3 small nucleolar RNA-associated protein 11

Chain UK:

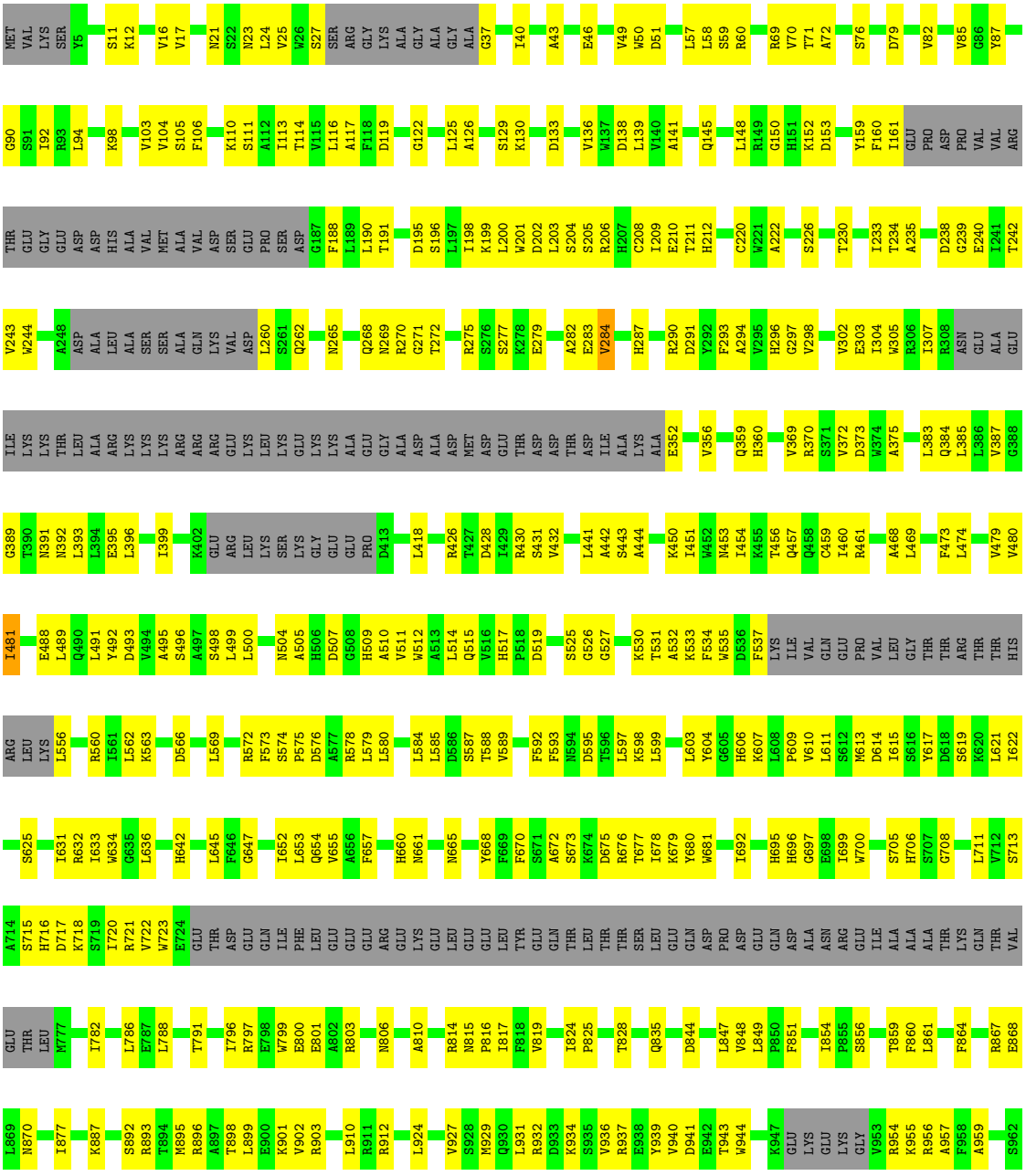




• Molecule 9: Utp12

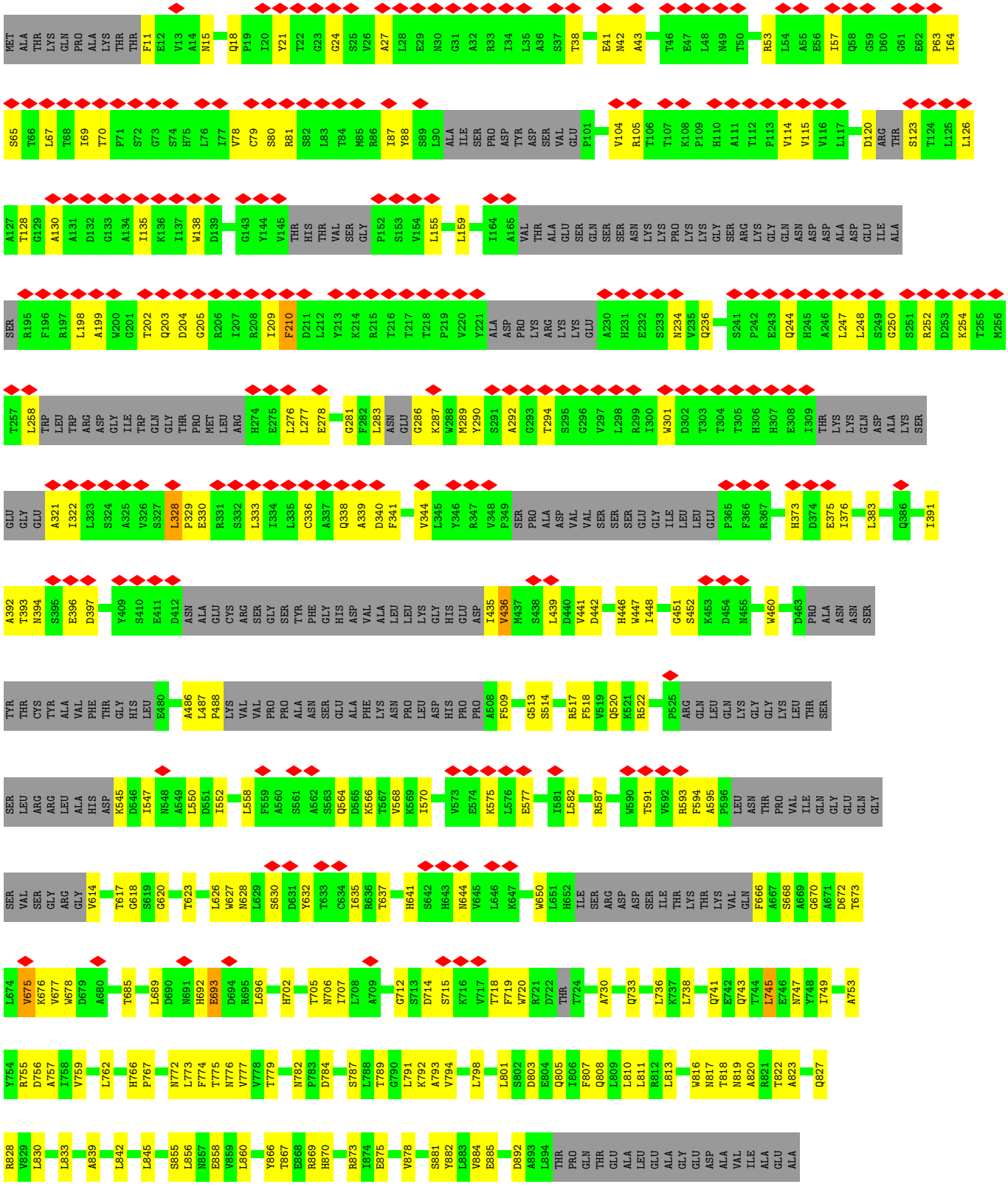
Chain UL:



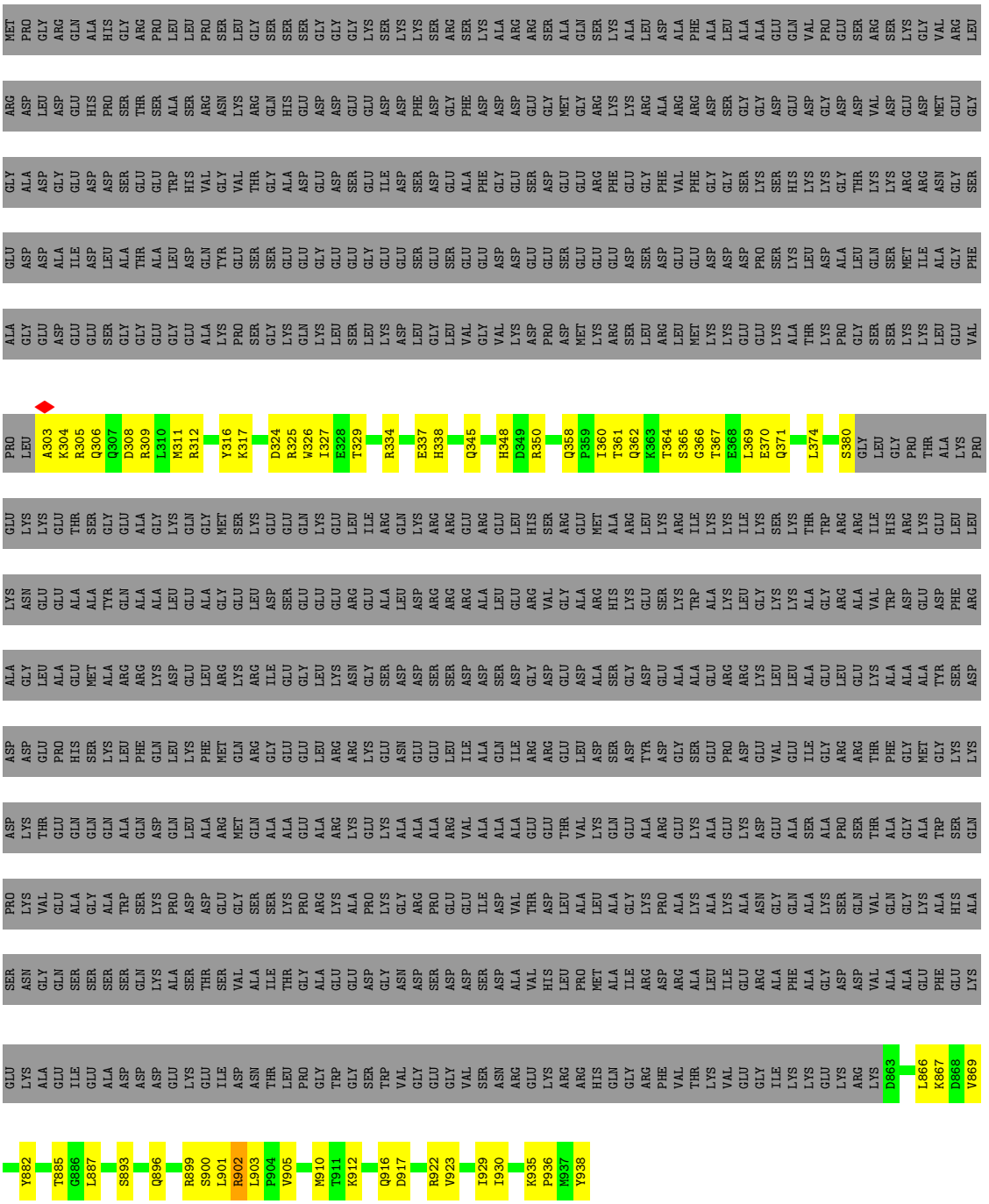
• Molecule 10: Utp13

Chain UM:



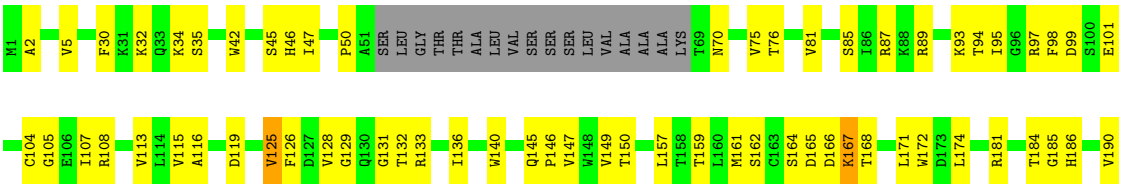
• Molecule 11: Utp14

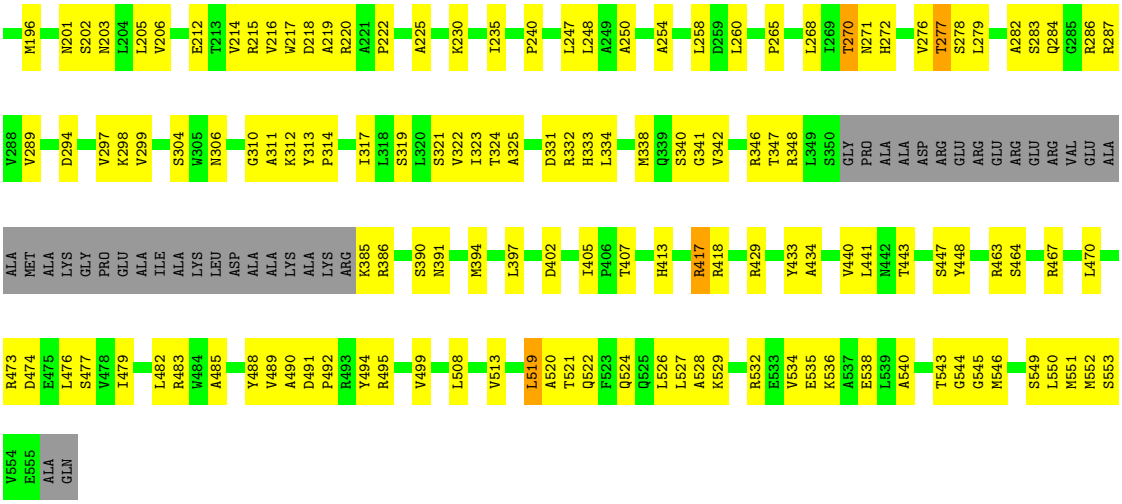
Chain UN: 10% 6% 84%



• Molecule 12: Utp15

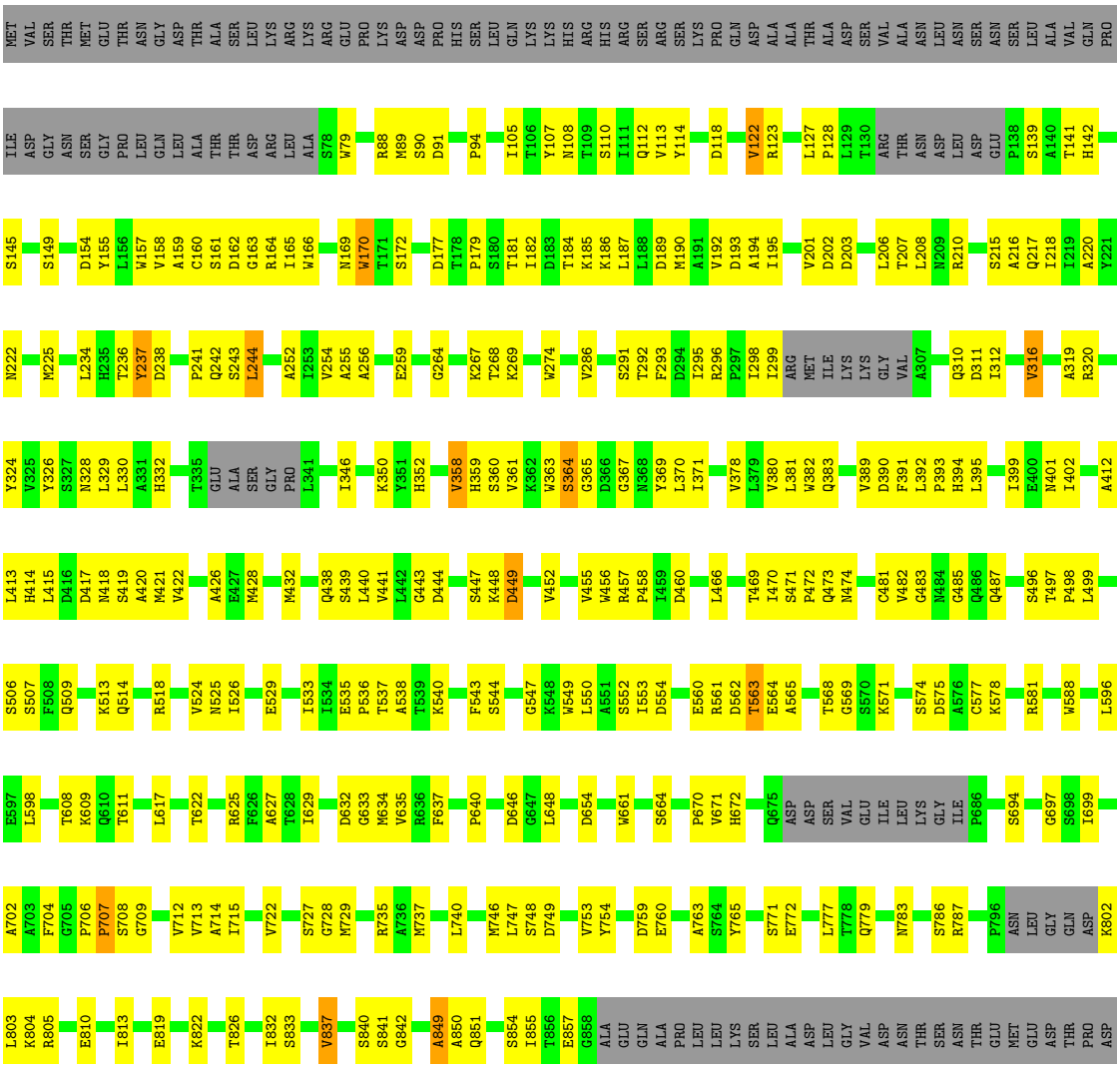
Chain UO:

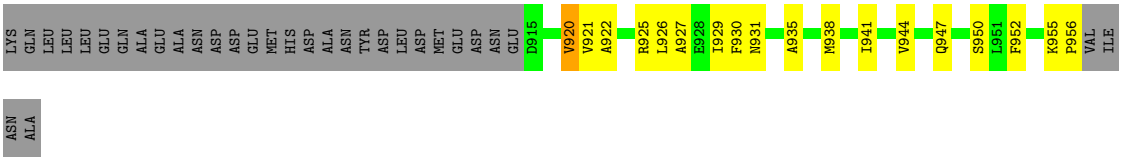




• Molecule 13: Utp17

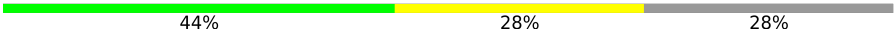
Chain UQ:

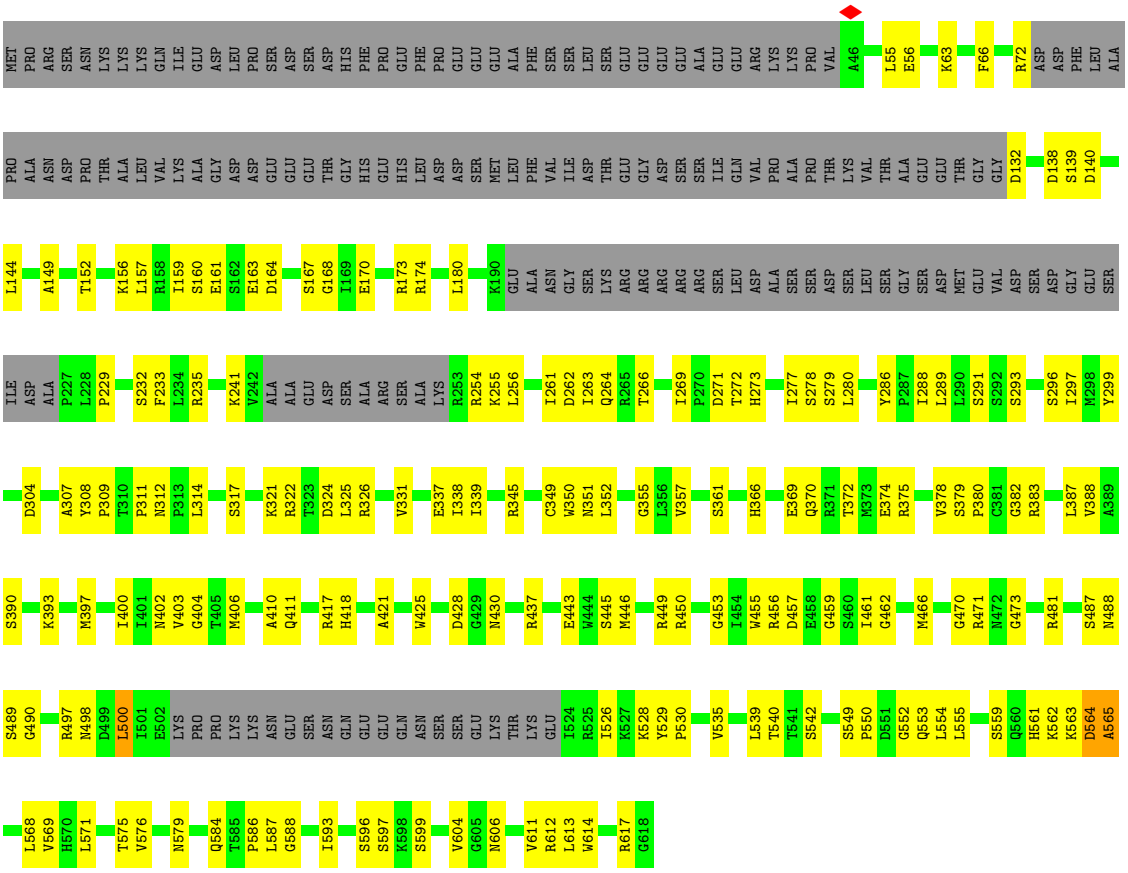





• Molecule 14: Utp18

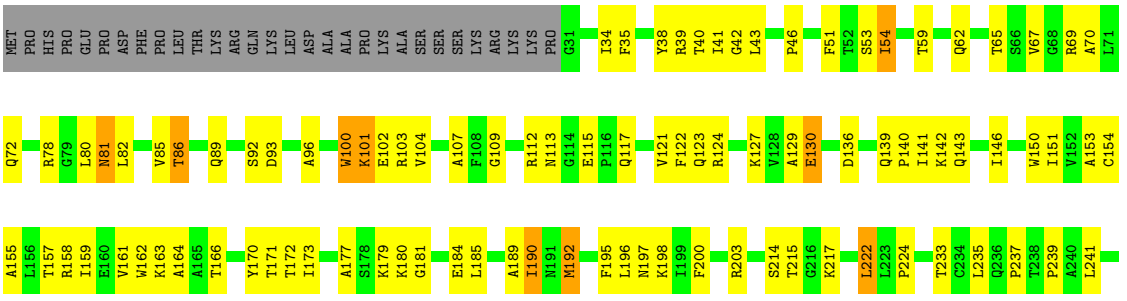
Chain UR:

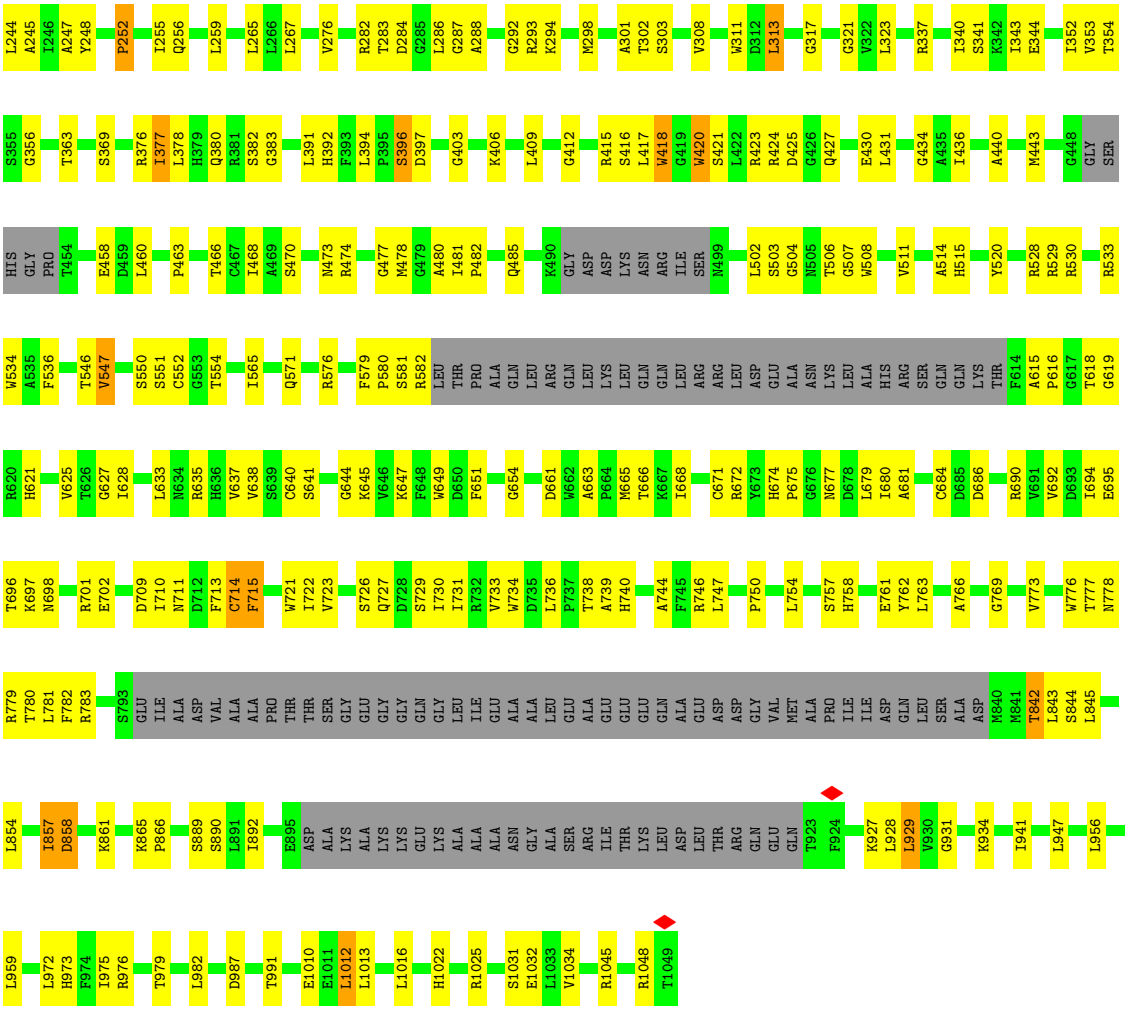



• Molecule 15: Utp21

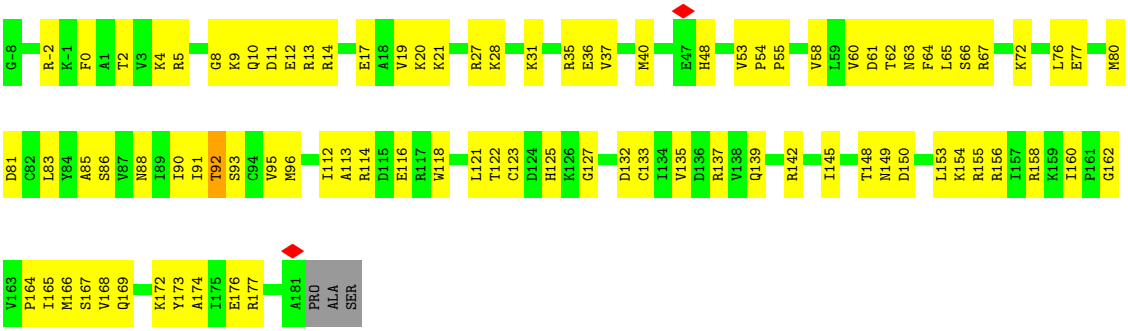
Chain UU:





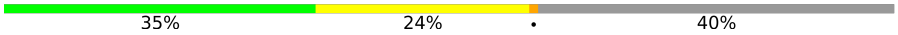
• Molecule 16: Utp24

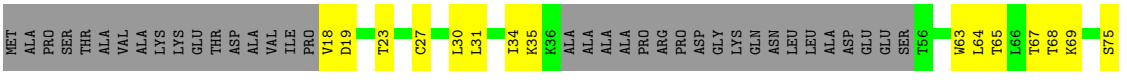
Chain UX:

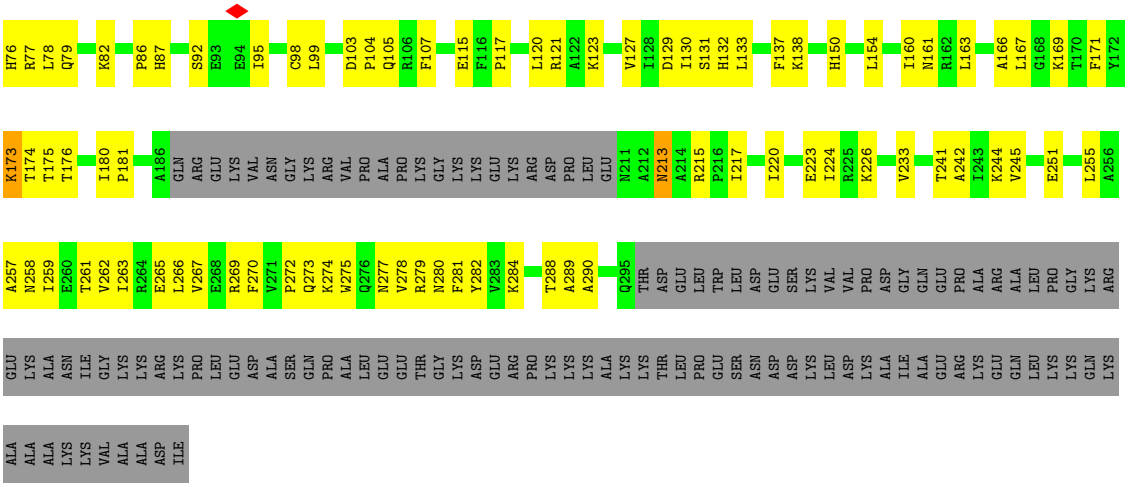


• Molecule 17: Utp30

Chain UZ:

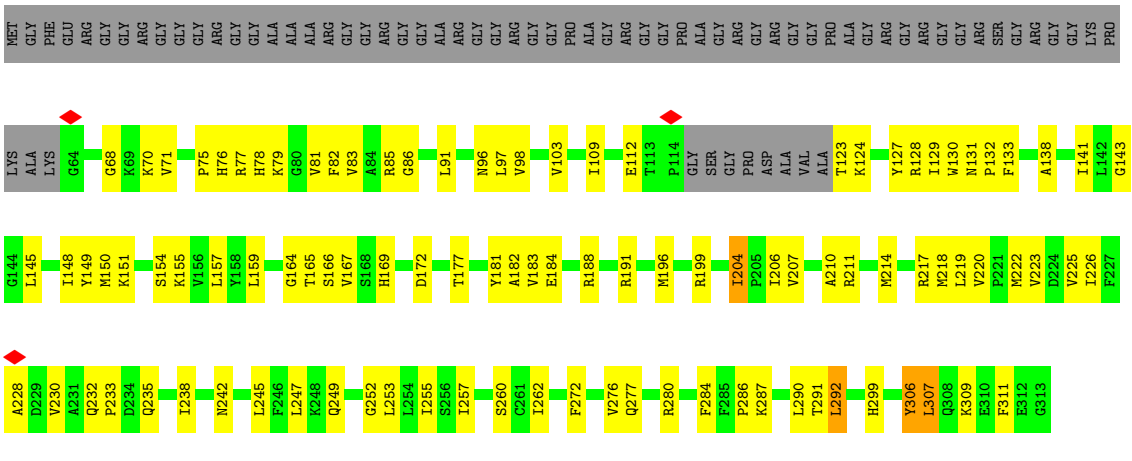




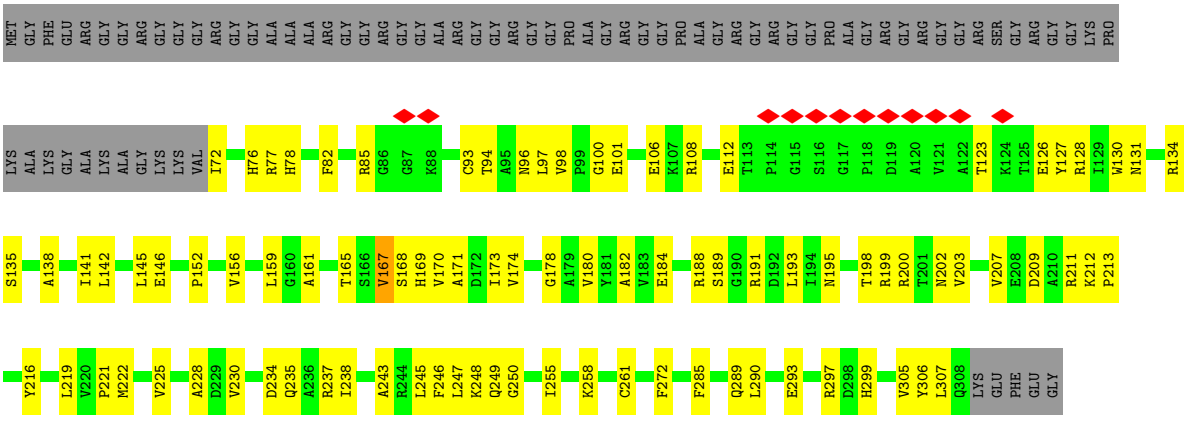
• Molecule 18: Nop1

Chain CA:



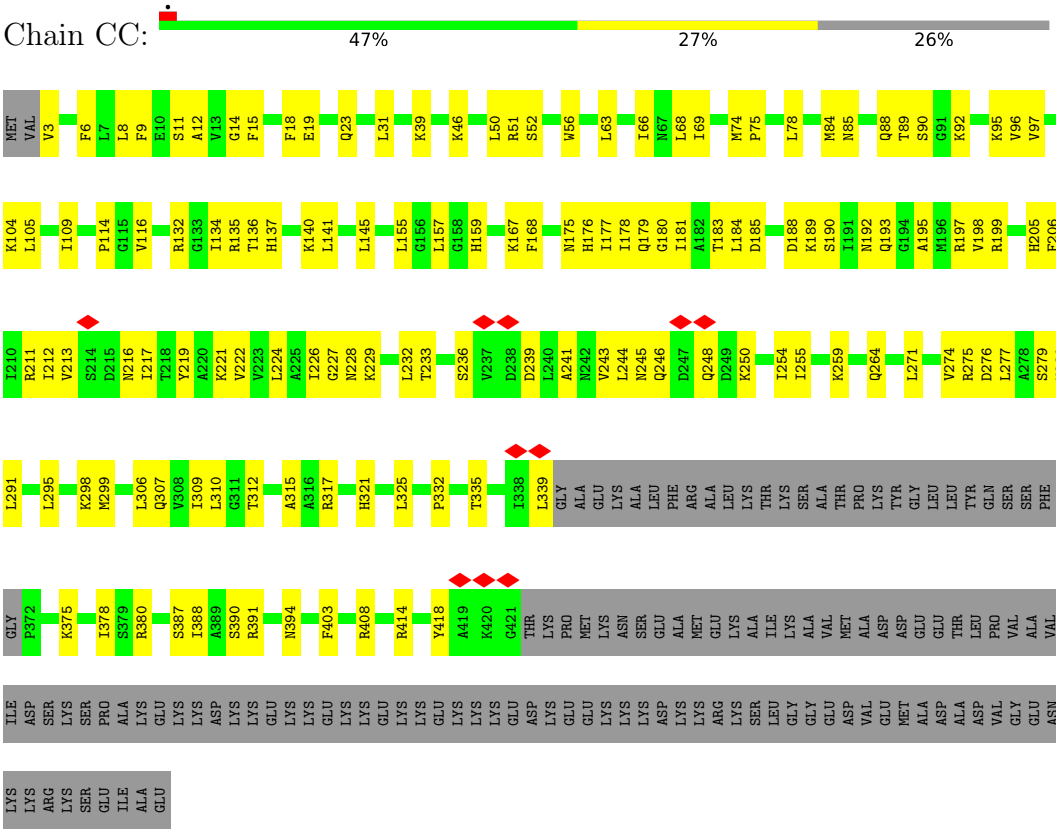
• Molecule 18: Nop1

Chain CB:



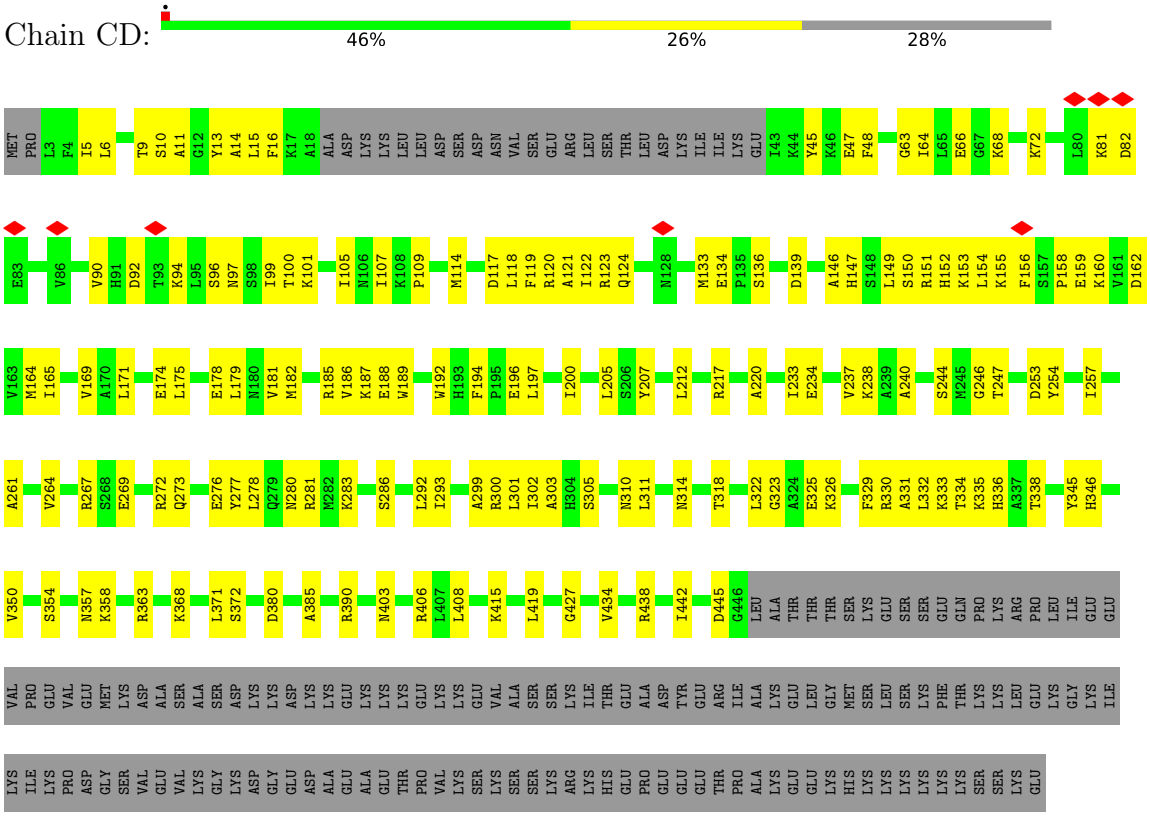
• Molecule 19: Nop56

Chain CC:



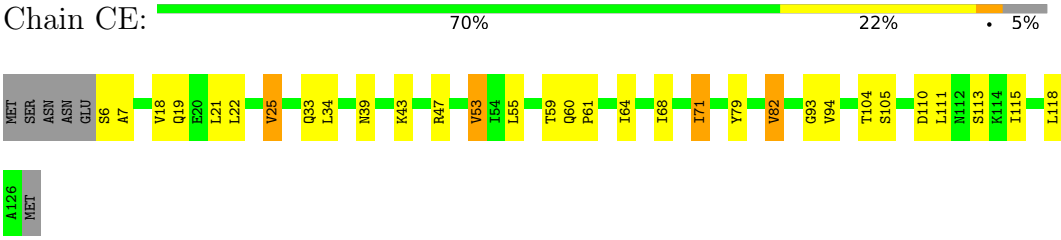

• Molecule 20: Nop58

Chain CD:



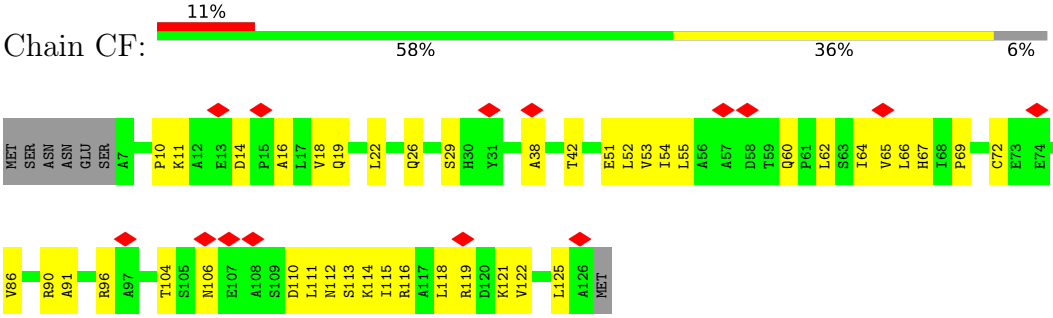
• Molecule 21: Snu13

Chain CE:



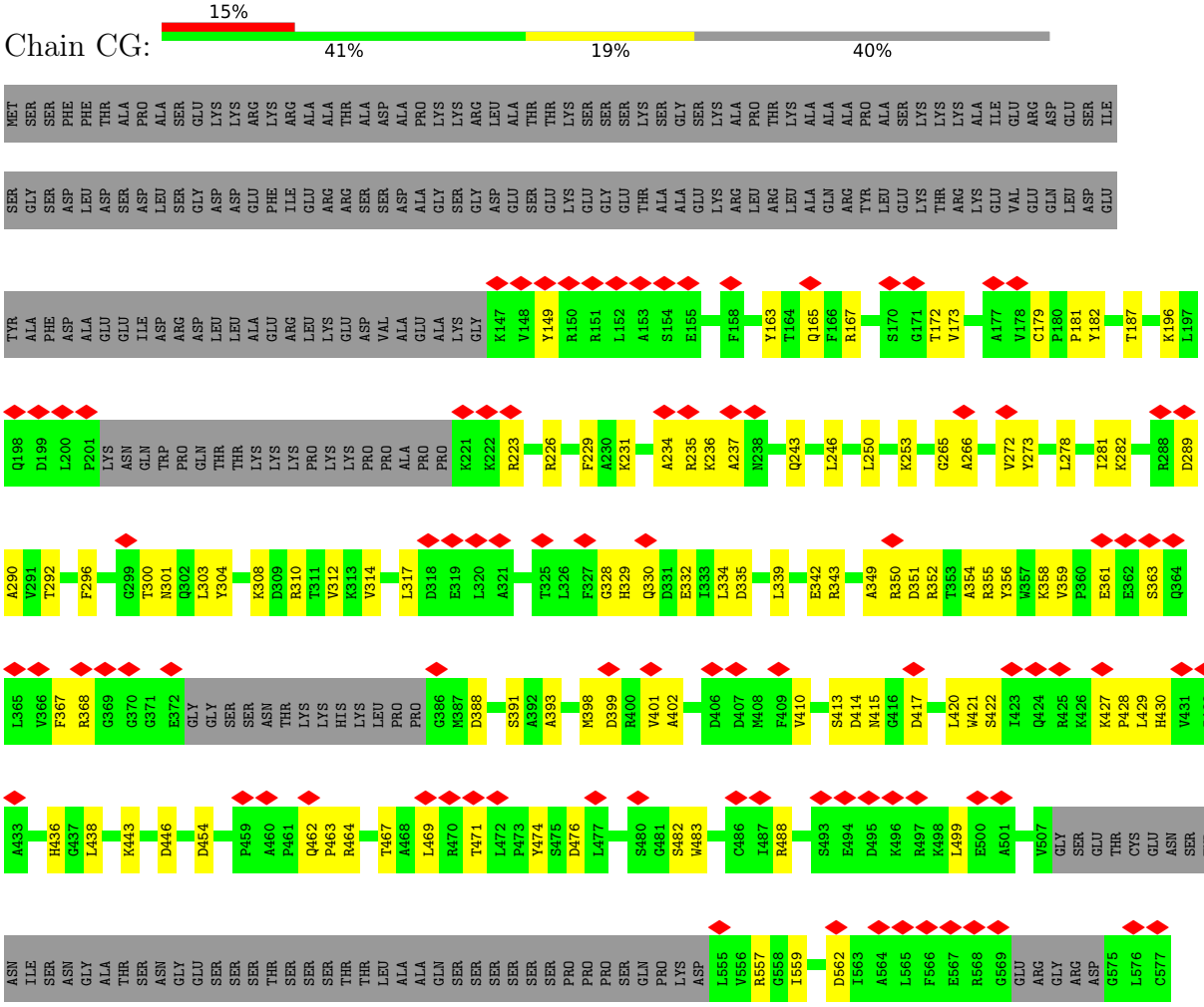

• Molecule 21: Snu13

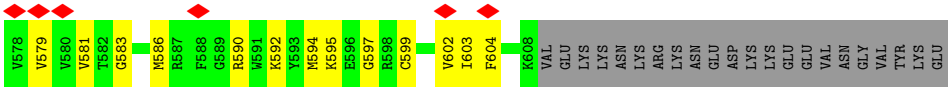
Chain CF:




• Molecule 22: Rrp9

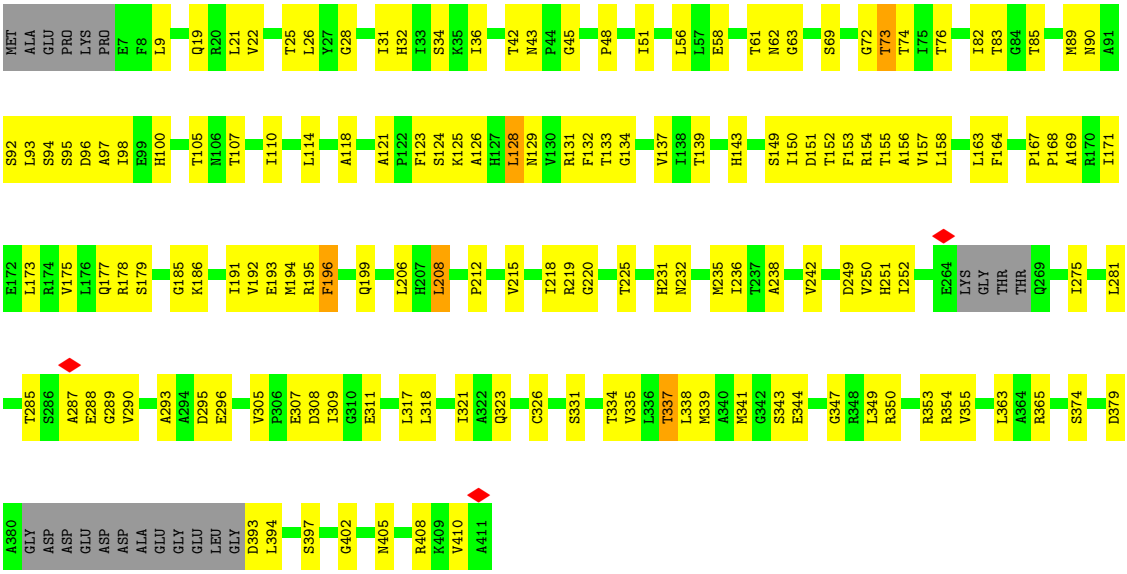
Chain CG:





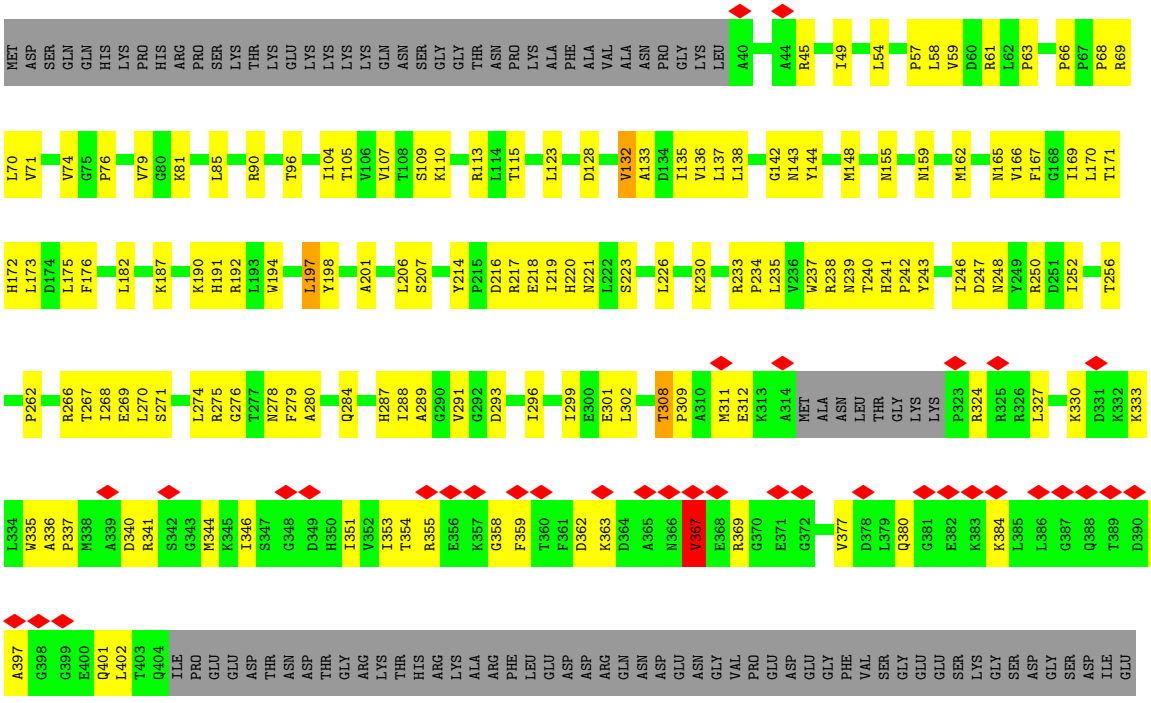

• Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

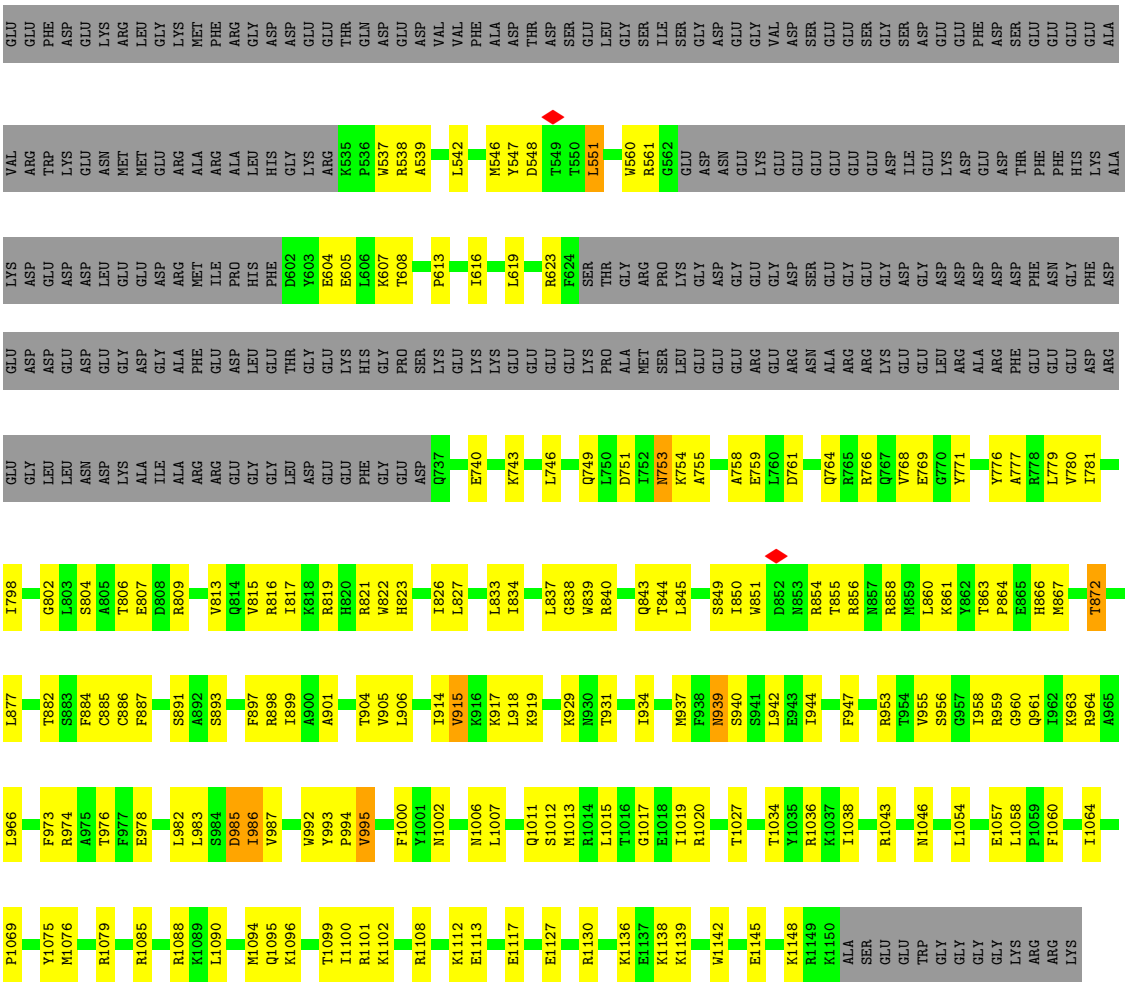
Chain CH:




• Molecule 24: Bms1

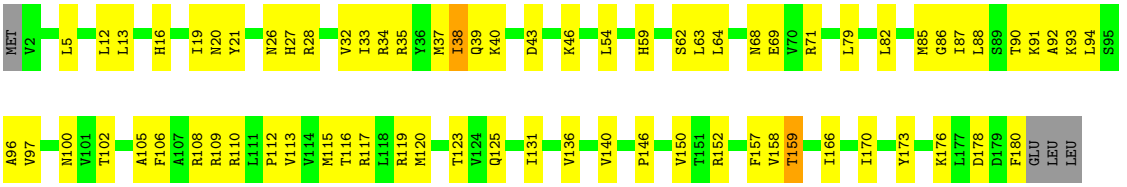
Chain CI:





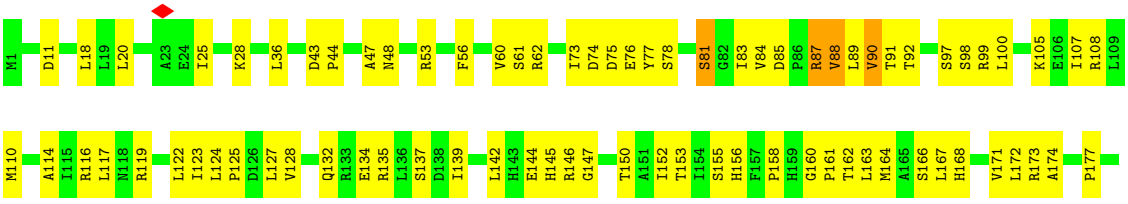
• Molecule 25: Imp3

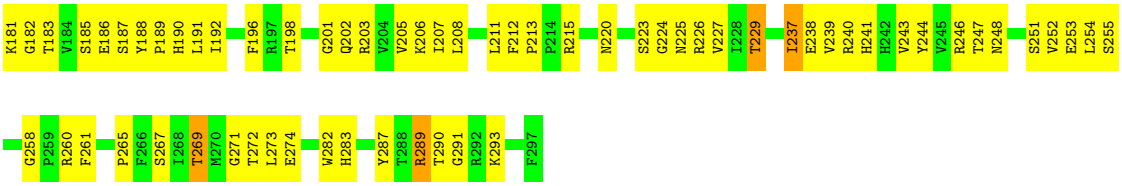
Chain CJ:



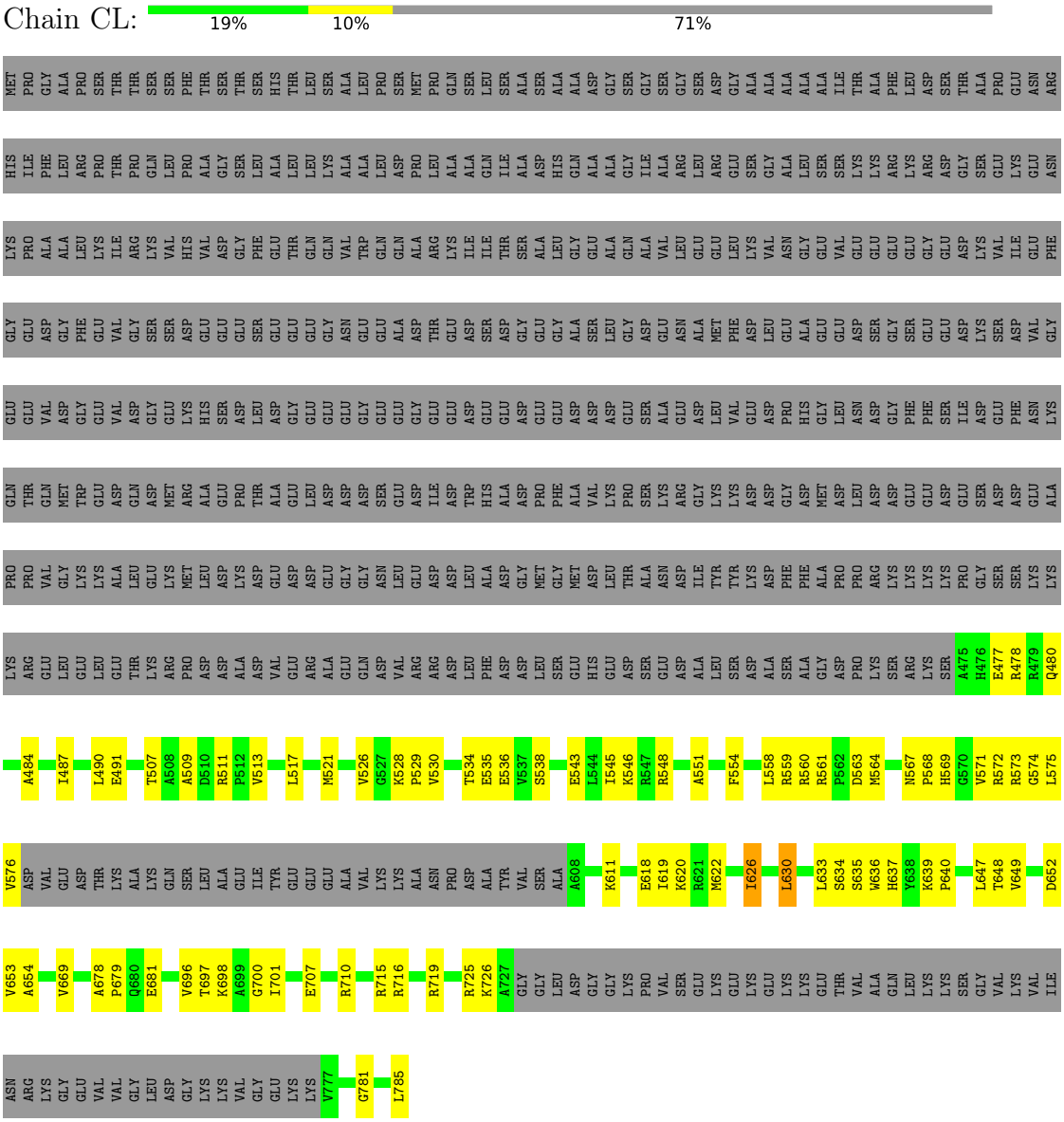
• Molecule 26: Imp4

Chain CK:

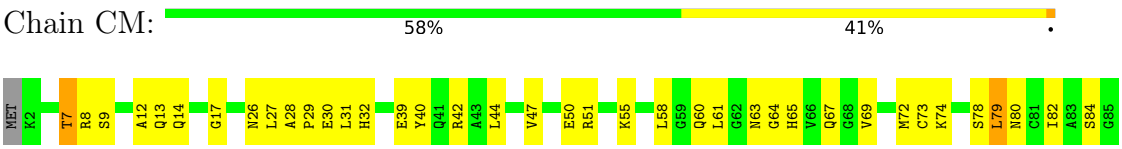


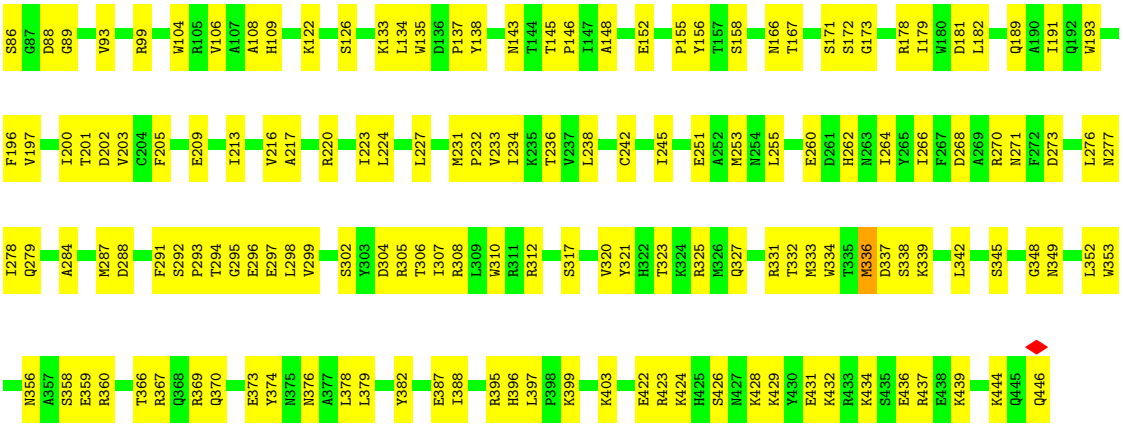



• Molecule 27: Mpp10



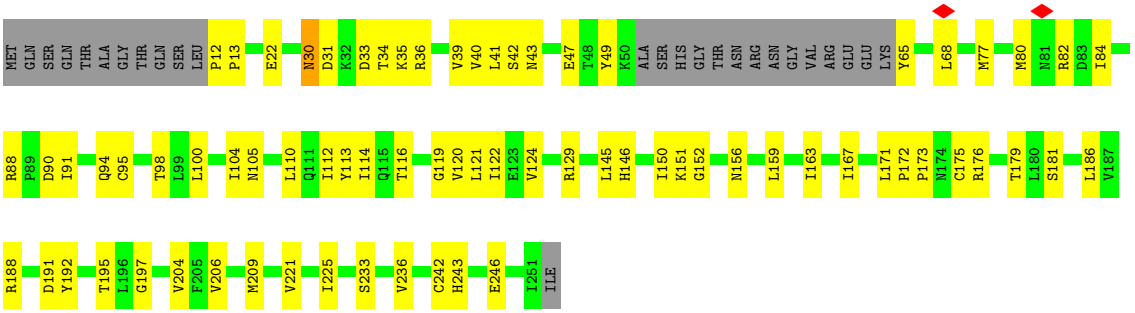

• Molecule 28: Sof1





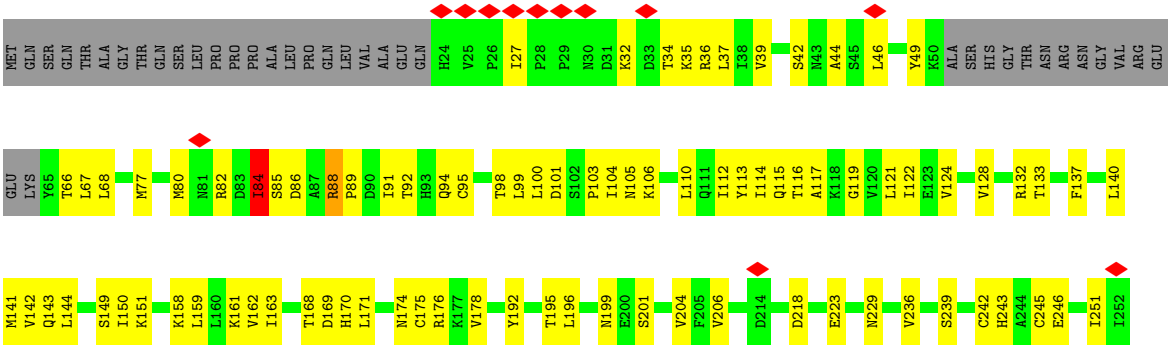
• Molecule 29: Emg1

Chain CN:



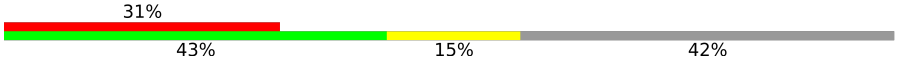
• Molecule 29: Emg1

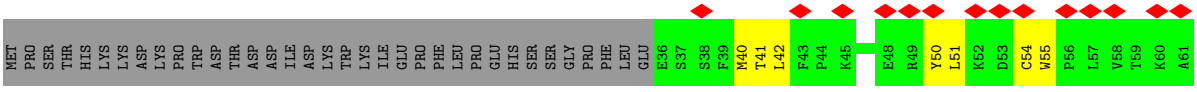
Chain CO:

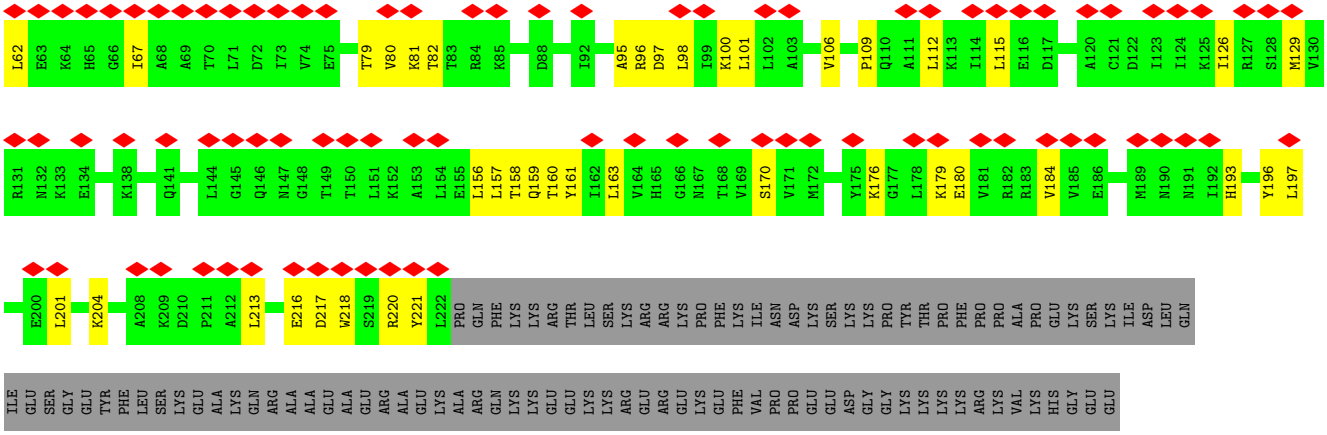


• Molecule 30: KRR1 small subunit processome component

Chain CP:







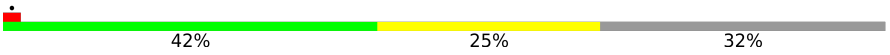


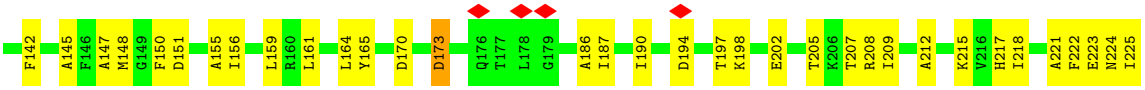


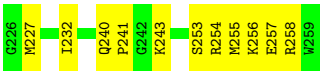


• Molecule 31: Pre-rRNA-processing protein PNO1

Chain CQ:

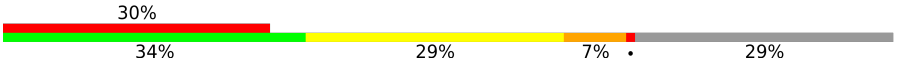


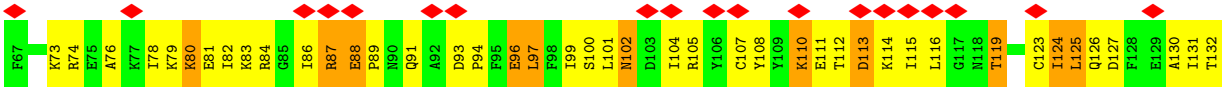


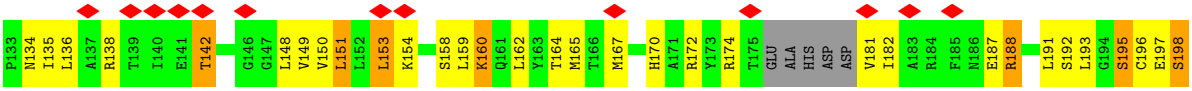


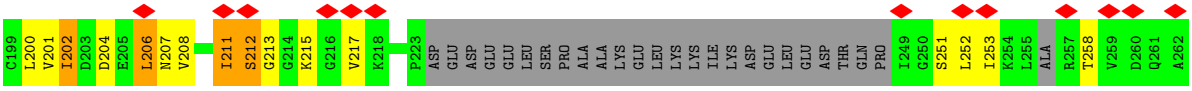
• Molecule 32: Kre33

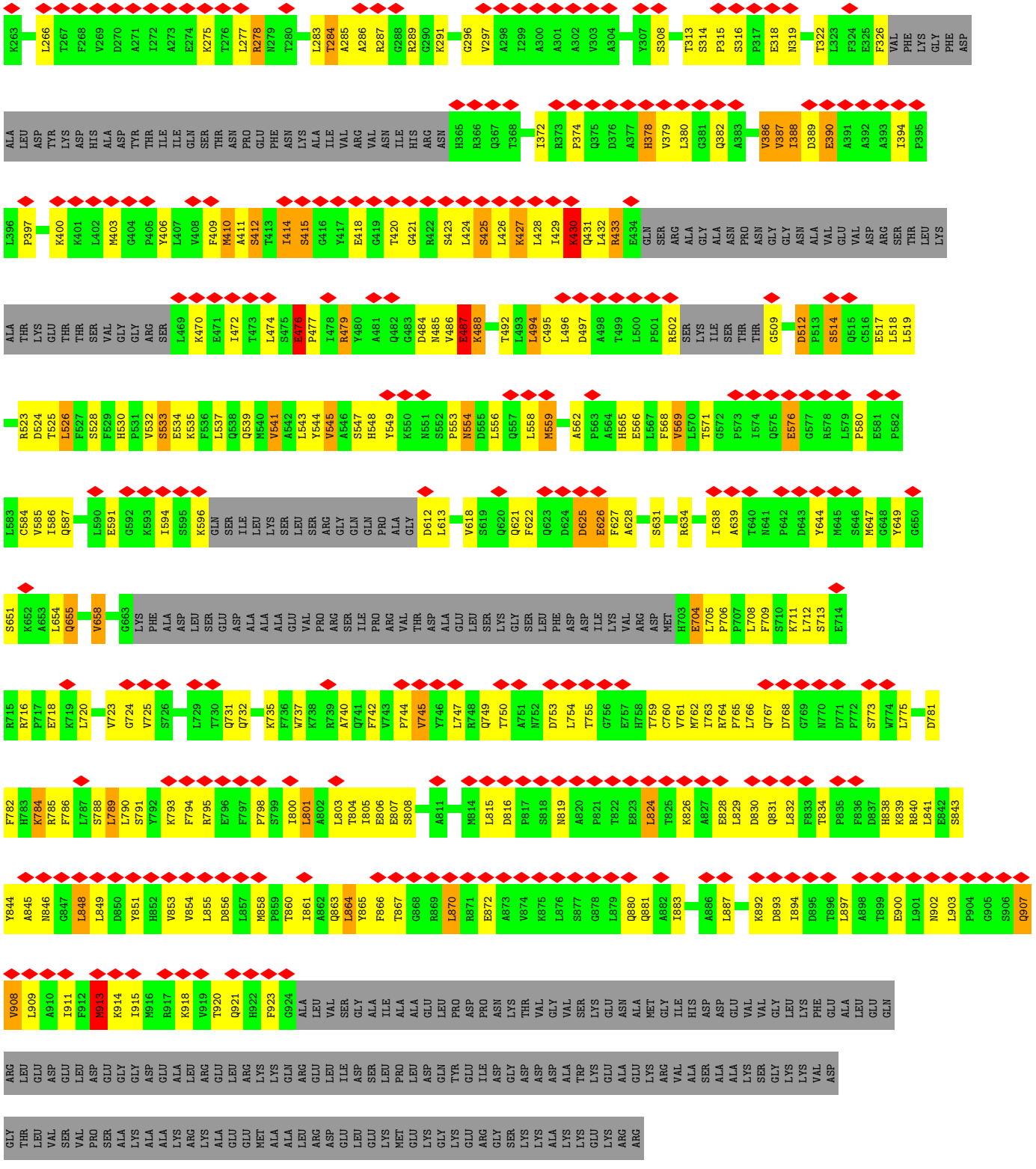
Chain CR:



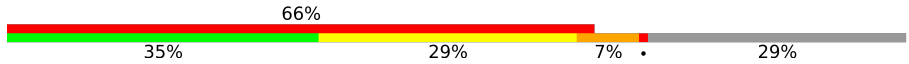


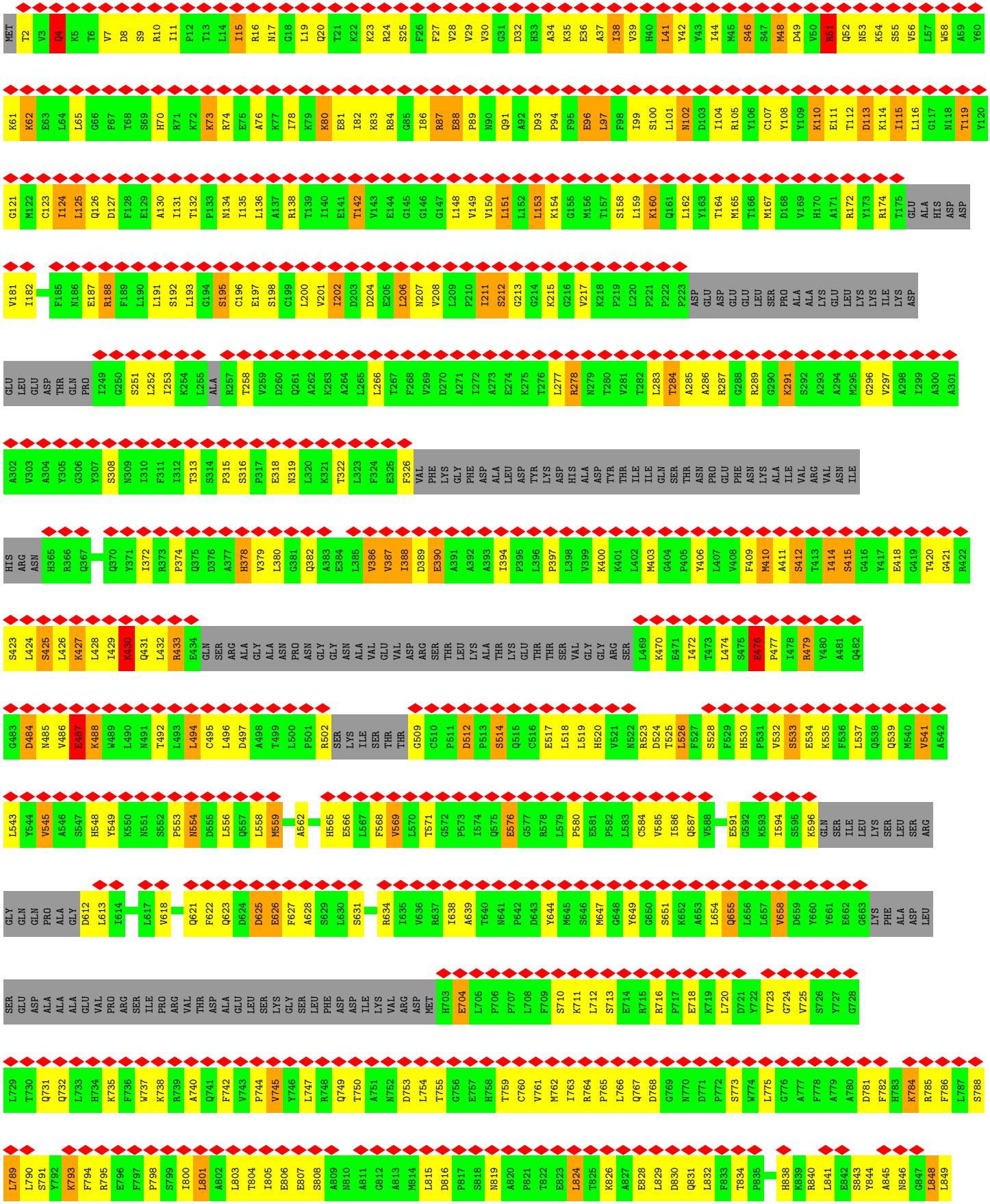






- Molecule 32: Kre33

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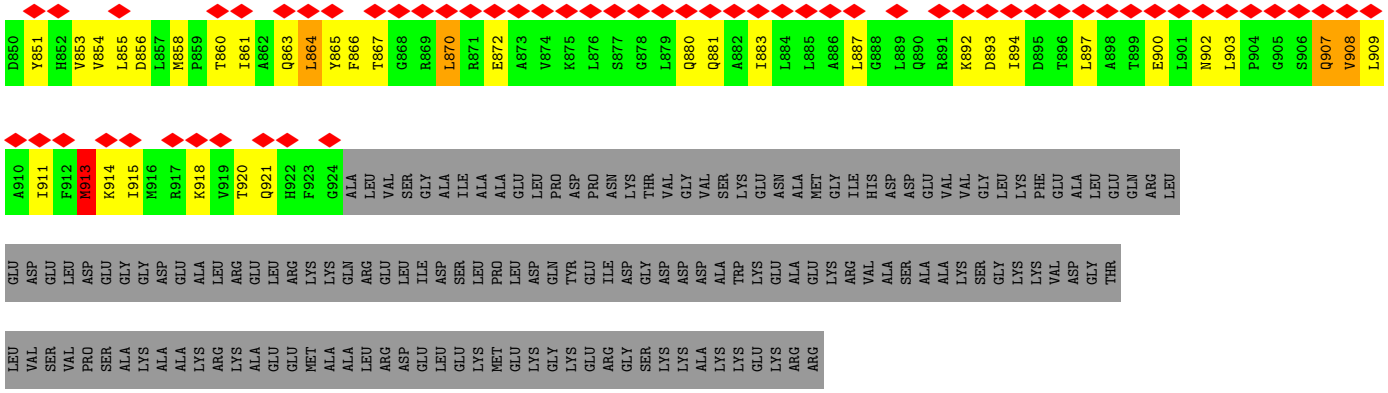
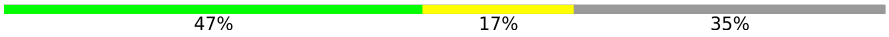
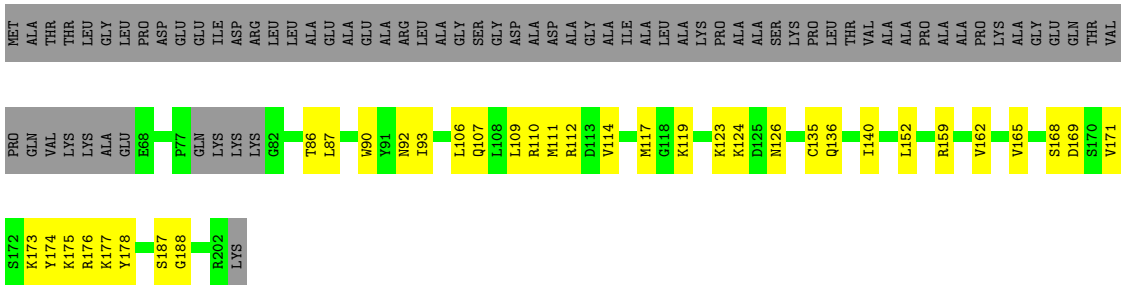
K61 K62 E63 L64 L65 G66 F67 T68 S69 H70 R71 K72 K73 R74 E75 A76 K77 I78 K79 K80 E81 I82 K83 R84 G85 I86 R87 E88 P89 N90 Q91 A92 D93 P94 F95 E96 L97 F98 I99 S100 L101 N102 D103 I104 R105 Y106 C107 Y108 Y109 K110 E111 T112 D113 K114 I115 L116 G117 N118 T119 Y120
G121 M122 C123 I124 L125 Q126 D127 F128 E129 A130 I131 T132 P133 N134 I135 L136 A137 R138 T139 I140 E141 T142 V143 E144 G145 G146 G147 L148 V149 V150 L151 L152 L153 K154 G155 M156 T157 S158 L159 K160 Q161 L162 Y163 T164 M165 T166 M167 D168 V169 H170 A171 R172 Y173 R174 T175 GLU ALA HIS ASP ASP
V181 I182 F185 N186 E187 R188 F189 L190 L191 S192 L193 G194 S195 C196 E197 S198 C199 L200 V201 I202 D203 D204 E205 L206 N207 V208 L209 P210 I211 S212 G213 G214 K215 G216 V217 K218 P219 L220 P221 P222 P223 ASP GLU ASP GLU GLU LEU SER PRO ALA ALA LYS GLU LEU LYS LYS ILE LYS ASP
GLU LEU GLU ASP THR GLN PRO T249 G250 S251 L252 I253 K254 L255 ALA R257 T258 V259 D260 Q261 A262 K263 A264 L265 L266 T267 F268 V269 D270 A271 I272 A273 E274 K275 T276 L277 R278 N279 T280 V281 T282 L283 T284 A285 A286 R287 G288 R289 G290 K291 S292 A293 A294 M295 G296 V297 A298 I299 A300 A301
A302 V303 A304 Y305 G306 Y307 S308 N309 I310 F311 I312 T313 S314 P315 S316 P317 E318 N319 L320 K321 T322 L323 F324 E325 F326 VAL PHE LYS GLY PHE ASP ALA LEU ASP TYR LYS ASP HIS ALA ASP TYR THR ILE ILE GLN SER THR ASN PRO GLU PHE ASN LYS ALA ILE VAL ARG VAL ASN ILE
HIS ARG ASN H365 R366 Q367 Q370 Y371 I372 R373 P374 Q375 D376 A377 H378 V379 L380 G381 Q382 A383 E384 L385 V386 V387 I388 D389 E390 A391 A392 A393 I394 P395 L396 P397 L398 V399 K400 K401 L402 M403 G404 P405 Y406 L407 V408 F409 M410 A411 S412 T413 I414 S415 G416 Y417 E418 G419 T420 G421 R422
S423 L424 S425 L426 K427 L428 I429 K430 Q431 L432 R433 E434 GLN SER ARG ALA GLY ALA ASN PRO ASN GLY GLY ASN ALA VAL GLU VAL ASP ARG SER THR LEU LYS ALA THR LYS GLU THR THR SER VAL GLY GLY ARG SER L469 K470 E471 I472 T473 L474 S475 E476 P477 I478 R479 Y480 A481 Q482
G483 D484 N485 V486 E487 K488 W489 L490 N491 T492 L493 L494 C495 L496 D497 A498 T499 L500 P501 R502 SER LYS ILE SER THR THR G509 C510 P511 D512 P513 S514 Q515 C516 E517 L518 L519 H520 V521 N522 R523 D524 T525 L526 F527 S528 F529 H530 P531 V532 S533 E534 K535 F536 L537 Q538 Q539 M540 V541 A542
L543 Y544 V545 A546 S547 H548 Y549 K550 N551 S552 P553 N554 D555 L556 Q557 L558 M559 A562 H565 E566 L567 F568 V569 L570 T571 G572 P573 I574 Q575 E576 G577 R578 L579 P580 E581 P582 L583 C584 V585 I586 Q587 V588 E591 G592 K593 I594 S595 K596 GLN SER ILE LEU LYS SER LEU SER ARG
GLY GLN GLN PRO ALA GLY D612 L613 I614 L617 V618 Q621 F622 Q623 D624 D625 E626 F627 A628 S629 L630 S631 R634 I635 V636 R637 I638 A639 T640 N641 P642 D643 Y644 M645 S646 M647 G648 Y649 G650 S651 K652 A653 L654 Q655 L656 L657 V658 D659 Y660 Y661 E662 G663 LYS PHE ALA ASP LEU
SER GLU ASP ALA ALA ALA GLU VAL PRO ARG SER ILE PRO ARG VAL THR ASP ALA GLU LEU SER LYS GLY SER LEU PHE ASP ASP ILE LYS VAL ARG ASP MET H703 E704 L705 P706 P707 L708 F709 S710 K711 L712 S713 E714 R715 R716 P717 E718 K719 L720 D721 Y722 V723 G724 V725 S726 Y727 G728
L729 T730 Q731 Q732 L733 H734 K735 F736 W737 K738 R739 A740 Q741 F742 V743 P744 V745 Y746 L747 R748 Q749 T750 A751 N752 D753 L754 T755 G756 E757 H758 T759 C760 V761 M762 I763 R764 P765 L766 Q767 D768 G769 N770 D771 P772 S773 W774 L775 G776 A777 F778 A779 A780 D781 F782 H783 K784 R785 F786 L787 S788
L789 L790 S791 Y792 K793 F794 R795 E796 F797 P798 S799 I800 L801 A802 L803 T804 I805 E806 E807 S808 A809 N810 A811 G812 A813 N814 L815 D816 P817 S818 N819 A820 P821 T822 E823 L824 T825 K826 A827 E828 L829 D830 Q831 L832 F833 T834 P835 H838 K839 R840 L841 E842 S843 Y844 A845 N846 Q847 L848 L849




• Molecule 33: Fcf2

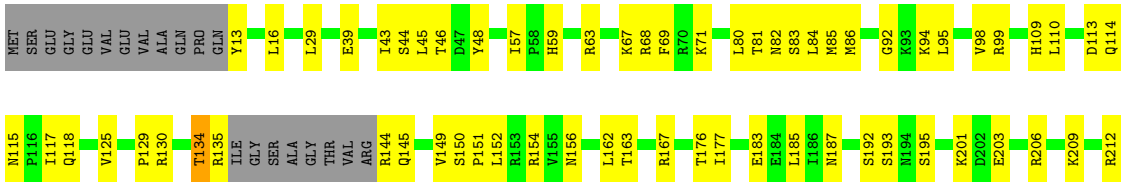
Chain CT:



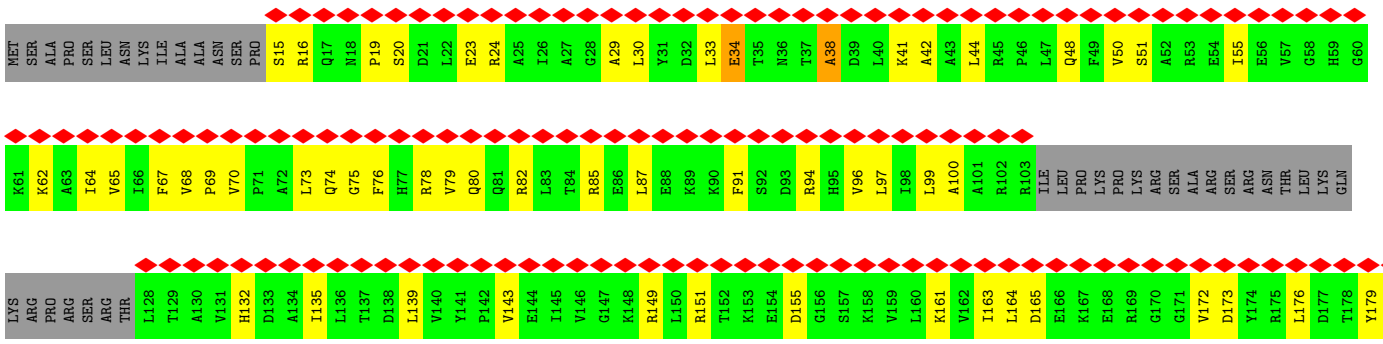

• Molecule 34: 40S ribosomal protein s5-like protein

Chain Cc:



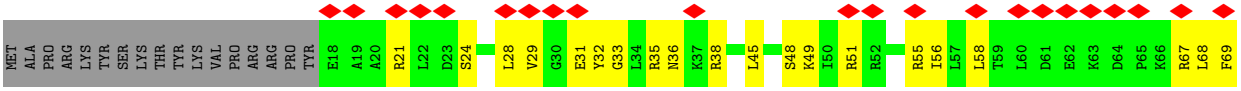

• Molecule 35: 40S ribosomal protein S7

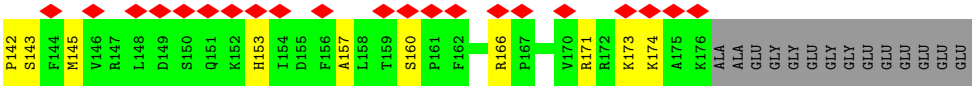
Chain Ce:



• Molecule 36: 40S ribosomal protein s9-like protein

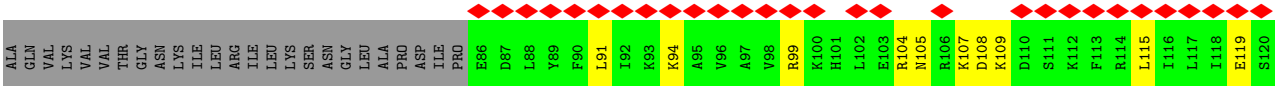
Chain Cg:

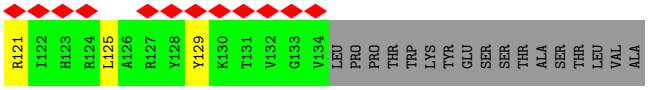





• Molecule 37: 40S ribosomal protein S13-like protein

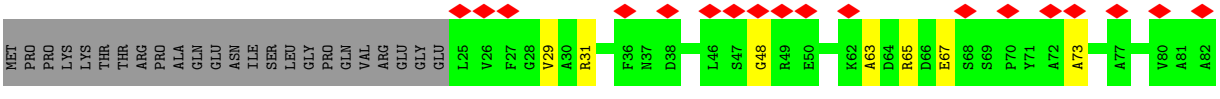
Chain Ch:

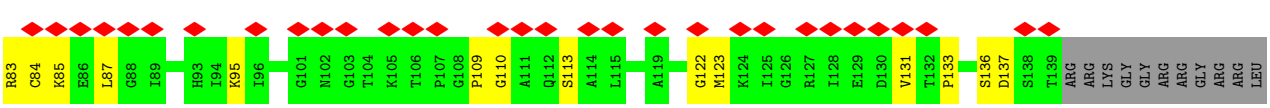



• Molecule 38: 40S ribosomal protein S14-like protein

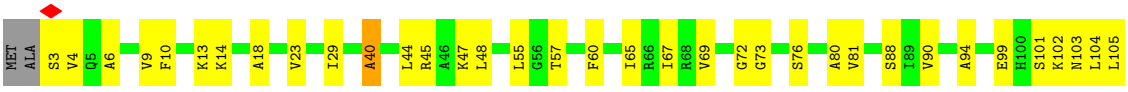
Chain Ci:



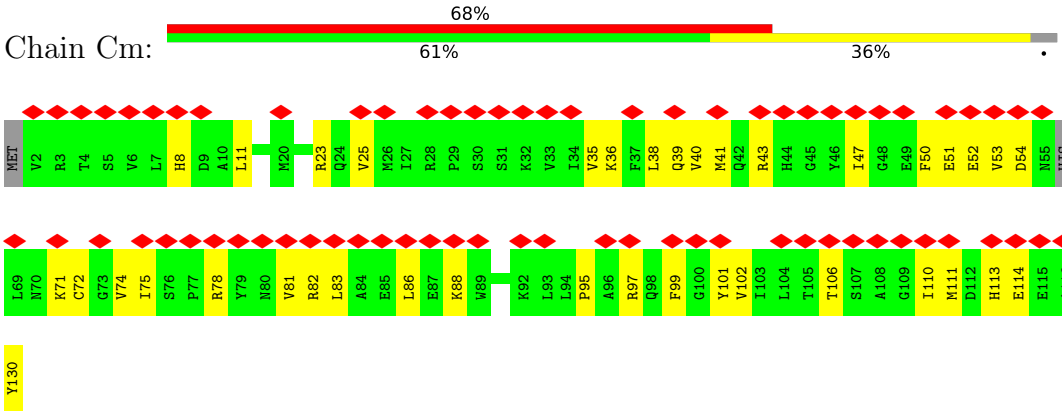

• Molecule 39: 40S ribosomal protein S16-like protein

Chain Cj:



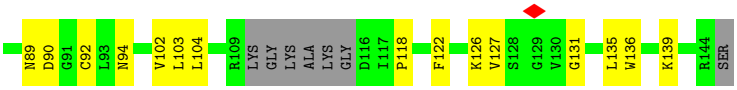
• Molecule 40: 40S ribosomal protein S22-like protein

Chain Cm:




• Molecule 41: 40S ribosomal protein s23-like protein

Chain Cn:

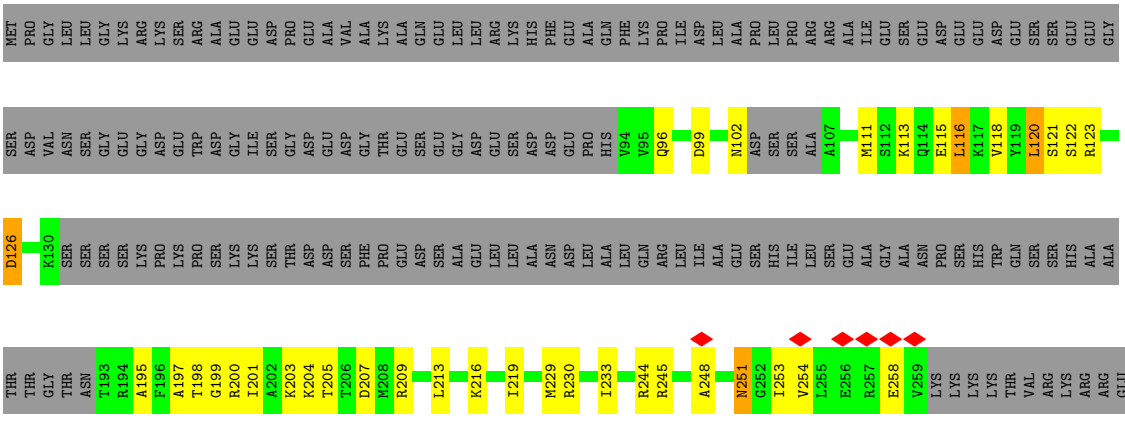


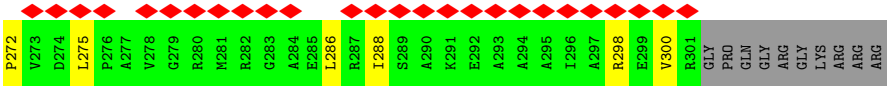

• Molecule 42: 40S ribosomal protein S28-like protein

Chain Cp:

• Molecule 43: Faf1

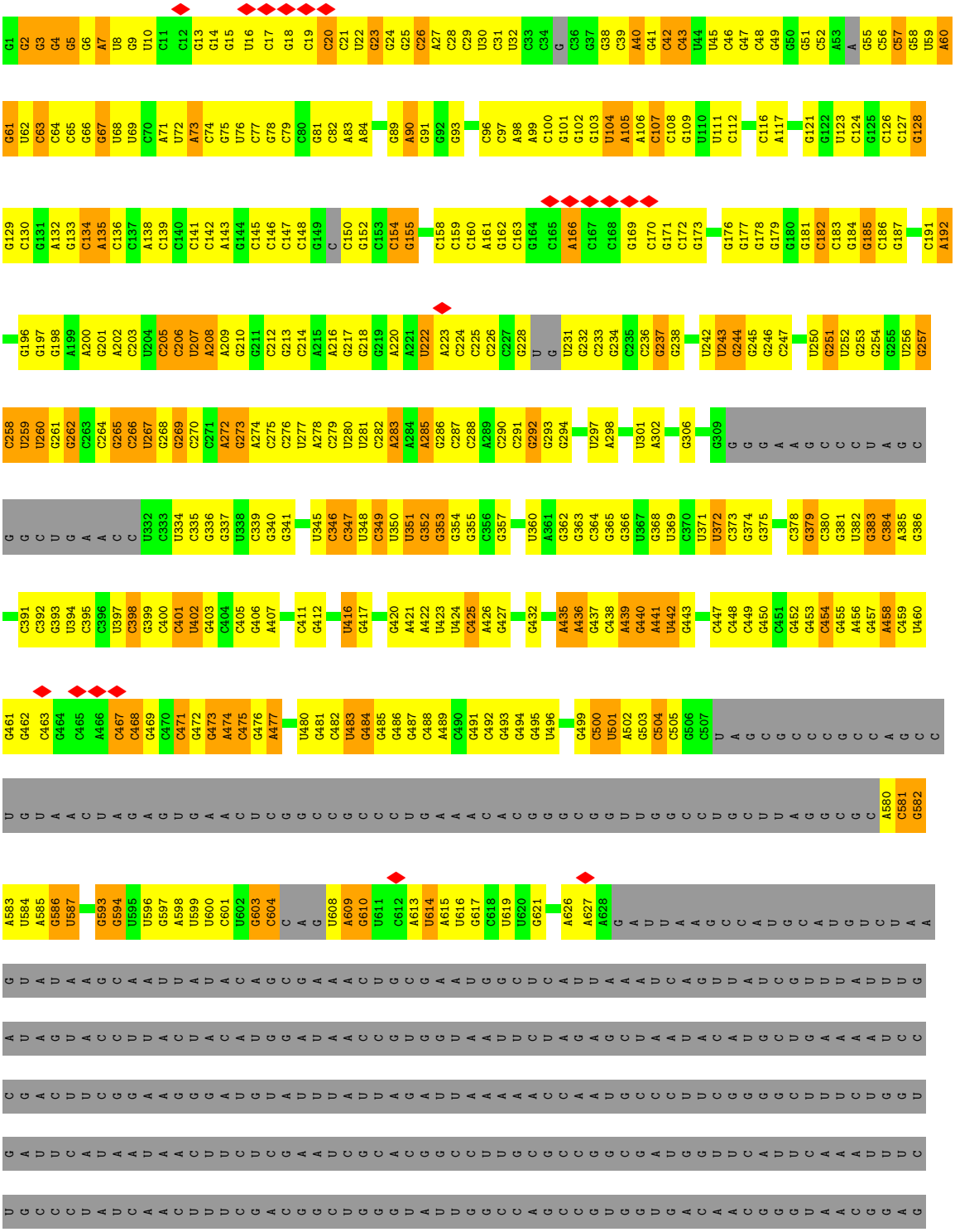
Chain CU:

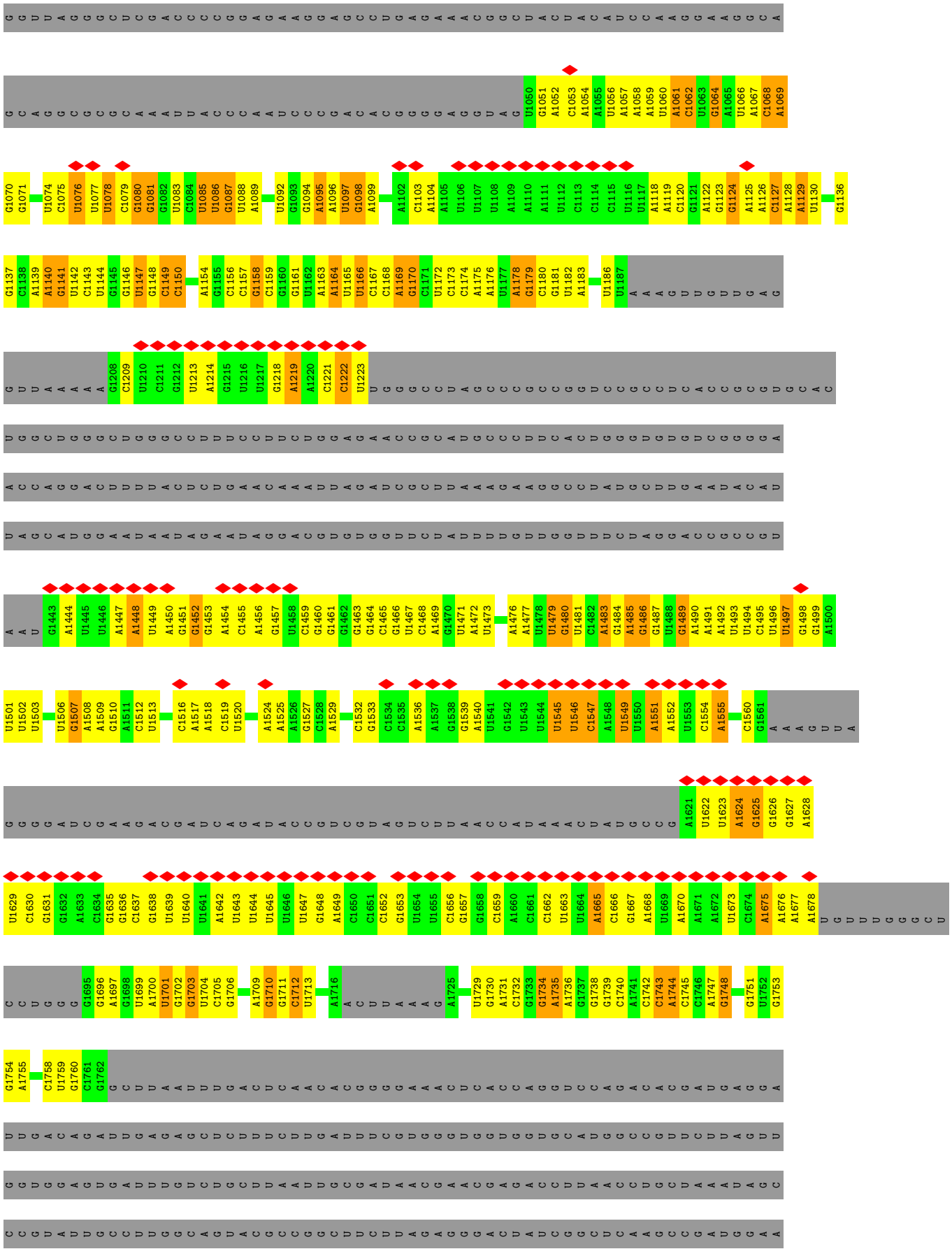


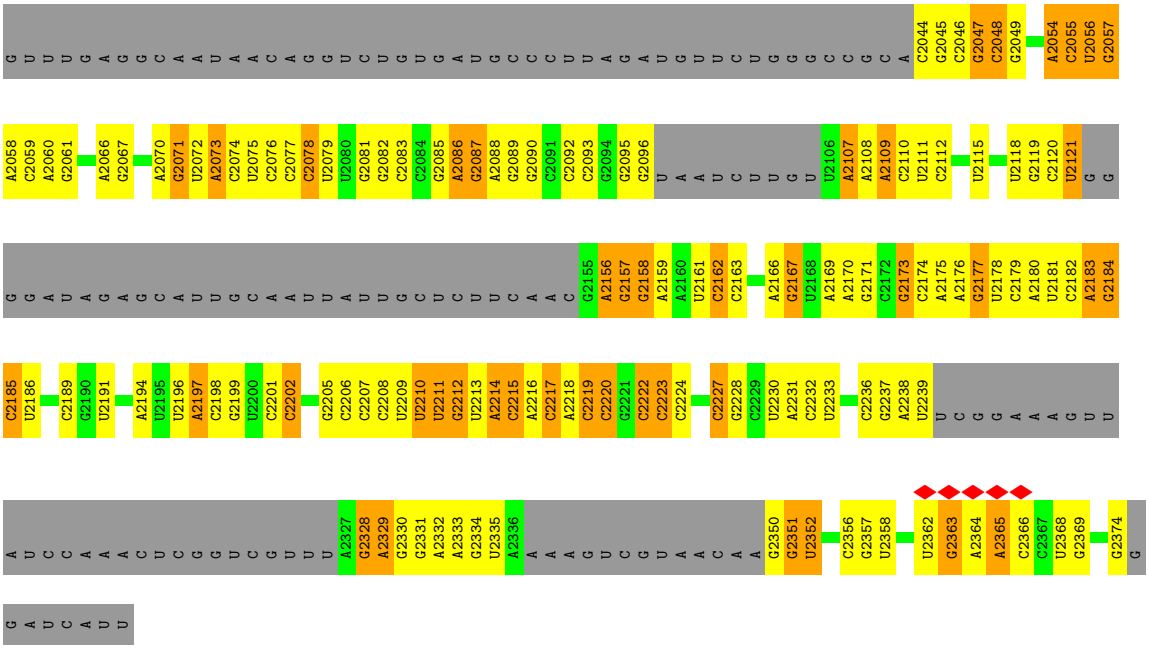


• Molecule 44: 35S rRNA

Chain C1:

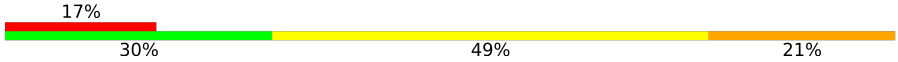


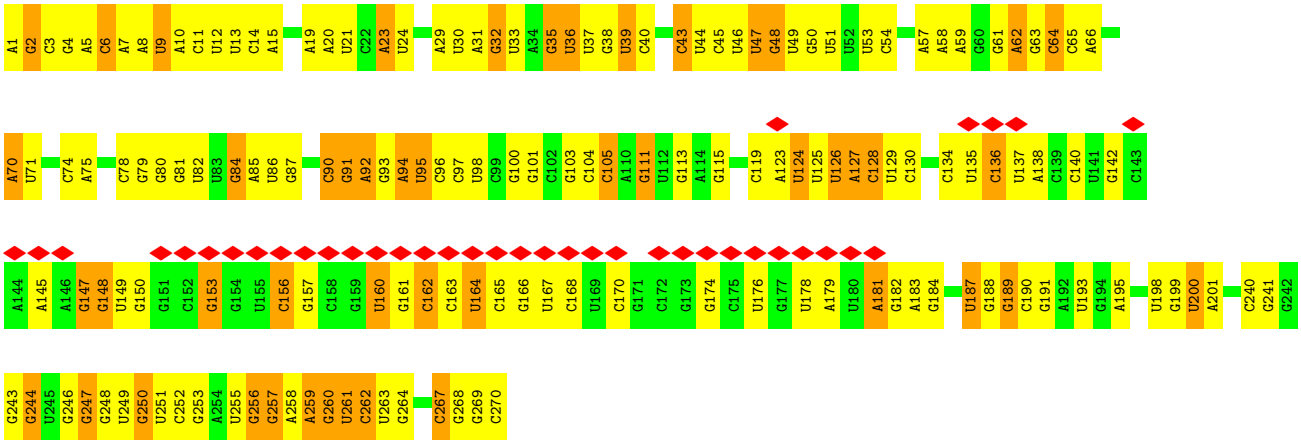




• Molecule 45: U3 snoRNA

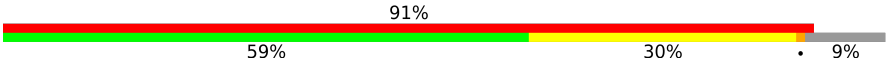
Chain C2:

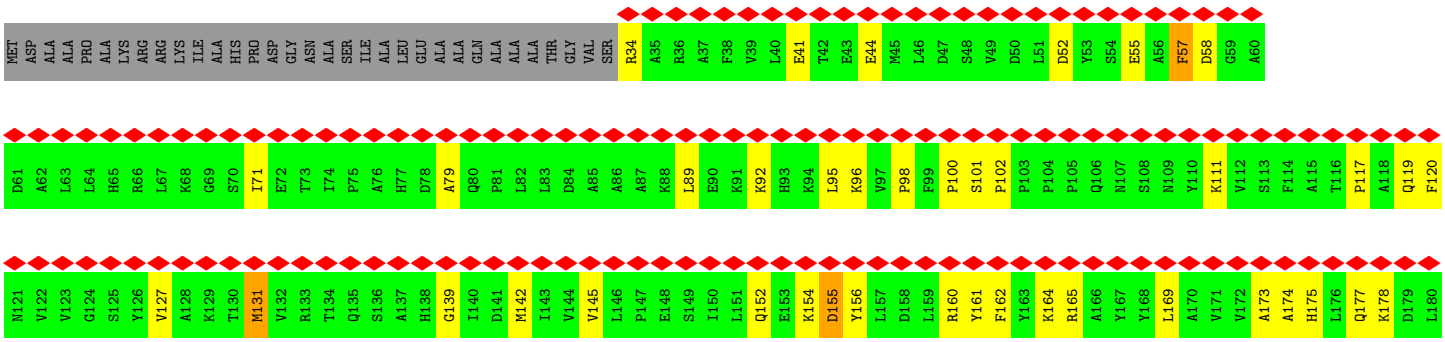


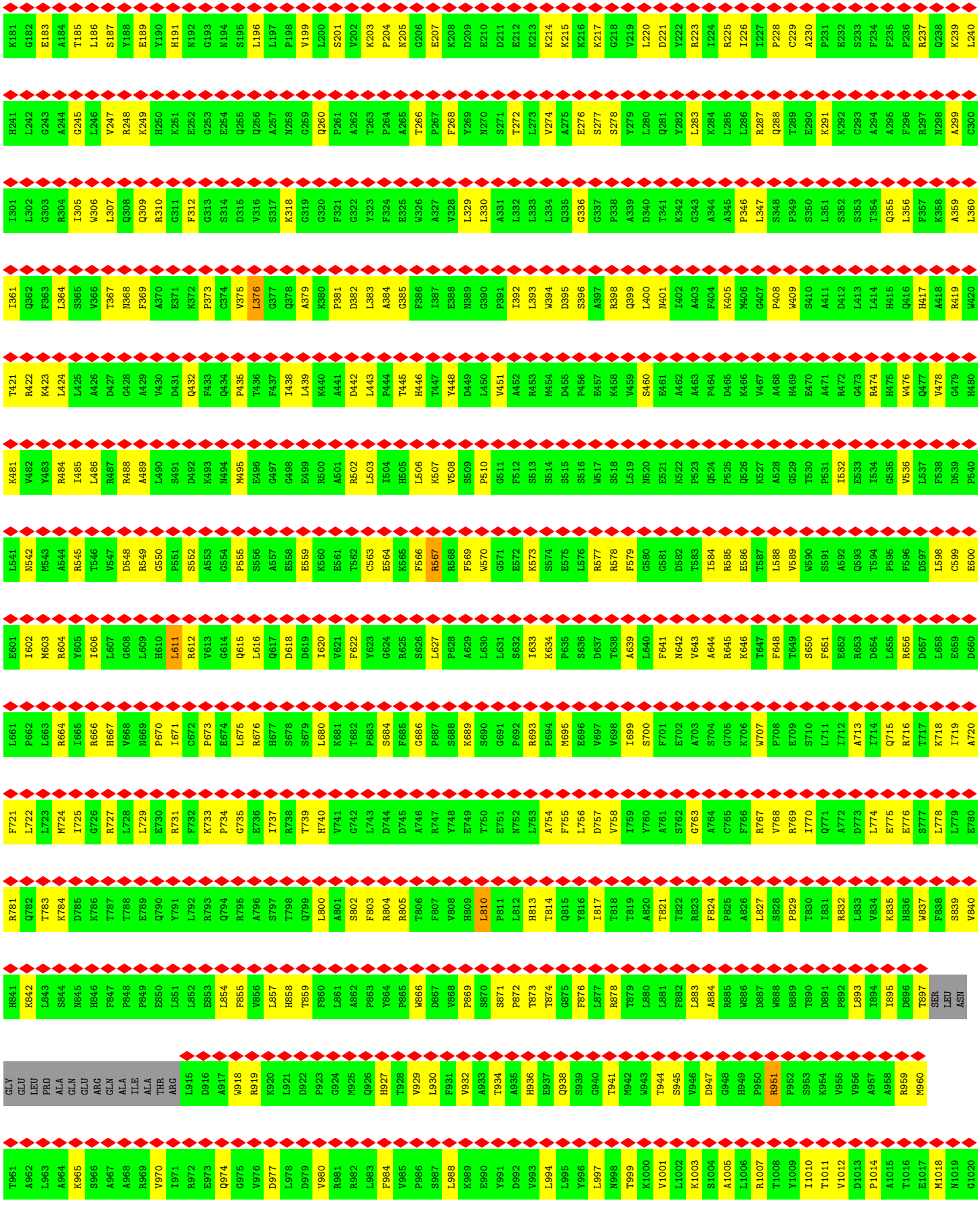



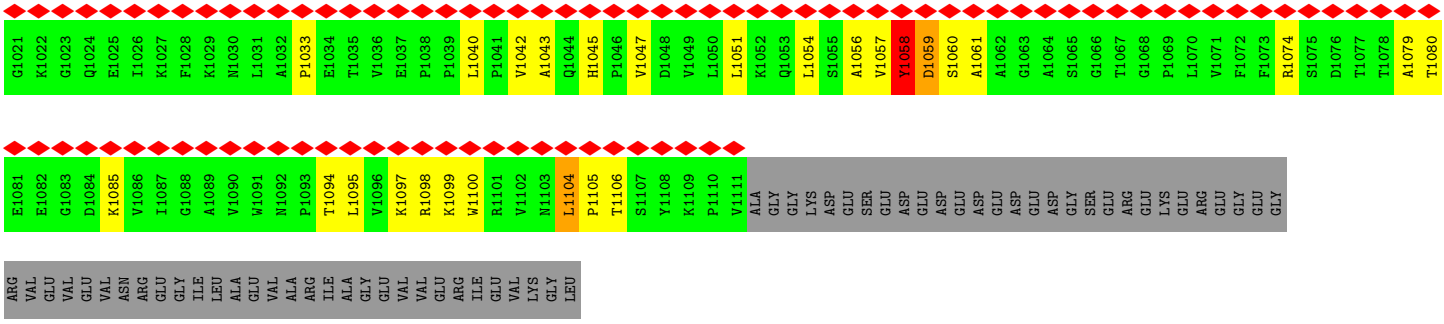
• Molecule 46: U3 small nucleolar RNA-associated protein 22

Chain UV:

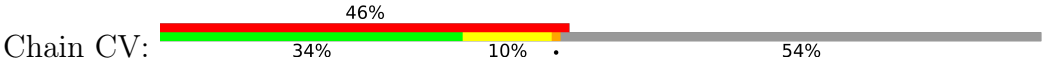


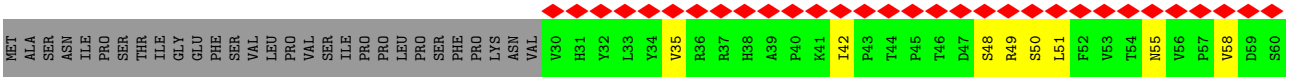



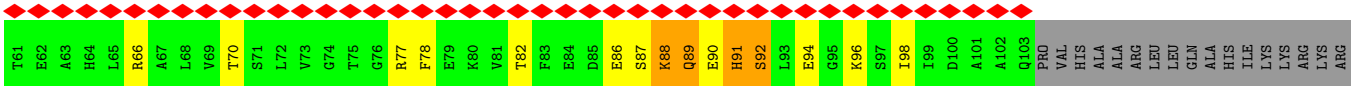

K181 G182 E183 A184 T185 L186 S187 Y188 E189 Y190 H191 N192 G193 N194 S195 L196 L197 P198 V199 L200 S201 V202 K203 P204 N205 G206 E207 K208 D209 E210 D211 E212 K213 K214 K215 K216 K217 G218 V219 L220 D221 Y222 R223 I224 R225 I226 I227 P228 C229 A230 P231 E232 S233 F234 F235 P236 R237 Q238 K239 L240
H241 L242 G243 A244 G245 L246 V247 R248 K249 H250 K251 E252 G253 E254 Q255 Q256 A257 N258 G259 Q260 P261 A262 T263 P264 A265 T266 P267 F268 Y269 N270 S271 T272 L273 V274 A275 E276 S277 S278 Y279 L280 Q281 Y282 L283 K284 L285 L286 R287 Q288 T289 E290 K291 K292 C293 A294 A295 F296 R297 N298 A299 C300
I301 L302 G303 R304 I305 W306 L307 Q308 Q309 R310 G311 F312 G313 S314 D315 V316 S317 K318 G319 G320 F321 G322 Y323 F324 E325 W326 A327 V328 L329 L330 A331 L332 L333 L334 Q335 G336 G337 P338 A339 D340 T341 K342 G343 A344 A345 P346 L347 S348 P349 S350 L351 S352 S353 T354 Q355 L356 F357 K358 A359 L360
I361 Q362 F363 L364 S365 V366 T367 N368 F369 A370 E371 K372 P373 C374 V375 L376 G377 Q378 A379 K380 P381 D382 L383 A384 G385 F386 I387 E388 N389 G390 P391 I392 L393 W394 D395 S396 A397 R398 Q399 L400 N401 I402 A403 F404 K405 M406 G407 P408 W409 S410 A411 D412 L413 L414 H415 Q416 H417 A418 R419 W420
T421 R422 K423 L424 L425 A426 D427 G428 A429 V430 D431 Q432 F433 Q434 P435 T436 F437 I438 L439 K440 A441 D442 L443 P444 T445 H446 T447 Y448 D449 L450 V451 A452 R453 M454 D455 P456 E457 K458 V459 S460 E461 A462 A463 P464 D465 K466 V467 A468 H469 E470 A471 R472 G473 R474 H475 W476 Q477 V478 G479 H480
K481 V482 Y483 R484 I485 L486 R487 R488 A489 L490 S491 D492 K493 N494 M495 E496 G497 G498 E499 R500 A501 R502 L503 I504 H505 L506 K507 V508 S509 P510 G511 F512 S513 S514 S515 S516 W517 S518 L519 N520 E521 K522 P523 Q524 P525 Q526 K527 A528 G529 T530 P531 I532 E533 I534 G535 V536 L537 F538 D539 P540
L541 N542 M543 A544 R545 T546 V547 D548 R549 G550 P551 S552 A553 G554 P555 S556 A557 E558 E559 K560 E561 T562 C563 E564 K565 F566 R567 R568 F569 W570 G571 E572 K573 S574 E575 L576 R577 R578 F579 G580 G581 D582 T583 I584 R585 E586 T587 L588 V589 W590 S591 A592 Q593 T594 P595 F596 D597 L598 C599 E600
E601 I602 M603 R604 Y605 I606 L607 G608 L609 H610 L611 R612 V613 G614 Q615 L616 Q617 D618 D619 I620 V621 F622 Y623 G624 R625 S626 L627 P628 A629 L630 L631 S632 I633 K634 P635 S636 D637 T638 A639 L640 F641 N642 V643 A644 R645 K646 T647 F648 T649 S650 F651 E652 R653 D654 L655 R656 D657 L658 E659 D660
L661 P662 L663 R664 I665 R666 H667 V668 N669 P670 I671 C672 P673 E674 L675 R676 H677 S678 S679 L680 K681 T682 P683 S684 F685 G686 P687 S688 K689 S690 G691 P692 R693 P694 M695 E696 V697 V698 I699 S700 F701 E702 A703 S704 G705 K706 W707 P708 E709 S710 L711 I712 A713 I714 Q715 R716 T717 K718 I719 A720
F721 L722 L723 M724 I725 G726 R727 L728 L729 E730 R731 F732 K733 P734 G735 E736 I737 R738 T739 H740 V741 G742 L743 D744 D745 A746 R747 Y748 E749 T750 E751 N752 L753 A754 F755 L756 D757 V758 I759 Y760 A761 S762 G763 A764 C765 F766 R767 V768 R769 I770 Q771 A772 D773 L774 E775 E776 S777 L778 L779 E780
R781 Q782 T783 K784 D785 K786 T787 T788 E789 Q790 Y791 L792 R793 Q794 R795 A796 S797 T798 Q799 L800 A801 S802 F803 R804 R805 T806 F807 V808 H809 L810 P811 L812 H813 T814 Q815 Y816 I817 T818 T819 A820 T821 T822 R823 F824 P825 A826 L827 S828 P829 T830 I831 R832 L833 V834 K835 H836 W837 F838 S839 V840
H841 K842 L843 S844 N845 H846 F847 P848 P849 E850 L851 L852 E853 L854 F855 V856 L857 H858 T859 F860 L861 A862 P863 Y864 P865 W866 D867 V868 P869 S870 S871 P872 T873 T874 G875 F876 L877 R878 T879 L880 L881 F882 L883 A884 R885 W886 D887 W888 R889 T890 D891 P892 L893 I894 I895 D896 T897 SER LEU ASN
GLY GLU LEU PRO ALA GLN GLU ARG GLN ALA ILE ALA THR ARG L915 D916 A917 W918 R919 K920 L921 D922 P923 G924 M925 Q926 H927 T928 V929 L930 F931 V932 A933 T934 A935 H936 E937 Q938 S939 G940 T941 M942 W943 T944 S945 V946 D947 G948 H949 P950 R951 P952 S953 K954 V955 V956 A957 A958 R959 M960
T961 A962 L963 A964 K965 S966 A967 A968 R969 V970 I971 R972 E973 Q974 G975 V976 D977 L978 D979 V980 R981 R982 L983 F984 V985 P986 S987 L988 K989 E990 Y991 D992 V993 L994 L995 Y996 L997 N998 T999 K1000 V1001 L1002 K1003 S1004 A1005 L1006 R1007 T1008 Y1009 I1010 T1011 V1012 D1013 P1014 A1015 T1016 E1017 M1018 W1019 G1020

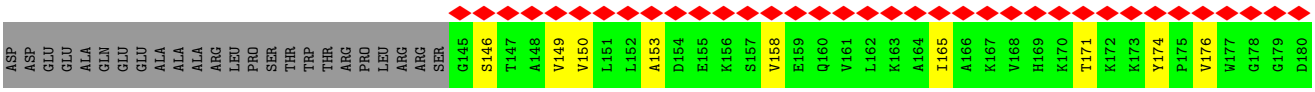


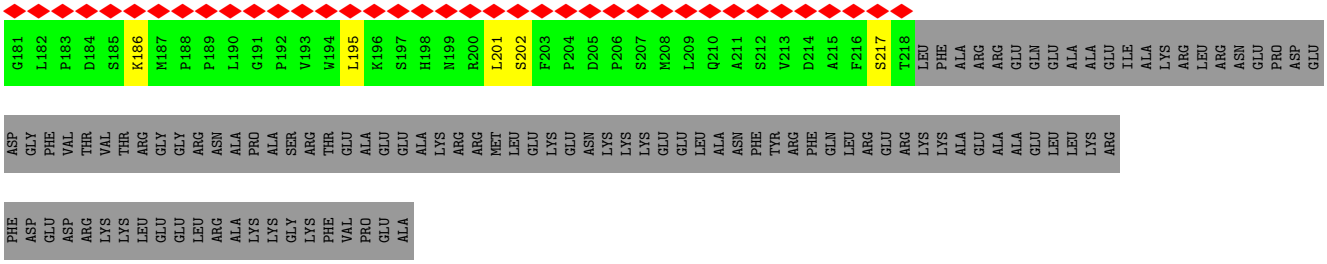

• Molecule 47: Rrp7



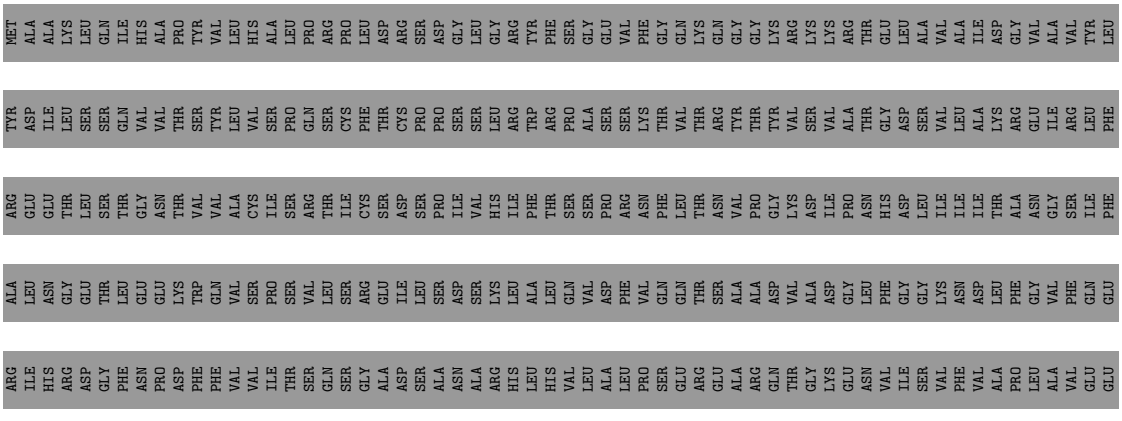



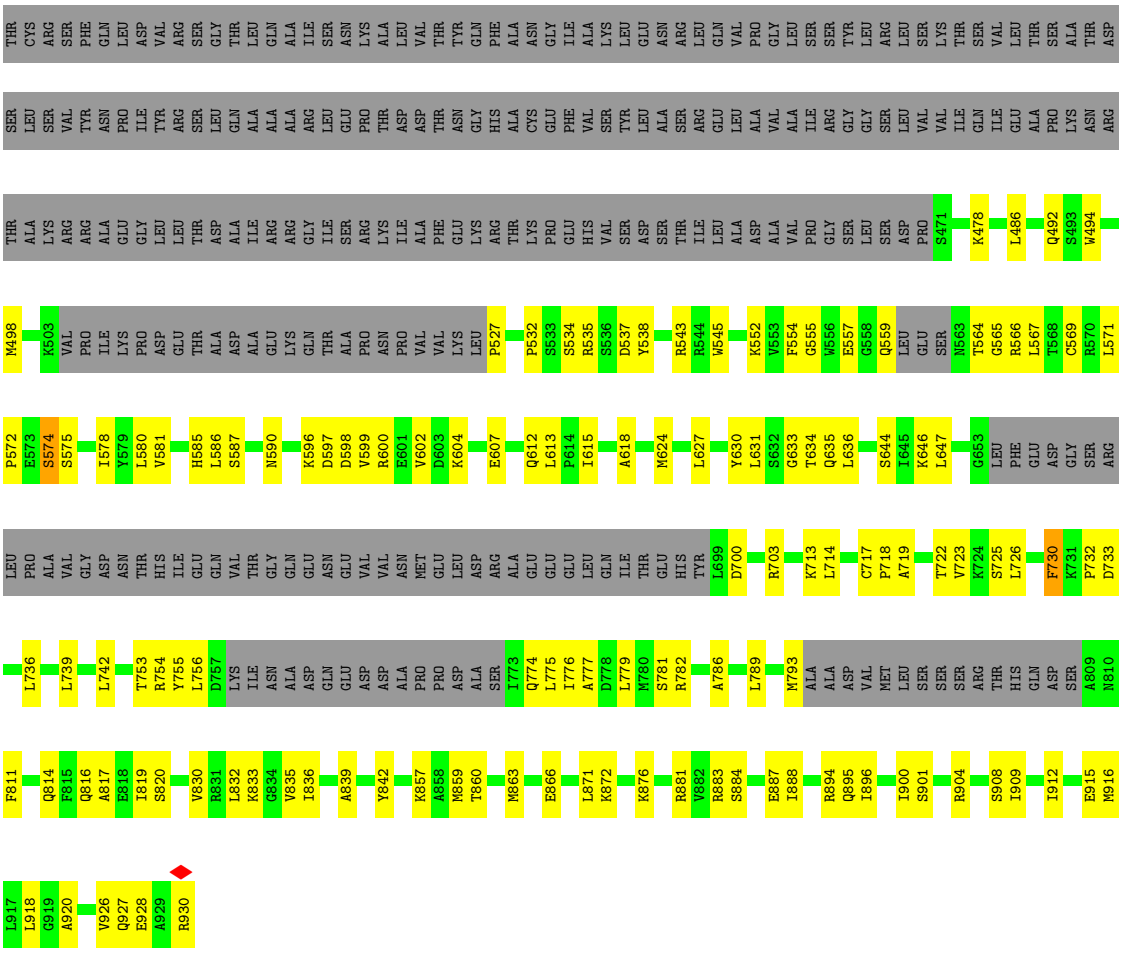



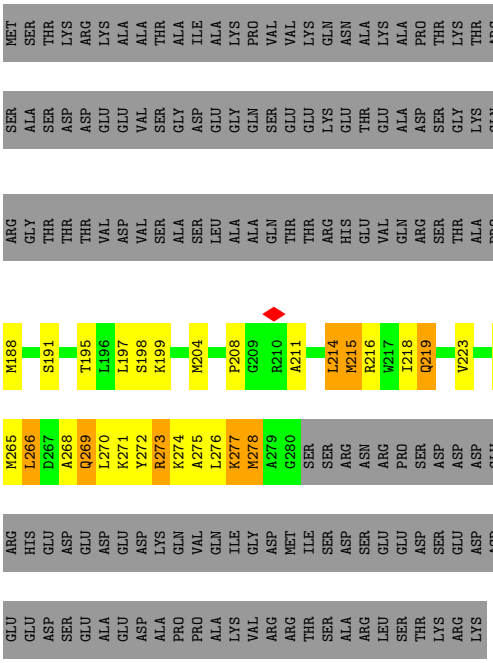

• Molecule 48: Utp8





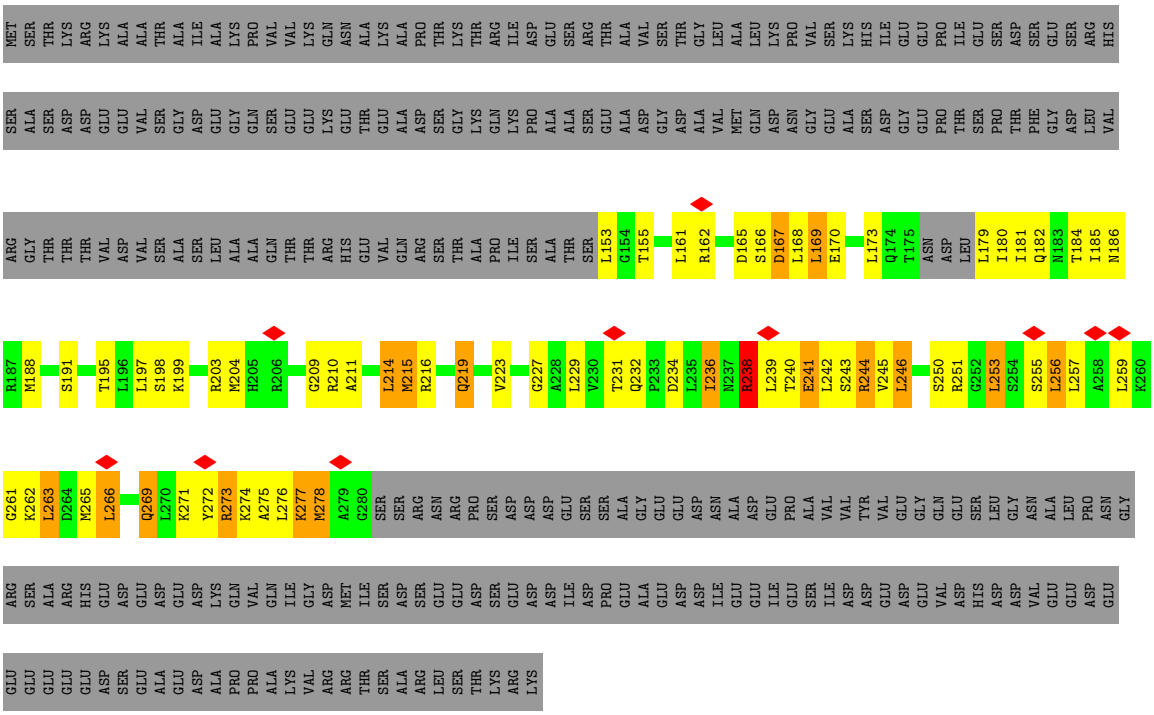
• Molecule 49: Utp5

Chain UE:



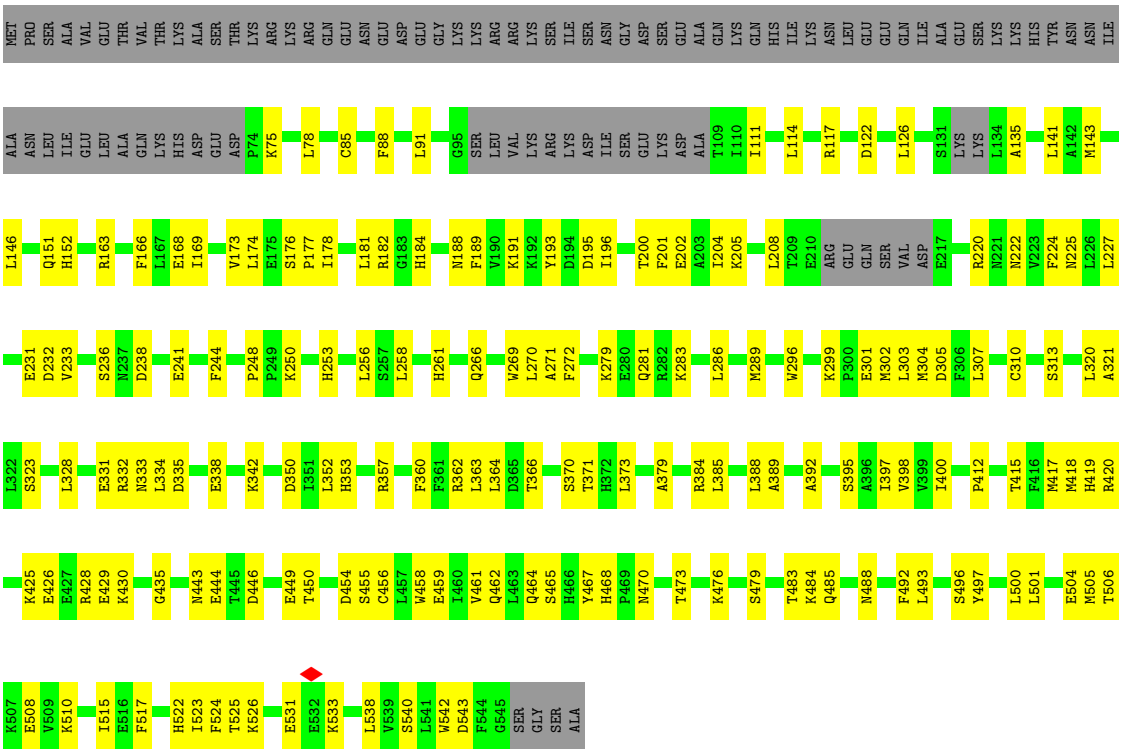
• Molecule 49: Utp5

Chain UI:



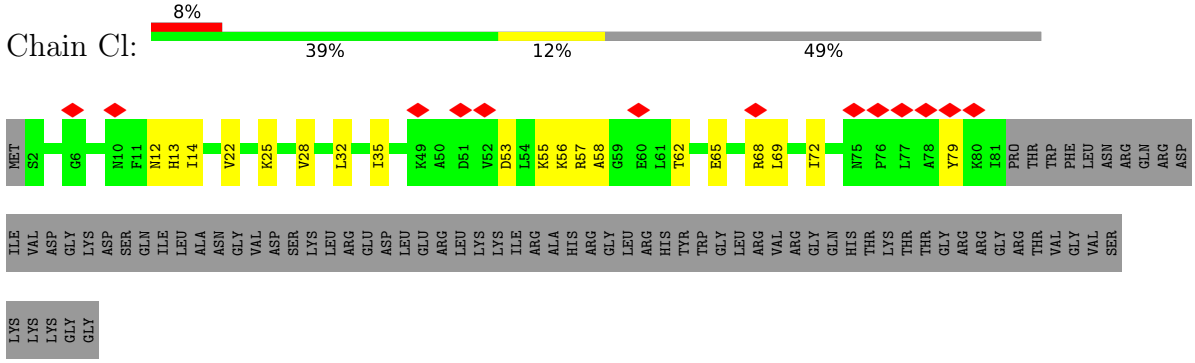

• Molecule 50: Noc4

Chain US:



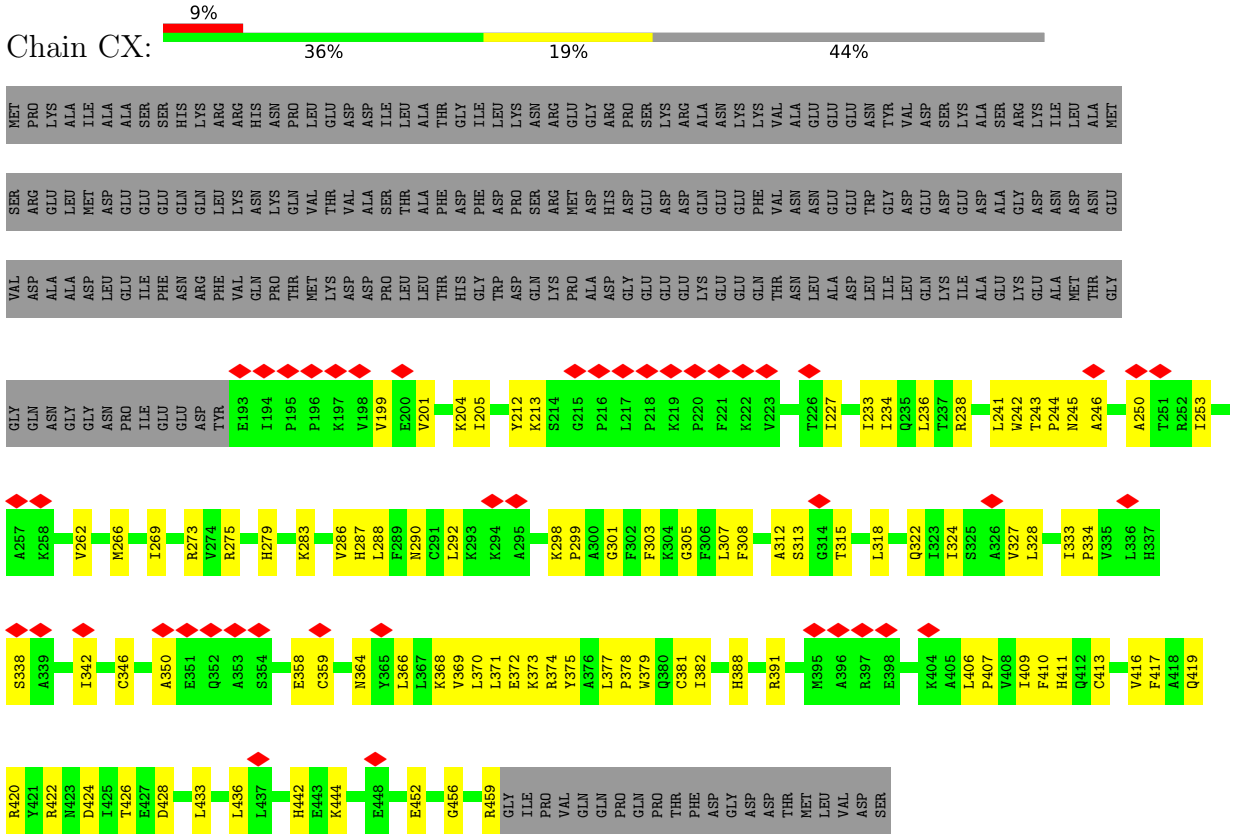
• Molecule 51: Rps18

Chain Cl:



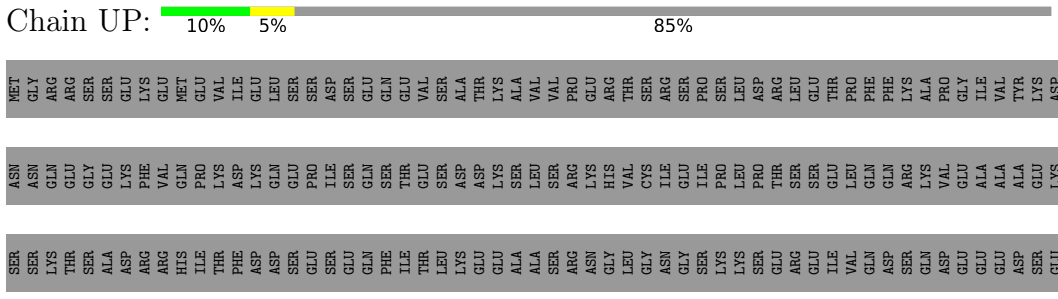

• Molecule 52: Enp1

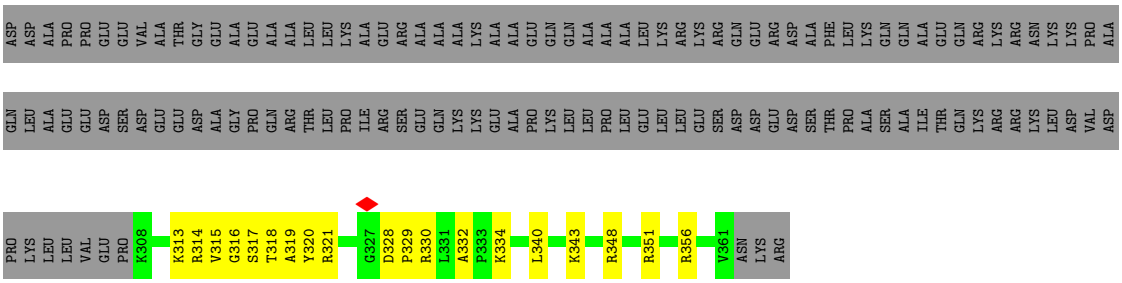
Chain CX:



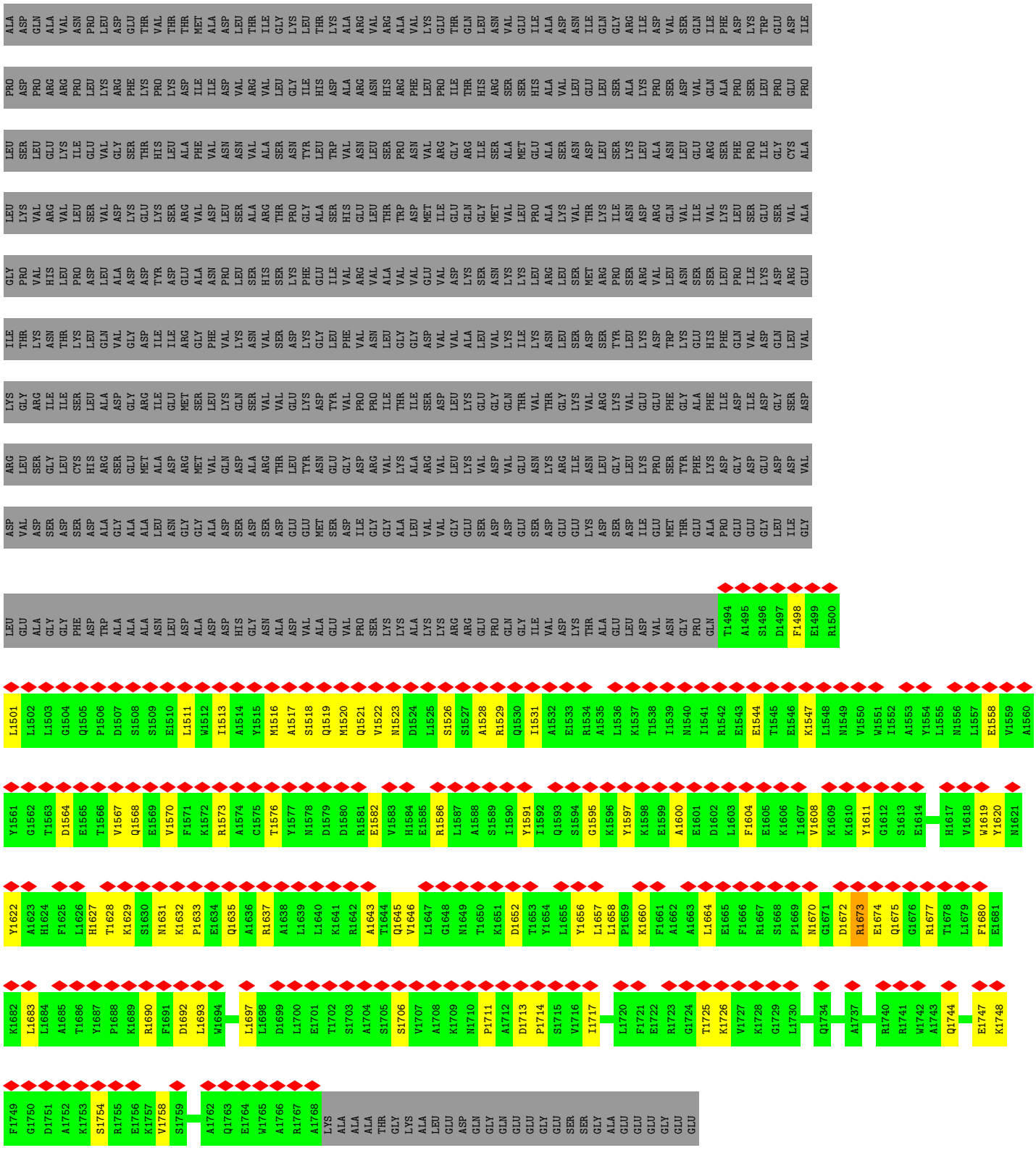

• Molecule 53: Utp16

Chain UP:






• Molecule 54: Rrp5


ALA ASP GLN ALA VAL ASN PRO LEU ASP GLU THR VAL THR THR MET ALA ASP LEU THR ILE GLY LYS LEU THR LYS ALA ARG VAL ARG ALA VAL LYS GLU THR GLN LEU ASN VAL GLU ILE ALA ASP ASN ILE GLN GLY ARG ILE ASP VAL SER GLN ILE PHE ASP LYS TRP GLU ASP ILE
PRO ASP PRO ARG ARG PRO LEU LYS ARG PHE LYS PRO LYS ASP ILE ILE ASP VAL ARG VAL LEU GLY ILE HIS ASP ALA ARG ASN HIS ARG PHE LEU PRO ILE THR HIS ARG SER SER HIS ALA VAL LEU GLU GLU LEU SER ALA SER LYS LEU ALA ASN LEU GLN ALA PRO SER PHE PRO ILE LEU PRO GLU PRO
LEU SER LEU GLU LYS ILE GLU VAL GLY SER THR HIS LEU ALA PHE VAL ASN ASN VAL ALA ALA SER ASN LEU TRP VAL ASN LEU SER PRO ASN VAL ARG GLY ARG ILE SER ALA MET GLU ALA SER ASN ASP ASP LEU GLU ARG SER PHE PRO ILE GLY CYS ALA
LEU LYS VAL ARG VAL LEU SER VAL ASP LYS GLU LYS SER ARG VAL ASP LEU SER ALA ARG THR PRO GLY ALA SER HIS GLU LEU THR TRP ASP MET ILE GLU GLN GLY MET VAL LEU PRO ALA LYS VAL THR LYS ILE ASN ASP ARG GLN VAL LEU ASN SER SER LEU PRO ILE LYS GLU SER VAL ALA
GLY PRO VAL HIS LEU PRO ASP LEU ALA ASP ASP TYR ASP GLU ALA ASN PRO LEU SER HIS SER LYS PHE GLU ILE VAL ARG VAL ALA ALA VAL GLU VAL GLU LYS LYS LEU ARG LEU SER MET ARG PRO SER ARG VAL LEU LEU PRO ILE ASP GLN LEU LEU VAL
ILE THR LYS ASN THR LYS LEU GLN VAL GLY ASP ILE ILE ARG GLY PHE VAL ASN LEU GLY GLY ASP VAL VAL ALA LEU VAL LYS ILE LYS ASN LEU SER ASP TYR LEU LEU LYS ASP TRP LYS GLU LEU PHE GLN VAL LEU ASP
LYS GLY ARG ILE ILE SER LEU ALA ASP GLY ARG ILE GLU MET SER LEU LYS GLN SER VAL VAL GLU LYS ASP PRO PRO ILE THR ILE SER ASP LEU LYS GLU GLY GLN THR VAL THR GLY LYS VAL GLY PHE GLY ALA PHE ILE ASP ILE ASP GLY SER ASP
ARG LEU SER GLY LEU CYS HIS ARG SER GLU MET ALA ASP ARG MET VAL GLN ASP ALA ARG THR LEU TYR ASN GLU GLY ASP ARG VAL LYS ALA LEU VAL LEU GLY LYS PRO SER ILE ASN LEU GLY LEU LYS ASP GLY ASP ASP VAL
ASP VAL ASP SER ASP SER ASP ALA ALA GLY ALA ALA LEU ASN GLY GLY ALA ASP SER ASP SER ASP GLU GLU MET SER ASP ILE GLY GLY LEU VAL ALA LYS ASP ASP ASP GLU SER ASP GLU GLU LYS ASP SER ASP ILE GLU MET THR GLU ALA PRO GLU GLU GLY LEU ILE GLY
LEU GLU ALA GLY GLY PHE ASP TRP ALA ALA ASN LEU ASP GLY HIS GLY ASN ALA ASP VAL ALA GLU VAL PRO SER LYS LYS ALA LYS LYS ARG ARG GLU PRO GLN GLY ILE VAL ASP LYS THR ALA GLU LEU ASP VAL ASN GLY PRO GLN T1494 A1495 S1496 D1497 F1498 E1499 R1500
L1501 L1502 L1503 G1504 Q1505 P1506 D1507 S1508 S1509 E1510 L1511 W1512 I1513 A1514 Y1515 M1516 A1517 S1518 Q1519 M1520 Q1521 V1522 N1523 D1524 L1525 S1526 S1527 A1528 R1529 Q1530 I1531 A1532 E1533 R1534 A1535 L1536 K1537 T1538 I1539 N1540 I1541 R1542 E1543 E1544 T1545 E1546 K1547 L1548 N1549 V1550 W1551 I1552 A1553 Y1554 L1555 N1556 L1557 E1558 V1559 A1560
Y1561 G1562 T1563 D1564 E1565 T1566 V1567 Q1568 E1569 V1570 F1571 K1572 R1573 A1574 C1575 T1576 Y1577 N1578 D1579 D1580 R1581 E1582 V1583 H1584 E1585 R1586 L1587 A1588 S1589 I1590 Y1591 I1592 Q1593 S1594 G1595 K1596 Y1597 K1598 E1599 A1600 E1601 D1602 L1603 F1604 E1605 K1606 I1607 V1608 K1609 K1610 Y1611 G1612 S1613 E1614 H1617 V1618 W1619 Y1620 N1621
Y1622 A1623 H1624 F1625 L1626 H1627 T1628 K1629 S1630 N1631 K1632 P1633 E1634 Q1635 A1636 R1637 A1638 L1639 L1640 K1641 R1642 A1643 T1644 Q1645 V1646 L1647 G1648 N1649 T1650 K1651 D1652 T1653 Y1654 L1655 Y1656 L1657 L1658 P1659 K1660 F1661 A1662 A1663 L1664 E1665 F1666 R1667 S1668 P1669 N1670 G1671 D1672 R1673 E1674 Q1675 G1676 R1677 T1678 L1679 F1680 E1681
K1682 L1683 L1684 A1685 T1686 Y1687 P1688 K1689 R1690 F1691 D1692 L1693 W1694 L1697 L1698 D1699 L1700 E1701 T1702 S1703 A1704 S1705 S1706 V1707 A1708 K1709 N1710 P1711 A1712 D1713 P1714 S1715 V1716 I1717 L1720 F1721 E1722 R1723 G1724 T1725 K1726 V1727 K1728 G1729 L1730 Q1734 A1737 R1740 R1741 W1742 A1743 Q1744 E1747 K1748
F1749 G1750 D1751 A1752 K1753 S1754 R1755 E1756 K1757 V1758 S1759 A1762 Q1763 E1764 W1765 A1766 R1767 A1768 LYS ALA ALA ALA THR GLY LYS ALA LEU GLU ASP GLN GLY GLN GLU GLU GLY GLU SER SER GLY ALA GLU GLU GLU GLY GLU GLU

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 20250 | 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 ($e^-/Å^2$) | 28 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.437 | Depositor |
| Minimum map value | -0.319 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.011 | Depositor |
| Recommended contour level | 0.03 | Depositor |
| Map size (Å) | 520.32, 520.32, 520.32 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.084, 1.084, 1.084 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | UA | 0.96 | 1/6521 (0.0%) | 1.01 | 10/8867 (0.1%) |
| 2 | UB | 0.46 | 0/4154 | 0.66 | 0/5583 |
| 3 | UC | 0.45 | 0/595 | 0.69 | 0/786 |
| 4 | UD | 0.65 | 2/6211 (0.0%) | 0.78 | 2/8408 (0.0%) |
| 5 | UF | 0.52 | 0/2657 | 0.69 | 0/3596 |
| 6 | UG | 0.91 | 3/3516 (0.1%) | 0.93 | 5/4761 (0.1%) |
| 7 | UJ | 0.52 | 0/6291 | 0.74 | 0/8543 |
| 8 | UK | 0.81 | 0/1701 | 0.90 | 5/2251 (0.2%) |
| 9 | UL | 0.45 | 0/6299 | 0.69 | 0/8531 |
| 10 | UM | 0.33 | 0/5366 | 0.63 | 0/7282 |
| 11 | UN | 0.60 | 0/1232 | 0.72 | 0/1662 |
| 12 | UO | 0.73 | 1/3903 (0.0%) | 0.84 | 4/5312 (0.1%) |
| 13 | UQ | 0.71 | 1/6136 (0.0%) | 0.85 | 4/8348 (0.0%) |
| 14 | UR | 0.95 | 2/3564 (0.1%) | 0.95 | 3/4816 (0.1%) |
| 15 | UU | 0.82 | 5/6903 (0.1%) | 0.89 | 7/9392 (0.1%) |
| 16 | UX | 0.64 | 0/1493 | 0.75 | 0/2011 |
| 17 | UZ | 0.44 | 0/1857 | 0.74 | 2/2526 (0.1%) |
| 18 | CA | 0.77 | 1/1814 (0.1%) | 0.86 | 0/2456 |
| 18 | CB | 0.44 | 0/1853 | 0.68 | 0/2511 |
| 19 | CC | 0.53 | 0/2911 | 0.72 | 0/3937 |
| 20 | CD | 0.55 | 0/3205 | 0.76 | 2/4338 (0.0%) |
| 21 | CE | 0.90 | 1/891 (0.1%) | 0.91 | 0/1214 |
| 21 | CF | 0.37 | 0/876 | 0.68 | 0/1195 |
| 22 | CG | 0.25 | 0/2983 | 0.58 | 0/4032 |
| 23 | CH | 0.51 | 0/2939 | 0.72 | 2/3988 (0.1%) |
| 24 | CI | 0.60 | 0/6631 | 0.77 | 9/8943 (0.1%) |
| 25 | CJ | 1.04 | 0/1462 | 1.00 | 0/1967 |
| 26 | CK | 0.96 | 1/2376 (0.0%) | 0.97 | 3/3214 (0.1%) |
| 27 | CL | 0.68 | 0/1812 | 0.76 | 0/2437 |
| 28 | CM | 0.71 | 0/3573 | 0.83 | 0/4829 |
| 29 | CN | 0.53 | 0/1797 | 0.73 | 0/2443 |
| 29 | CO | 0.39 | 0/1714 | 0.65 | 0/2325 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 30 | CP | 0.29 | 0/1528 | 0.77 | 1/2057 (0.0%) |
| 31 | CQ | 0.36 | 0/1379 | 0.62 | 0/1850 |
| 32 | CR | 0.37 | 1/6108 (0.0%) | 0.88 | 22/8266 (0.3%) |
| 32 | CS | 0.37 | 1/6108 (0.0%) | 0.88 | 22/8266 (0.3%) |
| 33 | CT | 0.63 | 0/1053 | 0.82 | 0/1413 |
| 34 | Cc | 0.82 | 0/1485 | 0.90 | 0/2008 |
| 35 | Ce | 0.36 | 0/1298 | 0.83 | 2/1750 (0.1%) |
| 36 | Cg | 0.33 | 0/1259 | 0.66 | 0/1687 |
| 37 | Ch | 0.23 | 0/422 | 0.71 | 0/561 |
| 38 | Ci | 0.27 | 0/801 | 0.74 | 1/1087 (0.1%) |
| 39 | Cj | 1.03 | 0/958 | 1.00 | 0/1293 |
| 40 | Cm | 0.30 | 0/1001 | 0.67 | 0/1345 |
| 41 | Cn | 0.60 | 0/712 | 0.75 | 0/954 |
| 42 | Cp | 0.58 | 0/458 | 0.79 | 0/617 |
| 43 | CU | 0.37 | 0/1015 | 0.65 | 0/1351 |
| 44 | C1 | 0.63 | 0/26369 | 0.61 | 4/41071 (0.0%) |
| 45 | C2 | 0.65 | 0/5459 | 0.66 | 7/8498 (0.1%) |
| 46 | UV | 0.32 | 0/8638 | 0.80 | 6/11725 (0.1%) |
| 47 | CV | 0.31 | 0/1172 | 0.76 | 1/1592 (0.1%) |
| 48 | UH | 0.48 | 1/2852 (0.0%) | 0.72 | 0/3846 |
| 49 | UE | 0.53 | 0/980 | 0.96 | 2/1316 (0.2%) |
| 49 | UI | 0.53 | 0/980 | 0.96 | 2/1316 (0.2%) |
| 50 | US | 0.50 | 0/3765 | 0.70 | 0/5100 |
| 51 | Cl | 0.38 | 0/638 | 0.74 | 0/857 |
| 52 | CX | 0.25 | 0/2180 | 0.62 | 0/2956 |
| 53 | UP | 0.56 | 0/428 | 0.74 | 0/570 |
| 54 | Cz | 0.26 | 0/2310 | 0.62 | 0/3120 |
| All | All | 0.61 | 21/186592 (0.0%) | 0.77 | 128/258976 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | UA | 0 | 4 |
| 4 | UD | 0 | 2 |
| 5 | UF | 0 | 1 |
| 6 | UG | 0 | 2 |
| 9 | UL | 0 | 1 |
| 10 | UM | 0 | 3 |
| 12 | UO | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 13 | UQ | 0 | 6 |
| 15 | UU | 0 | 8 |
| 17 | UZ | 0 | 3 |
| 18 | CA | 0 | 1 |
| 18 | CB | 0 | 1 |
| 21 | CF | 0 | 1 |
| 23 | CH | 0 | 1 |
| 24 | CI | 0 | 2 |
| 26 | CK | 0 | 1 |
| 29 | CO | 0 | 2 |
| 31 | CQ | 0 | 1 |
| 32 | CR | 0 | 2 |
| 32 | CS | 0 | 2 |
| 34 | Cc | 0 | 2 |
| 35 | Ce | 0 | 1 |
| 38 | Ci | 0 | 1 |
| 39 | Cj | 0 | 2 |
| 46 | UV | 0 | 5 |
| 47 | CV | 0 | 2 |
| 48 | UH | 0 | 2 |
| 50 | US | 0 | 1 |
| 51 | Cl | 0 | 1 |
| 54 | Cz | 0 | 1 |
| All | All | 0 | 64 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 13 | UQ | 394 | HIS | CA-CB | -17.11 | 1.23 | 1.53 |
| 15 | UU | 1048 | ARG | CA-CB | -10.32 | 1.39 | 1.52 |
| 1 | UA | 4 | ASN | CA-CB | -9.34 | 1.37 | 1.52 |
| 14 | UR | 565 | ALA | CA-CB | -8.64 | 1.40 | 1.52 |
| 26 | CK | 186 | GLU | CA-CB | -8.22 | 1.41 | 1.52 |
| 12 | UO | 417 | ARG | C-N | -7.87 | 1.20 | 1.33 |
| 18 | CA | 204 | ILE | C-N | -7.62 | 1.24 | 1.33 |
| 4 | UD | 496 | ALA | CA-CB | -6.14 | 1.45 | 1.53 |
| 15 | UU | 418 | TRP | CB-CG | -5.79 | 1.32 | 1.50 |
| 6 | UG | 154 | ALA | C-N | -5.71 | 1.28 | 1.33 |
| 32 | CR | 108 | TYR | CA-CB | 5.62 | 1.62 | 1.53 |
| 32 | CS | 108 | TYR | CA-CB | 5.55 | 1.62 | 1.53 |
| 15 | UU | 86 | THR | CB-CG2 | -5.45 | 1.34 | 1.52 |
| 6 | UG | 155 | GLY | CA-C | -5.26 | 1.48 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | UD | 25 | ALA | C-N | -5.25 | 1.25 | 1.33 |
| 21 | CE | 82 | VAL | C-N | -5.18 | 1.28 | 1.34 |
| 14 | UR | 530 | PRO | C-N | -5.13 | 1.24 | 1.33 |
| 48 | UH | 730 | PHE | C-N | -5.08 | 1.18 | 1.33 |
| 6 | UG | 464 | ASN | CA-CB | -5.06 | 1.40 | 1.53 |
| 15 | UU | 101 | LYS | C-N | -5.05 | 1.26 | 1.33 |
| 15 | UU | 420 | TRP | CB-CG | -5.02 | 1.34 | 1.50 |

All (128) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | C2 | 2 | G | OP1-P-OP2 | -13.18 | 80.07 | 119.60 |
| 24 | CI | 995 | VAL | CA-C-N | 12.59 | 151.76 | 122.31 |
| 24 | CI | 995 | VAL | C-N-CA | 12.59 | 151.76 | 122.31 |
| 45 | C2 | 2 | G | O5'-P-OP1 | -12.07 | 71.78 | 108.00 |
| 45 | C2 | 1 | A | OP2-P-O3' | -10.20 | 77.40 | 108.00 |
| 44 | C1 | 55 | G | OP1-P-O3' | -9.77 | 78.68 | 108.00 |
| 44 | C1 | 45 | U | OP1-P-O3' | -9.01 | 80.98 | 108.00 |
| 32 | CS | 372 | ILE | CA-C-N | 8.86 | 134.14 | 120.68 |
| 32 | CS | 372 | ILE | C-N-CA | 8.86 | 134.14 | 120.68 |
| 32 | CR | 372 | ILE | CA-C-N | 8.84 | 134.11 | 120.68 |
| 32 | CR | 372 | ILE | C-N-CA | 8.84 | 134.11 | 120.68 |
| 1 | UA | 199 | VAL | CA-C-N | -8.81 | 114.82 | 121.61 |
| 1 | UA | 199 | VAL | C-N-CA | -8.81 | 114.82 | 121.61 |
| 45 | C2 | 1 | A | OP1-P-O3' | 8.68 | 134.03 | 108.00 |
| 45 | C2 | 2 | G | O5'-P-OP2 | 8.52 | 133.54 | 108.00 |
| 44 | C1 | 45 | U | OP2-P-O3' | -8.07 | 83.80 | 108.00 |
| 32 | CS | 626 | GLU | CA-CB-CG | 7.67 | 129.44 | 114.10 |
| 32 | CR | 626 | GLU | CA-CB-CG | 7.67 | 129.44 | 114.10 |
| 46 | UV | 980 | VAL | N-CA-C | -7.62 | 105.28 | 112.83 |
| 13 | UQ | 352 | HIS | CA-C-N | -7.44 | 110.71 | 122.17 |
| 13 | UQ | 352 | HIS | C-N-CA | -7.44 | 110.71 | 122.17 |
| 32 | CS | 913 | MET | CB-CG-SD | 7.40 | 134.90 | 112.70 |
| 32 | CR | 913 | MET | CB-CG-SD | 7.40 | 134.89 | 112.70 |
| 32 | CS | 88 | GLU | CA-CB-CG | 7.24 | 128.59 | 114.10 |
| 32 | CR | 88 | GLU | CA-CB-CG | 7.23 | 128.56 | 114.10 |
| 35 | Ce | 38 | ALA | CA-C-N | 6.90 | 134.12 | 121.70 |
| 35 | Ce | 38 | ALA | C-N-CA | 6.90 | 134.12 | 121.70 |
| 32 | CS | 487 | GLU | CA-CB-CG | 6.83 | 127.76 | 114.10 |
| 32 | CR | 487 | GLU | CA-CB-CG | 6.83 | 127.75 | 114.10 |
| 47 | CV | 89 | GLN | N-CA-C | 6.72 | 121.19 | 113.19 |
| 24 | CI | 240 | THR | CA-C-N | -6.68 | 106.20 | 122.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | CI | 240 | THR | C-N-CA | -6.68 | 106.20 | 122.36 |
| 13 | UQ | 122 | VAL | N-CA-C | -6.60 | 106.58 | 112.12 |
| 32 | CS | 51 | ARG | CA-CB-CG | 6.56 | 127.22 | 114.10 |
| 32 | CR | 51 | ARG | CA-CB-CG | 6.55 | 127.21 | 114.10 |
| 32 | CR | 410 | MET | CB-CG-SD | 6.48 | 132.13 | 112.70 |
| 32 | CS | 410 | MET | CB-CG-SD | 6.47 | 132.12 | 112.70 |
| 12 | UO | 417 | ARG | CA-C-N | -6.42 | 112.08 | 122.48 |
| 12 | UO | 417 | ARG | C-N-CA | -6.42 | 112.08 | 122.48 |
| 44 | C1 | 55 | G | OP2-P-O3' | -6.32 | 89.05 | 108.00 |
| 1 | UA | 673 | VAL | CA-C-N | -6.17 | 114.48 | 123.00 |
| 1 | UA | 673 | VAL | C-N-CA | -6.17 | 114.48 | 123.00 |
| 49 | UE | 238 | ARG | NE-CZ-NH2 | 6.15 | 124.73 | 119.20 |
| 49 | UI | 238 | ARG | NE-CZ-NH2 | 6.14 | 124.73 | 119.20 |
| 49 | UI | 238 | ARG | CG-CD-NE | 6.09 | 125.40 | 112.00 |
| 1 | UA | 490 | ARG | CA-C-N | -6.08 | 112.26 | 122.29 |
| 1 | UA | 490 | ARG | C-N-CA | -6.08 | 112.26 | 122.29 |
| 49 | UE | 238 | ARG | CG-CD-NE | 6.07 | 125.36 | 112.00 |
| 15 | UU | 130 | GLU | CA-C-N | -6.06 | 107.95 | 122.74 |
| 15 | UU | 130 | GLU | C-N-CA | -6.06 | 107.95 | 122.74 |
| 8 | UK | 68 | MET | CA-C-N | -5.99 | 114.01 | 123.24 |
| 8 | UK | 68 | MET | C-N-CA | -5.99 | 114.01 | 123.24 |
| 1 | UA | 194 | HIS | CA-C-N | -5.96 | 112.95 | 122.08 |
| 1 | UA | 194 | HIS | C-N-CA | -5.96 | 112.95 | 122.08 |
| 32 | CS | 430 | LYS | CA-CB-CG | 5.96 | 126.03 | 114.10 |
| 32 | CR | 430 | LYS | CA-CB-CG | 5.95 | 126.00 | 114.10 |
| 24 | CI | 551 | LEU | CA-C-N | -5.94 | 111.65 | 120.68 |
| 24 | CI | 551 | LEU | C-N-CA | -5.94 | 111.65 | 120.68 |
| 6 | UG | 216 | HIS | N-CA-C | -5.91 | 102.17 | 110.50 |
| 14 | UR | 564 | ASP | CA-C-N | -5.83 | 114.14 | 122.77 |
| 14 | UR | 564 | ASP | C-N-CA | -5.83 | 114.14 | 122.77 |
| 26 | CK | 289 | ARG | NE-CZ-NH1 | -5.76 | 115.74 | 121.50 |
| 8 | UK | 79 | ARG | CA-C-N | -5.69 | 115.96 | 121.31 |
| 8 | UK | 79 | ARG | C-N-CA | -5.69 | 115.96 | 121.31 |
| 23 | CH | 85 | THR | CA-C-N | -5.69 | 117.17 | 123.43 |
| 23 | CH | 85 | THR | C-N-CA | -5.69 | 117.17 | 123.43 |
| 32 | CR | 88 | GLU | CB-CG-CD | 5.68 | 122.25 | 112.60 |
| 4 | UD | 190 | VAL | CA-C-N | -5.67 | 113.78 | 122.62 |
| 4 | UD | 190 | VAL | C-N-CA | -5.67 | 113.78 | 122.62 |
| 32 | CR | 188 | ARG | CG-CD-NE | 5.66 | 124.46 | 112.00 |
| 32 | CS | 88 | GLU | CB-CG-CD | 5.66 | 122.22 | 112.60 |
| 24 | CI | 367 | VAL | N-CA-C | -5.66 | 107.15 | 111.62 |
| 32 | CS | 188 | ARG | CG-CD-NE | 5.64 | 124.42 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | CS | 430 | LYS | CB-CA-C | -5.56 | 102.40 | 110.96 |
| 8 | UK | 51 | LEU | CA-CB-CG | -5.55 | 96.86 | 116.30 |
| 32 | CR | 430 | LYS | CB-CA-C | -5.52 | 102.46 | 110.96 |
| 32 | CS | 4 | GLN | CB-CG-CD | 5.52 | 121.98 | 112.60 |
| 32 | CS | 655 | GLN | CB-CG-CD | 5.51 | 121.96 | 112.60 |
| 32 | CR | 4 | GLN | CB-CG-CD | 5.50 | 121.94 | 112.60 |
| 32 | CR | 655 | GLN | CB-CG-CD | 5.49 | 121.94 | 112.60 |
| 15 | UU | 715 | PHE | CB-CA-C | -5.45 | 98.92 | 109.76 |
| 26 | CK | 211 | LEU | CA-C-N | 5.41 | 132.52 | 121.48 |
| 26 | CK | 211 | LEU | C-N-CA | 5.41 | 132.52 | 121.48 |
| 32 | CS | 410 | MET | CA-CB-CG | 5.38 | 124.85 | 114.10 |
| 32 | CR | 410 | MET | CA-CB-CG | 5.37 | 124.84 | 114.10 |
| 32 | CR | 430 | LYS | N-CA-CB | 5.36 | 117.73 | 109.91 |
| 12 | UO | 240 | PRO | CA-C-N | -5.35 | 111.21 | 123.15 |
| 12 | UO | 240 | PRO | C-N-CA | -5.35 | 111.21 | 123.15 |
| 32 | CR | 658 | VAL | CB-CA-C | -5.35 | 105.07 | 112.24 |
| 32 | CS | 430 | LYS | N-CA-CB | 5.34 | 117.70 | 109.91 |
| 32 | CR | 476 | GLU | CB-CG-CD | 5.33 | 121.67 | 112.60 |
| 1 | UA | 676 | SER | CA-C-N | -5.33 | 114.88 | 121.38 |
| 1 | UA | 676 | SER | C-N-CA | -5.33 | 114.88 | 121.38 |
| 32 | CS | 476 | GLU | CB-CG-CD | 5.32 | 121.64 | 112.60 |
| 32 | CS | 658 | VAL | CB-CA-C | -5.32 | 105.11 | 112.24 |
| 46 | UV | 1058 | TYR | N-CA-C | 5.30 | 116.92 | 111.03 |
| 24 | CI | 753 | ASN | CA-C-N | 5.23 | 131.53 | 121.54 |
| 24 | CI | 753 | ASN | C-N-CA | 5.23 | 131.53 | 121.54 |
| 46 | UV | 95 | LEU | CA-C-N | 5.23 | 128.51 | 120.82 |
| 46 | UV | 95 | LEU | C-N-CA | 5.23 | 128.51 | 120.82 |
| 20 | CD | 427 | GLY | CA-C-N | -5.22 | 110.09 | 122.31 |
| 20 | CD | 427 | GLY | C-N-CA | -5.22 | 110.09 | 122.31 |
| 17 | UZ | 18 | VAL | CA-C-N | -5.21 | 109.08 | 121.80 |
| 17 | UZ | 18 | VAL | C-N-CA | -5.21 | 109.08 | 121.80 |
| 32 | CR | 51 | ARG | CB-CG-CD | 5.15 | 123.15 | 111.30 |
| 32 | CS | 51 | ARG | CB-CG-CD | 5.15 | 123.14 | 111.30 |
| 32 | CS | 704 | GLU | CA-C-N | -5.12 | 112.56 | 122.70 |
| 32 | CS | 704 | GLU | C-N-CA | -5.12 | 112.56 | 122.70 |
| 30 | CP | 213 | LEU | CA-CB-CG | 5.12 | 134.22 | 116.30 |
| 32 | CS | 576 | GLU | CA-CB-CG | 5.12 | 124.33 | 114.10 |
| 32 | CR | 704 | GLU | CA-C-N | -5.11 | 112.58 | 122.70 |
| 32 | CR | 704 | GLU | C-N-CA | -5.11 | 112.58 | 122.70 |
| 15 | UU | 529 | ARG | CA-C-N | -5.11 | 114.24 | 122.82 |
| 15 | UU | 529 | ARG | C-N-CA | -5.11 | 114.24 | 122.82 |
| 46 | UV | 376 | LEU | N-CA-C | 5.09 | 116.55 | 110.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | UQ | 456 | TRP | CA-CB-CG | -5.08 | 103.95 | 113.60 |
| 45 | C2 | 1 | A | O3'-P-O5' | -5.08 | 96.38 | 104.00 |
| 14 | UR | 587 | LEU | CA-CB-CG | -5.08 | 98.53 | 116.30 |
| 32 | CR | 576 | GLU | CA-CB-CG | 5.07 | 124.25 | 114.10 |
| 38 | Ci | 122 | GLY | N-CA-C | 5.07 | 125.20 | 113.18 |
| 46 | UV | 1058 | TYR | CB-CA-C | -5.07 | 103.10 | 110.95 |
| 15 | UU | 102 | GLU | N-CA-C | -5.05 | 108.14 | 114.56 |
| 6 | UG | 175 | GLN | CA-C-N | 5.04 | 131.16 | 121.54 |
| 6 | UG | 175 | GLN | C-N-CA | 5.04 | 131.16 | 121.54 |
| 6 | UG | 129 | LYS | CA-C-N | -5.03 | 113.56 | 122.20 |
| 6 | UG | 129 | LYS | C-N-CA | -5.03 | 113.56 | 122.20 |
| 45 | C2 | 23 | A | P-O3'-C3' | 5.03 | 127.74 | 120.20 |
| 15 | UU | 321 | GLY | N-CA-C | 5.02 | 117.90 | 110.42 |

There are no chirality outliers.

All (64) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 18 | CA | 306 | TYR | Peptide |
| 18 | CB | 293 | GLU | Peptide |
| 21 | CF | 60 | GLN | Peptide |
| 23 | CH | 143 | HIS | Peptide |
| 24 | CI | 132 | VAL | Peptide |
| 24 | CI | 851 | TRP | Peptide |
| 26 | CK | 261 | PHE | Peptide |
| 29 | CO | 84 | ILE | Peptide |
| 29 | CO | 88 | ARG | Peptide |
| 31 | CQ | 173 | ASP | Peptide |
| 32 | CR | 48 | MET | Peptide |
| 32 | CR | 866 | PHE | Peptide |
| 32 | CS | 48 | MET | Peptide |
| 32 | CS | 866 | PHE | Peptide |
| 47 | CV | 88 | LYS | Peptide |
| 47 | CV | 91 | HIS | Peptide |
| 34 | Cc | 13 | TYR | Peptide |
| 34 | Cc | 86 | MET | Peptide |
| 35 | Ce | 38 | ALA | Peptide |
| 38 | Ci | 137 | ASP | Peptide |
| 39 | Cj | 126 | PRO | Peptide |
| 39 | Cj | 40 | ALA | Peptide |
| 51 | Cl | 79 | TYR | Peptide |
| 54 | Cz | 1628 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | UA | 214 | SER | Peptide |
| 1 | UA | 386 | THR | Peptide |
| 1 | UA | 667 | ARG | Peptide |
| 1 | UA | 8 | SER | Peptide |
| 4 | UD | 309 | GLN | Peptide |
| 4 | UD | 387 | TRP | Peptide |
| 5 | UF | 120 | VAL | Peptide |
| 6 | UG | 126 | ALA | Peptide |
| 6 | UG | 258 | HIS | Peptide |
| 48 | UH | 753 | THR | Peptide |
| 48 | UH | 857 | LYS | Peptide |
| 9 | UL | 17 | VAL | Peptide |
| 10 | UM | 204 | ASP | Peptide |
| 10 | UM | 328 | LEU | Peptide |
| 10 | UM | 693 | GLU | Peptide |
| 12 | UO | 167 | LYS | Peptide |
| 12 | UO | 282 | ALA | Peptide |
| 13 | UQ | 170 | TRP | Peptide |
| 13 | UQ | 237 | TYR | Peptide |
| 13 | UQ | 364 | SER | Peptide |
| 13 | UQ | 563 | THR | Peptide |
| 13 | UQ | 707 | PRO | Peptide |
| 13 | UQ | 849 | ALA | Peptide |
| 50 | US | 510 | LYS | Peptide |
| 15 | UU | 100 | TRP | Peptide |
| 15 | UU | 252 | PRO | Peptide |
| 15 | UU | 313 | LEU | Peptide |
| 15 | UU | 369 | SER | Peptide |
| 15 | UU | 378 | LEU | Peptide |
| 15 | UU | 396 | SER | Peptide |
| 15 | UU | 397 | ASP | Peptide |
| 15 | UU | 857 | ILE | Peptide |
| 46 | UV | 1058 | TYR | Peptide |
| 46 | UV | 1104 | LEU | Peptide |
| 46 | UV | 57 | PHE | Peptide |
| 46 | UV | 611 | LEU | Peptide |
| 46 | UV | 951 | ARG | Peptide |
| 17 | UZ | 103 | ASP | Peptide |
| 17 | UZ | 173 | LYS | Peptide |
| 17 | UZ | 273 | GLN | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | UA | 6366 | 0 | 6273 | 209 | 0 |
| 2 | UB | 4079 | 0 | 4201 | 125 | 0 |
| 3 | UC | 588 | 0 | 647 | 18 | 0 |
| 4 | UD | 6071 | 0 | 6080 | 232 | 0 |
| 5 | UF | 2591 | 0 | 2642 | 80 | 0 |
| 6 | UG | 3444 | 0 | 3454 | 135 | 0 |
| 7 | UJ | 6180 | 0 | 6341 | 188 | 0 |
| 8 | UK | 1687 | 0 | 1820 | 62 | 0 |
| 9 | UL | 6175 | 0 | 6188 | 260 | 0 |
| 10 | UM | 5273 | 0 | 5284 | 169 | 0 |
| 11 | UN | 1209 | 0 | 1234 | 58 | 0 |
| 12 | UO | 3819 | 0 | 3873 | 154 | 0 |
| 13 | UQ | 6008 | 0 | 6033 | 228 | 0 |
| 14 | UR | 3491 | 0 | 3507 | 129 | 0 |
| 15 | UU | 6734 | 0 | 6745 | 248 | 0 |
| 16 | UX | 1470 | 0 | 1533 | 80 | 0 |
| 17 | UZ | 1815 | 0 | 1896 | 69 | 0 |
| 18 | CA | 1778 | 0 | 1830 | 82 | 0 |
| 18 | CB | 1816 | 0 | 1847 | 68 | 0 |
| 19 | CC | 2866 | 0 | 2960 | 108 | 0 |
| 20 | CD | 3150 | 0 | 3262 | 117 | 0 |
| 21 | CE | 879 | 0 | 918 | 22 | 0 |
| 21 | CF | 864 | 0 | 900 | 34 | 0 |
| 22 | CG | 2922 | 0 | 2939 | 87 | 0 |
| 23 | CH | 2888 | 0 | 2979 | 118 | 0 |
| 24 | CI | 6486 | 0 | 6650 | 261 | 0 |
| 25 | CJ | 1434 | 0 | 1482 | 63 | 0 |
| 26 | CK | 2329 | 0 | 2373 | 110 | 0 |
| 27 | CL | 1786 | 0 | 1826 | 78 | 0 |
| 28 | CM | 3501 | 0 | 3498 | 144 | 0 |
| 29 | CN | 1762 | 0 | 1807 | 52 | 0 |
| 29 | CO | 1683 | 0 | 1726 | 62 | 0 |
| 30 | CP | 1504 | 0 | 1596 | 33 | 0 |
| 31 | CQ | 1361 | 0 | 1431 | 47 | 0 |
| 32 | CR | 5989 | 0 | 6130 | 202 | 0 |
| 32 | CS | 5989 | 0 | 6130 | 192 | 0 |
| 33 | CT | 1035 | 0 | 1063 | 32 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 34 | Cc | 1464 | 0 | 1504 | 53 | 0 |
| 35 | Ce | 1279 | 0 | 1322 | 43 | 0 |
| 36 | Cg | 1242 | 0 | 1354 | 49 | 0 |
| 37 | Ch | 416 | 0 | 451 | 11 | 0 |
| 38 | Ci | 791 | 0 | 795 | 13 | 0 |
| 39 | Cj | 943 | 0 | 1002 | 28 | 0 |
| 40 | Cm | 985 | 0 | 1021 | 31 | 0 |
| 41 | Cn | 702 | 0 | 750 | 19 | 0 |
| 42 | Cp | 455 | 0 | 482 | 15 | 0 |
| 43 | CU | 1009 | 0 | 1070 | 39 | 0 |
| 44 | C1 | 23604 | 0 | 11955 | 691 | 0 |
| 45 | C2 | 4891 | 0 | 2476 | 136 | 0 |
| 46 | UV | 8424 | 0 | 8502 | 254 | 0 |
| 47 | CV | 1145 | 0 | 1155 | 33 | 0 |
| 48 | UH | 2809 | 0 | 2843 | 122 | 0 |
| 49 | UE | 972 | 0 | 1032 | 61 | 0 |
| 49 | UI | 972 | 0 | 1032 | 68 | 0 |
| 50 | US | 3672 | 0 | 3679 | 121 | 0 |
| 51 | Cl | 633 | 0 | 676 | 14 | 0 |
| 52 | CX | 2130 | 0 | 2219 | 59 | 0 |
| 53 | UP | 422 | 0 | 457 | 19 | 0 |
| 54 | Cz | 2259 | 0 | 2235 | 54 | 0 |
| 55 | UX | 1 | 0 | 0 | 0 | 0 |
| All | All | 180242 | 0 | 169110 | 5636 | 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 16.

All (5636) 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) |
|---|---|---|---|
| 48:UH:555:GLY:O | 48:UH:567:LEU:HA | 1.43 | 1.17 |
| 48:UH:557:GLU:O | 48:UH:565:GLY:HA2 | 1.45 | 1.16 |
| 44:C1:2238:A:N6 | 44:C1:2328:G:N3 | 1.97 | 1.10 |
| 17:UZ:133:LEU:O | 17:UZ:137:PHE:HB2 | 1.52 | 1.07 |
| 44:C1:2238:A:H62 | 44:C1:2328:G:N2 | 1.53 | 1.07 |
| 44:C1:2237:G:H1 | 44:C1:2329:A:N6 | 1.53 | 1.04 |
| 14:UR:559:SER:O | 14:UR:565:ALA:HB3 | 1.58 | 1.03 |
| 48:UH:557:GLU:O | 48:UH:565:GLY:CA | 2.08 | 1.02 |
| 44:C1:306:G:H1 | 44:C1:334:U:H3 | 1.03 | 0.99 |
| 44:C1:1702:G:H1 | 45:C2:7:A:N6 | 1.61 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:559:GLU:O | 46:UV:563:CYS:HB2 | 1.65 | 0.97 |
| 44:C1:2238:A:N6 | 44:C1:2328:G:C2 | 2.33 | 0.96 |
| 44:C1:1702:G:H1 | 45:C2:7:A:H61 | 1.00 | 0.95 |
| 10:UM:666:PHE:HB2 | 10:UM:678:TRP:O | 1.66 | 0.95 |
| 45:C2:85:A:N6 | 45:C2:264:G:N3 | 2.15 | 0.94 |
| 44:C1:5:G:H1 | 44:C1:30:U:H3 | 1.15 | 0.94 |
| 24:CI:269:GLU:HA | 24:CI:779:LEU:O | 1.70 | 0.92 |
| 44:C1:619:U:O2 | 44:C1:1052:A:N6 | 2.04 | 0.91 |
| 45:C2:137:U:H3 | 45:C2:150:G:H1 | 0.95 | 0.90 |
| 45:C2:103:G:O6 | 45:C2:250:G:C6 | 2.24 | 0.90 |
| 32:CS:509:GLY:N | 32:CS:644:TYR:HH | 1.68 | 0.90 |
| 15:UU:189:ALA:HA | 15:UU:200:PHE:O | 1.70 | 0.89 |
| 49:UE:268:ALA:HB1 | 49:UI:223:VAL:HG22 | 1.54 | 0.89 |
| 44:C1:2237:G:H1 | 44:C1:2329:A:H61 | 0.89 | 0.89 |
| 15:UU:715:PHE:CE2 | 15:UU:722:ILE:HD12 | 2.08 | 0.89 |
| 32:CR:509:GLY:N | 32:CR:644:TYR:HH | 1.72 | 0.88 |
| 44:C1:2238:A:N6 | 44:C1:2328:G:N2 | 2.22 | 0.88 |
| 5:UF:2:ALA:N | 45:C2:39:U:HO2' | 1.72 | 0.87 |
| 9:UL:713:SER:O | 9:UL:720:ILE:HA | 1.75 | 0.87 |
| 15:UU:715:PHE:HE2 | 15:UU:722:ILE:HD12 | 1.36 | 0.87 |
| 14:UR:430:ASN:O | 14:UR:446:MET:HB3 | 1.74 | 0.87 |
| 27:CL:781:GLY:O | 27:CL:785:LEU:HB2 | 1.76 | 0.85 |
| 44:C1:619:U:C2 | 44:C1:1052:A:N6 | 2.44 | 0.85 |
| 24:CI:914:ILE:HB | 24:CI:995:VAL:O | 1.78 | 0.84 |
| 44:C1:2238:A:N6 | 44:C1:2328:G:H21 | 1.74 | 0.83 |
| 45:C2:103:G:C6 | 45:C2:250:G:C6 | 2.65 | 0.83 |
| 46:UV:1058:TYR:HB2 | 47:CV:91:HIS:HA | 1.60 | 0.83 |
| 44:C1:2358:U:H3 | 44:C1:2369:G:H1 | 0.83 | 0.83 |
| 54:Cz:1652:ASP:O | 54:Cz:1656:TYR:HB3 | 1.79 | 0.83 |
| 48:UH:781:SER:HB2 | 49:UI:262:LYS:HD3 | 1.59 | 0.82 |
| 21:CE:39:ASN:ND2 | 45:C2:84:G:N7 | 2.26 | 0.82 |
| 29:CO:133:THR:O | 29:CO:137:PHE:HB2 | 1.79 | 0.82 |
| 23:CH:219:ARG:HH22 | 23:CH:249:ASP:HB2 | 1.46 | 0.81 |
| 39:Cj:9:VAL:HG21 | 39:Cj:88:SER:HA | 1.62 | 0.81 |
| 9:UL:534:PHE:HB2 | 9:UL:560:ARG:O | 1.80 | 0.81 |
| 1:UA:419:THR:O | 44:C1:2214:A:N6 | 2.15 | 0.80 |
| 9:UL:511:VAL:HA | 9:UL:527:GLY:HA2 | 1.62 | 0.80 |
| 44:C1:460:U:H3 | 44:C1:472:G:H1 | 1.30 | 0.79 |
| 31:CQ:86:PRO:HA | 31:CQ:120:LYS:O | 1.81 | 0.79 |
| 8:UK:97:SER:HG | 44:C1:233:C:HO2' | 1.31 | 0.78 |
| 16:UX:55:PRO:HA | 16:UX:86:SER:O | 1.84 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:CC:179:GLN:HE21 | 20:CD:185:ARG:HD3 | 1.49 | 0.78 |
| 29:CN:112:ILE:HB | 29:CN:124:VAL:HB | 1.64 | 0.78 |
| 33:CT:124:LYS:HB3 | 33:CT:126:ASN:HD21 | 1.47 | 0.78 |
| 44:C1:495:G:N7 | 44:C1:503:G:N1 | 2.31 | 0.77 |
| 35:Ce:163:ILE:HA | 35:Ce:194:GLU:O | 1.83 | 0.77 |
| 13:UQ:737:MET:HG2 | 13:UQ:746:MET:HB3 | 1.66 | 0.77 |
| 15:UU:190:ILE:CD1 | 15:UU:237:PRO:HD3 | 2.14 | 0.77 |
| 32:CR:880:GLN:HE21 | 32:CR:915:ILE:HG12 | 1.50 | 0.77 |
| 12:UO:534:VAL:HG11 | 49:UE:260:LYS:HE2 | 1.67 | 0.77 |
| 45:C2:87:G:C2 | 45:C2:263:U:O2 | 2.37 | 0.77 |
| 49:UI:278:MET:N | 49:UI:278:MET:SD | 2.58 | 0.76 |
| 28:CM:233:VAL:HG12 | 28:CM:234:ILE:HG12 | 1.68 | 0.76 |
| 45:C2:127:A:N7 | 45:C2:187:U:O4 | 2.18 | 0.76 |
| 14:UR:261:ILE:H | 14:UR:579:ASN:HD21 | 1.32 | 0.76 |
| 15:UU:224:PRO:HB3 | 15:UU:248:TYR:OH | 1.85 | 0.76 |
| 6:UG:95:ASN:H | 6:UG:427:ASN:HD21 | 1.33 | 0.76 |
| 49:UE:278:MET:N | 49:UE:278:MET:SD | 2.58 | 0.76 |
| 9:UL:443:SER:HB3 | 9:UL:450:LYS:O | 1.85 | 0.76 |
| 1:UA:563:ARG:HH22 | 16:UX:-2:ARG:HB2 | 1.49 | 0.76 |
| 18:CB:250:GLY:HA2 | 18:CB:306:TYR:O | 1.86 | 0.76 |
| 7:UJ:603:PRO:HA | 7:UJ:671:GLU:HG2 | 1.68 | 0.75 |
| 8:UK:126:LEU:HB3 | 8:UK:223:VAL:HG12 | 1.66 | 0.75 |
| 32:CS:880:GLN:HE21 | 32:CS:915:ILE:HG12 | 1.50 | 0.75 |
| 44:C1:1166:U:H1' | 44:C1:1169:A:H62 | 1.51 | 0.75 |
| 44:C1:1625:G:N2 | 44:C1:1663:U:O2 | 2.19 | 0.75 |
| 9:UL:929:MET:SD | 9:UL:932:ARG:NH2 | 2.60 | 0.75 |
| 2:UB:89:GLU:HG2 | 27:CL:535:GLU:HG3 | 1.67 | 0.75 |
| 20:CD:346:HIS:NE2 | 45:C2:90:C:N3 | 2.35 | 0.75 |
| 15:UU:190:ILE:HD13 | 15:UU:237:PRO:HD3 | 1.66 | 0.74 |
| 15:UU:224:PRO:HB3 | 15:UU:248:TYR:CZ | 2.22 | 0.74 |
| 16:UX:133:CYS:SG | 16:UX:137:ARG:NH2 | 2.59 | 0.74 |
| 44:C1:1448:A:N6 | 44:C1:1549:U:C4 | 2.55 | 0.74 |
| 7:UJ:715:VAL:HG12 | 7:UJ:748:LEU:HG | 1.68 | 0.74 |
| 54:Cz:1706:SER:HB2 | 54:Cz:1711:PRO:HD2 | 1.69 | 0.74 |
| 46:UV:71:ILE:HG22 | 46:UV:117:PRO:HG3 | 1.69 | 0.74 |
| 41:Cn:102:VAL:HG22 | 41:Cn:127:VAL:HG22 | 1.68 | 0.74 |
| 4:UD:506:ARG:NH1 | 4:UD:507:VAL:O | 2.20 | 0.74 |
| 6:UG:198:LYS:NZ | 44:C1:290:C:N3 | 2.36 | 0.74 |
| 16:UX:123:CYS:HB3 | 16:UX:137:ARG:HH22 | 1.53 | 0.74 |
| 1:UA:448:PHE:HB2 | 26:CK:135:ARG:HH11 | 1.53 | 0.73 |
| 44:C1:1546:U:H2' | 44:C1:1547:C:H5 | 1.54 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:UB:796:ARG:HH12 | 50:US:435:GLY:HA2 | 1.51 | 0.73 |
| 13:UQ:112:GLN:NE2 | 13:UQ:114:TYR:OH | 2.21 | 0.73 |
| 24:CI:59:VAL:HG23 | 24:CI:239:ASN:HD22 | 1.53 | 0.73 |
| 9:UL:291:ASP:HB3 | 9:UL:307:ILE:HB | 1.71 | 0.73 |
| 24:CI:1108:ARG:NH1 | 44:C1:1071:G:N7 | 2.37 | 0.73 |
| 45:C2:86:U:O4 | 45:C2:264:G:N2 | 2.20 | 0.73 |
| 45:C2:200:U:H3 | 45:C2:246:G:H1 | 1.36 | 0.73 |
| 15:UU:244:LEU:O | 15:UU:255:ILE:HA | 1.88 | 0.73 |
| 22:CG:586:MET:HE1 | 22:CG:592:LYS:H | 1.52 | 0.73 |
| 8:UK:268:ARG:NH1 | 14:UR:539:LEU:O | 2.21 | 0.73 |
| 9:UL:201:TRP:HA | 9:UL:208:CYS:HA | 1.71 | 0.73 |
| 10:UM:762:LEU:HD11 | 10:UM:805:GLN:HB3 | 1.71 | 0.73 |
| 15:UU:96:ALA:HB3 | 15:UU:107:ALA:HB3 | 1.69 | 0.73 |
| 2:UB:584:LEU:HG | 2:UB:625:LYS:HD2 | 1.70 | 0.73 |
| 35:Ce:76:PHE:O | 35:Ce:80:GLN:HB2 | 1.89 | 0.73 |
| 1:UA:170:SER:OG | 1:UA:171:LYS:N | 2.22 | 0.73 |
| 44:C1:619:U:H3 | 44:C1:1052:A:H62 | 1.36 | 0.73 |
| 25:CJ:96:ALA:O | 25:CJ:100:ASN:HB3 | 1.89 | 0.73 |
| 48:UH:555:GLY:O | 48:UH:567:LEU:CA | 2.31 | 0.73 |
| 18:CA:222:MET:HE3 | 19:CC:135:ARG:HD2 | 1.71 | 0.72 |
| 28:CM:122:LYS:HD3 | 28:CM:138:TYR:HB2 | 1.71 | 0.72 |
| 28:CM:156:TYR:HA | 28:CM:172:SER:HA | 1.70 | 0.72 |
| 1:UA:544:GLN:OE1 | 39:Cj:114:ARG:NH2 | 2.22 | 0.72 |
| 12:UO:214:VAL:HG13 | 12:UO:235:ILE:HD13 | 1.70 | 0.72 |
| 18:CB:156:VAL:HG22 | 18:CB:225:VAL:HB | 1.71 | 0.72 |
| 24:CI:537:TRP:HB3 | 24:CI:561:ARG:HA | 1.71 | 0.72 |
| 18:CA:182:ALA:O | 18:CA:206:ILE:HB | 1.89 | 0.72 |
| 15:UU:671:CYS:O | 15:UU:672:ARG:NH2 | 2.21 | 0.72 |
| 26:CK:47:ALA:O | 26:CK:53:ARG:NH2 | 2.23 | 0.72 |
| 2:UB:534:ILE:HG12 | 2:UB:552:LEU:HD21 | 1.71 | 0.72 |
| 23:CH:251:HIS:HB3 | 43:CU:111:MET:HG2 | 1.71 | 0.72 |
| 1:UA:258:LEU:HA | 1:UA:274:PHE:HA | 1.71 | 0.72 |
| 29:CO:161:LYS:NZ | 29:CO:162:VAL:O | 2.23 | 0.72 |
| 7:UJ:780:ASP:HA | 7:UJ:812:ARG:HE | 1.54 | 0.72 |
| 21:CE:43:LYS:NZ | 45:C2:263:U:OP2 | 2.21 | 0.72 |
| 46:UV:1054:LEU:HA | 47:CV:90:GLU:HB3 | 1.70 | 0.72 |
| 14:UR:170:GLU:HG3 | 14:UR:173:ARG:HH22 | 1.55 | 0.72 |
| 32:CR:111:GLU:O | 32:CR:114:LYS:NZ | 2.23 | 0.72 |
| 46:UV:55:GLU:HG2 | 46:UV:217:LYS:HD2 | 1.71 | 0.72 |
| 44:C1:1472:A:H2 | 44:C1:1510:G:H1 | 1.32 | 0.72 |
| 2:UB:759:HIS:O | 2:UB:765:ASN:ND2 | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:UD:378:PRO:HB3 | 4:UD:841:ILE:HA | 1.70 | 0.71 |
| 44:C1:1735:A:H2' | 44:C1:1736:A:H8 | 1.54 | 0.71 |
| 1:UA:356:VAL:HG21 | 1:UA:397:LEU:HD11 | 1.72 | 0.71 |
| 49:UE:269:GLN:HA | 49:UE:272:TYR:HB3 | 1.71 | 0.71 |
| 14:UR:400:ILE:HB | 14:UR:410:ALA:HB3 | 1.70 | 0.71 |
| 15:UU:282:ARG:NE | 15:UU:284:ASP:OD2 | 2.22 | 0.71 |
| 19:CC:212:ILE:HG23 | 19:CC:213:VAL:HG13 | 1.71 | 0.71 |
| 44:C1:1213:U:O2 | 44:C1:1555:A:N7 | 2.24 | 0.71 |
| 45:C2:65:C:H2' | 45:C2:66:A:H8 | 1.54 | 0.71 |
| 24:CI:754:LYS:O | 24:CI:758:ALA:HB2 | 1.90 | 0.71 |
| 31:CQ:92:MET:SD | 31:CQ:120:LYS:NZ | 2.63 | 0.71 |
| 4:UD:118:LYS:HD2 | 53:UP:330:ARG:HH22 | 1.55 | 0.71 |
| 8:UK:1:MET:HG2 | 8:UK:4:LEU:HG | 1.73 | 0.71 |
| 15:UU:412:GLY:O | 15:UU:415:ARG:N | 2.23 | 0.71 |
| 24:CI:173:LEU:HB2 | 24:CI:207:SER:HA | 1.72 | 0.71 |
| 33:CT:173:LYS:HG2 | 33:CT:176:ARG:HH11 | 1.56 | 0.71 |
| 29:CN:175:CYS:SG | 29:CN:176:ARG:N | 2.64 | 0.71 |
| 44:C1:2175:A:H2' | 44:C1:2176:A:C8 | 2.26 | 0.71 |
| 29:CO:99:LEU:HD13 | 29:CO:112:ILE:HG12 | 1.73 | 0.71 |
| 44:C1:26:C:C4 | 44:C1:27:A:N6 | 2.59 | 0.71 |
| 44:C1:1759:U:O4 | 44:C1:2047:G:O6 | 2.08 | 0.71 |
| 10:UM:486:ALA:HB1 | 10:UM:552:ILE:HG23 | 1.73 | 0.70 |
| 12:UO:532:ARG:O | 12:UO:536:LYS:NZ | 2.24 | 0.70 |
| 9:UL:633:ILE:O | 9:UL:642:HIS:N | 2.23 | 0.70 |
| 12:UO:543:THR:HG22 | 12:UO:546:MET:HE2 | 1.71 | 0.70 |
| 26:CK:173:ARG:HH21 | 26:CK:181:LYS:HB2 | 1.56 | 0.70 |
| 46:UV:408:PRO:HG2 | 46:UV:484:ARG:HH22 | 1.53 | 0.70 |
| 3:UC:636:SER:O | 33:CT:123:LYS:NZ | 2.20 | 0.70 |
| 25:CJ:64:LEU:HD23 | 25:CJ:71:ARG:HB2 | 1.73 | 0.70 |
| 46:UV:566:PHE:O | 46:UV:569:PHE:N | 2.23 | 0.70 |
| 6:UG:403:PHE:O | 28:CM:8:ARG:NH2 | 2.25 | 0.70 |
| 13:UQ:298:ILE:O | 13:UQ:310:GLN:N | 2.23 | 0.70 |
| 49:UI:269:GLN:HA | 49:UI:272:TYR:HB3 | 1.71 | 0.70 |
| 4:UD:139:PRO:HA | 4:UD:152:ARG:HH21 | 1.57 | 0.70 |
| 32:CR:116:LEU:HB3 | 32:CR:287:ARG:HH11 | 1.57 | 0.70 |
| 16:UX:155:ARG:NH2 | 44:C1:603:G:O2' | 2.24 | 0.70 |
| 18:CA:238:ILE:O | 18:CA:242:ASN:ND2 | 2.22 | 0.70 |
| 31:CQ:190:ILE:HG12 | 31:CQ:232:ILE:HD11 | 1.72 | 0.70 |
| 2:UB:828:ASN:HD21 | 2:UB:831:ARG:HH21 | 1.39 | 0.70 |
| 23:CH:218:ILE:HB | 23:CH:250:VAL:HG12 | 1.72 | 0.70 |
| 24:CI:90:ARG:HH22 | 32:CR:91:GLN:HA | 1.55 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:1745:C:H1' | 44:C1:2202:C:H42 | 1.55 | 0.70 |
| 13:UQ:160:CYS:SG | 13:UQ:161:SER:N | 2.63 | 0.70 |
| 15:UU:252:PRO:HA | 15:UU:267:LEU:O | 1.92 | 0.70 |
| 5:UF:338:HIS:O | 5:UF:363:ARG:NH1 | 2.24 | 0.70 |
| 32:CS:111:GLU:O | 32:CS:114:LYS:NZ | 2.23 | 0.70 |
| 32:CS:116:LEU:HB3 | 32:CS:287:ARG:HH11 | 1.57 | 0.70 |
| 12:UO:332:ARG:HG3 | 12:UO:333:HIS:HD2 | 1.56 | 0.70 |
| 29:CO:128:VAL:HB | 29:CO:159:LEU:HB3 | 1.74 | 0.70 |
| 7:UJ:259:MET:O | 7:UJ:268:GLN:NE2 | 2.24 | 0.69 |
| 44:C1:2175:A:H2' | 44:C1:2176:A:H8 | 1.55 | 0.69 |
| 1:UA:827:ARG:HG3 | 1:UA:831:ARG:HD3 | 1.75 | 0.69 |
| 6:UG:313:ARG:HG3 | 6:UG:373:LYS:HE2 | 1.74 | 0.69 |
| 24:CI:816:ARG:NH2 | 41:Cn:94:ASN:O | 2.25 | 0.69 |
| 28:CM:55:LYS:NZ | 45:C2:35:G:OP2 | 2.26 | 0.69 |
| 1:UA:558:ARG:HH11 | 1:UA:565:THR:HA | 1.55 | 0.69 |
| 4:UD:686:ARG:NH1 | 44:C1:63:C:O2 | 2.26 | 0.69 |
| 8:UK:28:LEU:O | 8:UK:30:LYS:NZ | 2.25 | 0.69 |
| 8:UK:246:LYS:HD2 | 44:C1:213:G:H4' | 1.74 | 0.69 |
| 15:UU:858:ASP:N | 15:UU:858:ASP:OD1 | 2.24 | 0.69 |
| 19:CC:155:LEU:O | 19:CC:159:HIS:ND1 | 2.23 | 0.69 |
| 29:CO:144:LEU:HD13 | 29:CO:150:ILE:HG12 | 1.73 | 0.69 |
| 12:UO:247:LEU:HB2 | 12:UO:260:LEU:HD11 | 1.74 | 0.69 |
| 12:UO:270:THR:OG1 | 49:UE:162:ARG:NH2 | 2.25 | 0.69 |
| 12:UO:495:ARG:HD2 | 49:UE:252:GLY:HA3 | 1.73 | 0.69 |
| 28:CM:143:ASN:ND2 | 28:CM:145:THR:O | 2.26 | 0.69 |
| 1:UA:68:ASN:OD1 | 1:UA:68:ASN:N | 2.25 | 0.69 |
| 15:UU:136:ASP:O | 15:UU:158:ARG:NH1 | 2.24 | 0.69 |
| 44:C1:1665:A:N3 | 44:C1:1666:C:N4 | 2.39 | 0.69 |
| 6:UG:209:GLU:N | 16:UX:5:ARG:O | 2.25 | 0.69 |
| 6:UG:284:LEU:HB2 | 6:UG:294:VAL:HG22 | 1.72 | 0.69 |
| 14:UR:487:SER:HG | 14:UR:490:GLY:H | 1.39 | 0.69 |
| 15:UU:235:LEU:HA | 15:UU:245:ALA:O | 1.92 | 0.69 |
| 44:C1:2048:C:H2' | 44:C1:2049:G:H8 | 1.58 | 0.69 |
| 9:UL:94:LEU:O | 9:UL:103:VAL:N | 2.25 | 0.69 |
| 21:CF:51:GLU:H | 21:CF:104:THR:HA | 1.58 | 0.68 |
| 32:CS:892:LYS:NZ | 32:CS:900:GLU:OE1 | 2.26 | 0.68 |
| 51:Cl:32:LEU:HA | 51:Cl:35:ILE:HD12 | 1.75 | 0.68 |
| 9:UL:488:GLU:HG2 | 9:UL:504:ASN:HA | 1.74 | 0.68 |
| 10:UM:104:VAL:HG12 | 10:UM:105:ARG:HG3 | 1.76 | 0.68 |
| 19:CC:179:GLN:HE22 | 20:CD:188:GLU:HB2 | 1.57 | 0.68 |
| 35:Ce:67:PHE:HA | 35:Ce:99:LEU:O | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:UD:619:LYS:HA | 4:UD:622:MET:HE2 | 1.74 | 0.68 |
| 6:UG:310:ARG:NH1 | 28:CM:30:GLU:O | 2.22 | 0.68 |
| 4:UD:647:LEU:O | 4:UD:658:ILE:HA | 1.94 | 0.68 |
| 15:UU:112:ARG:HH11 | 15:UU:140:PRO:HG3 | 1.58 | 0.68 |
| 16:UX:162:GLY:H | 16:UX:177:ARG:HH22 | 1.42 | 0.68 |
| 29:CN:179:THR:HG22 | 29:CN:221:VAL:HG11 | 1.75 | 0.68 |
| 48:UH:883:ARG:NH2 | 48:UH:884:SER:O | 2.25 | 0.68 |
| 2:UB:701:GLN:HB3 | 50:US:543:ASP:HB2 | 1.74 | 0.68 |
| 4:UD:707:LEU:O | 4:UD:828:HIS:HA | 1.91 | 0.68 |
| 18:CA:247:LEU:O | 19:CC:132:ARG:NH2 | 2.24 | 0.68 |
| 24:CI:861:LYS:NZ | 44:C1:1161:G:N7 | 2.41 | 0.68 |
| 46:UV:1059:ASP:N | 47:CV:92:SER:O | 2.24 | 0.68 |
| 9:UL:864:PHE:O | 9:UL:868:GLU:HA | 1.93 | 0.68 |
| 18:CA:157:LEU:HB2 | 18:CA:223:VAL:HG21 | 1.74 | 0.68 |
| 50:US:302:MET:SD | 50:US:302:MET:N | 2.65 | 0.68 |
| 10:UM:545:LYS:HE3 | 10:UM:564:GLN:HB2 | 1.75 | 0.68 |
| 29:CN:80:MET:O | 29:CN:82:ARG:NH1 | 2.27 | 0.68 |
| 32:CR:58:TRP:HB2 | 32:CR:104:ILE:HD11 | 1.76 | 0.68 |
| 44:C1:301:U:H2' | 44:C1:302:A:H8 | 1.58 | 0.68 |
| 44:C1:460:U:O2 | 44:C1:472:G:N2 | 2.26 | 0.68 |
| 12:UO:433:TYR:OH | 12:UO:463:ARG:NH2 | 2.26 | 0.68 |
| 32:CS:58:TRP:HB2 | 32:CS:104:ILE:HD11 | 1.76 | 0.68 |
| 49:UI:179:LEU:N | 49:UI:182:GLN:OE1 | 2.27 | 0.68 |
| 3:UC:644:LYS:NZ | 18:CA:143:GLY:O | 2.27 | 0.68 |
| 15:UU:731:ILE:O | 15:UU:744:ALA:HA | 1.93 | 0.68 |
| 17:UZ:64:LEU:HD11 | 17:UZ:281:PHE:HB3 | 1.76 | 0.68 |
| 17:UZ:265:GLU:O | 17:UZ:269:ARG:HB3 | 1.94 | 0.68 |
| 23:CH:154:ARG:HA | 23:CH:158:LEU:HD23 | 1.76 | 0.68 |
| 24:CI:964:ARG:NH2 | 44:C1:2182:C:OP1 | 2.27 | 0.68 |
| 25:CJ:96:ALA:O | 25:CJ:100:ASN:CB | 2.42 | 0.68 |
| 29:CN:43:ASN:ND2 | 29:CN:209:MET:SD | 2.66 | 0.68 |
| 46:UV:1058:TYR:N | 47:CV:90:GLU:O | 2.26 | 0.68 |
| 49:UE:236:ILE:O | 49:UE:240:THR:N | 2.27 | 0.68 |
| 17:UZ:138:LYS:NZ | 44:C1:2107:A:OP1 | 2.27 | 0.67 |
| 18:CA:230:VAL:O | 18:CA:235:GLN:NE2 | 2.27 | 0.67 |
| 31:CQ:212:ALA:HB3 | 31:CQ:215:LYS:HE3 | 1.76 | 0.67 |
| 32:CR:892:LYS:NZ | 32:CR:900:GLU:OE1 | 2.26 | 0.67 |
| 44:C1:5:G:N2 | 44:C1:30:U:O2 | 2.27 | 0.67 |
| 44:C1:1452:G:H1 | 44:C1:1546:U:H3 | 1.41 | 0.67 |
| 49:UE:159:GLN:NE2 | 50:US:335:ASP:O | 2.26 | 0.67 |
| 49:UI:236:ILE:O | 49:UI:240:THR:N | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:UH:585:HIS:O | 48:UH:590:ASN:ND2 | 2.26 | 0.67 |
| 36:Cg:118:LYS:H | 36:Cg:122:HIS:HD2 | 1.40 | 0.67 |
| 44:C1:2363:G:N7 | 44:C1:2365:A:N6 | 2.42 | 0.67 |
| 49:UE:179:LEU:N | 49:UE:182:GLN:OE1 | 2.27 | 0.67 |
| 4:UD:443:LEU:HB3 | 4:UD:454:PHE:HB2 | 1.77 | 0.67 |
| 9:UL:305:TRP:HA | 9:UL:360:HIS:H | 1.58 | 0.67 |
| 10:UM:64:ILE:HA | 10:UM:80:SER:HA | 1.75 | 0.67 |
| 13:UQ:926:LEU:HA | 13:UQ:929:ILE:HD12 | 1.77 | 0.67 |
| 24:CI:866:HIS:O | 44:C1:1156:C:N4 | 2.27 | 0.67 |
| 30:CP:50:TYR:O | 30:CP:54:CYS:HB2 | 1.93 | 0.67 |
| 31:CQ:91:ARG:NH2 | 31:CQ:150:PHE:O | 2.28 | 0.67 |
| 43:CU:126:ASP:N | 43:CU:126:ASP:OD1 | 2.28 | 0.67 |
| 44:C1:619:U:N3 | 44:C1:1052:A:N6 | 2.41 | 0.67 |
| 44:C1:2167:G:N2 | 44:C1:2194:A:OP2 | 2.27 | 0.67 |
| 1:UA:393:LYS:NZ | 1:UA:436:SER:O | 2.27 | 0.67 |
| 10:UM:396:GLU:OE1 | 10:UM:435:ILE:N | 2.27 | 0.67 |
| 14:UR:304:ASP:H | 14:UR:312:ASN:HD22 | 1.41 | 0.67 |
| 15:UU:53:SER:HA | 15:UU:62:GLN:O | 1.93 | 0.67 |
| 26:CK:223:SER:OG | 26:CK:224:GLY:N | 2.26 | 0.67 |
| 44:C1:1472:A:N1 | 44:C1:1510:G:C6 | 2.62 | 0.67 |
| 46:UV:330:LEU:HD13 | 46:UV:360:LEU:HD12 | 1.76 | 0.67 |
| 2:UB:652:ARG:HD3 | 50:US:467:TYR:HA | 1.76 | 0.67 |
| 4:UD:690:LYS:NZ | 4:UD:836:MET:O | 2.27 | 0.67 |
| 16:UX:114:ARG:NH2 | 28:CM:63:ASN:O | 2.28 | 0.67 |
| 18:CB:159:LEU:HB2 | 18:CB:228:ALA:HA | 1.75 | 0.67 |
| 18:CB:243:ALA:O | 20:CD:120:ARG:NH2 | 2.26 | 0.67 |
| 19:CC:178:ILE:HA | 19:CC:181:ILE:HD12 | 1.75 | 0.67 |
| 32:CR:495:CYS:HB3 | 32:CR:541:VAL:HG21 | 1.76 | 0.67 |
| 44:C1:75:G:H5' | 44:C1:76:U:H5" | 1.76 | 0.67 |
| 44:C1:1472:A:N1 | 44:C1:1510:G:O6 | 2.27 | 0.67 |
| 44:C1:2358:U:O2 | 44:C1:2369:G:N2 | 2.23 | 0.67 |
| 52:CX:371:LEU:HD21 | 52:CX:417:PHE:HB2 | 1.77 | 0.67 |
| 4:UD:684:ASP:HB2 | 4:UD:734:ARG:HD3 | 1.75 | 0.67 |
| 5:UF:284:ASP:O | 5:UF:288:LYS:NZ | 2.28 | 0.67 |
| 13:UQ:364:SER:O | 13:UQ:367:GLY:N | 2.28 | 0.67 |
| 15:UU:417:LEU:HD23 | 15:UU:431:LEU:HD22 | 1.75 | 0.67 |
| 24:CI:885:CYS:SG | 24:CI:886:CYS:N | 2.68 | 0.67 |
| 46:UV:656:ARG:HH22 | 46:UV:768:VAL:HG11 | 1.59 | 0.67 |
| 1:UA:706:PHE:O | 15:UU:677:ASN:ND2 | 2.28 | 0.67 |
| 9:UL:23:ASN:ND2 | 9:UL:71:THR:O | 2.28 | 0.67 |
| 9:UL:70:VAL:HA | 9:UL:87:TYR:HA | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:UU:713:PHE:C | 15:UU:714:CYS:SG | 2.78 | 0.67 |
| 24:CI:819:ARG:NH1 | 24:CI:823:HIS:O | 2.28 | 0.67 |
| 6:UG:139:PRO:HA | 6:UG:412:ASN:HA | 1.76 | 0.67 |
| 32:CS:495:CYS:HB3 | 32:CS:541:VAL:HG21 | 1.77 | 0.67 |
| 7:UJ:62:LEU:HD22 | 7:UJ:108:ARG:HE | 1.59 | 0.67 |
| 8:UK:86:THR:HG22 | 24:CI:1064:ILE:HB | 1.76 | 0.67 |
| 9:UL:117:ALA:HB3 | 9:UL:126:ALA:HB3 | 1.76 | 0.67 |
| 11:UN:929:ILE:HG23 | 28:CM:336:MET:HB3 | 1.77 | 0.67 |
| 16:UX:83:LEU:O | 36:Cg:51:ARG:NH1 | 2.28 | 0.67 |
| 51:Cl:14:ILE:HD12 | 51:Cl:22:VAL:HG13 | 1.76 | 0.67 |
| 1:UA:337:GLN:O | 1:UA:365:LYS:NZ | 2.28 | 0.66 |
| 7:UJ:16:SER:O | 7:UJ:159:ARG:NH2 | 2.28 | 0.66 |
| 9:UL:673:SER:OG | 9:UL:677:THR:OG1 | 2.13 | 0.66 |
| 19:CC:227:GLY:HA2 | 19:CC:275:ARG:HH22 | 1.60 | 0.66 |
| 49:UI:266:LEU:HA | 49:UI:269:GLN:HE22 | 1.60 | 0.66 |
| 1:UA:256:ALA:HB1 | 1:UA:275:SER:HB2 | 1.78 | 0.66 |
| 2:UB:572:ARG:NH1 | 50:US:508:GLU:O | 2.28 | 0.66 |
| 2:UB:723:ILE:HG23 | 2:UB:773:LEU:HD11 | 1.76 | 0.66 |
| 15:UU:424:ARG:NH1 | 44:C1:256:U:OP2 | 2.28 | 0.66 |
| 24:CI:380:GLN:NE2 | 32:CR:207:ASN:OD1 | 2.27 | 0.66 |
| 29:CO:114:ILE:HB | 29:CO:122:ILE:HB | 1.77 | 0.66 |
| 44:C1:253:G:H2' | 44:C1:254:G:C8 | 2.30 | 0.66 |
| 44:C1:265:G:C6 | 44:C1:274:A:N1 | 2.63 | 0.66 |
| 4:UD:309:GLN:HE21 | 4:UD:312:ARG:HG3 | 1.61 | 0.66 |
| 4:UD:395:HIS:HB2 | 4:UD:420:LEU:HD22 | 1.76 | 0.66 |
| 9:UL:589:VAL:HB | 9:UL:603:LEU:HB2 | 1.77 | 0.66 |
| 13:UQ:760:GLU:HA | 48:UH:543:ARG:HH22 | 1.59 | 0.66 |
| 23:CH:374:SER:HB3 | 24:CI:768:VAL:HG22 | 1.76 | 0.66 |
| 13:UQ:617:LEU:HA | 13:UQ:627:ALA:O | 1.95 | 0.66 |
| 17:UZ:284:LYS:NZ | 17:UZ:288:THR:O | 2.28 | 0.66 |
| 18:CB:245:LEU:O | 20:CD:123:ARG:NH2 | 2.26 | 0.66 |
| 20:CD:272:ARG:NH1 | 20:CD:273:GLN:OE1 | 2.27 | 0.66 |
| 26:CK:134:GLU:OE2 | 39:Cj:128:LYS:NZ | 2.27 | 0.66 |
| 44:C1:2057:G:H2' | 44:C1:2058:A:H8 | 1.61 | 0.66 |
| 47:CV:66:ARG:HH21 | 47:CV:78:PHE:HB2 | 1.60 | 0.66 |
| 9:UL:587:SER:HA | 9:UL:609:PRO:HA | 1.77 | 0.66 |
| 15:UU:463:PRO:O | 15:UU:515:HIS:ND1 | 2.28 | 0.66 |
| 24:CI:749:GLN:HE21 | 24:CI:753:ASN:HD22 | 1.43 | 0.66 |
| 1:UA:574:ASN:N | 1:UA:574:ASN:OD1 | 2.27 | 0.66 |
| 2:UB:3:GLY:O | 2:UB:8:ARG:NH2 | 2.28 | 0.66 |
| 2:UB:111:ASN:OD1 | 2:UB:111:ASN:N | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:UO:489:VAL:O | 12:UO:495:ARG:NH1 | 2.29 | 0.66 |
| 28:CM:271:ASN:ND2 | 28:CM:273:ASP:OD2 | 2.26 | 0.66 |
| 47:CV:49:ARG:HB2 | 47:CV:158:VAL:HG21 | 1.78 | 0.66 |
| 1:UA:336:GLN:NE2 | 1:UA:374:CYS:SG | 2.69 | 0.66 |
| 9:UL:563:LYS:HB3 | 43:CU:99:ASP:HA | 1.77 | 0.66 |
| 10:UM:749:ILE:HD12 | 10:UM:773:LEU:HD21 | 1.77 | 0.66 |
| 27:CL:636:TRP:O | 27:CL:637:HIS:ND1 | 2.29 | 0.66 |
| 44:C1:253:G:H2' | 44:C1:254:G:H8 | 1.60 | 0.66 |
| 1:UA:143:ARG:NH1 | 44:C1:261:G:OP2 | 2.29 | 0.66 |
| 4:UD:549:VAL:HA | 4:UD:565:ASP:HA | 1.78 | 0.66 |
| 12:UO:99:ASP:O | 51:Cl:57:ARG:NH1 | 2.27 | 0.66 |
| 18:CB:156:VAL:HA | 18:CB:225:VAL:O | 1.96 | 0.66 |
| 26:CK:152:ILE:HG23 | 26:CK:167:LEU:HD11 | 1.78 | 0.66 |
| 32:CR:512:ASP:OD2 | 32:CR:514:SER:OG | 2.13 | 0.66 |
| 32:CR:585:VAL:HG23 | 32:CR:639:ALA:HB3 | 1.78 | 0.66 |
| 45:C2:137:U:O2 | 45:C2:150:G:N2 | 2.25 | 0.66 |
| 4:UD:209:ILE:HB | 4:UD:223:MET:HB2 | 1.78 | 0.66 |
| 7:UJ:740:THR:HG22 | 7:UJ:742:THR:H | 1.60 | 0.66 |
| 18:CB:219:LEU:HD21 | 20:CD:149:LEU:HD21 | 1.78 | 0.66 |
| 23:CH:218:ILE:O | 23:CH:219:ARG:NH1 | 2.28 | 0.66 |
| 24:CI:864:PRO:HB2 | 24:CI:867:MET:HB3 | 1.76 | 0.66 |
| 36:Cg:78:LEU:HB3 | 36:Cg:84:LEU:HD23 | 1.78 | 0.66 |
| 46:UV:577:ARG:HH21 | 46:UV:589:VAL:HG22 | 1.61 | 0.66 |
| 46:UV:689:LYS:NZ | 46:UV:1040:LEU:O | 2.29 | 0.66 |
| 49:UE:153:LEU:N | 50:US:305:ASP:OD2 | 2.29 | 0.66 |
| 2:UB:572:ARG:NH2 | 50:US:504:GLU:O | 2.28 | 0.66 |
| 16:UX:114:ARG:NH1 | 28:CM:65:HIS:O | 2.29 | 0.66 |
| 26:CK:150:THR:O | 26:CK:167:LEU:N | 2.27 | 0.66 |
| 30:CP:95:ALA:HA | 30:CP:98:LEU:HD12 | 1.78 | 0.66 |
| 44:C1:181:G:H3' | 44:C1:182:C:H4' | 1.78 | 0.66 |
| 44:C1:191:C:O2' | 44:C1:192:A:N7 | 2.29 | 0.66 |
| 44:C1:1735:A:H2' | 44:C1:1736:A:C8 | 2.30 | 0.66 |
| 44:C1:2048:C:H2' | 44:C1:2049:G:C8 | 2.31 | 0.66 |
| 7:UJ:189:ARG:NH2 | 45:C2:70:A:OP1 | 2.29 | 0.65 |
| 18:CA:68:GLY:H | 33:CT:140:ILE:HB | 1.61 | 0.65 |
| 23:CH:339:MET:HE1 | 23:CH:349:LEU:HB2 | 1.78 | 0.65 |
| 24:CI:939:ASN:HD22 | 27:CL:513:VAL:HA | 1.61 | 0.65 |
| 32:CS:512:ASP:OD2 | 32:CS:514:SER:OG | 2.13 | 0.65 |
| 46:UV:79:ALA:HB1 | 46:UV:111:LYS:HD3 | 1.78 | 0.65 |
| 49:UE:182:GLN:O | 49:UE:186:ASN:ND2 | 2.26 | 0.65 |
| 49:UE:241:GLU:O | 49:UE:245:VAL:N | 2.28 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:407:ARG:HE | 1:UA:416:ASN:HD22 | 1.44 | 0.65 |
| 9:UL:799:TRP:NE1 | 9:UL:810:ALA:O | 2.27 | 0.65 |
| 29:CO:67:LEU:HD11 | 29:CO:141:MET:HB2 | 1.78 | 0.65 |
| 29:CO:113:TYR:HA | 29:CO:122:ILE:O | 1.96 | 0.65 |
| 48:UH:928:GLU:O | 48:UH:930:ARG:NH1 | 2.27 | 0.65 |
| 49:UI:241:GLU:O | 49:UI:245:VAL:N | 2.28 | 0.65 |
| 1:UA:519:ARG:NH1 | 1:UA:524:GLN:OE1 | 2.29 | 0.65 |
| 15:UU:982:LEU:HD22 | 15:UU:1022:HIS:HB3 | 1.77 | 0.65 |
| 21:CE:33:GLN:NE2 | 21:CE:104:THR:O | 2.30 | 0.65 |
| 21:CF:111:LEU:HA | 21:CF:114:LYS:HD2 | 1.77 | 0.65 |
| 23:CH:9:LEU:HB3 | 23:CH:31:ILE:HG22 | 1.76 | 0.65 |
| 24:CI:267:THR:HA | 24:CI:781:ILE:O | 1.96 | 0.65 |
| 49:UE:266:LEU:HA | 49:UE:269:GLN:HE22 | 1.60 | 0.65 |
| 3:UC:616:ARG:NH1 | 44:C1:1086:U:OP2 | 2.30 | 0.65 |
| 14:UR:430:ASN:O | 14:UR:446:MET:CB | 2.43 | 0.65 |
| 26:CK:76:GLU:OE2 | 26:CK:203:ARG:NH2 | 2.29 | 0.65 |
| 32:CS:585:VAL:HG23 | 32:CS:639:ALA:HB3 | 1.78 | 0.65 |
| 12:UO:385:LYS:NZ | 12:UO:386:ARG:O | 2.29 | 0.65 |
| 15:UU:192:MET:HE2 | 15:UU:192:MET:HA | 1.78 | 0.65 |
| 32:CS:278:ARG:NH2 | 32:CS:433:ARG:O | 2.27 | 0.65 |
| 12:UO:98:PHE:O | 51:Cl:57:ARG:NH2 | 2.29 | 0.65 |
| 24:CI:953:ARG:NH1 | 44:C1:1141:G:OP1 | 2.29 | 0.65 |
| 45:C2:259:A:N3 | 45:C2:260:G:N1 | 2.44 | 0.65 |
| 46:UV:716:ARG:HA | 46:UV:719:ILE:HD12 | 1.79 | 0.65 |
| 50:US:524:PHE:O | 50:US:526:LYS:NZ | 2.23 | 0.65 |
| 1:UA:404:GLY:O | 1:UA:421:THR:HG22 | 1.96 | 0.65 |
| 4:UD:765:GLY:O | 4:UD:768:TRP:NE1 | 2.30 | 0.65 |
| 9:UL:678:ILE:HB | 9:UL:692:ILE:HB | 1.78 | 0.65 |
| 15:UU:192:MET:HE2 | 15:UU:192:MET:CA | 2.27 | 0.65 |
| 33:CT:187:SER:OG | 33:CT:188:GLY:N | 2.27 | 0.65 |
| 1:UA:112:VAL:HG22 | 1:UA:157:LEU:HD13 | 1.79 | 0.65 |
| 4:UD:188:LYS:NZ | 44:C1:191:C:OP1 | 2.30 | 0.65 |
| 10:UM:15:ASN:H | 10:UM:719:PHE:HB2 | 1.62 | 0.65 |
| 16:UX:58:VAL:HG12 | 16:UX:145:ILE:HB | 1.77 | 0.65 |
| 23:CH:154:ARG:NH1 | 43:CU:121:SER:O | 2.29 | 0.65 |
| 26:CK:238:GLU:OE2 | 26:CK:240:ARG:NH2 | 2.30 | 0.65 |
| 4:UD:274:SER:OG | 4:UD:275:HIS:N | 2.27 | 0.65 |
| 4:UD:686:ARG:NH2 | 4:UD:745:SER:OG | 2.25 | 0.65 |
| 9:UL:49:VAL:HG13 | 9:UL:58:LEU:HB2 | 1.77 | 0.65 |
| 16:UX:77:GLU:O | 36:Cg:55:ARG:NH1 | 2.29 | 0.65 |
| 44:C1:22:U:H2' | 44:C1:23:G:H8 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:345:U:N3 | 44:C1:346:C:N4 | 2.44 | 0.65 |
| 44:C1:1625:G:H2' | 44:C1:1626:G:C8 | 2.32 | 0.65 |
| 44:C1:1747:A:N3 | 44:C1:2196:U:O2' | 2.29 | 0.65 |
| 46:UV:829:PRO:HA | 46:UV:832:ARG:HD2 | 1.79 | 0.65 |
| 2:UB:557:HIS:HD1 | 2:UB:600:THR:HG22 | 1.62 | 0.65 |
| 6:UG:125:VAL:HG23 | 6:UG:128:LYS:HD2 | 1.79 | 0.65 |
| 7:UJ:817:TRP:O | 7:UJ:825:LYS:NZ | 2.30 | 0.65 |
| 13:UQ:371:ILE:HG22 | 13:UQ:381:LEU:HG | 1.79 | 0.65 |
| 28:CM:193:TRP:HB3 | 28:CM:196:PHE:HB2 | 1.79 | 0.65 |
| 44:C1:1180:C:H2' | 44:C1:1181:G:H8 | 1.62 | 0.65 |
| 8:UK:113:ARG:NH2 | 45:C2:264:G:OP1 | 2.29 | 0.64 |
| 15:UU:302:THR:OG1 | 15:UU:303:SER:N | 2.29 | 0.64 |
| 17:UZ:63:TRP:HB3 | 17:UZ:244:LYS:HA | 1.79 | 0.64 |
| 20:CD:220:ALA:O | 20:CD:238:LYS:NZ | 2.30 | 0.64 |
| 46:UV:1056:ALA:N | 47:CV:91:HIS:O | 2.30 | 0.64 |
| 51:Cl:25:LYS:HA | 51:Cl:58:ALA:HB3 | 1.79 | 0.64 |
| 1:UA:203:PHE:HA | 1:UA:210:ILE:HG22 | 1.79 | 0.64 |
| 12:UO:126:PHE:HB3 | 12:UO:136:ILE:HA | 1.79 | 0.64 |
| 15:UU:141:ILE:HA | 15:UU:155:ALA:HA | 1.80 | 0.64 |
| 15:UU:197:ASN:ND2 | 20:CD:445:ASP:O | 2.30 | 0.64 |
| 15:UU:723:VAL:HG13 | 15:UU:733:VAL:HG22 | 1.78 | 0.64 |
| 25:CJ:110:ARG:NH2 | 25:CJ:146:PRO:O | 2.31 | 0.64 |
| 43:CU:198:THR:HA | 43:CU:201:ILE:HD12 | 1.79 | 0.64 |
| 15:UU:581:SER:OG | 15:UU:582:ARG:N | 2.28 | 0.64 |
| 18:CA:96:ASN:HB2 | 18:CA:128:ARG:HG3 | 1.79 | 0.64 |
| 18:CB:222:MET:SD | 20:CD:123:ARG:NH2 | 2.70 | 0.64 |
| 39:Cj:6:ALA:HA | 39:Cj:23:VAL:HG12 | 1.79 | 0.64 |
| 1:UA:548:VAL:HG23 | 1:UA:604:MET:HE3 | 1.78 | 0.64 |
| 6:UG:355:LEU:HD12 | 6:UG:423:ALA:HB2 | 1.79 | 0.64 |
| 14:UR:462:GLY:O | 14:UR:488:ASN:N | 2.30 | 0.64 |
| 17:UZ:175:THR:OG1 | 17:UZ:176:THR:N | 2.30 | 0.64 |
| 20:CD:354:SER:H | 20:CD:357:ASN:HB2 | 1.61 | 0.64 |
| 23:CH:97:ALA:HA | 23:CH:129:ASN:HB3 | 1.79 | 0.64 |
| 25:CJ:33:ILE:HG12 | 25:CJ:38:ILE:HD12 | 1.79 | 0.64 |
| 28:CM:288:ASP:OD2 | 28:CM:331:ARG:NH1 | 2.30 | 0.64 |
| 32:CS:82:ILE:HD12 | 32:CS:89:PRO:HA | 1.79 | 0.64 |
| 36:Cg:133:ARG:HB3 | 36:Cg:138:ILE:HD13 | 1.79 | 0.64 |
| 1:UA:619:SER:OG | 1:UA:620:GLY:N | 2.30 | 0.64 |
| 18:CB:250:GLY:CA | 18:CB:306:TYR:O | 2.46 | 0.64 |
| 29:CO:112:ILE:HB | 29:CO:124:VAL:HB | 1.79 | 0.64 |
| 31:CQ:209:ILE:HG22 | 31:CQ:218:ILE:HG23 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 43:CU:205:THR:HG23 | 43:CU:209:ARG:HH22 | 1.60 | 0.64 |
| 44:C1:103:G:N2 | 44:C1:106:A:OP2 | 2.30 | 0.64 |
| 46:UV:237:ARG:HE | 46:UV:398:ARG:HD3 | 1.61 | 0.64 |
| 4:UD:646:ASP:HB3 | 4:UD:658:ILE:HD11 | 1.78 | 0.64 |
| 9:UL:451:ILE:HG12 | 9:UL:461:ARG:HB2 | 1.80 | 0.64 |
| 12:UO:418:ARG:NH2 | 44:C1:75:G:N7 | 2.45 | 0.64 |
| 18:CA:277:GLN:HE22 | 18:CA:280:ARG:HD2 | 1.62 | 0.64 |
| 24:CI:248:ASN:HD22 | 24:CI:337:PRO:HB2 | 1.62 | 0.64 |
| 26:CK:188:TYR:O | 26:CK:215:ARG:NH1 | 2.30 | 0.64 |
| 28:CM:220:ARG:NH1 | 28:CM:238:LEU:O | 2.31 | 0.64 |
| 32:CR:754:LEU:HG | 32:CR:755:THR:HG23 | 1.79 | 0.64 |
| 18:CB:174:VAL:HB | 18:CB:178:GLY:HA3 | 1.78 | 0.64 |
| 23:CH:152:THR:O | 23:CH:156:ALA:HB3 | 1.98 | 0.64 |
| 25:CJ:90:THR:OG1 | 25:CJ:91:LYS:N | 2.26 | 0.64 |
| 9:UL:200:LEU:HB3 | 9:UL:210:GLU:HB2 | 1.78 | 0.64 |
| 9:UL:673:SER:OG | 9:UL:675:ASP:OD1 | 2.16 | 0.64 |
| 46:UV:567:ARG:HH11 | 46:UV:586:GLU:HG2 | 1.62 | 0.64 |
| 46:UV:884:ALA:O | 46:UV:965:LYS:NZ | 2.27 | 0.64 |
| 10:UM:336:CYS:HB3 | 10:UM:344:VAL:HB | 1.79 | 0.64 |
| 16:UX:14:ARG:NH2 | 25:CJ:26:ASN:O | 2.30 | 0.64 |
| 18:CA:287:LYS:NZ | 18:CA:309:LYS:O | 2.27 | 0.64 |
| 18:CB:152:PRO:HA | 18:CB:174:VAL:HA | 1.80 | 0.64 |
| 45:C2:87:G:N1 | 45:C2:263:U:C2 | 2.66 | 0.64 |
| 5:UF:135:ARG:NH2 | 19:CC:85:ASN:O | 2.30 | 0.64 |
| 24:CI:262:PRO:O | 24:CI:266:ARG:NH2 | 2.31 | 0.64 |
| 26:CK:246:ARG:HA | 26:CK:252:VAL:HG23 | 1.80 | 0.64 |
| 28:CM:50:GLU:OE2 | 28:CM:51:ARG:NH2 | 2.31 | 0.64 |
| 50:US:258:LEU:HA | 50:US:261:HIS:HD2 | 1.63 | 0.64 |
| 1:UA:55:ARG:NH1 | 1:UA:614:VAL:O | 2.31 | 0.63 |
| 29:CN:49:TYR:O | 29:CN:65:TYR:HA | 1.98 | 0.63 |
| 34:Cc:99:ARG:NH2 | 44:C1:2112:C:OP2 | 2.31 | 0.63 |
| 4:UD:633:LEU:HD13 | 4:UD:649:VAL:HG22 | 1.78 | 0.63 |
| 4:UD:690:LYS:H | 4:UD:703:GLY:HA2 | 1.62 | 0.63 |
| 6:UG:332:PHE:HB3 | 11:UN:869:VAL:HG21 | 1.78 | 0.63 |
| 8:UK:67:MET:HE1 | 25:CJ:170:ILE:HG12 | 1.81 | 0.63 |
| 11:UN:366:GLY:N | 11:UN:370:GLU:OE1 | 2.30 | 0.63 |
| 21:CF:90:ARG:HH22 | 22:CG:586:MET:HG2 | 1.61 | 0.63 |
| 2:UB:330:LYS:O | 2:UB:333:GLN:NE2 | 2.31 | 0.63 |
| 7:UJ:309:LEU:HA | 7:UJ:312:LEU:HD12 | 1.79 | 0.63 |
| 18:CA:96:ASN:ND2 | 18:CA:98:VAL:O | 2.28 | 0.63 |
| 29:CO:103:PRO:HA | 29:CO:106:LYS:HB2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:453:TRP:HD1 | 1:UA:460:LEU:HA | 1.63 | 0.63 |
| 12:UO:407:THR:HG22 | 14:UR:321:LYS:HB3 | 1.80 | 0.63 |
| 15:UU:161:VAL:HG23 | 15:UU:170:TYR:HB3 | 1.81 | 0.63 |
| 24:CI:1015:LEU:HD23 | 24:CI:1017:GLY:H | 1.63 | 0.63 |
| 44:C1:250:U:H2' | 44:C1:251:G:H8 | 1.64 | 0.63 |
| 49:UE:238:ARG:HG2 | 49:UE:238:ARG:HH21 | 1.63 | 0.63 |
| 15:UU:550:SER:OG | 15:UU:551:SER:N | 2.31 | 0.63 |
| 17:UZ:160:ILE:HA | 17:UZ:163:LEU:HD12 | 1.78 | 0.63 |
| 20:CD:217:ARG:NH2 | 20:CD:246:GLY:O | 2.32 | 0.63 |
| 22:CG:273:TYR:HB3 | 22:CG:281:ILE:H | 1.62 | 0.63 |
| 22:CG:301:ASN:HB3 | 22:CG:317:LEU:HB3 | 1.79 | 0.63 |
| 32:CR:82:ILE:HD12 | 32:CR:89:PRO:HA | 1.79 | 0.63 |
| 32:CS:754:LEU:HG | 32:CS:755:THR:HG23 | 1.80 | 0.63 |
| 1:UA:646:SER:O | 1:UA:651:ARG:NH2 | 2.32 | 0.63 |
| 24:CI:944:ILE:HD13 | 24:CI:973:PHE:HB3 | 1.80 | 0.63 |
| 24:CI:963:LYS:NZ | 44:C1:2181:U:OP2 | 2.28 | 0.63 |
| 47:CV:94:GLU:HG3 | 47:CV:98:ILE:HG13 | 1.81 | 0.63 |
| 1:UA:831:ARG:NH1 | 10:UM:875:GLU:OE2 | 2.32 | 0.63 |
| 4:UD:87:ASP:OD2 | 4:UD:97:HIS:ND1 | 2.31 | 0.63 |
| 4:UD:363:ARG:NH2 | 4:UD:686:ARG:O | 2.32 | 0.63 |
| 9:UL:473:PHE:HA | 9:UL:480:VAL:HA | 1.81 | 0.63 |
| 25:CJ:131:ILE:HG22 | 25:CJ:136:VAL:HG21 | 1.81 | 0.63 |
| 1:UA:626:ASN:HB3 | 44:C1:256:U:H2' | 1.80 | 0.63 |
| 2:UB:574:ARG:HG2 | 2:UB:593:ILE:HD13 | 1.81 | 0.63 |
| 7:UJ:77:GLN:HG3 | 14:UR:66:PHE:HB2 | 1.79 | 0.63 |
| 9:UL:955:LYS:O | 9:UL:956:ARG:NH1 | 2.31 | 0.63 |
| 10:UM:64:ILE:HD11 | 10:UM:78:VAL:HB | 1.80 | 0.63 |
| 32:CR:315:PRO:HA | 32:CR:374:PRO:HG3 | 1.81 | 0.63 |
| 44:C1:1480:G:H1 | 44:C1:1502:U:H3 | 1.46 | 0.63 |
| 45:C2:160:U:H2' | 45:C2:161:G:H8 | 1.61 | 0.63 |
| 1:UA:15:TYR:OH | 1:UA:18:GLY:O | 2.14 | 0.63 |
| 4:UD:366:PRO:HG3 | 4:UD:704:VAL:HG21 | 1.81 | 0.63 |
| 12:UO:89:ARG:NH2 | 12:UO:347:THR:OG1 | 2.32 | 0.63 |
| 13:UQ:524:VAL:HG12 | 13:UQ:526:ILE:H | 1.63 | 0.63 |
| 24:CI:619:LEU:O | 24:CI:623:ARG:HB2 | 1.99 | 0.63 |
| 43:CU:197:ALA:HA | 43:CU:200:ARG:HD2 | 1.80 | 0.63 |
| 4:UD:7:ARG:NH2 | 48:UH:901:SER:O | 2.32 | 0.62 |
| 10:UM:43:ALA:HB1 | 10:UM:67:LEU:HD21 | 1.80 | 0.62 |
| 11:UN:305:ARG:HH12 | 11:UN:309:ARG:HD2 | 1.64 | 0.62 |
| 32:CS:315:PRO:HA | 32:CS:374:PRO:HG3 | 1.81 | 0.62 |
| 44:C1:2216:A:N6 | 44:C1:2217:C:N3 | 2.46 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:165:ARG:NH2 | 46:UV:196:LEU:O | 2.32 | 0.62 |
| 2:UB:770:PRO:HD2 | 2:UB:773:LEU:HD12 | 1.81 | 0.62 |
| 6:UG:318:THR:HG21 | 6:UG:345:ALA:HB3 | 1.81 | 0.62 |
| 27:CL:477:GLU:OE1 | 27:CL:478:ARG:NH2 | 2.32 | 0.62 |
| 29:CO:246:GLU:HG2 | 29:CO:251:ILE:HB | 1.80 | 0.62 |
| 32:CS:202:ILE:HD11 | 32:CS:206:LEU:HD22 | 1.81 | 0.62 |
| 52:CX:422:ARG:NH2 | 52:CX:452:GLU:OE2 | 2.32 | 0.62 |
| 10:UM:341:PHE:HB2 | 10:UM:373:HIS:HB3 | 1.79 | 0.62 |
| 12:UO:70:ASN:O | 12:UO:87:ARG:NH1 | 2.31 | 0.62 |
| 12:UO:464:SER:OG | 13:UQ:562:ASP:OD1 | 2.15 | 0.62 |
| 15:UU:192:MET:HA | 15:UU:192:MET:CE | 2.14 | 0.62 |
| 16:UX:8:GLY:O | 16:UX:14:ARG:NH1 | 2.32 | 0.62 |
| 16:UX:54:PRO:HB3 | 16:UX:85:ALA:HB1 | 1.81 | 0.62 |
| 27:CL:536:GLU:OE1 | 27:CL:536:GLU:N | 2.32 | 0.62 |
| 27:CL:543:GLU:HA | 27:CL:546:LYS:HE2 | 1.81 | 0.62 |
| 30:CP:156:LEU:O | 30:CP:159:GLN:NE2 | 2.32 | 0.62 |
| 32:CR:197:GLU:HB3 | 32:CR:485:ASN:HD21 | 1.63 | 0.62 |
| 32:CS:197:GLU:HB3 | 32:CS:485:ASN:HD21 | 1.64 | 0.62 |
| 44:C1:616:U:H2' | 44:C1:617:G:C8 | 2.34 | 0.62 |
| 46:UV:552:SER:HA | 46:UV:585:ARG:HG2 | 1.81 | 0.62 |
| 4:UD:188:LYS:N | 4:UD:205:SER:OG | 2.28 | 0.62 |
| 19:CC:243:VAL:HG12 | 19:CC:244:LEU:HG | 1.82 | 0.62 |
| 20:CD:155:LYS:NZ | 20:CD:159:GLU:O | 2.31 | 0.62 |
| 26:CK:119:ARG:HH22 | 26:CK:124:LEU:HD13 | 1.64 | 0.62 |
| 32:CR:798:PRO:HB2 | 32:CR:801:LEU:HB2 | 1.81 | 0.62 |
| 32:CS:798:PRO:HB2 | 32:CS:801:LEU:HB2 | 1.81 | 0.62 |
| 34:Cc:203:GLU:HA | 34:Cc:206:ARG:HE | 1.64 | 0.62 |
| 46:UV:680:LEU:HD22 | 46:UV:835:LYS:HG3 | 1.80 | 0.62 |
| 49:UI:238:ARG:HH21 | 49:UI:238:ARG:HG2 | 1.63 | 0.62 |
| 20:CD:380:ASP:N | 20:CD:380:ASP:OD1 | 2.32 | 0.62 |
| 44:C1:4:G:N1 | 44:C1:32:U:N3 | 2.48 | 0.62 |
| 44:C1:392:C:H2' | 44:C1:393:G:H8 | 1.64 | 0.62 |
| 44:C1:616:U:H2' | 44:C1:617:G:H8 | 1.64 | 0.62 |
| 44:C1:1448:A:C6 | 44:C1:1549:U:O4 | 2.52 | 0.62 |
| 4:UD:381:ARG:NH2 | 4:UD:398:ASN:O | 2.32 | 0.62 |
| 5:UF:135:ARG:HG2 | 19:CC:84:MET:HE1 | 1.81 | 0.62 |
| 7:UJ:387:LEU:HD23 | 7:UJ:391:GLN:HB3 | 1.81 | 0.62 |
| 13:UQ:139:SER:OG | 44:C1:46:C:N3 | 2.28 | 0.62 |
| 17:UZ:99:LEU:HB2 | 17:UZ:127:VAL:HG12 | 1.82 | 0.62 |
| 29:CO:100:LEU:O | 29:CO:105:ASN:ND2 | 2.32 | 0.62 |
| 44:C1:202:A:H2 | 44:C1:206:C:H41 | 1.47 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:351:U:C4 | 44:C1:353:G:C6 | 2.88 | 0.62 |
| 48:UH:624:MET:SD | 48:UH:703:ARG:NH1 | 2.73 | 0.62 |
| 2:UB:795:ARG:O | 2:UB:796:ARG:NH1 | 2.33 | 0.62 |
| 9:UL:531:THR:HA | 9:UL:562:LEU:O | 2.00 | 0.62 |
| 10:UM:566:LYS:HG2 | 10:UM:587:ARG:HA | 1.81 | 0.62 |
| 18:CA:76:HIS:HB3 | 18:CA:81:VAL:HG13 | 1.82 | 0.62 |
| 23:CH:281:LEU:HB3 | 23:CH:317:LEU:HD22 | 1.82 | 0.62 |
| 29:CO:49:TYR:N | 29:CO:66:THR:O | 2.27 | 0.62 |
| 48:UH:634:THR:O | 48:UH:713:LYS:NZ | 2.33 | 0.62 |
| 4:UD:162:ASN:HB3 | 4:UD:181:ARG:HB3 | 1.81 | 0.62 |
| 9:UL:25:VAL:HB | 9:UL:40:ILE:HB | 1.81 | 0.62 |
| 12:UO:543:THR:HA | 12:UO:546:MET:HG3 | 1.82 | 0.62 |
| 32:CR:202:ILE:HD11 | 32:CR:206:LEU:HD22 | 1.81 | 0.62 |
| 5:UF:105:GLY:HA2 | 5:UF:137:HIS:HE1 | 1.65 | 0.62 |
| 25:CJ:63:LEU:HD22 | 43:CU:203:LYS:HE2 | 1.81 | 0.62 |
| 31:CQ:165:TYR:HD2 | 31:CQ:222:PHE:HB3 | 1.65 | 0.62 |
| 32:CR:278:ARG:NH2 | 32:CR:433:ARG:O | 2.27 | 0.62 |
| 45:C2:74:C:H2' | 45:C2:75:A:H8 | 1.64 | 0.62 |
| 2:UB:574:ARG:NH2 | 2:UB:577:GLU:OE1 | 2.32 | 0.62 |
| 4:UD:876:TYR:CZ | 53:UP:348:ARG:HD3 | 2.35 | 0.62 |
| 13:UQ:195:ILE:O | 13:UQ:201:VAL:HA | 2.00 | 0.62 |
| 15:UU:157:THR:HG22 | 15:UU:184:GLU:HA | 1.82 | 0.62 |
| 26:CK:283:HIS:NE2 | 44:C1:1147:U:O2' | 2.33 | 0.62 |
| 44:C1:1453:G:N2 | 44:C1:1545:U:O2 | 2.33 | 0.62 |
| 49:UI:182:GLN:O | 49:UI:186:ASN:ND2 | 2.26 | 0.62 |
| 1:UA:52:PHE:HB3 | 1:UA:89:VAL:HG21 | 1.79 | 0.61 |
| 1:UA:296:SER:OG | 1:UA:321:GLN:NE2 | 2.33 | 0.61 |
| 1:UA:642:GLN:NE2 | 1:UA:650:ASP:O | 2.32 | 0.61 |
| 6:UG:309:ASP:HA | 6:UG:350:ILE:HD11 | 1.82 | 0.61 |
| 7:UJ:332:VAL:HG11 | 7:UJ:358:LEU:HD22 | 1.83 | 0.61 |
| 9:UL:835:GLN:OE1 | 9:UL:870:ASN:ND2 | 2.33 | 0.61 |
| 13:UQ:413:LEU:O | 13:UQ:420:ALA:HA | 1.99 | 0.61 |
| 15:UU:255:ILE:HD11 | 15:UU:265:LEU:HB2 | 1.81 | 0.61 |
| 17:UZ:163:LEU:HA | 17:UZ:166:ALA:HB3 | 1.82 | 0.61 |
| 32:CR:42:TYR:O | 32:CR:46:SER:OG | 2.18 | 0.61 |
| 44:C1:398:C:H2' | 44:C1:399:G:H8 | 1.64 | 0.61 |
| 52:CX:301:GLY:O | 52:CX:305:GLY:CA | 2.47 | 0.61 |
| 1:UA:418:ARG:NH2 | 1:UA:455:VAL:O | 2.33 | 0.61 |
| 4:UD:160:ASP:OD1 | 4:UD:160:ASP:N | 2.32 | 0.61 |
| 19:CC:19:GLU:OE1 | 19:CC:51:ARG:NH1 | 2.32 | 0.61 |
| 22:CG:273:TYR:HA | 22:CG:281:ILE:HG12 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:CK:185:SER:O | 26:CK:226:ARG:NH1 | 2.33 | 0.61 |
| 44:C1:381:G:N2 | 44:C1:385:A:H62 | 1.98 | 0.61 |
| 45:C2:101:G:O6 | 45:C2:251:U:O4 | 2.16 | 0.61 |
| 1:UA:9:ASN:ND2 | 1:UA:10:LEU:O | 2.33 | 0.61 |
| 2:UB:26:LYS:NZ | 9:UL:110:LYS:O | 2.33 | 0.61 |
| 2:UB:550:GLU:HG3 | 50:US:523:ILE:HB | 1.81 | 0.61 |
| 4:UD:527:HIS:O | 4:UD:616:ARG:NH2 | 2.32 | 0.61 |
| 6:UG:158:GLY:O | 6:UG:175:GLN:O | 2.18 | 0.61 |
| 8:UK:2:SER:OG | 8:UK:10:ARG:NH2 | 2.33 | 0.61 |
| 12:UO:284:GLN:HB2 | 12:UO:286:ARG:HE | 1.65 | 0.61 |
| 16:UX:122:THR:OG1 | 16:UX:123:CYS:N | 2.31 | 0.61 |
| 22:CG:310:ARG:NH2 | 22:CG:332:GLU:OE1 | 2.33 | 0.61 |
| 24:CI:1013:MET:HE3 | 27:CL:491:GLU:HG3 | 1.81 | 0.61 |
| 24:CI:1136:LYS:HA | 24:CI:1139:LYS:HE2 | 1.83 | 0.61 |
| 25:CJ:40:LYS:O | 25:CJ:43:ASP:N | 2.32 | 0.61 |
| 25:CJ:54:LEU:HD21 | 25:CJ:82:LEU:HD11 | 1.82 | 0.61 |
| 44:C1:472:G:H2' | 44:C1:473:G:H8 | 1.65 | 0.61 |
| 46:UV:778:LEU:HA | 46:UV:781:ARG:HG3 | 1.80 | 0.61 |
| 2:UB:84:ILE:HG21 | 2:UB:87:ARG:HE | 1.66 | 0.61 |
| 8:UK:249:LYS:NZ | 45:C2:267:C:OP1 | 2.24 | 0.61 |
| 10:UM:675:VAL:HG22 | 10:UM:689:LEU:HB2 | 1.81 | 0.61 |
| 13:UQ:482:VAL:O | 13:UQ:499:LEU:HB2 | 2.00 | 0.61 |
| 14:UR:379:SER:OG | 14:UR:382:GLY:N | 2.34 | 0.61 |
| 24:CI:1127:GLU:OE1 | 24:CI:1130:ARG:NH2 | 2.34 | 0.61 |
| 34:Cc:29:LEU:HD23 | 34:Cc:117:ILE:HD11 | 1.83 | 0.61 |
| 35:Ce:42:ALA:HB1 | 35:Ce:78:ARG:HH12 | 1.65 | 0.61 |
| 44:C1:1122:A:H1' | 44:C1:1124:G:H22 | 1.65 | 0.61 |
| 2:UB:615:MET:HA | 2:UB:618:ILE:HD12 | 1.82 | 0.61 |
| 2:UB:799:GLU:HA | 50:US:419:HIS:HA | 1.83 | 0.61 |
| 7:UJ:797:VAL:HG22 | 7:UJ:809:ILE:HD12 | 1.83 | 0.61 |
| 9:UL:12:LYS:HD3 | 9:UL:457:GLN:HB3 | 1.80 | 0.61 |
| 9:UL:27:SER:O | 9:UL:37:GLY:N | 2.34 | 0.61 |
| 12:UO:145:GLN:HG3 | 12:UO:165:ASP:HB3 | 1.82 | 0.61 |
| 15:UU:731:ILE:HD11 | 15:UU:747:LEU:HD11 | 1.80 | 0.61 |
| 19:CC:332:PRO:O | 19:CC:335:THR:OG1 | 2.18 | 0.61 |
| 24:CI:843:GLN:HB3 | 24:CI:1002:ASN:HB3 | 1.83 | 0.61 |
| 28:CM:369:ARG:NH1 | 44:C1:439:A:OP2 | 2.26 | 0.61 |
| 32:CR:289:ARG:HB3 | 32:CR:474:LEU:HD22 | 1.83 | 0.61 |
| 35:Ce:20:SER:H | 35:Ce:23:GLU:HB3 | 1.65 | 0.61 |
| 40:Cm:75:ILE:HG23 | 43:CU:288:ILE:HD13 | 1.81 | 0.61 |
| 12:UO:540:ALA:O | 12:UO:544:GLY:N | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:UR:562:LYS:NZ | 44:C1:237:G:OP1 | 2.32 | 0.61 |
| 23:CH:208:LEU:HD23 | 23:CH:350:ARG:H | 1.64 | 0.61 |
| 24:CI:807:GLU:O | 24:CI:840:ARG:NH2 | 2.33 | 0.61 |
| 25:CJ:120:MET:HE1 | 25:CJ:159:THR:HA | 1.83 | 0.61 |
| 37:Ch:109:LYS:HD3 | 44:C1:1560:C:H5' | 1.81 | 0.61 |
| 44:C1:1701:U:H2' | 44:C1:1702:G:C8 | 2.36 | 0.61 |
| 2:UB:551:GLN:HE22 | 2:UB:554:ARG:HD3 | 1.64 | 0.61 |
| 10:UM:447:TRP:HD1 | 10:UM:460:TRP:HB2 | 1.62 | 0.61 |
| 11:UN:930:ILE:HB | 28:CM:293:PRO:HB2 | 1.81 | 0.61 |
| 23:CH:215:VAL:HA | 23:CH:285:THR:HA | 1.82 | 0.61 |
| 32:CR:845:ALA:HB2 | 32:CR:920:THR:HG21 | 1.83 | 0.61 |
| 37:Ch:129:TYR:OH | 44:C1:1547:C:O2 | 2.18 | 0.61 |
| 44:C1:1182:U:H2' | 44:C1:1183:A:H8 | 1.66 | 0.61 |
| 44:C1:1626:G:H2' | 44:C1:1627:G:C8 | 2.36 | 0.61 |
| 46:UV:930:LEU:HD21 | 46:UV:960:MET:HE1 | 1.81 | 0.61 |
| 1:UA:45:ASN:OD1 | 1:UA:45:ASN:N | 2.32 | 0.61 |
| 9:UL:941:ASP:OD1 | 9:UL:943:THR:OG1 | 2.18 | 0.61 |
| 14:UR:584:GLN:OE1 | 44:C1:244:G:O2' | 2.17 | 0.61 |
| 15:UU:730:ILE:HD11 | 15:UU:746:ARG:HH11 | 1.64 | 0.61 |
| 22:CG:352:ARG:HB2 | 22:CG:368:ARG:HH21 | 1.66 | 0.61 |
| 29:CO:32:LYS:NZ | 29:CO:170:HIS:O | 2.34 | 0.61 |
| 32:CS:613:LEU:HD22 | 32:CS:634:ARG:HD2 | 1.83 | 0.61 |
| 44:C1:2358:U:O4 | 44:C1:2369:G:O6 | 2.18 | 0.61 |
| 48:UH:777:ALA:HA | 49:UI:259:LEU:HD13 | 1.83 | 0.61 |
| 1:UA:21:LEU:HD12 | 1:UA:61:ILE:HG22 | 1.82 | 0.61 |
| 1:UA:278:ILE:HA | 1:UA:294:SER:HA | 1.83 | 0.61 |
| 2:UB:605:ASP:O | 2:UB:652:ARG:NH2 | 2.34 | 0.61 |
| 9:UL:136:VAL:HG13 | 9:UL:145:GLN:HB2 | 1.81 | 0.61 |
| 9:UL:797:ARG:NH1 | 9:UL:801:GLU:OE1 | 2.33 | 0.61 |
| 12:UO:306:ASN:ND2 | 13:UQ:646:ASP:O | 2.33 | 0.61 |
| 13:UQ:190:MET:HA | 13:UQ:206:LEU:O | 1.99 | 0.61 |
| 13:UQ:439:SER:OG | 13:UQ:440:LEU:N | 2.33 | 0.61 |
| 24:CI:974:ARG:HD2 | 44:C1:2183:A:H2 | 1.66 | 0.61 |
| 28:CM:40:TYR:OH | 28:CM:387:GLU:OE1 | 2.19 | 0.61 |
| 46:UV:684:SER:HB2 | 46:UV:1011:THR:HG21 | 1.83 | 0.61 |
| 14:UR:593:ILE:HG22 | 14:UR:604:VAL:HG13 | 1.82 | 0.61 |
| 15:UU:842:THR:OG1 | 15:UU:843:LEU:N | 2.34 | 0.61 |
| 19:CC:88:GLN:NE2 | 44:C1:455:G:OP1 | 2.31 | 0.61 |
| 22:CG:438:LEU:HA | 22:CG:463:PRO:HA | 1.81 | 0.61 |
| 26:CK:272:THR:OG1 | 26:CK:273:LEU:N | 2.30 | 0.61 |
| 28:CM:73:CYS:SG | 28:CM:74:LYS:N | 2.74 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:CO:178:VAL:HG12 | 29:CO:223:GLU:HB2 | 1.83 | 0.61 |
| 32:CS:289:ARG:HB3 | 32:CS:474:LEU:HD22 | 1.83 | 0.61 |
| 44:C1:484:G:H2' | 44:C1:485:G:C8 | 2.36 | 0.61 |
| 45:C2:91:G:OP1 | 45:C2:91:G:N2 | 2.33 | 0.61 |
| 46:UV:318:LYS:NZ | 46:UV:442:ASP:OD1 | 2.34 | 0.61 |
| 48:UH:781:SER:HB3 | 49:UI:259:LEU:HA | 1.83 | 0.61 |
| 4:UD:162:ASN:N | 4:UD:162:ASN:OD1 | 2.34 | 0.60 |
| 5:UF:165:LEU:HD11 | 11:UN:360:ILE:HG13 | 1.82 | 0.60 |
| 6:UG:411:HIS:NE2 | 6:UG:416:SER:OG | 2.34 | 0.60 |
| 14:UR:322:ARG:HD3 | 44:C1:133:G:H22 | 1.65 | 0.60 |
| 18:CA:130:TRP:HE3 | 18:CA:138:ALA:HB2 | 1.66 | 0.60 |
| 34:Cc:152:LEU:O | 34:Cc:156:ASN:ND2 | 2.34 | 0.60 |
| 44:C1:495:G:H8 | 44:C1:503:G:H22 | 1.47 | 0.60 |
| 44:C1:1640:U:H3 | 44:C1:1648:G:H1 | 1.46 | 0.60 |
| 45:C2:49:U:H2' | 45:C2:50:G:H8 | 1.64 | 0.60 |
| 46:UV:727:ARG:HD2 | 46:UV:731:ARG:HH12 | 1.66 | 0.60 |
| 51:Cl:69:LEU:HD13 | 51:Cl:72:ILE:HD11 | 1.83 | 0.60 |
| 4:UD:29:VAL:HB | 4:UD:33:LYS:HD2 | 1.83 | 0.60 |
| 4:UD:153:LYS:HD2 | 4:UD:165:LEU:HD21 | 1.83 | 0.60 |
| 9:UL:572:ARG:NH2 | 9:UL:613:MET:O | 2.35 | 0.60 |
| 24:CI:915:VAL:HG11 | 24:CI:992:TRP:HB3 | 1.82 | 0.60 |
| 24:CI:1085:ARG:NH2 | 44:C1:391:C:OP1 | 2.34 | 0.60 |
| 25:CJ:35:ARG:NH1 | 44:C1:351:U:O4 | 2.34 | 0.60 |
| 49:UI:263:LEU:HA | 49:UI:266:LEU:HD23 | 1.83 | 0.60 |
| 7:UJ:287:ASN:N | 7:UJ:287:ASN:OD1 | 2.33 | 0.60 |
| 9:UL:507:ASP:OD1 | 9:UL:509:HIS:ND1 | 2.34 | 0.60 |
| 20:CD:305:SER:O | 20:CD:310:ASN:ND2 | 2.34 | 0.60 |
| 24:CI:1043:ARG:NH2 | 44:C1:2072:U:O2' | 2.33 | 0.60 |
| 31:CQ:113:VAL:O | 31:CQ:114:ARG:NH1 | 2.33 | 0.60 |
| 32:CS:745:VAL:HG23 | 32:CS:761:VAL:HG13 | 1.83 | 0.60 |
| 44:C1:1182:U:H2' | 44:C1:1183:A:C8 | 2.36 | 0.60 |
| 48:UH:756:LEU:HD21 | 49:UI:170:GLU:HA | 1.83 | 0.60 |
| 49:UE:263:LEU:HA | 49:UE:266:LEU:HD23 | 1.83 | 0.60 |
| 52:CX:419:GLN:O | 52:CX:422:ARG:NH2 | 2.34 | 0.60 |
| 7:UJ:259:MET:HE2 | 7:UJ:275:VAL:HG11 | 1.83 | 0.60 |
| 9:UL:199:LYS:HD3 | 9:UL:211:THR:HG22 | 1.83 | 0.60 |
| 9:UL:233:ILE:HG22 | 9:UL:243:VAL:HG12 | 1.83 | 0.60 |
| 9:UL:461:ARG:NH1 | 9:UL:495:ALA:O | 2.30 | 0.60 |
| 15:UU:51:PHE:HB2 | 15:UU:65:THR:HG22 | 1.83 | 0.60 |
| 15:UU:282:ARG:NH1 | 15:UU:286:LEU:O | 2.34 | 0.60 |
| 31:CQ:112:GLN:HG3 | 31:CQ:125:ARG:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:CS:523:ARG:NH1 | 32:CS:559:MET:O | 2.35 | 0.60 |
| 32:CS:845:ALA:HB2 | 32:CS:920:THR:HG21 | 1.83 | 0.60 |
| 44:C1:265:G:O6 | 44:C1:274:A:N1 | 2.34 | 0.60 |
| 48:UH:754:ARG:HA | 49:UI:209:GLY:HA3 | 1.83 | 0.60 |
| 48:UH:754:ARG:HB3 | 49:UI:210:ARG:HD3 | 1.83 | 0.60 |
| 2:UB:539:ASP:OD1 | 2:UB:540:ARG:NH1 | 2.34 | 0.60 |
| 4:UD:668:GLU:HA | 4:UD:671:ARG:HG2 | 1.84 | 0.60 |
| 9:UL:244:TRP:HA | 9:UL:268:GLN:O | 2.01 | 0.60 |
| 12:UO:332:ARG:HG3 | 12:UO:333:HIS:CD2 | 2.36 | 0.60 |
| 13:UQ:449:ASP:OD2 | 13:UQ:487:GLN:NE2 | 2.34 | 0.60 |
| 15:UU:690:ARG:NH2 | 15:UU:702:GLU:OE1 | 2.35 | 0.60 |
| 30:CP:204:LYS:HD3 | 44:C1:1489:G:H21 | 1.66 | 0.60 |
| 36:Cg:58:LEU:HA | 36:Cg:67:ARG:HH21 | 1.66 | 0.60 |
| 1:UA:149:GLN:HE21 | 44:C1:266:C:H3' | 1.66 | 0.60 |
| 4:UD:550:SER:N | 4:UD:564:ALA:O | 2.34 | 0.60 |
| 6:UG:55:GLY:O | 11:UN:902:ARG:NH2 | 2.32 | 0.60 |
| 9:UL:130:LYS:HG2 | 44:C1:2333:A:H4' | 1.82 | 0.60 |
| 12:UO:50:PRO:HD3 | 12:UO:107:ILE:HD11 | 1.84 | 0.60 |
| 15:UU:619:GLY:O | 15:UU:647:LYS:NZ | 2.33 | 0.60 |
| 23:CH:26:LEU:HD12 | 23:CH:341:MET:HE3 | 1.83 | 0.60 |
| 23:CH:139:THR:HB | 23:CH:150:ILE:HD13 | 1.82 | 0.60 |
| 26:CK:198:THR:OG1 | 26:CK:201:GLY:N | 2.31 | 0.60 |
| 29:CO:49:TYR:O | 29:CO:66:THR:N | 2.28 | 0.60 |
| 44:C1:496:U:C4 | 44:C1:503:G:C6 | 2.90 | 0.60 |
| 52:CX:286:VAL:O | 52:CX:290:ASN:ND2 | 2.34 | 0.60 |
| 54:Cz:1632:LYS:HB3 | 54:Cz:1635:GLN:HB2 | 1.83 | 0.60 |
| 4:UD:19:VAL:HG22 | 4:UD:46:ILE:HG12 | 1.81 | 0.60 |
| 4:UD:269:ALA:O | 4:UD:312:ARG:NH1 | 2.31 | 0.60 |
| 4:UD:456:LEU:HG | 4:UD:469:ILE:HG22 | 1.84 | 0.60 |
| 4:UD:489:ASP:OD2 | 4:UD:491:ARG:NE | 2.35 | 0.60 |
| 4:UD:663:ARG:HD3 | 4:UD:665:MET:HE2 | 1.84 | 0.60 |
| 7:UJ:727:LEU:HA | 7:UJ:730:LEU:HG | 1.84 | 0.60 |
| 8:UK:72:GLY:O | 8:UK:79:ARG:NH1 | 2.33 | 0.60 |
| 13:UQ:312:ILE:HG13 | 13:UQ:329:LEU:HB2 | 1.83 | 0.60 |
| 18:CA:222:MET:HG3 | 19:CC:136:THR:HA | 1.83 | 0.60 |
| 24:CI:123:LEU:HD22 | 24:CI:898:ARG:HD2 | 1.82 | 0.60 |
| 27:CL:719:ARG:NH2 | 44:C1:2224:C:OP2 | 2.34 | 0.60 |
| 32:CR:58:TRP:HE1 | 32:CR:126:GLN:HE21 | 1.50 | 0.60 |
| 50:US:538:LEU:O | 50:US:542:TRP:HB2 | 2.02 | 0.60 |
| 7:UJ:44:THR:OG1 | 7:UJ:45:PHE:N | 2.35 | 0.60 |
| 8:UK:9:GLN:NE2 | 44:C1:1156:C:OP2 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:UL:275:ARG:NH2 | 9:UL:277:SER:OG | 2.35 | 0.60 |
| 12:UO:93:LYS:HD2 | 12:UO:132:THR:HA | 1.83 | 0.60 |
| 18:CB:94:THR:O | 18:CB:127:TYR:HA | 2.02 | 0.60 |
| 44:C1:197:G:H2' | 44:C1:198:G:H8 | 1.66 | 0.60 |
| 45:C2:103:G:C5 | 45:C2:250:G:N1 | 2.70 | 0.60 |
| 1:UA:643:GLY:HA3 | 6:UG:179:THR:HG21 | 1.83 | 0.60 |
| 6:UG:403:PHE:HB3 | 28:CM:8:ARG:HH22 | 1.66 | 0.60 |
| 7:UJ:129:GLU:HG2 | 7:UJ:156:PRO:HG2 | 1.84 | 0.60 |
| 7:UJ:170:TYR:O | 7:UJ:173:SER:O | 2.19 | 0.60 |
| 8:UK:161:LYS:HZ3 | 18:CB:290:LEU:HB2 | 1.66 | 0.60 |
| 10:UM:244:GLN:HB3 | 10:UM:287:LYS:HZ1 | 1.67 | 0.60 |
| 13:UQ:550:LEU:O | 13:UQ:588:TRP:HB2 | 2.02 | 0.60 |
| 16:UX:62:THR:HG22 | 16:UX:95:VAL:HG13 | 1.83 | 0.60 |
| 18:CB:285:PHE:HB2 | 18:CB:305:VAL:HG12 | 1.84 | 0.60 |
| 28:CM:423:ARG:NH2 | 28:CM:428:LYS:O | 2.34 | 0.60 |
| 7:UJ:771:VAL:HA | 7:UJ:774:ILE:HD12 | 1.83 | 0.60 |
| 9:UL:474:LEU:HB2 | 9:UL:479:VAL:HG23 | 1.83 | 0.60 |
| 15:UU:546:THR:HG21 | 15:UU:627:GLY:H | 1.65 | 0.60 |
| 26:CK:289:ARG:HG3 | 26:CK:290:THR:HG23 | 1.84 | 0.60 |
| 32:CR:523:ARG:NH1 | 32:CR:559:MET:O | 2.35 | 0.60 |
| 44:C1:26:C:N4 | 44:C1:27:A:N6 | 2.50 | 0.60 |
| 44:C1:619:U:H3 | 44:C1:1052:A:N6 | 1.99 | 0.60 |
| 46:UV:278:SER:HB2 | 46:UV:398:ARG:HD2 | 1.84 | 0.60 |
| 50:US:286:LEU:HD11 | 50:US:321:ALA:HA | 1.84 | 0.60 |
| 6:UG:188:ASN:HB2 | 6:UG:190:GLN:H | 1.66 | 0.59 |
| 7:UJ:555:TYR:HA | 7:UJ:558:VAL:HG12 | 1.83 | 0.59 |
| 9:UL:70:VAL:HG21 | 9:UL:85:VAL:HB | 1.84 | 0.59 |
| 10:UM:558:LEU:HD23 | 10:UM:570:ILE:HD11 | 1.84 | 0.59 |
| 13:UQ:292:THR:OG1 | 13:UQ:293:PHE:N | 2.35 | 0.59 |
| 13:UQ:292:THR:HG21 | 13:UQ:360:SER:HA | 1.84 | 0.59 |
| 31:CQ:205:THR:O | 31:CQ:224:ASN:ND2 | 2.35 | 0.59 |
| 32:CR:613:LEU:HD22 | 32:CR:634:ARG:HD2 | 1.83 | 0.59 |
| 39:Cj:102:LYS:NZ | 39:Cj:103:ASN:OD1 | 2.35 | 0.59 |
| 46:UV:272:THR:OG1 | 46:UV:474:ARG:NH2 | 2.35 | 0.59 |
| 48:UH:883:ARG:NH2 | 48:UH:887:GLU:OE2 | 2.35 | 0.59 |
| 52:CX:442:HIS:HE1 | 52:CX:444:LYS:HE2 | 1.67 | 0.59 |
| 54:Cz:1519:GLN:HA | 54:Cz:1522:VAL:HG22 | 1.83 | 0.59 |
| 1:UA:8:SER:OG | 1:UA:699:SER:N | 2.35 | 0.59 |
| 2:UB:670:PRO:HB3 | 2:UB:691:ILE:HD11 | 1.84 | 0.59 |
| 9:UL:239:GLY:HA2 | 9:UL:275:ARG:HE | 1.68 | 0.59 |
| 9:UL:537:PHE:HB3 | 9:UL:556:LEU:HB3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:UM:668:SER:O | 10:UM:675:VAL:HA | 2.02 | 0.59 |
| 14:UR:456:ARG:HH11 | 14:UR:529:TYR:HE1 | 1.50 | 0.59 |
| 32:CS:27:PHE:HB2 | 32:CS:148:LEU:HD11 | 1.82 | 0.59 |
| 34:Cc:135:ARG:HD3 | 34:Cc:144:ARG:HB3 | 1.83 | 0.59 |
| 52:CX:359:CYS:SG | 52:CX:391:ARG:NH2 | 2.73 | 0.59 |
| 1:UA:96:LYS:NZ | 44:C1:260:U:OP1 | 2.35 | 0.59 |
| 4:UD:446:SER:HA | 4:UD:451:VAL:HG12 | 1.85 | 0.59 |
| 6:UG:56:PRO:HG2 | 11:UN:899:ARG:HD3 | 1.83 | 0.59 |
| 6:UG:65:ASP:OD2 | 44:C1:582:G:N2 | 2.35 | 0.59 |
| 10:UM:115:VAL:HG21 | 10:UM:155:LEU:HD11 | 1.83 | 0.59 |
| 10:UM:810:LEU:HA | 10:UM:813:LEU:HD12 | 1.84 | 0.59 |
| 17:UZ:87:HIS:HE1 | 17:UZ:257:ALA:HB3 | 1.66 | 0.59 |
| 23:CH:152:THR:O | 23:CH:156:ALA:CB | 2.50 | 0.59 |
| 28:CM:152:GLU:O | 28:CM:156:TYR:OH | 2.20 | 0.59 |
| 31:CQ:253:SER:OG | 31:CQ:254:ARG:NH1 | 2.34 | 0.59 |
| 46:UV:173:ALA:O | 46:UV:177:GLN:NE2 | 2.31 | 0.59 |
| 4:UD:456:LEU:HD23 | 4:UD:467:LEU:HD21 | 1.84 | 0.59 |
| 10:UM:448:ILE:HD13 | 10:UM:487:LEU:HD11 | 1.84 | 0.59 |
| 14:UR:564:ASP:N | 14:UR:588:GLY:O | 2.30 | 0.59 |
| 16:UX:81:ASP:HA | 36:Cg:55:ARG:HE | 1.68 | 0.59 |
| 18:CB:248:LYS:HB2 | 20:CD:124:GLN:HE22 | 1.66 | 0.59 |
| 19:CC:205:HIS:ND1 | 19:CC:264:GLN:O | 2.33 | 0.59 |
| 32:CS:58:TRP:HE1 | 32:CS:126:GLN:HE21 | 1.50 | 0.59 |
| 46:UV:495:MET:HG2 | 46:UV:585:ARG:HH11 | 1.66 | 0.59 |
| 49:UI:253:LEU:HA | 49:UI:256:LEU:HB2 | 1.84 | 0.59 |
| 1:UA:209:THR:HG22 | 1:UA:223:LYS:HG2 | 1.84 | 0.59 |
| 14:UR:428:ASP:OD1 | 14:UR:428:ASP:N | 2.34 | 0.59 |
| 15:UU:645:LYS:HG2 | 15:UU:661:ASP:HA | 1.84 | 0.59 |
| 17:UZ:105:GLN:HG3 | 17:UZ:129:ASP:H | 1.66 | 0.59 |
| 24:CI:90:ARG:HD2 | 24:CI:96:THR:HG22 | 1.85 | 0.59 |
| 29:CO:104:ILE:HD13 | 29:CO:242:CYS:HB2 | 1.83 | 0.59 |
| 32:CR:843:SER:HA | 32:CR:846:ASN:HD22 | 1.67 | 0.59 |
| 43:CU:205:THR:OG1 | 43:CU:209:ARG:NH1 | 2.35 | 0.59 |
| 44:C1:362:G:H2' | 44:C1:363:G:H8 | 1.68 | 0.59 |
| 51:Cl:14:ILE:HG23 | 51:Cl:22:VAL:HA | 1.85 | 0.59 |
| 4:UD:528:ARG:NH1 | 4:UD:547:ARG:O | 2.34 | 0.59 |
| 7:UJ:556:LEU:HD21 | 7:UJ:592:ILE:HG23 | 1.85 | 0.59 |
| 10:UM:236:GLN:HG2 | 10:UM:252:ARG:HH11 | 1.67 | 0.59 |
| 13:UQ:238:ASP:OD1 | 13:UQ:238:ASP:N | 2.31 | 0.59 |
| 13:UQ:735:ARG:HB2 | 13:UQ:747:LEU:HG | 1.84 | 0.59 |
| 19:CC:3:VAL:HG23 | 19:CC:23:GLN:HE22 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:CG:562:ASP:HB3 | 22:CG:581:VAL:HB | 1.84 | 0.59 |
| 27:CL:484:ALA:HA | 27:CL:487:ILE:HD12 | 1.85 | 0.59 |
| 34:Cc:82:ASN:ND2 | 44:C1:2194:A:O3' | 2.36 | 0.59 |
| 44:C1:496:U:O4 | 44:C1:503:G:O6 | 2.20 | 0.59 |
| 46:UV:671:ILE:O | 46:UV:676:ARG:NH1 | 2.34 | 0.59 |
| 1:UA:626:ASN:ND2 | 44:C1:257:G:OP1 | 2.35 | 0.59 |
| 1:UA:707:ASP:HA | 15:UU:677:ASN:HD21 | 1.66 | 0.59 |
| 2:UB:592:VAL:O | 2:UB:595:THR:OG1 | 2.19 | 0.59 |
| 9:UL:11:SER:N | 9:UL:722:VAL:O | 2.30 | 0.59 |
| 13:UQ:449:ASP:OD1 | 13:UQ:449:ASP:N | 2.24 | 0.59 |
| 13:UQ:538:ALA:HA | 13:UQ:554:ASP:HA | 1.85 | 0.59 |
| 15:UU:423:ARG:NH1 | 44:C1:258:C:N3 | 2.51 | 0.59 |
| 18:CB:234:ASP:OD1 | 18:CB:237:ARG:NH2 | 2.35 | 0.59 |
| 29:CO:116:THR:O | 29:CO:119:GLY:N | 2.34 | 0.59 |
| 32:CR:27:PHE:HB2 | 32:CR:148:LEU:HD11 | 1.82 | 0.59 |
| 52:CX:234:ILE:HD12 | 52:CX:269:ILE:HD11 | 1.83 | 0.59 |
| 6:UG:172:CYS:SG | 6:UG:173:GLU:N | 2.76 | 0.59 |
| 9:UL:676:ARG:NH1 | 9:UL:696:HIS:O | 2.34 | 0.59 |
| 12:UO:181:ARG:HD3 | 12:UO:222:PRO:HG3 | 1.84 | 0.59 |
| 13:UQ:90:SER:OG | 13:UQ:91:ASP:N | 2.34 | 0.59 |
| 13:UQ:244:LEU:HA | 13:UQ:254:VAL:O | 2.02 | 0.59 |
| 15:UU:416:SER:OG | 15:UU:417:LEU:N | 2.36 | 0.59 |
| 35:Ce:149:ARG:HD3 | 40:Cm:53:VAL:HG12 | 1.84 | 0.59 |
| 45:C2:113:G:H1' | 45:C2:195:A:H61 | 1.68 | 0.59 |
| 1:UA:10:LEU:HD12 | 1:UA:11:LEU:H | 1.67 | 0.59 |
| 1:UA:762:VAL:HG21 | 1:UA:796:ALA:HB1 | 1.84 | 0.59 |
| 4:UD:33:LYS:HB3 | 4:UD:36:LEU:HD12 | 1.83 | 0.59 |
| 5:UF:280:ILE:HD11 | 5:UF:316:ILE:HG22 | 1.85 | 0.59 |
| 9:UL:275:ARG:NH1 | 9:UL:279:GLU:O | 2.35 | 0.59 |
| 12:UO:101:GLU:HB2 | 12:UO:119:ASP:HB2 | 1.85 | 0.59 |
| 13:UQ:252:ALA:HA | 13:UQ:264:GLY:O | 2.03 | 0.59 |
| 13:UQ:563:THR:O | 13:UQ:565:ALA:N | 2.35 | 0.59 |
| 29:CN:151:LYS:NZ | 29:CN:156:ASN:O | 2.35 | 0.59 |
| 40:Cm:40:VAL:HG13 | 40:Cm:43:ARG:HH21 | 1.67 | 0.59 |
| 44:C1:212:C:H2' | 44:C1:213:G:H8 | 1.68 | 0.59 |
| 44:C1:2095:G:H2' | 44:C1:2096:G:C8 | 2.38 | 0.59 |
| 45:C2:5:A:O2' | 45:C2:6:C:O5' | 2.20 | 0.59 |
| 45:C2:103:G:C6 | 45:C2:250:G:N1 | 2.71 | 0.59 |
| 3:UC:613:LYS:HE2 | 3:UC:616:ARG:HH12 | 1.68 | 0.59 |
| 5:UF:310:LEU:HB2 | 5:UF:313:HIS:HB3 | 1.85 | 0.59 |
| 6:UG:442:ARG:NH1 | 44:C1:426:A:OP1 | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:UJ:107:SER:OG | 7:UJ:108:ARG:N | 2.36 | 0.59 |
| 9:UL:903:ARG:HD2 | 10:UM:885:GLU:HG3 | 1.83 | 0.59 |
| 10:UM:289:MET:HB3 | 10:UM:301:TRP:HB2 | 1.85 | 0.59 |
| 15:UU:179:LYS:HG3 | 15:UU:181:GLY:H | 1.68 | 0.59 |
| 26:CK:85:ASP:OD1 | 27:CL:559:ARG:NH2 | 2.35 | 0.59 |
| 26:CK:100:LEU:HD22 | 26:CK:144:GLU:HB3 | 1.85 | 0.59 |
| 45:C2:188:G:N1 | 45:C2:189:G:O6 | 2.36 | 0.59 |
| 46:UV:394:TRP:HE1 | 46:UV:399:GLN:HG2 | 1.67 | 0.59 |
| 54:Cz:1558:GLU:HG3 | 54:Cz:1567:VAL:HG12 | 1.84 | 0.59 |
| 15:UU:473:ASN:ND2 | 15:UU:552:CYS:O | 2.26 | 0.58 |
| 17:UZ:223:GLU:HA | 17:UZ:226:LYS:HD2 | 1.84 | 0.58 |
| 19:CC:198:VAL:HB | 19:CC:277:LEU:HD22 | 1.85 | 0.58 |
| 22:CG:334:LEU:HD12 | 22:CG:399:ASP:HA | 1.85 | 0.58 |
| 24:CI:69:ARG:NH1 | 24:CI:230:LYS:O | 2.36 | 0.58 |
| 25:CJ:71:ARG:NE | 26:CK:61:SER:OG | 2.36 | 0.58 |
| 32:CR:745:VAL:HG23 | 32:CR:761:VAL:HG13 | 1.83 | 0.58 |
| 32:CR:883:ILE:HD13 | 32:CR:911:ILE:HG21 | 1.85 | 0.58 |
| 32:CS:843:SER:HA | 32:CS:846:ASN:HD22 | 1.67 | 0.58 |
| 32:CS:883:ILE:HD13 | 32:CS:911:ILE:HG21 | 1.85 | 0.58 |
| 34:Cc:48:TYR:HD1 | 34:Cc:152:LEU:HD13 | 1.68 | 0.58 |
| 46:UV:934:THR:HG23 | 46:UV:936:HIS:H | 1.67 | 0.58 |
| 12:UO:196:MET:HB3 | 12:UO:201:ASN:HB3 | 1.85 | 0.58 |
| 12:UO:248:LEU:HD13 | 12:UO:279:LEU:HD13 | 1.85 | 0.58 |
| 13:UQ:145:SER:HB3 | 13:UQ:190:MET:HG3 | 1.85 | 0.58 |
| 13:UQ:529:GLU:OE1 | 13:UQ:561:ARG:NH1 | 2.34 | 0.58 |
| 14:UR:331:VAL:HG22 | 14:UR:378:VAL:HG11 | 1.85 | 0.58 |
| 15:UU:124:ARG:NH1 | 44:C1:260:U:O2 | 2.30 | 0.58 |
| 18:CA:123:THR:OG1 | 18:CA:124:LYS:N | 2.36 | 0.58 |
| 19:CC:179:GLN:NE2 | 20:CD:185:ARG:O | 2.36 | 0.58 |
| 20:CD:162:ASP:OD1 | 20:CD:162:ASP:N | 2.34 | 0.58 |
| 29:CN:47:GLU:HB2 | 29:CN:68:LEU:HB3 | 1.84 | 0.58 |
| 33:CT:168:SER:OG | 33:CT:169:ASP:N | 2.36 | 0.58 |
| 40:Cm:23:ARG:O | 40:Cm:64:GLN:NE2 | 2.35 | 0.58 |
| 40:Cm:78:ARG:HB3 | 40:Cm:124:LYS:HD3 | 1.85 | 0.58 |
| 44:C1:336:G:H2' | 44:C1:337:G:H8 | 1.68 | 0.58 |
| 2:UB:84:ILE:HD13 | 2:UB:87:ARG:HH21 | 1.67 | 0.58 |
| 4:UD:358:GLY:O | 4:UD:751:SER:OG | 2.18 | 0.58 |
| 8:UK:161:LYS:HD3 | 18:CB:290:LEU:HD13 | 1.85 | 0.58 |
| 9:UL:647:GLY:O | 9:UL:679:LYS:NZ | 2.33 | 0.58 |
| 18:CA:257:ILE:O | 18:CA:299:HIS:HA | 2.02 | 0.58 |
| 24:CI:858:ARG:NH1 | 44:C1:1157:C:O2' | 2.35 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:CK:269:THR:OG1 | 26:CK:271:GLY:O | 2.21 | 0.58 |
| 44:C1:186:C:H2' | 44:C1:187:G:H8 | 1.68 | 0.58 |
| 44:C1:1487:G:N2 | 44:C1:1493:U:O4 | 2.36 | 0.58 |
| 44:C1:2057:G:H2' | 44:C1:2058:A:C8 | 2.39 | 0.58 |
| 45:C2:153:G:O6 | 45:C2:176:U:O2 | 2.20 | 0.58 |
| 46:UV:545:ARG:HH11 | 46:UV:548:ASP:HA | 1.68 | 0.58 |
| 50:US:301:GLU:OE2 | 50:US:332:ARG:NE | 2.36 | 0.58 |
| 4:UD:552:ILE:HG22 | 4:UD:563:VAL:HG12 | 1.85 | 0.58 |
| 11:UN:866:LEU:N | 44:C1:283:A:OP1 | 2.36 | 0.58 |
| 19:CC:46:LYS:NZ | 44:C1:437:G:O3' | 2.36 | 0.58 |
| 48:UH:793:MET:HG2 | 49:UI:273:ARG:NH2 | 2.18 | 0.58 |
| 49:UE:253:LEU:HA | 49:UE:256:LEU:HB2 | 1.84 | 0.58 |
| 1:UA:78:GLN:HG3 | 44:C1:257:G:N2 | 2.18 | 0.58 |
| 1:UA:260:CYS:SG | 1:UA:303:VAL:N | 2.75 | 0.58 |
| 4:UD:71:GLY:O | 4:UD:430:HIS:ND1 | 2.36 | 0.58 |
| 13:UQ:637:PHE:O | 13:UQ:664:SER:N | 2.36 | 0.58 |
| 23:CH:121:ALA:HB3 | 23:CH:196:PHE:HD2 | 1.66 | 0.58 |
| 26:CK:110:MET:O | 26:CK:226:ARG:NH2 | 2.36 | 0.58 |
| 28:CM:60:GLN:NE2 | 28:CM:349:ASN:OD1 | 2.36 | 0.58 |
| 35:Ce:62:LYS:HB2 | 35:Ce:94:ARG:HD2 | 1.84 | 0.58 |
| 44:C1:2171:G:H1 | 44:C1:2191:U:H3 | 1.51 | 0.58 |
| 9:UL:453:ASN:HD22 | 9:UL:456:THR:H | 1.50 | 0.58 |
| 9:UL:535:TRP:HB3 | 9:UL:556:LEU:HD13 | 1.84 | 0.58 |
| 10:UM:798:LEU:HA | 10:UM:801:LEU:HG | 1.86 | 0.58 |
| 23:CH:365:ARG:NE | 24:CI:546:MET:O | 2.36 | 0.58 |
| 24:CI:271:SER:HB2 | 24:CI:776:TYR:HE2 | 1.68 | 0.58 |
| 31:CQ:218:ILE:HG22 | 31:CQ:225:ILE:HD12 | 1.85 | 0.58 |
| 32:CR:764:ARG:HG2 | 32:CR:766:LEU:HD22 | 1.86 | 0.58 |
| 35:Ce:51:SER:HB2 | 35:Ce:67:PHE:HB2 | 1.84 | 0.58 |
| 44:C1:597:G:H2' | 44:C1:598:A:C8 | 2.39 | 0.58 |
| 45:C2:65:C:H2' | 45:C2:66:A:C8 | 2.36 | 0.58 |
| 50:US:114:LEU:HA | 50:US:117:ARG:HD2 | 1.86 | 0.58 |
| 1:UA:685:ASN:HA | 1:UA:700:LEU:HD13 | 1.85 | 0.58 |
| 4:UD:620:ALA:HA | 4:UD:623:ILE:HD12 | 1.84 | 0.58 |
| 9:UL:428:ASP:OD2 | 9:UL:430:ARG:NH2 | 2.37 | 0.58 |
| 14:UR:167:SER:OG | 14:UR:170:GLU:OE1 | 2.22 | 0.58 |
| 18:CB:211:ARG:HG2 | 18:CB:238:ILE:HG12 | 1.85 | 0.58 |
| 24:CI:1088:ARG:NH2 | 44:C1:369:U:OP2 | 2.36 | 0.58 |
| 29:CN:100:LEU:HD11 | 29:CN:129:ARG:HA | 1.84 | 0.58 |
| 32:CS:764:ARG:HG2 | 32:CS:766:LEU:HD22 | 1.86 | 0.58 |
| 44:C1:335:C:H2' | 44:C1:336:G:H8 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:392:C:H2' | 44:C1:393:G:C8 | 2.38 | 0.58 |
| 44:C1:1509:A:O2' | 54:Cz:1645:GLN:O | 2.20 | 0.58 |
| 48:UH:733:ASP:OD1 | 48:UH:733:ASP:N | 2.35 | 0.58 |
| 12:UO:550:LEU:O | 12:UO:553:SER:OG | 2.21 | 0.58 |
| 22:CG:167:ARG:NH2 | 22:CG:599:CYS:SG | 2.71 | 0.58 |
| 23:CH:124:SER:OG | 23:CH:126:ALA:O | 2.19 | 0.58 |
| 24:CI:68:PRO:O | 24:CI:275:ARG:NH2 | 2.30 | 0.58 |
| 29:CO:27:ILE:HG21 | 29:CO:36:ARG:HE | 1.69 | 0.58 |
| 44:C1:2237:G:N2 | 44:C1:2329:A:N1 | 2.46 | 0.58 |
| 10:UM:776:ASN:O | 10:UM:779:THR:C | 2.47 | 0.58 |
| 15:UU:440:ALA:O | 15:UU:443:MET:C | 2.47 | 0.58 |
| 27:CL:548:ARG:O | 27:CL:551:ALA:O | 2.22 | 0.58 |
| 44:C1:6:G:C2 | 44:C1:30:U:C2 | 2.91 | 0.58 |
| 44:C1:57:C:H2' | 44:C1:58:G:C8 | 2.39 | 0.58 |
| 44:C1:336:G:H2' | 44:C1:337:G:C8 | 2.39 | 0.58 |
| 44:C1:1702:G:N2 | 45:C2:7:A:N1 | 2.48 | 0.58 |
| 48:UH:624:MET:HA | 48:UH:627:LEU:HD23 | 1.86 | 0.58 |
| 1:UA:105:SER:HG | 1:UA:163:SER:HG | 1.50 | 0.58 |
| 4:UD:695:GLN:HG2 | 4:UD:856:PRO:HD2 | 1.86 | 0.58 |
| 11:UN:326:TRP:NE1 | 28:CM:209:GLU:OE1 | 2.36 | 0.58 |
| 14:UR:160:SER:OG | 14:UR:161:GLU:N | 2.37 | 0.58 |
| 18:CA:211:ARG:NH2 | 18:CA:232:GLN:OE1 | 2.37 | 0.58 |
| 22:CG:422:SER:HB3 | 22:CG:429:LEU:HD22 | 1.85 | 0.58 |
| 26:CK:290:THR:HB | 26:CK:293:LYS:HB2 | 1.84 | 0.58 |
| 28:CM:205:PHE:HA | 28:CM:213:ILE:HG12 | 1.86 | 0.58 |
| 47:CV:87:SER:H | 47:CV:146:SER:HB3 | 1.68 | 0.58 |
| 52:CX:368:LYS:HZ1 | 52:CX:372:GLU:HB2 | 1.68 | 0.58 |
| 4:UD:548:ASN:OD1 | 4:UD:548:ASN:N | 2.37 | 0.57 |
| 10:UM:375:GLU:OE2 | 10:UM:394:ASN:ND2 | 2.37 | 0.57 |
| 12:UO:325:ALA:HB2 | 12:UO:332:ARG:HB2 | 1.85 | 0.57 |
| 12:UO:331:ASP:N | 12:UO:331:ASP:OD1 | 2.34 | 0.57 |
| 13:UQ:163:GLY:O | 13:UQ:181:THR:HA | 2.04 | 0.57 |
| 13:UQ:193:ASP:O | 13:UQ:203:ASP:HA | 2.04 | 0.57 |
| 15:UU:701:ARG:NH1 | 15:UU:736:LEU:O | 2.37 | 0.57 |
| 20:CD:357:ASN:HB3 | 20:CD:408:LEU:HD13 | 1.86 | 0.57 |
| 24:CI:538:ARG:O | 24:CI:560:TRP:NE1 | 2.30 | 0.57 |
| 32:CS:386:VAL:HG12 | 32:CS:406:TYR:HE2 | 1.69 | 0.57 |
| 44:C1:306:G:O6 | 44:C1:334:U:O4 | 2.22 | 0.57 |
| 44:C1:1472:A:C2 | 44:C1:1510:G:N1 | 2.54 | 0.57 |
| 46:UV:424:LEU:HD13 | 46:UV:432:GLN:HG3 | 1.86 | 0.57 |
| 9:UL:92:ILE:O | 9:UL:105:SER:HA | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:UL:238:ASP:HB3 | 9:UL:240:GLU:HG2 | 1.86 | 0.57 |
| 12:UO:529:LYS:NZ | 44:C1:112:C:O2' | 2.37 | 0.57 |
| 13:UQ:813:ILE:O | 13:UQ:822:LYS:N | 2.37 | 0.57 |
| 18:CA:70:LYS:NZ | 33:CT:159:ARG:O | 2.32 | 0.57 |
| 31:CQ:92:MET:HA | 31:CQ:95:LEU:HD12 | 1.84 | 0.57 |
| 32:CR:386:VAL:HG12 | 32:CR:406:TYR:HE2 | 1.69 | 0.57 |
| 44:C1:2333:A:H2' | 44:C1:2334:G:C8 | 2.39 | 0.57 |
| 48:UH:756:LEU:HD11 | 49:UI:170:GLU:HG2 | 1.85 | 0.57 |
| 52:CX:424:ASP:O | 52:CX:459:ARG:NH1 | 2.35 | 0.57 |
| 6:UG:417:SER:O | 6:UG:417:SER:OG | 2.21 | 0.57 |
| 7:UJ:669:LEU:HD23 | 7:UJ:670:HIS:HB2 | 1.86 | 0.57 |
| 10:UM:202:THR:O | 10:UM:205:GLY:HA2 | 2.04 | 0.57 |
| 10:UM:488:PRO:HG2 | 10:UM:509:PHE:HB2 | 1.87 | 0.57 |
| 12:UO:45:SER:O | 12:UO:319:SER:OG | 2.22 | 0.57 |
| 13:UQ:350:LYS:NZ | 44:C1:69:U:O2' | 2.38 | 0.57 |
| 16:UX:10:GLN:HE22 | 25:CJ:34:ARG:HH22 | 1.52 | 0.57 |
| 25:CJ:28:ARG:NH2 | 44:C1:349:C:OP1 | 2.38 | 0.57 |
| 46:UV:1098:ARG:HH12 | 46:UV:1104:LEU:HB2 | 1.68 | 0.57 |
| 50:US:379:ALA:HB1 | 50:US:417:MET:HE1 | 1.86 | 0.57 |
| 54:Cz:1573:ARG:HA | 54:Cz:1576:THR:HG22 | 1.86 | 0.57 |
| 1:UA:800:LYS:O | 1:UA:800:LYS:NZ | 2.38 | 0.57 |
| 6:UG:256:THR:HG21 | 6:UG:277:GLN:HE22 | 1.69 | 0.57 |
| 10:UM:772:ASN:O | 10:UM:776:ASN:ND2 | 2.37 | 0.57 |
| 10:UM:839:ALA:HA | 10:UM:842:LEU:HB2 | 1.85 | 0.57 |
| 13:UQ:568:THR:OG1 | 13:UQ:569:GLY:N | 2.37 | 0.57 |
| 19:CC:307:GLN:HG3 | 19:CC:312:THR:HB | 1.86 | 0.57 |
| 23:CH:131:ARG:NH1 | 23:CH:193:GLU:OE1 | 2.37 | 0.57 |
| 24:CI:70:LEU:HD22 | 24:CI:133:ALA:HA | 1.86 | 0.57 |
| 29:CN:121:LEU:HB2 | 29:CN:163:ILE:O | 2.03 | 0.57 |
| 34:Cc:39:GLU:N | 34:Cc:118:GLN:OE1 | 2.37 | 0.57 |
| 45:C2:259:A:H1' | 45:C2:260:G:C2 | 2.40 | 0.57 |
| 46:UV:185:THR:HG23 | 46:UV:203:LYS:HB2 | 1.87 | 0.57 |
| 48:UH:832:LEU:HA | 48:UH:835:VAL:HG22 | 1.85 | 0.57 |
| 2:UB:587:THR:OG1 | 2:UB:588:VAL:N | 2.29 | 0.57 |
| 2:UB:685:PRO:HG2 | 2:UB:690:ARG:HH21 | 1.70 | 0.57 |
| 2:UB:894:ASN:ND2 | 45:C2:9:U:OP1 | 2.37 | 0.57 |
| 7:UJ:256:SER:HA | 7:UJ:295:GLN:HE22 | 1.68 | 0.57 |
| 10:UM:587:ARG:HH21 | 10:UM:644:ASN:HD21 | 1.53 | 0.57 |
| 13:UQ:207:THR:O | 13:UQ:218:ILE:HA | 2.04 | 0.57 |
| 13:UQ:296:ARG:HD2 | 13:UQ:363:TRP:CD2 | 2.39 | 0.57 |
| 20:CD:139:ASP:N | 20:CD:139:ASP:OD1 | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:CF:96:ARG:NH1 | 22:CG:590:ARG:O | 2.37 | 0.57 |
| 32:CS:42:TYR:O | 32:CS:46:SER:OG | 2.18 | 0.57 |
| 39:Cj:55:LEU:HG | 39:Cj:105:LEU:HD11 | 1.85 | 0.57 |
| 44:C1:381:G:O5' | 44:C1:383:G:N2 | 2.38 | 0.57 |
| 45:C2:115:G:O2' | 45:C2:195:A:N3 | 2.37 | 0.57 |
| 46:UV:1012:VAL:HG12 | 46:UV:1014:PRO:HD3 | 1.86 | 0.57 |
| 52:CX:199:VAL:HA | 52:CX:236:LEU:HD21 | 1.86 | 0.57 |
| 7:UJ:782:VAL:O | 7:UJ:812:ARG:NH2 | 2.37 | 0.57 |
| 8:UK:164:PHE:HE1 | 53:UP:321:ARG:HH11 | 1.53 | 0.57 |
| 12:UO:473:ARG:HD2 | 12:UO:477:SER:HB2 | 1.86 | 0.57 |
| 12:UO:483:ARG:NH2 | 44:C1:112:C:OP1 | 2.37 | 0.57 |
| 15:UU:627:GLY:O | 15:UU:640:CYS:HB3 | 2.04 | 0.57 |
| 16:UX:0:PHE:HE2 | 45:C2:59:A:H2 | 1.52 | 0.57 |
| 16:UX:54:PRO:HG2 | 36:Cg:96:ALA:HA | 1.87 | 0.57 |
| 17:UZ:288:THR:O | 44:C1:2081:G:O2' | 2.22 | 0.57 |
| 21:CF:52:LEU:HG | 21:CF:78:PRO:HB2 | 1.87 | 0.57 |
| 24:CI:882:THR:H | 24:CI:905:VAL:HG12 | 1.69 | 0.57 |
| 32:CR:119:THR:HA | 32:CR:479:ARG:HH22 | 1.70 | 0.57 |
| 32:CR:134:ASN:HD22 | 32:CR:554:ASN:HB3 | 1.70 | 0.57 |
| 44:C1:369:U:O4 | 44:C1:398:C:N3 | 2.38 | 0.57 |
| 44:C1:597:G:H2' | 44:C1:598:A:H8 | 1.68 | 0.57 |
| 53:UP:328:ASP:OD1 | 53:UP:328:ASP:N | 2.34 | 0.57 |
| 4:UD:83:VAL:N | 4:UD:101:ARG:O | 2.37 | 0.57 |
| 4:UD:546:ASP:N | 4:UD:546:ASP:OD1 | 2.37 | 0.57 |
| 15:UU:341:SER:H | 15:UU:356:GLY:HA2 | 1.69 | 0.57 |
| 21:CF:26:GLN:OE1 | 21:CF:29:SER:OG | 2.21 | 0.57 |
| 24:CI:919:LYS:NZ | 44:C1:1140:A:N3 | 2.47 | 0.57 |
| 29:CO:151:LYS:HA | 29:CO:158:LYS:HA | 1.85 | 0.57 |
| 35:Ce:139:LEU:HD21 | 35:Ce:179:TYR:HB3 | 1.85 | 0.57 |
| 38:Ci:29:VAL:HG13 | 38:Ci:95:LYS:HD3 | 1.85 | 0.57 |
| 46:UV:306:TRP:HE1 | 46:UV:421:THR:HG21 | 1.69 | 0.57 |
| 46:UV:656:ARG:HH12 | 46:UV:768:VAL:HG21 | 1.69 | 0.57 |
| 7:UJ:49:TYR:OH | 7:UJ:74:PHE:O | 2.15 | 0.57 |
| 15:UU:710:ILE:HA | 15:UU:726:SER:HA | 1.87 | 0.57 |
| 17:UZ:104:PRO:HB2 | 17:UZ:107:PHE:HB3 | 1.85 | 0.57 |
| 22:CG:482:SER:OG | 22:CG:483:TRP:N | 2.37 | 0.57 |
| 24:CI:344:MET:HG2 | 24:CI:353:ILE:HG22 | 1.87 | 0.57 |
| 24:CI:393:VAL:HB | 32:CR:708:LEU:HB2 | 1.85 | 0.57 |
| 25:CJ:28:ARG:NH2 | 44:C1:349:C:O4' | 2.38 | 0.57 |
| 28:CM:397:LEU:O | 44:C1:593:G:N1 | 2.25 | 0.57 |
| 34:Cc:82:ASN:HA | 34:Cc:85:MET:HE3 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:C2:103:G:O6 | 45:C2:250:G:O6 | 2.22 | 0.57 |
| 46:UV:217:LYS:HE3 | 46:UV:220:LEU:HB2 | 1.86 | 0.57 |
| 54:Cz:1513:ILE:HA | 54:Cz:1516:MET:HG2 | 1.85 | 0.57 |
| 21:CE:104:THR:OG1 | 21:CE:105:SER:N | 2.30 | 0.57 |
| 24:CI:288:ILE:HG23 | 24:CI:291:VAL:HB | 1.86 | 0.57 |
| 32:CS:849:LEU:HD12 | 32:CS:853:VAL:HG13 | 1.86 | 0.57 |
| 46:UV:217:LYS:HB3 | 46:UV:221:ASP:HB2 | 1.86 | 0.57 |
| 52:CX:301:GLY:O | 52:CX:305:GLY:HA3 | 2.04 | 0.57 |
| 4:UD:188:LYS:HB2 | 4:UD:205:SER:HB3 | 1.86 | 0.57 |
| 7:UJ:165:ARG:NH1 | 20:CD:419:LEU:O | 2.35 | 0.57 |
| 14:UR:296:SER:HA | 14:UR:325:LEU:HD23 | 1.87 | 0.57 |
| 15:UU:482:PRO:HD2 | 15:UU:502:LEU:HD21 | 1.86 | 0.57 |
| 16:UX:2:THR:O | 25:CJ:39:GLN:NE2 | 2.38 | 0.57 |
| 28:CM:78:SER:OG | 28:CM:79:LEU:N | 2.30 | 0.57 |
| 32:CR:851:TYR:HA | 32:CR:854:VAL:HG12 | 1.86 | 0.57 |
| 34:Cc:177:ILE:HD11 | 44:C1:2056:U:H5' | 1.85 | 0.57 |
| 46:UV:432:GLN:NE2 | 46:UV:435:PRO:O | 2.31 | 0.57 |
| 1:UA:259:ARG:NH1 | 1:UA:299:GLU:OE2 | 2.38 | 0.56 |
| 4:UD:230:THR:OG1 | 4:UD:231:GLY:N | 2.35 | 0.56 |
| 6:UG:54:ARG:HH11 | 28:CM:29:PRO:HB3 | 1.70 | 0.56 |
| 17:UZ:282:TYR:HB3 | 17:UZ:290:ALA:HB1 | 1.87 | 0.56 |
| 28:CM:245:ILE:HD11 | 28:CM:255:LEU:HD12 | 1.87 | 0.56 |
| 32:CR:849:LEU:HD12 | 32:CR:853:VAL:HG13 | 1.86 | 0.56 |
| 46:UV:829:PRO:HB2 | 46:UV:872:PRO:HB3 | 1.86 | 0.56 |
| 50:US:531:GLU:HG3 | 50:US:533:LYS:H | 1.68 | 0.56 |
| 1:UA:593:SER:OG | 1:UA:594:LYS:N | 2.35 | 0.56 |
| 2:UB:882:ILE:HG22 | 41:Cn:68:ILE:HG21 | 1.87 | 0.56 |
| 13:UQ:163:GLY:HA3 | 13:UQ:182:ILE:HG22 | 1.87 | 0.56 |
| 15:UU:43:LEU:HD22 | 15:UU:67:VAL:HG13 | 1.87 | 0.56 |
| 17:UZ:217:ILE:HA | 17:UZ:220:ILE:HB | 1.88 | 0.56 |
| 18:CB:188:ARG:HA | 18:CB:191:ARG:HD2 | 1.86 | 0.56 |
| 22:CG:179:CYS:HB3 | 22:CG:182:TYR:HB2 | 1.86 | 0.56 |
| 24:CI:268:ILE:O | 24:CI:780:VAL:HA | 2.06 | 0.56 |
| 29:CO:44:ALA:HB1 | 29:CO:46:LEU:HD23 | 1.86 | 0.56 |
| 36:Cg:68:LEU:O | 36:Cg:72:ASN:ND2 | 2.38 | 0.56 |
| 46:UV:34:ARG:HH12 | 46:UV:432:GLN:HB3 | 1.70 | 0.56 |
| 1:UA:162:ASP:OD2 | 1:UA:164:ARG:NE | 2.38 | 0.56 |
| 1:UA:444:SER:OG | 1:UA:447:SER:O | 2.19 | 0.56 |
| 1:UA:617:SER:OG | 1:UA:618:LEU:N | 2.37 | 0.56 |
| 4:UD:708:PHE:HA | 4:UD:827:TRP:O | 2.04 | 0.56 |
| 6:UG:305:SER:OG | 6:UG:346:THR:O | 2.22 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:UL:848:VAL:HG23 | 42:Cp:17:LEU:HD13 | 1.86 | 0.56 |
| 12:UO:108:ARG:NH1 | 34:Cc:110:LEU:O | 2.35 | 0.56 |
| 12:UO:429:ARG:NH2 | 44:C1:73:A:OP1 | 2.23 | 0.56 |
| 13:UQ:381:LEU:HB2 | 13:UQ:390:ASP:O | 2.06 | 0.56 |
| 13:UQ:927:ALA:O | 13:UQ:931:ASN:ND2 | 2.39 | 0.56 |
| 15:UU:255:ILE:HG13 | 15:UU:265:LEU:H | 1.69 | 0.56 |
| 21:CF:38:ALA:O | 21:CF:42:THR:OG1 | 2.20 | 0.56 |
| 28:CM:80:ASN:N | 28:CM:80:ASN:OD1 | 2.37 | 0.56 |
| 31:CQ:151:ASP:O | 31:CQ:155:ALA:HB2 | 2.04 | 0.56 |
| 32:CS:17:ASN:HA | 32:CS:20:GLN:HE21 | 1.70 | 0.56 |
| 32:CS:93:ASP:HB3 | 32:CS:96:GLU:HB2 | 1.88 | 0.56 |
| 32:CS:851:TYR:HA | 32:CS:854:VAL:HG12 | 1.86 | 0.56 |
| 34:Cc:84:LEU:O | 34:Cc:167:ARG:NH2 | 2.38 | 0.56 |
| 35:Ce:70:VAL:HA | 35:Ce:73:LEU:HD23 | 1.86 | 0.56 |
| 44:C1:6:G:N1 | 44:C1:30:U:C2 | 2.73 | 0.56 |
| 44:C1:420:G:H2' | 44:C1:421:A:H8 | 1.71 | 0.56 |
| 44:C1:1623:U:O2' | 44:C1:1675:A:N7 | 2.39 | 0.56 |
| 44:C1:1734:G:H2' | 44:C1:1735:A:H8 | 1.70 | 0.56 |
| 46:UV:375:VAL:HG23 | 46:UV:376:LEU:HG | 1.87 | 0.56 |
| 46:UV:945:SER:HA | 46:UV:951:ARG:HH22 | 1.69 | 0.56 |
| 47:CV:66:ARG:HE | 47:CV:70:THR:HG23 | 1.68 | 0.56 |
| 48:UH:492:GLN:HG3 | 48:UH:527:PRO:HG3 | 1.87 | 0.56 |
| 1:UA:645:ALA:O | 1:UA:651:ARG:NH1 | 2.39 | 0.56 |
| 12:UO:492:PRO:HD3 | 49:UE:249:ARG:HH21 | 1.71 | 0.56 |
| 15:UU:78:ARG:O | 15:UU:81:ASN:ND2 | 2.38 | 0.56 |
| 32:CR:17:ASN:HA | 32:CR:20:GLN:HE21 | 1.70 | 0.56 |
| 42:Cp:16:VAL:HA | 42:Cp:29:VAL:HG23 | 1.88 | 0.56 |
| 44:C1:123:U:H2' | 44:C1:124:C:C6 | 2.40 | 0.56 |
| 1:UA:334:LEU:HD12 | 1:UA:336:GLN:HG2 | 1.86 | 0.56 |
| 2:UB:531:ILE:HA | 2:UB:534:ILE:HD12 | 1.88 | 0.56 |
| 4:UD:381:ARG:NH1 | 4:UD:842:GLU:O | 2.35 | 0.56 |
| 6:UG:387:THR:OG1 | 6:UG:388:TRP:N | 2.36 | 0.56 |
| 13:UQ:149:SER:HB3 | 13:UQ:155:TYR:HB2 | 1.87 | 0.56 |
| 13:UQ:208:LEU:HD21 | 13:UQ:241:PRO:HB2 | 1.86 | 0.56 |
| 18:CB:249:GLN:NE2 | 18:CB:307:LEU:O | 2.35 | 0.56 |
| 19:CC:190:SER:O | 19:CC:193:GLN:NE2 | 2.38 | 0.56 |
| 20:CD:14:ALA:HA | 20:CD:48:PHE:HA | 1.86 | 0.56 |
| 21:CE:6:SER:OG | 21:CE:7:ALA:N | 2.38 | 0.56 |
| 21:CF:53:VAL:O | 21:CF:79:TYR:HA | 2.05 | 0.56 |
| 28:CM:155:PRO:O | 28:CM:173:GLY:N | 2.38 | 0.56 |
| 29:CO:174:ASN:ND2 | 29:CO:199:ASN:O | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:CR:424:LEU:HA | 32:CR:427:LYS:HG2 | 1.88 | 0.56 |
| 32:CS:119:THR:HA | 32:CS:479:ARG:HH22 | 1.70 | 0.56 |
| 40:Cm:8:HIS:HB2 | 40:Cm:74:VAL:HG11 | 1.88 | 0.56 |
| 44:C1:411:C:H2' | 44:C1:412:G:H8 | 1.70 | 0.56 |
| 45:C2:252:C:H2' | 45:C2:253:G:H8 | 1.70 | 0.56 |
| 45:C2:257:G:H2' | 45:C2:258:A:C8 | 2.39 | 0.56 |
| 46:UV:716:ARG:NH2 | 47:CV:217:SER:OG | 2.38 | 0.56 |
| 46:UV:718:LYS:HD3 | 46:UV:769:ARG:HH22 | 1.70 | 0.56 |
| 46:UV:737:ILE:HD11 | 46:UV:758:VAL:HB | 1.87 | 0.56 |
| 4:UD:48:ARG:HB2 | 4:UD:52:ASP:HB3 | 1.87 | 0.56 |
| 6:UG:267:ASN:ND2 | 6:UG:270:ASN:OD1 | 2.36 | 0.56 |
| 9:UL:49:VAL:O | 9:UL:58:LEU:N | 2.38 | 0.56 |
| 9:UL:815:ASN:HD22 | 9:UL:817:ILE:HG22 | 1.70 | 0.56 |
| 13:UQ:89:MET:HE2 | 13:UQ:414:HIS:HD2 | 1.71 | 0.56 |
| 15:UU:288:ALA:N | 15:UU:294:LYS:O | 2.39 | 0.56 |
| 46:UV:120:PHE:HE1 | 46:UV:142:MET:HB2 | 1.70 | 0.56 |
| 1:UA:35:ASN:ND2 | 1:UA:54:HIS:O | 2.39 | 0.56 |
| 6:UG:130:PHE:H | 6:UG:417:SER:HG | 1.53 | 0.56 |
| 9:UL:579:LEU:HD13 | 9:UL:593:PHE:HA | 1.88 | 0.56 |
| 13:UQ:169:ASN:O | 13:UQ:172:SER:OG | 2.24 | 0.56 |
| 13:UQ:215:SER:OG | 13:UQ:216:ALA:N | 2.39 | 0.56 |
| 15:UU:709:ASP:O | 15:UU:727:GLN:N | 2.37 | 0.56 |
| 16:UX:148:THR:OG1 | 16:UX:149:ASN:N | 2.38 | 0.56 |
| 17:UZ:87:HIS:HB2 | 17:UZ:258:ASN:HD21 | 1.70 | 0.56 |
| 19:CC:176:HIS:HA | 20:CD:189:TRP:HZ3 | 1.71 | 0.56 |
| 19:CC:380:ARG:NH2 | 45:C2:111:G:O6 | 2.39 | 0.56 |
| 24:CI:54:LEU:HD13 | 41:Cn:77:ILE:HB | 1.88 | 0.56 |
| 26:CK:48:ASN:HD21 | 43:CU:216:LYS:H | 1.51 | 0.56 |
| 45:C2:149:U:H2' | 45:C2:150:G:H8 | 1.70 | 0.56 |
| 52:CX:346:CYS:O | 52:CX:388:HIS:ND1 | 2.38 | 0.56 |
| 1:UA:578:ILE:HD12 | 1:UA:587:LEU:HD21 | 1.87 | 0.56 |
| 2:UB:654:VAL:HG12 | 2:UB:657:MET:H | 1.71 | 0.56 |
| 2:UB:729:ALA:HA | 2:UB:732:ILE:HD12 | 1.88 | 0.56 |
| 6:UG:477:ARG:NH1 | 44:C1:587:U:O2 | 2.39 | 0.56 |
| 8:UK:22:ARG:NH2 | 24:CI:983:LEU:O | 2.39 | 0.56 |
| 9:UL:92:ILE:HB | 9:UL:106:PHE:HB2 | 1.86 | 0.56 |
| 9:UL:119:ASP:HB3 | 9:UL:122:GLY:H | 1.71 | 0.56 |
| 12:UO:164:SER:OG | 12:UO:166:ASP:OD1 | 2.22 | 0.56 |
| 12:UO:440:VAL:HG12 | 12:UO:441:LEU:HD23 | 1.87 | 0.56 |
| 13:UQ:498:PRO:HG3 | 13:UQ:535:GLU:HG2 | 1.88 | 0.56 |
| 15:UU:35:PHE:HB3 | 15:UU:776:TRP:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:CD:16:PHE:HA | 20:CD:45:TYR:HA | 1.87 | 0.56 |
| 24:CI:821:ARG:NH1 | 41:Cn:139:LYS:O | 2.39 | 0.56 |
| 32:CR:744:PRO:HD3 | 32:CR:762:MET:HE3 | 1.87 | 0.56 |
| 40:Cm:81:VAL:HG21 | 40:Cm:125:ILE:HG12 | 1.86 | 0.56 |
| 46:UV:207:GLU:HG2 | 46:UV:215:LYS:HB2 | 1.88 | 0.56 |
| 48:UH:535:ARG:HH11 | 48:UH:633:GLY:HA3 | 1.69 | 0.56 |
| 1:UA:111:PHE:CE1 | 1:UA:122:TRP:HB2 | 2.41 | 0.56 |
| 4:UD:366:PRO:HB3 | 4:UD:704:VAL:HG11 | 1.86 | 0.56 |
| 9:UL:574:SER:HA | 9:UL:615:ILE:HD11 | 1.86 | 0.56 |
| 10:UM:435:ILE:O | 10:UM:452:SER:N | 2.38 | 0.56 |
| 10:UM:620:GLY:O | 10:UM:644:ASN:ND2 | 2.38 | 0.56 |
| 13:UQ:107:TYR:HB2 | 13:UQ:110:SER:HB2 | 1.88 | 0.56 |
| 17:UZ:133:LEU:HA | 17:UZ:137:PHE:HD2 | 1.70 | 0.56 |
| 17:UZ:288:THR:OG1 | 17:UZ:289:ALA:N | 2.39 | 0.56 |
| 20:CD:179:LEU:HD21 | 20:CD:267:ARG:HB3 | 1.88 | 0.56 |
| 24:CI:54:LEU:HD11 | 41:Cn:78:LYS:HB2 | 1.87 | 0.56 |
| 24:CI:346:ILE:HA | 24:CI:351:ILE:HG22 | 1.88 | 0.56 |
| 24:CI:804:SER:OG | 24:CI:806:THR:OG1 | 2.19 | 0.56 |
| 25:CJ:105:ALA:HA | 25:CJ:108:ARG:HG2 | 1.87 | 0.56 |
| 26:CK:75:ASP:OD2 | 26:CK:77:TYR:N | 2.34 | 0.56 |
| 40:Cm:88:LYS:HD2 | 43:CU:300:VAL:HG12 | 1.88 | 0.56 |
| 44:C1:69:U:N3 | 48:UH:884:SER:OG | 2.37 | 0.56 |
| 44:C1:472:G:H2' | 44:C1:473:G:C8 | 2.41 | 0.56 |
| 44:C1:1630:C:H2' | 44:C1:1631:G:H8 | 1.71 | 0.56 |
| 2:UB:104:LEU:HB2 | 2:UB:858:PHE:HZ | 1.71 | 0.56 |
| 4:UD:158:THR:OG1 | 4:UD:159:VAL:N | 2.34 | 0.56 |
| 6:UG:283:THR:OG1 | 6:UG:285:TRP:NE1 | 2.39 | 0.56 |
| 7:UJ:826:TYR:HA | 7:UJ:865:ILE:HD11 | 1.86 | 0.56 |
| 10:UM:666:PHE:O | 10:UM:677:VAL:HA | 2.06 | 0.56 |
| 13:UQ:88:ARG:HB2 | 13:UQ:850:ALA:HB3 | 1.88 | 0.56 |
| 13:UQ:455:VAL:HA | 48:UH:888:ILE:HD11 | 1.88 | 0.56 |
| 15:UU:192:MET:HE2 | 15:UU:192:MET:N | 2.21 | 0.56 |
| 15:UU:987:ASP:O | 15:UU:991:THR:OG1 | 2.14 | 0.56 |
| 22:CG:303:LEU:O | 22:CG:314:VAL:HA | 2.06 | 0.56 |
| 23:CH:48:PRO:HA | 23:CH:51:ILE:HG22 | 1.87 | 0.56 |
| 24:CI:109:SER:HA | 24:CI:327:LEU:HD11 | 1.88 | 0.56 |
| 24:CI:235:LEU:HD23 | 24:CI:238:ARG:HG3 | 1.87 | 0.56 |
| 28:CM:396:HIS:ND1 | 44:C1:594:G:O6 | 2.38 | 0.56 |
| 28:CM:432:LYS:HZ2 | 28:CM:434:LYS:HG3 | 1.71 | 0.56 |
| 32:CS:35:LYS:HA | 32:CS:38:ILE:HG13 | 1.88 | 0.56 |
| 32:CS:424:LEU:HA | 32:CS:427:LYS:HG2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:CS:744:PRO:HD3 | 32:CS:762:MET:HE3 | 1.87 | 0.56 |
| 36:Cg:106:ARG:HH22 | 36:Cg:142:PRO:HG2 | 1.70 | 0.56 |
| 44:C1:2351:G:H1' | 44:C1:2352:U:H5 | 1.71 | 0.56 |
| 50:US:362:ARG:HE | 50:US:493:LEU:HD13 | 1.71 | 0.56 |
| 4:UD:253:ASP:OD1 | 4:UD:257:GLN:N | 2.38 | 0.55 |
| 9:UL:243:VAL:HG23 | 9:UL:270:ARG:HG3 | 1.88 | 0.55 |
| 9:UL:861:LEU:HD21 | 9:UL:877:ILE:HD11 | 1.87 | 0.55 |
| 13:UQ:514:GLN:NE2 | 13:UQ:596:LEU:O | 2.39 | 0.55 |
| 13:UQ:671:VAL:HG22 | 48:UH:718:PRO:HD3 | 1.88 | 0.55 |
| 14:UR:159:ILE:N | 14:UR:163:GLU:OE1 | 2.40 | 0.55 |
| 19:CC:232:LEU:HD11 | 19:CC:259:LYS:HZ2 | 1.70 | 0.55 |
| 20:CD:64:ILE:O | 20:CD:94:LYS:NZ | 2.27 | 0.55 |
| 20:CD:192:TRP:NE1 | 20:CD:247:THR:OG1 | 2.39 | 0.55 |
| 24:CI:246:ILE:HG13 | 24:CI:270:LEU:HD13 | 1.88 | 0.55 |
| 24:CI:1076:MET:HA | 24:CI:1079:ARG:HG2 | 1.89 | 0.55 |
| 28:CM:31:LEU:O | 28:CM:32:HIS:ND1 | 2.39 | 0.55 |
| 44:C1:2089:G:H2' | 44:C1:2090:G:C8 | 2.40 | 0.55 |
| 4:UD:685:THR:O | 44:C1:63:C:O2' | 2.23 | 0.55 |
| 7:UJ:637:LEU:HB2 | 7:UJ:642:GLY:HA2 | 1.87 | 0.55 |
| 7:UJ:647:LEU:HD13 | 7:UJ:652:LEU:HB3 | 1.89 | 0.55 |
| 7:UJ:720:LEU:HB3 | 7:UJ:767:GLU:HG2 | 1.88 | 0.55 |
| 15:UU:38:TYR:HB2 | 15:UU:777:THR:HG23 | 1.88 | 0.55 |
| 15:UU:481:ILE:O | 15:UU:485:GLN:NE2 | 2.38 | 0.55 |
| 15:UU:644:GLY:HA2 | 15:UU:663:ALA:HA | 1.86 | 0.55 |
| 22:CG:173:VAL:HG13 | 22:CG:581:VAL:HG13 | 1.89 | 0.55 |
| 22:CG:226:ARG:NH2 | 45:C2:126:U:O4 | 2.39 | 0.55 |
| 22:CG:342:GLU:HG3 | 22:CG:359:VAL:HB | 1.87 | 0.55 |
| 23:CH:168:PRO:HA | 23:CH:171:ILE:HB | 1.88 | 0.55 |
| 24:CI:197:LEU:HD12 | 24:CI:198:TYR:H | 1.71 | 0.55 |
| 32:CS:414:ILE:HG23 | 32:CS:415:SER:HB2 | 1.88 | 0.55 |
| 44:C1:4:G:C2 | 44:C1:32:U:C2 | 2.94 | 0.55 |
| 44:C1:1453:G:H2' | 44:C1:1454:A:H8 | 1.70 | 0.55 |
| 50:US:455:SER:OG | 50:US:456:CYS:N | 2.38 | 0.55 |
| 52:CX:243:THR:HG23 | 52:CX:246:ALA:H | 1.70 | 0.55 |
| 54:Cz:1652:ASP:O | 54:Cz:1656:TYR:CB | 2.54 | 0.55 |
| 1:UA:407:ARG:HG2 | 1:UA:419:THR:HG22 | 1.88 | 0.55 |
| 2:UB:820:ASP:OD2 | 2:UB:825:TYR:OH | 2.25 | 0.55 |
| 8:UK:250:THR:O | 8:UK:252:THR:OG1 | 2.24 | 0.55 |
| 12:UO:277:THR:OG1 | 12:UO:278:SER:N | 2.38 | 0.55 |
| 15:UU:470:SER:HB2 | 15:UU:511:VAL:HG22 | 1.86 | 0.55 |
| 16:UX:142:ARG:HH21 | 16:UX:160:ILE:HD12 | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:CB:180:VAL:O | 18:CB:203:VAL:HA | 2.06 | 0.55 |
| 19:CC:185:ASP:OD1 | 19:CC:317:ARG:NH2 | 2.40 | 0.55 |
| 24:CI:63:PRO:HG2 | 24:CI:66:PRO:HA | 1.88 | 0.55 |
| 24:CI:605:GLU:O | 24:CI:608:THR:OG1 | 2.23 | 0.55 |
| 28:CM:39:GLU:HG2 | 28:CM:382:TYR:HE2 | 1.70 | 0.55 |
| 32:CR:113:ASP:OD1 | 32:CR:113:ASP:N | 2.37 | 0.55 |
| 38:Ci:85:LYS:HZ1 | 38:Ci:123:MET:HB3 | 1.71 | 0.55 |
| 43:CU:272:PRO:HB2 | 43:CU:275:LEU:HD23 | 1.88 | 0.55 |
| 44:C1:1456:A:H2' | 44:C1:1457:G:C8 | 2.41 | 0.55 |
| 1:UA:326:GLU:OE2 | 1:UA:327:TRP:N | 2.39 | 0.55 |
| 6:UG:245:THR:O | 25:CJ:21:TYR:OH | 2.20 | 0.55 |
| 7:UJ:232:MET:HB3 | 7:UJ:243:ASN:HB3 | 1.88 | 0.55 |
| 8:UK:172:GLN:HA | 8:UK:175:LEU:HD12 | 1.88 | 0.55 |
| 10:UM:733:GLN:HA | 10:UM:736:LEU:HG | 1.89 | 0.55 |
| 12:UO:202:SER:OG | 12:UO:203:ASN:N | 2.39 | 0.55 |
| 13:UQ:259:GLU:O | 13:UQ:286:VAL:N | 2.40 | 0.55 |
| 15:UU:54:ILE:HG13 | 15:UU:62:GLN:HB2 | 1.88 | 0.55 |
| 24:CI:45:ARG:NH2 | 44:C1:615:A:OP1 | 2.37 | 0.55 |
| 24:CI:110:LYS:NZ | 24:CI:324:ARG:O | 2.40 | 0.55 |
| 27:CL:572:ARG:NH2 | 44:C1:2215:C:OP2 | 2.40 | 0.55 |
| 32:CR:93:ASP:HB3 | 32:CR:96:GLU:HB2 | 1.88 | 0.55 |
| 32:CR:414:ILE:HG23 | 32:CR:415:SER:HB2 | 1.88 | 0.55 |
| 32:CS:116:LEU:HD21 | 32:CS:138:ARG:HE | 1.71 | 0.55 |
| 32:CS:125:LEU:HD12 | 32:CS:151:LEU:HD12 | 1.89 | 0.55 |
| 39:Cj:13:LYS:HG3 | 39:Cj:14:LYS:H | 1.71 | 0.55 |
| 44:C1:1744:A:H2' | 44:C1:1745:C:H6 | 1.72 | 0.55 |
| 45:C2:243:G:H2' | 45:C2:244:G:C8 | 2.42 | 0.55 |
| 46:UV:191:HIS:HB2 | 46:UV:199:VAL:HG21 | 1.87 | 0.55 |
| 46:UV:355:GLN:NE2 | 54:Cz:1522:VAL:O | 2.39 | 0.55 |
| 50:US:426:GLU:O | 50:US:430:LYS:NZ | 2.39 | 0.55 |
| 1:UA:420:PHE:HE1 | 1:UA:458:GLY:HA2 | 1.70 | 0.55 |
| 1:UA:536:PHE:HB2 | 1:UA:546:SER:HB2 | 1.87 | 0.55 |
| 4:UD:381:ARG:HB2 | 4:UD:395:HIS:HE1 | 1.70 | 0.55 |
| 10:UM:628:ASN:ND2 | 10:UM:630:SER:OG | 2.39 | 0.55 |
| 13:UQ:447:SER:OG | 13:UQ:449:ASP:OD1 | 2.24 | 0.55 |
| 18:CB:77:ARG:NH1 | 18:CB:146:GLU:O | 2.37 | 0.55 |
| 18:CB:167:VAL:HA | 18:CB:170:VAL:HG22 | 1.87 | 0.55 |
| 20:CD:9:THR:HG23 | 20:CD:11:ALA:H | 1.72 | 0.55 |
| 23:CH:95:SER:O | 23:CH:195:ARG:NH2 | 2.40 | 0.55 |
| 24:CI:929:LYS:NZ | 44:C1:2071:G:O6 | 2.40 | 0.55 |
| 24:CI:937:MET:O | 27:CL:511:ARG:NH2 | 2.34 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:Cg:114:LEU:HD22 | 36:Cg:116:LEU:HG | 1.89 | 0.55 |
| 44:C1:488:C:H2' | 44:C1:489:A:H8 | 1.72 | 0.55 |
| 44:C1:1139:A:O3' | 44:C1:1158:G:N2 | 2.39 | 0.55 |
| 46:UV:824:PHE:HE1 | 46:UV:869:PRO:HD2 | 1.71 | 0.55 |
| 6:UG:41:ARG:HH22 | 6:UG:45:TYR:HB2 | 1.69 | 0.55 |
| 7:UJ:542:ARG:HE | 7:UJ:578:ARG:HE | 1.53 | 0.55 |
| 8:UK:268:ARG:HH11 | 14:UR:540:THR:HA | 1.72 | 0.55 |
| 9:UL:451:ILE:HG13 | 9:UL:460:ILE:HG23 | 1.89 | 0.55 |
| 11:UN:901:LEU:O | 11:UN:903:LEU:N | 2.40 | 0.55 |
| 16:UX:125:HIS:HD1 | 16:UX:127:GLY:H | 1.54 | 0.55 |
| 23:CH:177:GLN:HB3 | 23:CH:191:ILE:H | 1.71 | 0.55 |
| 24:CI:891:SER:O | 24:CI:898:ARG:NE | 2.33 | 0.55 |
| 26:CK:269:THR:OG1 | 26:CK:269:THR:O | 2.25 | 0.55 |
| 32:CR:4:GLN:HA | 32:CR:4:GLN:HE21 | 1.71 | 0.55 |
| 32:CR:116:LEU:HD21 | 32:CR:138:ARG:HE | 1.71 | 0.55 |
| 44:C1:205:C:O2' | 44:C1:206:C:O2 | 2.21 | 0.55 |
| 44:C1:244:G:H2' | 44:C1:245:G:H8 | 1.71 | 0.55 |
| 44:C1:440:G:H4' | 44:C1:441:A:H5" | 1.87 | 0.55 |
| 44:C1:496:U:C4 | 44:C1:503:G:N1 | 2.75 | 0.55 |
| 46:UV:199:VAL:HG11 | 46:UV:225:ARG:HG2 | 1.89 | 0.55 |
| 48:UH:557:GLU:O | 48:UH:565:GLY:HA3 | 2.02 | 0.55 |
| 4:UD:445:ALA:O | 4:UD:451:VAL:HA | 2.06 | 0.55 |
| 7:UJ:259:MET:HG2 | 7:UJ:271:SER:HB2 | 1.89 | 0.55 |
| 7:UJ:421:GLY:HA3 | 7:UJ:456:LEU:HG | 1.89 | 0.55 |
| 9:UL:222:ALA:HB3 | 9:UL:235:ALA:HB3 | 1.88 | 0.55 |
| 9:UL:507:ASP:OD1 | 9:UL:507:ASP:N | 2.38 | 0.55 |
| 14:UR:138:ASP:OD2 | 15:UU:198:LYS:NZ | 2.38 | 0.55 |
| 14:UR:497:ARG:HA | 14:UR:500:LEU:HB2 | 1.89 | 0.55 |
| 21:CE:25:VAL:HG13 | 21:CE:34:LEU:HD11 | 1.89 | 0.55 |
| 21:CF:64:ILE:HA | 21:CF:67:HIS:HD2 | 1.70 | 0.55 |
| 23:CH:19:GLN:OE1 | 23:CH:19:GLN:N | 2.39 | 0.55 |
| 23:CH:22:VAL:O | 23:CH:25:THR:OG1 | 2.20 | 0.55 |
| 24:CI:815:VAL:HG23 | 24:CI:905:VAL:HA | 1.89 | 0.55 |
| 29:CN:242:CYS:SG | 29:CN:243:HIS:N | 2.79 | 0.55 |
| 31:CQ:156:ILE:HA | 31:CQ:159:LEU:HD12 | 1.89 | 0.55 |
| 32:CR:8:ASP:OD1 | 32:CR:10:ARG:NE | 2.38 | 0.55 |
| 41:Cn:79:ASN:HB3 | 41:Cn:81:LYS:HG3 | 1.88 | 0.55 |
| 44:C1:486:G:H2' | 44:C1:487:G:H8 | 1.71 | 0.55 |
| 45:C2:43:C:H2' | 45:C2:44:U:H6 | 1.72 | 0.55 |
| 46:UV:478:VAL:HA | 46:UV:481:LYS:HD2 | 1.89 | 0.55 |
| 46:UV:689:LYS:HE2 | 46:UV:1043:ALA:HB3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:149:GLN:NE2 | 44:C1:267:U:OP2 | 2.39 | 0.55 |
| 4:UD:108:THR:O | 4:UD:132:ILE:N | 2.36 | 0.55 |
| 4:UD:673:ASN:HD21 | 4:UD:715:ASP:HA | 1.70 | 0.55 |
| 9:UL:24:LEU:HB2 | 9:UL:373:ASP:HB2 | 1.88 | 0.55 |
| 10:UM:114:VAL:HA | 10:UM:130:ALA:HA | 1.89 | 0.55 |
| 12:UO:527:LEU:HD13 | 49:UE:263:LEU:HB3 | 1.89 | 0.55 |
| 25:CJ:20:ASN:OD1 | 25:CJ:20:ASN:N | 2.36 | 0.55 |
| 28:CM:296:GLU:OE2 | 28:CM:312:ARG:NH1 | 2.40 | 0.55 |
| 30:CP:157:LEU:HB3 | 30:CP:201:LEU:HD22 | 1.88 | 0.55 |
| 32:CR:731:GLN:HE22 | 32:CR:735:LYS:HE2 | 1.72 | 0.55 |
| 42:Cp:44:ASN:ND2 | 42:Cp:65:ARG:O | 2.40 | 0.55 |
| 44:C1:1758:C:H4' | 44:C1:2184:G:C2 | 2.42 | 0.55 |
| 44:C1:2230:U:H2' | 44:C1:2231:A:C8 | 2.41 | 0.55 |
| 49:UE:234:ASP:OD1 | 49:UE:234:ASP:N | 2.39 | 0.55 |
| 50:US:303:LEU:O | 50:US:307:LEU:HB2 | 2.05 | 0.55 |
| 50:US:370:SER:OG | 50:US:371:THR:N | 2.39 | 0.55 |
| 49:UI:234:ASP:N | 49:UI:234:ASP:OD1 | 2.39 | 0.55 |
| 1:UA:21:LEU:HD13 | 1:UA:63:LEU:HB2 | 1.88 | 0.55 |
| 2:UB:521:GLU:HG2 | 2:UB:522:ARG:HE | 1.72 | 0.55 |
| 4:UD:78:ASP:HB3 | 4:UD:105:ILE:HD11 | 1.89 | 0.55 |
| 4:UD:625:LYS:HB3 | 7:UJ:670:HIS:CE1 | 2.42 | 0.55 |
| 9:UL:283:GLU:HB3 | 9:UL:296:HIS:HE1 | 1.72 | 0.55 |
| 9:UL:940:VAL:HG11 | 31:CQ:197:THR:HG23 | 1.89 | 0.55 |
| 22:CG:172:THR:HG23 | 22:CG:583:GLY:HA3 | 1.88 | 0.55 |
| 22:CG:557:ARG:HG3 | 22:CG:597:GLY:HA2 | 1.87 | 0.55 |
| 23:CH:128:LEU:O | 23:CH:195:ARG:HA | 2.06 | 0.55 |
| 24:CI:395:LEU:HD13 | 32:CR:709:PHE:HD2 | 1.72 | 0.55 |
| 29:CN:181:SER:N | 29:CN:225:ILE:O | 2.40 | 0.55 |
| 29:CO:34:THR:O | 29:CO:201:SER:OG | 2.25 | 0.55 |
| 43:CU:244:ARG:HH21 | 43:CU:245:ARG:HE | 1.53 | 0.55 |
| 44:C1:274:A:H2' | 44:C1:275:C:C6 | 2.42 | 0.55 |
| 46:UV:934:THR:O | 46:UV:938:GLN:NE2 | 2.40 | 0.55 |
| 2:UB:60:PHE:HB3 | 2:UB:87:ARG:HG3 | 1.88 | 0.55 |
| 4:UD:59:LEU:HB3 | 4:UD:62:GLY:HA3 | 1.88 | 0.55 |
| 4:UD:504:ILE:O | 4:UD:524:HIS:N | 2.37 | 0.55 |
| 9:UL:284:VAL:HA | 9:UL:294:ALA:O | 2.06 | 0.55 |
| 10:UM:126:LEU:HD23 | 10:UM:138:TRP:HB2 | 1.89 | 0.55 |
| 10:UM:276:LEU:HB3 | 10:UM:294:THR:H | 1.72 | 0.55 |
| 14:UR:138:ASP:OD1 | 14:UR:139:SER:N | 2.40 | 0.55 |
| 14:UR:397:MET:HG3 | 14:UR:411:GLN:HE21 | 1.71 | 0.55 |
| 15:UU:729:SER:HB2 | 15:UU:750:PRO:HG3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:CC:19:GLU:HG2 | 19:CC:51:ARG:HB2 | 1.89 | 0.55 |
| 24:CI:247:ASP:N | 24:CI:271:SER:O | 2.37 | 0.55 |
| 28:CM:373:GLU:OE1 | 44:C1:440:G:N2 | 2.30 | 0.55 |
| 32:CR:125:LEU:HD12 | 32:CR:151:LEU:HD12 | 1.89 | 0.55 |
| 34:Cc:176:THR:OG1 | 34:Cc:177:ILE:N | 2.38 | 0.55 |
| 35:Ce:163:ILE:HB | 35:Ce:196:PRO:HD3 | 1.89 | 0.55 |
| 44:C1:1652:C:H2' | 44:C1:1653:G:H8 | 1.72 | 0.55 |
| 48:UH:615:ILE:HD13 | 48:UH:647:LEU:HD11 | 1.89 | 0.55 |
| 1:UA:162:ASP:H | 1:UA:207:GLN:HE22 | 1.54 | 0.54 |
| 5:UF:285:VAL:HA | 5:UF:288:LYS:HZ3 | 1.71 | 0.54 |
| 6:UG:478:GLN:HG2 | 6:UG:481:ARG:HH12 | 1.72 | 0.54 |
| 13:UQ:922:ALA:HB3 | 13:UQ:925:ARG:HG2 | 1.90 | 0.54 |
| 18:CA:228:ALA:HB3 | 18:CA:255:ILE:HG13 | 1.90 | 0.54 |
| 20:CD:300:ARG:NH2 | 45:C2:93:G:OP2 | 2.40 | 0.54 |
| 21:CF:55:LEU:HD12 | 21:CF:65:VAL:HG12 | 1.88 | 0.54 |
| 23:CH:94:SER:OG | 23:CH:95:SER:N | 2.39 | 0.54 |
| 26:CK:25:ILE:HA | 26:CK:28:LYS:HE3 | 1.89 | 0.54 |
| 26:CK:172:LEU:HB3 | 26:CK:174:ALA:H | 1.73 | 0.54 |
| 27:CL:715:ARG:HH11 | 44:C1:2224:C:H5" | 1.72 | 0.54 |
| 32:CR:35:LYS:HA | 32:CR:38:ILE:HG13 | 1.88 | 0.54 |
| 32:CR:378:HIS:HD2 | 32:CS:378:HIS:HB3 | 1.73 | 0.54 |
| 32:CR:474:LEU:HD23 | 32:CR:476:GLU:H | 1.72 | 0.54 |
| 32:CR:519:LEU:HB3 | 32:CR:569:VAL:HG12 | 1.89 | 0.54 |
| 32:CS:134:ASN:HD22 | 32:CS:554:ASN:HB3 | 1.70 | 0.54 |
| 38:Ci:31:ARG:HD3 | 44:C1:1503:U:H4' | 1.89 | 0.54 |
| 48:UH:927:GLN:HB2 | 48:UH:930:ARG:HH12 | 1.73 | 0.54 |
| 1:UA:127:THR:OG1 | 1:UA:130:THR:N | 2.39 | 0.54 |
| 5:UF:127:ARG:O | 5:UF:131:THR:OG1 | 2.25 | 0.54 |
| 7:UJ:455:LYS:HD3 | 7:UJ:456:LEU:HD22 | 1.89 | 0.54 |
| 10:UM:803:ASP:N | 10:UM:803:ASP:OD1 | 2.40 | 0.54 |
| 12:UO:250:ALA:HB2 | 12:UO:279:LEU:HD11 | 1.90 | 0.54 |
| 19:CC:208:GLU:HA | 19:CC:211:ARG:HE | 1.72 | 0.54 |
| 22:CG:253:LYS:HG3 | 22:CG:296:PHE:HD2 | 1.73 | 0.54 |
| 26:CK:105:LYS:NZ | 44:C1:2163:C:OP1 | 2.36 | 0.54 |
| 26:CK:139:ILE:HG22 | 26:CK:155:SER:HB2 | 1.89 | 0.54 |
| 29:CO:42:SER:OG | 29:CO:206:VAL:O | 2.22 | 0.54 |
| 32:CS:775:LEU:HD21 | 32:CS:815:LEU:HD11 | 1.89 | 0.54 |
| 39:Cj:73:GLY:O | 39:Cj:76:SER:OG | 2.24 | 0.54 |
| 44:C1:1169:A:O2' | 44:C1:1170:G:N2 | 2.40 | 0.54 |
| 46:UV:622:PHE:HB2 | 46:UV:873:THR:HG22 | 1.89 | 0.54 |
| 49:UI:261:GLY:O | 49:UI:265:MET:N | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:UB:559:LEU:HA | 2:UB:562:THR:HG22 | 1.88 | 0.54 |
| 2:UB:806:LEU:N | 29:CN:22:GLU:O | 2.40 | 0.54 |
| 5:UF:330:ASN:OD1 | 5:UF:335:TRP:NE1 | 2.38 | 0.54 |
| 6:UG:211:HIS:HB3 | 25:CJ:27:HIS:HE1 | 1.72 | 0.54 |
| 9:UL:491:LEU:O | 9:UL:500:LEU:N | 2.37 | 0.54 |
| 10:UM:755:ARG:HG3 | 10:UM:793:ALA:HB1 | 1.90 | 0.54 |
| 13:UQ:417:ASP:OD2 | 13:UQ:417:ASP:N | 2.38 | 0.54 |
| 15:UU:972:LEU:HA | 15:UU:975:ILE:HD12 | 1.90 | 0.54 |
| 23:CH:331:SER:O | 23:CH:334:THR:OG1 | 2.16 | 0.54 |
| 32:CR:559:MET:SD | 32:CR:587:GLN:NE2 | 2.81 | 0.54 |
| 32:CS:474:LEU:HD23 | 32:CS:476:GLU:H | 1.72 | 0.54 |
| 32:CS:559:MET:SD | 32:CS:587:GLN:NE2 | 2.81 | 0.54 |
| 32:CS:731:GLN:HE22 | 32:CS:735:LYS:HE2 | 1.72 | 0.54 |
| 44:C1:454:C:H3' | 44:C1:455:G:H8 | 1.71 | 0.54 |
| 44:C1:488:C:H2' | 44:C1:489:A:C8 | 2.41 | 0.54 |
| 44:C1:2086:A:H5" | 44:C1:2087:G:H8 | 1.72 | 0.54 |
| 48:UH:597:ASP:N | 48:UH:597:ASP:OD1 | 2.41 | 0.54 |
| 48:UH:777:ALA:HB1 | 49:UI:259:LEU:HB2 | 1.90 | 0.54 |
| 3:UC:582:GLN:O | 3:UC:585:LYS:O | 2.26 | 0.54 |
| 5:UF:272:PRO:HG2 | 5:UF:274:LEU:HB3 | 1.89 | 0.54 |
| 11:UN:362:GLN:NE2 | 11:UN:365:SER:OG | 2.40 | 0.54 |
| 43:CU:116:LEU:HG | 43:CU:120:LEU:HD21 | 1.88 | 0.54 |
| 44:C1:335:C:H2' | 44:C1:336:G:C8 | 2.43 | 0.54 |
| 46:UV:361:ILE:HD13 | 46:UV:421:THR:HB | 1.90 | 0.54 |
| 46:UV:997:LEU:HB2 | 46:UV:1085:LYS:HE2 | 1.89 | 0.54 |
| 48:UH:598:ASP:N | 48:UH:598:ASP:OD1 | 2.37 | 0.54 |
| 2:UB:6:LEU:HD11 | 26:CK:225:ASN:HB3 | 1.89 | 0.54 |
| 4:UD:54:GLU:OE1 | 4:UD:56:TRP:NE1 | 2.37 | 0.54 |
| 7:UJ:170:TYR:O | 7:UJ:173:SER:C | 2.50 | 0.54 |
| 9:UL:851:PHE:HA | 9:UL:854:ILE:HG12 | 1.89 | 0.54 |
| 11:UN:350:ARG:NH2 | 44:C1:452:G:O3' | 2.38 | 0.54 |
| 12:UO:85:SER:OG | 12:UO:89:ARG:N | 2.40 | 0.54 |
| 15:UU:508:TRP:CD2 | 15:UU:571:GLN:HB2 | 2.42 | 0.54 |
| 23:CH:347:GLY:O | 23:CH:397:SER:HA | 2.08 | 0.54 |
| 44:C1:293:G:H2' | 44:C1:294:G:C8 | 2.42 | 0.54 |
| 45:C2:103:G:O6 | 45:C2:249:U:C4 | 2.60 | 0.54 |
| 46:UV:1060:SER:OG | 46:UV:1105:PRO:O | 2.26 | 0.54 |
| 48:UH:580:LEU:HB3 | 48:UH:586:LEU:HD21 | 1.89 | 0.54 |
| 1:UA:149:GLN:HG2 | 44:C1:266:C:H5" | 1.90 | 0.54 |
| 5:UF:331:HIS:ND1 | 5:UF:333:CYS:SG | 2.81 | 0.54 |
| 5:UF:404:HIS:HA | 5:UF:407:ARG:HH11 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:UG:63:VAL:O | 6:UG:69:ARG:NH2 | 2.41 | 0.54 |
| 7:UJ:854:GLU:O | 7:UJ:858:LYS:HG2 | 2.08 | 0.54 |
| 10:UM:817:ASN:HD21 | 10:UM:867:THR:HG23 | 1.73 | 0.54 |
| 15:UU:70:ALA:HB2 | 15:UU:89:GLN:HG2 | 1.90 | 0.54 |
| 17:UZ:259:ILE:HA | 17:UZ:262:VAL:HG22 | 1.90 | 0.54 |
| 22:CG:413:SER:HB3 | 22:CG:417:ASP:HB2 | 1.89 | 0.54 |
| 26:CK:173:ARG:NH2 | 26:CK:182:GLY:O | 2.41 | 0.54 |
| 32:CR:816:ASP:HB2 | 32:CR:819:ASN:HB2 | 1.90 | 0.54 |
| 44:C1:4:G:N1 | 44:C1:32:U:C2 | 2.76 | 0.54 |
| 44:C1:1068:C:H2' | 44:C1:1069:A:H8 | 1.70 | 0.54 |
| 46:UV:854:LEU:HD11 | 46:UV:897:THR:HG21 | 1.90 | 0.54 |
| 52:CX:422:ARG:HB2 | 52:CX:456:GLY:HA3 | 1.89 | 0.54 |
| 1:UA:355:ILE:HD11 | 1:UA:695:LEU:HD21 | 1.88 | 0.54 |
| 4:UD:27:PRO:O | 4:UD:37:GLN:NE2 | 2.41 | 0.54 |
| 6:UG:452:ASN:HD21 | 28:CM:42:ARG:HE | 1.54 | 0.54 |
| 8:UK:58:ARG:NE | 24:CI:1057:GLU:O | 2.41 | 0.54 |
| 10:UM:18:GLN:OE1 | 10:UM:53:ARG:NH1 | 2.41 | 0.54 |
| 10:UM:705:THR:OG1 | 10:UM:706:ASN:N | 2.39 | 0.54 |
| 11:UN:362:GLN:NE2 | 11:UN:371:GLN:OE1 | 2.31 | 0.54 |
| 13:UQ:672:HIS:HB3 | 48:UH:635:GLN:HB3 | 1.88 | 0.54 |
| 20:CD:92:ASP:OD1 | 20:CD:92:ASP:N | 2.36 | 0.54 |
| 24:CI:934:ILE:HD13 | 24:CI:987:VAL:HG11 | 1.89 | 0.54 |
| 28:CM:308:ARG:HG2 | 28:CM:320:VAL:HG12 | 1.90 | 0.54 |
| 29:CN:30:ASN:N | 29:CN:30:ASN:OD1 | 2.39 | 0.54 |
| 44:C1:10:U:O2 | 44:C1:25:G:N2 | 2.41 | 0.54 |
| 44:C1:495:G:O6 | 44:C1:503:G:O6 | 2.25 | 0.54 |
| 44:C1:1068:C:H2' | 44:C1:1069:A:C8 | 2.43 | 0.54 |
| 1:UA:766:PRO:HB2 | 1:UA:769:TYR:HD2 | 1.72 | 0.54 |
| 2:UB:708:LEU:O | 2:UB:710:LYS:NZ | 2.41 | 0.54 |
| 4:UD:291:ILE:HB | 4:UD:303:TYR:HB2 | 1.88 | 0.54 |
| 4:UD:410:PRO:HD2 | 4:UD:411:LEU:HD23 | 1.89 | 0.54 |
| 4:UD:491:ARG:NH1 | 4:UD:612:GLU:OE2 | 2.41 | 0.54 |
| 5:UF:111:LEU:HA | 5:UF:114:LEU:HD12 | 1.89 | 0.54 |
| 9:UL:442:ALA:HA | 9:UL:451:ILE:HG22 | 1.90 | 0.54 |
| 23:CH:225:THR:O | 23:CH:275:ILE:HA | 2.06 | 0.54 |
| 28:CM:9:SER:OG | 28:CM:12:ALA:N | 2.38 | 0.54 |
| 39:Cj:57:THR:O | 39:Cj:60:PHE:N | 2.40 | 0.54 |
| 40:Cm:82:ARG:O | 40:Cm:86:LEU:N | 2.41 | 0.54 |
| 44:C1:398:C:H2' | 44:C1:399:G:C8 | 2.41 | 0.54 |
| 44:C1:2054:A:N6 | 44:C1:2121:U:O2 | 2.41 | 0.54 |
| 45:C2:95:U:H2' | 45:C2:96:C:C6 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:438:ILE:HB | 46:UV:866:TRP:HE1 | 1.71 | 0.54 |
| 1:UA:198:VAL:HA | 1:UA:214:SER:HA | 1.90 | 0.54 |
| 5:UF:135:ARG:O | 19:CC:52:SER:OG | 2.17 | 0.54 |
| 9:UL:59:SER:OG | 9:UL:60:ARG:N | 2.41 | 0.54 |
| 9:UL:125:LEU:HB2 | 9:UL:139:LEU:HD11 | 1.90 | 0.54 |
| 13:UQ:237:TYR:CZ | 13:UQ:241:PRO:HB3 | 2.43 | 0.54 |
| 13:UQ:759:ASP:OD1 | 48:UH:543:ARG:NH1 | 2.41 | 0.54 |
| 15:UU:92:SER:OG | 15:UU:93:ASP:O | 2.26 | 0.54 |
| 15:UU:713:PHE:C | 15:UU:714:CYS:HG | 2.16 | 0.54 |
| 16:UX:149:ASN:OD1 | 16:UX:167:SER:OG | 2.25 | 0.54 |
| 17:UZ:65:THR:HA | 17:UZ:242:ALA:HA | 1.90 | 0.54 |
| 19:CC:31:LEU:HD11 | 28:CM:58:LEU:HD11 | 1.89 | 0.54 |
| 24:CI:81:LYS:H | 24:CI:81:LYS:HZ3 | 1.56 | 0.54 |
| 24:CI:1145:GLU:HA | 24:CI:1148:LYS:HD2 | 1.87 | 0.54 |
| 26:CK:153:THR:HG23 | 26:CK:164:MET:HG2 | 1.89 | 0.54 |
| 35:Ce:149:ARG:NH2 | 40:Cm:54:ASP:H | 2.05 | 0.54 |
| 46:UV:1001:VAL:HB | 46:UV:1005:ALA:HB3 | 1.90 | 0.54 |
| 48:UH:618:ALA:HA | 48:UH:627:LEU:HD21 | 1.90 | 0.54 |
| 54:Cz:1690:ARG:HE | 54:Cz:1692:ASP:H | 1.54 | 0.54 |
| 1:UA:138:PHE:HE1 | 15:UU:39:ARG:HD2 | 1.73 | 0.54 |
| 2:UB:19:ILE:HD13 | 26:CK:247:THR:HA | 1.90 | 0.54 |
| 2:UB:821:PRO:HG3 | 29:CN:146:HIS:CE1 | 2.43 | 0.54 |
| 9:UL:532:ALA:O | 9:UL:562:LEU:HB2 | 2.08 | 0.54 |
| 10:UM:784:ASP:HB2 | 10:UM:787:SER:HB3 | 1.89 | 0.54 |
| 15:UU:308:VAL:HG22 | 15:UU:323:LEU:HB3 | 1.88 | 0.54 |
| 35:Ce:184:ARG:HE | 35:Ce:190:ASN:HA | 1.73 | 0.54 |
| 44:C1:10:U:O2 | 44:C1:25:G:C2 | 2.61 | 0.54 |
| 44:C1:42:C:H2' | 44:C1:43:C:C6 | 2.43 | 0.54 |
| 44:C1:460:U:H2' | 44:C1:461:G:C8 | 2.43 | 0.54 |
| 54:Cz:1501:LEU:HD13 | 54:Cz:1511:LEU:HD13 | 1.89 | 0.54 |
| 9:UL:898:THR:HA | 9:UL:901:LYS:HD2 | 1.90 | 0.53 |
| 10:UM:830:LEU:HA | 10:UM:833:LEU:HB2 | 1.90 | 0.53 |
| 13:UQ:89:MET:HE1 | 13:UQ:420:ALA:HB2 | 1.90 | 0.53 |
| 14:UR:317:SER:O | 14:UR:317:SER:OG | 2.24 | 0.53 |
| 15:UU:171:THR:OG1 | 15:UU:172:THR:N | 2.41 | 0.53 |
| 18:CA:184:GLU:O | 18:CA:207:VAL:HA | 2.08 | 0.53 |
| 28:CM:294:THR:HG23 | 28:CM:296:GLU:H | 1.73 | 0.53 |
| 30:CP:51:LEU:O | 30:CP:55:TRP:HB2 | 2.09 | 0.53 |
| 32:CS:4:GLN:HA | 32:CS:4:GLN:HE21 | 1.71 | 0.53 |
| 32:CS:519:LEU:HB3 | 32:CS:569:VAL:HG12 | 1.89 | 0.53 |
| 44:C1:425:C:H2' | 44:C1:426:A:H8 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:2158:G:H2' | 44:C1:2159:A:C8 | 2.42 | 0.53 |
| 44:C1:2185:C:H2' | 44:C1:2186:U:C6 | 2.43 | 0.53 |
| 45:C2:96:C:H2' | 45:C2:97:C:C6 | 2.43 | 0.53 |
| 46:UV:1099:LYS:HD3 | 46:UV:1100:TRP:H | 1.71 | 0.53 |
| 48:UH:631:LEU:HA | 48:UH:636:LEU:HD11 | 1.89 | 0.53 |
| 1:UA:254:ASN:O | 44:C1:286:G:N2 | 2.41 | 0.53 |
| 2:UB:113:VAL:HG13 | 23:CH:63:GLY:HA2 | 1.89 | 0.53 |
| 4:UD:322:HIS:CE1 | 4:UD:326:VAL:HG12 | 2.43 | 0.53 |
| 6:UG:208:VAL:HA | 16:UX:5:ARG:HB3 | 1.89 | 0.53 |
| 10:UM:776:ASN:O | 10:UM:779:THR:O | 2.27 | 0.53 |
| 12:UO:184:THR:OG1 | 12:UO:185:GLY:N | 2.37 | 0.53 |
| 12:UO:405:ILE:HD13 | 14:UR:357:VAL:HG11 | 1.90 | 0.53 |
| 13:UQ:483:GLY:HA2 | 13:UQ:498:PRO:HD2 | 1.90 | 0.53 |
| 15:UU:478:MET:O | 15:UU:480:ALA:N | 2.39 | 0.53 |
| 18:CB:141:ILE:HA | 18:CB:145:LEU:HB3 | 1.90 | 0.53 |
| 26:CK:187:SER:O | 26:CK:226:ARG:NH1 | 2.41 | 0.53 |
| 29:CN:105:ASN:HB2 | 29:CN:110:LEU:HD23 | 1.90 | 0.53 |
| 32:CR:174:ARG:NH2 | 32:CR:524:ASP:OD2 | 2.40 | 0.53 |
| 35:Ce:19:PRO:HB3 | 35:Ce:24:ARG:HE | 1.73 | 0.53 |
| 44:C1:420:G:H2' | 44:C1:421:A:C8 | 2.43 | 0.53 |
| 44:C1:485:G:H2' | 44:C1:486:G:C8 | 2.44 | 0.53 |
| 46:UV:486:LEU:HD23 | 46:UV:506:LEU:HD11 | 1.88 | 0.53 |
| 46:UV:1104:LEU:HD11 | 47:CV:55:ASN:HD21 | 1.73 | 0.53 |
| 49:UE:261:GLY:O | 49:UE:265:MET:N | 2.39 | 0.53 |
| 1:UA:758:ILE:HD11 | 1:UA:793:TRP:HA | 1.90 | 0.53 |
| 2:UB:762:THR:OG1 | 2:UB:765:ASN:ND2 | 2.41 | 0.53 |
| 4:UD:64:TYR:HE1 | 4:UD:370:GLN:HG2 | 1.72 | 0.53 |
| 4:UD:413:LEU:HD11 | 48:UH:926:VAL:HG12 | 1.90 | 0.53 |
| 7:UJ:50:SER:OG | 7:UJ:51:GLN:N | 2.40 | 0.53 |
| 9:UL:387:VAL:HG23 | 9:UL:395:GLU:HB2 | 1.90 | 0.53 |
| 9:UL:653:LEU:N | 9:UL:672:ALA:O | 2.41 | 0.53 |
| 14:UR:606:ASN:OD1 | 14:UR:606:ASN:N | 2.39 | 0.53 |
| 15:UU:139:GLN:NE2 | 15:UU:157:THR:OG1 | 2.42 | 0.53 |
| 19:CC:375:LYS:HD3 | 19:CC:378:ILE:HD11 | 1.89 | 0.53 |
| 25:CJ:43:ASP:HA | 25:CJ:46:LYS:HD2 | 1.90 | 0.53 |
| 28:CM:395:ARG:HD3 | 45:C2:31:A:H61 | 1.72 | 0.53 |
| 29:CN:236:VAL:HG11 | 29:CO:101:ASP:HB3 | 1.90 | 0.53 |
| 31:CQ:240:GLN:OE1 | 31:CQ:243:LYS:N | 2.42 | 0.53 |
| 32:CS:838:HIS:HD2 | 32:CS:841:LEU:HD22 | 1.74 | 0.53 |
| 40:Cm:83:LEU:HA | 40:Cm:86:LEU:HG | 1.90 | 0.53 |
| 2:UB:693:ASP:HA | 2:UB:768:HIS:HA | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:UD:500:SER:HB2 | 4:UD:528:ARG:HH22 | 1.73 | 0.53 |
| 10:UM:517:ARG:HA | 10:UM:547:ILE:HG13 | 1.90 | 0.53 |
| 13:UQ:443:GLY:N | 13:UQ:460:ASP:OD2 | 2.39 | 0.53 |
| 14:UR:144:LEU:O | 14:UR:168:GLY:N | 2.41 | 0.53 |
| 15:UU:721:TRP:HZ3 | 15:UU:778:ASN:HD21 | 1.55 | 0.53 |
| 23:CH:337:THR:HG23 | 23:CH:363:LEU:HD11 | 1.90 | 0.53 |
| 24:CI:171:THR:OG1 | 24:CI:172:HIS:N | 2.41 | 0.53 |
| 32:CS:518:LEU:HD22 | 32:CS:568:PHE:HB3 | 1.91 | 0.53 |
| 34:Cc:192:SER:OG | 34:Cc:193:SER:N | 2.39 | 0.53 |
| 36:Cg:106:ARG:HH12 | 36:Cg:142:PRO:HB2 | 1.73 | 0.53 |
| 44:C1:1064:G:H1 | 44:C1:1092:U:H3 | 1.56 | 0.53 |
| 44:C1:1466:G:OP1 | 54:Cz:1611:TYR:OH | 2.22 | 0.53 |
| 50:US:473:THR:HA | 50:US:476:LYS:HD2 | 1.90 | 0.53 |
| 1:UA:503:THR:OG1 | 1:UA:504:SER:N | 2.39 | 0.53 |
| 2:UB:648:ASP:N | 2:UB:648:ASP:OD1 | 2.37 | 0.53 |
| 7:UJ:439:ARG:HA | 7:UJ:442:ILE:HD12 | 1.90 | 0.53 |
| 8:UK:10:ARG:NH1 | 44:C1:1136:G:O6 | 2.40 | 0.53 |
| 9:UL:303:GLU:HB3 | 9:UL:305:TRP:HE1 | 1.74 | 0.53 |
| 9:UL:575:PRO:HD3 | 9:UL:615:ILE:HD11 | 1.91 | 0.53 |
| 9:UL:576:ASP:OD1 | 9:UL:619:SER:OG | 2.22 | 0.53 |
| 12:UO:250:ALA:HB1 | 12:UO:276:VAL:HG21 | 1.90 | 0.53 |
| 13:UQ:242:GLN:N | 13:UQ:256:ALA:O | 2.36 | 0.53 |
| 23:CH:151:ASP:N | 23:CH:151:ASP:OD1 | 2.42 | 0.53 |
| 28:CM:422:GLU:O | 28:CM:426:SER:OG | 2.27 | 0.53 |
| 32:CR:397:PRO:HA | 32:CR:400:LYS:HG2 | 1.91 | 0.53 |
| 32:CR:855:LEU:HD22 | 32:CS:793:LYS:HE2 | 1.90 | 0.53 |
| 32:CS:174:ARG:NH2 | 32:CS:524:ASP:OD2 | 2.40 | 0.53 |
| 32:CS:816:ASP:HB2 | 32:CS:819:ASN:HB2 | 1.90 | 0.53 |
| 46:UV:1057:VAL:HB | 47:CV:90:GLU:O | 2.08 | 0.53 |
| 48:UH:816:GLN:NE2 | 49:UI:263:LEU:O | 2.42 | 0.53 |
| 49:UE:236:ILE:HA | 49:UE:239:LEU:HD12 | 1.90 | 0.53 |
| 50:US:461:VAL:HA | 50:US:464:GLN:HG3 | 1.90 | 0.53 |
| 9:UL:283:GLU:HB3 | 9:UL:296:HIS:CE1 | 2.43 | 0.53 |
| 9:UL:697:GLY:O | 9:UL:715:SER:OG | 2.27 | 0.53 |
| 9:UL:864:PHE:O | 9:UL:867:ARG:O | 2.27 | 0.53 |
| 12:UO:108:ARG:NE | 12:UO:157:LEU:HD12 | 2.24 | 0.53 |
| 12:UO:171:LEU:HD13 | 12:UO:181:ARG:HB2 | 1.89 | 0.53 |
| 28:CM:253:MET:SD | 28:CM:253:MET:N | 2.70 | 0.53 |
| 28:CM:358:SER:O | 28:CM:360:ARG:NH1 | 2.42 | 0.53 |
| 52:CX:328:LEU:HD22 | 52:CX:369:VAL:HG13 | 1.90 | 0.53 |
| 2:UB:21:PRO:HB3 | 44:C1:1732:C:H1' | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:UD:6:CYS:HB2 | 4:UD:863:ILE:HG12 | 1.90 | 0.53 |
| 4:UD:82:TRP:CD2 | 4:UD:102:LEU:HD13 | 2.43 | 0.53 |
| 4:UD:673:ASN:HA | 4:UD:677:LYS:HD2 | 1.90 | 0.53 |
| 7:UJ:752:TRP:O | 7:UJ:802:ARG:NH2 | 2.36 | 0.53 |
| 15:UU:353:VAL:HG22 | 15:UU:363:THR:HG22 | 1.91 | 0.53 |
| 15:UU:696:THR:OG1 | 15:UU:698:ASN:OD1 | 2.13 | 0.53 |
| 18:CA:235:GLN:HA | 18:CA:238:ILE:HD12 | 1.90 | 0.53 |
| 20:CD:276:GLU:O | 20:CD:280:ASN:ND2 | 2.42 | 0.53 |
| 23:CH:171:ILE:HG23 | 23:CH:196:PHE:HE1 | 1.74 | 0.53 |
| 24:CI:74:VAL:HG13 | 24:CI:138:LEU:HD13 | 1.91 | 0.53 |
| 28:CM:338:SER:O | 28:CM:338:SER:OG | 2.24 | 0.53 |
| 32:CS:8:ASP:OD1 | 32:CS:10:ARG:NE | 2.38 | 0.53 |
| 32:CS:200:LEU:HG | 32:CS:202:ILE:HG22 | 1.91 | 0.53 |
| 34:Cc:183:GLU:OE1 | 34:Cc:187:ASN:ND2 | 2.41 | 0.53 |
| 36:Cg:107:LEU:HD23 | 36:Cg:142:PRO:HA | 1.91 | 0.53 |
| 36:Cg:142:PRO:HD2 | 44:C1:1058:A:H5” | 1.89 | 0.53 |
| 39:Cj:126:PRO:HB3 | 44:C1:2166:A:H5” | 1.89 | 0.53 |
| 5:UF:377:LEU:HA | 5:UF:380:LYS:HD2 | 1.90 | 0.53 |
| 6:UG:477:ARG:HH22 | 44:C1:587:U:H1’ | 1.74 | 0.53 |
| 7:UJ:32:SER:OG | 7:UJ:33:LEU:N | 2.42 | 0.53 |
| 7:UJ:809:ILE:HG13 | 7:UJ:810:PHE:HD2 | 1.74 | 0.53 |
| 12:UO:35:SER:O | 12:UO:35:SER:OG | 2.23 | 0.53 |
| 14:UR:331:VAL:HG21 | 14:UR:339:ILE:HD12 | 1.90 | 0.53 |
| 14:UR:417:ARG:O | 14:UR:418:HIS:ND1 | 2.41 | 0.53 |
| 15:UU:222:LEU:HD11 | 15:UU:256:GLN:OE1 | 2.08 | 0.53 |
| 24:CI:137:LEU:HD13 | 24:CI:167:PHE:HB2 | 1.89 | 0.53 |
| 24:CI:942:LEU:HB3 | 27:CL:517:LEU:HD21 | 1.89 | 0.53 |
| 30:CP:109:PRO:HG2 | 43:CU:253:ILE:HG13 | 1.90 | 0.53 |
| 32:CR:518:LEU:HD22 | 32:CR:568:PHE:HB3 | 1.91 | 0.53 |
| 32:CS:74:ARG:HH12 | 32:CS:100:SER:HB3 | 1.73 | 0.53 |
| 32:CS:397:PRO:HA | 32:CS:400:LYS:HG2 | 1.91 | 0.53 |
| 44:C1:101:G:H2’ | 44:C1:102:G:H8 | 1.72 | 0.53 |
| 44:C1:297:U:O2’ | 44:C1:298:A:N7 | 2.33 | 0.53 |
| 44:C1:1629:U:O2 | 44:C1:1659:C:N4 | 2.41 | 0.53 |
| 48:UH:756:LEU:HB3 | 49:UI:210:ARG:HH22 | 1.73 | 0.53 |
| 6:UG:179:THR:OG1 | 6:UG:180:VAL:N | 2.41 | 0.53 |
| 9:UL:372:VAL:HG12 | 9:UL:387:VAL:HG12 | 1.91 | 0.53 |
| 9:UL:603:LEU:HD13 | 9:UL:634:TRP:CE2 | 2.44 | 0.53 |
| 10:UM:328:LEU:HD23 | 10:UM:333:LEU:H | 1.74 | 0.53 |
| 10:UM:675:VAL:HG12 | 10:UM:696:LEU:HD21 | 1.90 | 0.53 |
| 10:UM:756:ASP:HA | 10:UM:759:VAL:HG22 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:UU:70:ALA:HB1 | 15:UU:86:THR:HB | 1.91 | 0.53 |
| 15:UU:434:GLY:O | 15:UU:436:ILE:N | 2.41 | 0.53 |
| 18:CA:130:TRP:CZ2 | 18:CA:169:HIS:HB3 | 2.44 | 0.53 |
| 22:CG:330:GLN:HB2 | 22:CG:351:ASP:HB3 | 1.90 | 0.53 |
| 29:CN:77:MET:HE2 | 29:CN:82:ARG:H | 1.73 | 0.53 |
| 32:CR:74:ARG:HH12 | 32:CR:100:SER:HB3 | 1.73 | 0.53 |
| 32:CR:775:LEU:HD21 | 32:CR:815:LEU:HD11 | 1.90 | 0.53 |
| 54:Cz:1619:TRP:CZ2 | 54:Cz:1646:VAL:HG21 | 2.44 | 0.53 |
| 1:UA:558:ARG:HB2 | 1:UA:566:ALA:HB2 | 1.90 | 0.53 |
| 5:UF:286:ALA:HA | 5:UF:289:GLN:HG2 | 1.91 | 0.53 |
| 11:UN:901:LEU:HD12 | 11:UN:902:ARG:H | 1.73 | 0.53 |
| 13:UQ:577:CYS:SG | 13:UQ:578:LYS:N | 2.81 | 0.53 |
| 15:UU:681:ALA:HB2 | 15:UU:715:PHE:CE2 | 2.44 | 0.53 |
| 15:UU:757:SER:OG | 15:UU:758:HIS:N | 2.41 | 0.53 |
| 17:UZ:213:ASN:OD1 | 17:UZ:213:ASN:N | 2.32 | 0.53 |
| 24:CI:961:GLN:NE2 | 27:CL:526:VAL:O | 2.41 | 0.53 |
| 27:CL:725:ARG:NH2 | 44:C1:1731:A:OP2 | 2.41 | 0.53 |
| 32:CS:427:LYS:HA | 32:CS:430:LYS:HD2 | 1.91 | 0.53 |
| 35:Ce:132:HIS:HA | 35:Ce:135:ILE:HD12 | 1.90 | 0.53 |
| 44:C1:365:G:H2' | 44:C1:366:G:H8 | 1.74 | 0.53 |
| 46:UV:247:VAL:HG22 | 46:UV:266:THR:HG21 | 1.91 | 0.53 |
| 48:UH:756:LEU:HD13 | 49:UI:203:ARG:HE | 1.74 | 0.53 |
| 50:US:332:ARG:O | 50:US:334:LEU:N | 2.36 | 0.53 |
| 52:CX:199:VAL:HG13 | 52:CX:236:LEU:HD11 | 1.91 | 0.53 |
| 1:UA:661:ARG:HG3 | 1:UA:662:GLY:H | 1.72 | 0.52 |
| 2:UB:327:GLU:HA | 2:UB:330:LYS:HE2 | 1.91 | 0.52 |
| 6:UG:155:GLY:O | 6:UG:158:GLY:N | 2.27 | 0.52 |
| 6:UG:176:LEU:HG | 16:UX:4:LYS:HZ1 | 1.73 | 0.52 |
| 7:UJ:573:GLU:HA | 7:UJ:576:LYS:HE2 | 1.90 | 0.52 |
| 9:UL:234:THR:OG1 | 9:UL:242:THR:OG1 | 2.22 | 0.52 |
| 12:UO:434:ALA:HA | 12:UO:473:ARG:HH22 | 1.74 | 0.52 |
| 13:UQ:89:MET:HE2 | 13:UQ:414:HIS:CD2 | 2.44 | 0.52 |
| 13:UQ:753:VAL:HB | 13:UQ:763:ALA:HB3 | 1.92 | 0.52 |
| 14:UR:443:GLU:CD | 14:UR:455:TRP:HE1 | 2.16 | 0.52 |
| 18:CB:100:GLY:H | 18:CB:126:GLU:CD | 2.16 | 0.52 |
| 20:CD:326:LYS:HB2 | 45:C2:94:A:H2 | 1.73 | 0.52 |
| 25:CJ:157:PHE:O | 25:CJ:159:THR:OG1 | 2.23 | 0.52 |
| 29:CO:239:SER:O | 29:CO:243:HIS:ND1 | 2.42 | 0.52 |
| 32:CR:200:LEU:HG | 32:CR:202:ILE:HG22 | 1.91 | 0.52 |
| 44:C1:626:A:O2' | 44:C1:1051:G:N2 | 2.33 | 0.52 |
| 48:UH:559:GLN:NE2 | 48:UH:564:THR:O | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:UH:604:LYS:HG3 | 48:UH:607:GLU:HB3 | 1.91 | 0.52 |
| 50:US:357:ARG:NH1 | 50:US:395:SER:OG | 2.37 | 0.52 |
| 1:UA:627:SER:OG | 1:UA:628:LYS:N | 2.41 | 0.52 |
| 2:UB:744:PRO:O | 2:UB:795:ARG:NH1 | 2.42 | 0.52 |
| 4:UD:103:PHE:HE1 | 4:UD:173:LEU:HD13 | 1.74 | 0.52 |
| 4:UD:134:CYS:HB2 | 4:UD:192:ILE:HG22 | 1.91 | 0.52 |
| 4:UD:276:THR:OG1 | 4:UD:277:GLN:N | 2.41 | 0.52 |
| 4:UD:644:ASP:OD1 | 4:UD:645:TYR:N | 2.40 | 0.52 |
| 11:UN:312:ARG:NH1 | 28:CM:446:GLN:O | 2.42 | 0.52 |
| 15:UU:151:ILE:HG23 | 15:UU:164:ALA:HB2 | 1.91 | 0.52 |
| 15:UU:520:TYR:HA | 15:UU:536:PHE:O | 2.08 | 0.52 |
| 18:CB:101:GLU:HG2 | 18:CB:199:ARG:HH22 | 1.72 | 0.52 |
| 28:CM:178:ARG:HA | 28:CM:189:GLN:O | 2.09 | 0.52 |
| 29:CO:176:ARG:HE | 29:CO:196:LEU:HD22 | 1.74 | 0.52 |
| 36:Cg:129:GLN:OE1 | 44:C1:1097:U:O2' | 2.24 | 0.52 |
| 45:C2:49:U:H2' | 45:C2:50:G:C8 | 2.45 | 0.52 |
| 50:US:196:ILE:O | 50:US:200:THR:OG1 | 2.20 | 0.52 |
| 1:UA:39:VAL:O | 1:UA:47:SER:HA | 2.10 | 0.52 |
| 2:UB:745:ALA:O | 2:UB:749:SER:OG | 2.21 | 0.52 |
| 2:UB:853:ARG:NH1 | 44:C1:1760:G:OP1 | 2.27 | 0.52 |
| 5:UF:74:ARG:NH1 | 14:UR:56:GLU:OE2 | 2.42 | 0.52 |
| 5:UF:159:ARG:O | 5:UF:163:HIS:ND1 | 2.42 | 0.52 |
| 6:UG:274:HIS:CE1 | 6:UG:284:LEU:HD21 | 2.43 | 0.52 |
| 10:UM:393:THR:OG1 | 10:UM:397:ASP:OD1 | 2.27 | 0.52 |
| 13:UQ:177:ASP:N | 13:UQ:177:ASP:OD1 | 2.40 | 0.52 |
| 13:UQ:419:SER:OG | 13:UQ:420:ALA:N | 2.42 | 0.52 |
| 13:UQ:715:ILE:HG22 | 13:UQ:722:VAL:HA | 1.91 | 0.52 |
| 14:UR:586:PRO:O | 14:UR:612:ARG:NH1 | 2.42 | 0.52 |
| 18:CA:141:ILE:HD11 | 18:CA:148:ILE:HD13 | 1.90 | 0.52 |
| 21:CE:110:ASP:O | 21:CE:113:SER:OG | 2.17 | 0.52 |
| 23:CH:139:THR:HG21 | 23:CH:178:ARG:HA | 1.91 | 0.52 |
| 24:CI:302:LEU:HG | 24:CI:776:TYR:HB3 | 1.91 | 0.52 |
| 26:CK:75:ASP:HB3 | 26:CK:78:SER:H | 1.75 | 0.52 |
| 26:CK:166:SER:OG | 26:CK:167:LEU:N | 2.41 | 0.52 |
| 29:CO:149:SER:HB2 | 29:CO:158:LYS:HD3 | 1.90 | 0.52 |
| 32:CR:387:VAL:HG23 | 32:CR:409:PHE:HD2 | 1.75 | 0.52 |
| 32:CR:427:LYS:HA | 32:CR:430:LYS:HD2 | 1.91 | 0.52 |
| 34:Cc:68:ARG:HB3 | 34:Cc:69:PHE:CD2 | 2.44 | 0.52 |
| 44:C1:62:U:O2' | 44:C1:64:C:OP2 | 2.28 | 0.52 |
| 46:UV:245:GLY:HA2 | 46:UV:266:THR:HG22 | 1.91 | 0.52 |
| 48:UH:777:ALA:HA | 49:UI:259:LEU:HD22 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:Cz:1631:ASN:HD22 | 54:Cz:1670:ASN:HD22 | 1.55 | 0.52 |
| 2:UB:528:GLN:O | 2:UB:532:HIS:ND1 | 2.33 | 0.52 |
| 2:UB:754:LEU:HD21 | 2:UB:784:LEU:HB3 | 1.92 | 0.52 |
| 4:UD:687:ASP:OD2 | 4:UD:705:ALA:N | 2.31 | 0.52 |
| 12:UO:513:VAL:HA | 12:UO:519:LEU:HD11 | 1.90 | 0.52 |
| 14:UR:549:SER:O | 14:UR:552:GLY:N | 2.42 | 0.52 |
| 15:UU:956:LEU:HD13 | 15:UU:959:LEU:HD11 | 1.91 | 0.52 |
| 20:CD:323:GLY:O | 20:CD:325:GLU:N | 2.42 | 0.52 |
| 24:CI:354:THR:OG1 | 32:CR:4:GLN:NE2 | 2.38 | 0.52 |
| 26:CK:291:GLY:O | 27:CL:528:LYS:NZ | 2.42 | 0.52 |
| 29:CN:42:SER:OG | 29:CN:43:ASN:N | 2.41 | 0.52 |
| 30:CP:217:ASP:O | 30:CP:220:ARG:NH2 | 2.42 | 0.52 |
| 32:CR:191:LEU:O | 32:CR:195:SER:OG | 2.28 | 0.52 |
| 33:CT:135:CYS:SG | 33:CT:136:GLN:N | 2.83 | 0.52 |
| 44:C1:154:C:H2' | 44:C1:155:G:H8 | 1.75 | 0.52 |
| 44:C1:301:U:H2' | 44:C1:302:A:C8 | 2.42 | 0.52 |
| 44:C1:1551:A:N6 | 44:C1:1552:A:N6 | 2.58 | 0.52 |
| 45:C2:134:C:O2' | 45:C2:181:A:N6 | 2.43 | 0.52 |
| 48:UH:700:ASP:OD1 | 48:UH:700:ASP:N | 2.42 | 0.52 |
| 5:UF:5:ALA:HA | 5:UF:45:HIS:HE1 | 1.75 | 0.52 |
| 8:UK:1:MET:HG3 | 8:UK:3:SER:H | 1.75 | 0.52 |
| 9:UL:786:LEU:HD21 | 9:UL:856:SER:HB2 | 1.90 | 0.52 |
| 10:UM:753:ALA:O | 10:UM:757:ALA:HB2 | 2.10 | 0.52 |
| 13:UQ:79:TRP:HZ3 | 13:UQ:842:GLY:HA2 | 1.75 | 0.52 |
| 13:UQ:578:LYS:O | 13:UQ:581:ARG:NE | 2.39 | 0.52 |
| 15:UU:158:ARG:HE | 15:UU:172:THR:HG21 | 1.74 | 0.52 |
| 15:UU:392:HIS:HB3 | 15:UU:468:ILE:HD11 | 1.91 | 0.52 |
| 24:CI:104:ILE:O | 24:CI:115:THR:HA | 2.09 | 0.52 |
| 28:CM:133:LYS:HB2 | 28:CM:135:TRP:CH2 | 2.45 | 0.52 |
| 44:C1:274:A:C6 | 44:C1:275:C:N4 | 2.77 | 0.52 |
| 44:C1:496:U:N3 | 44:C1:503:G:C6 | 2.77 | 0.52 |
| 44:C1:500:C:O2' | 44:C1:501:U:O4' | 2.27 | 0.52 |
| 44:C1:1086:U:H2' | 44:C1:1087:G:H8 | 1.75 | 0.52 |
| 54:Cz:1570:VAL:HA | 54:Cz:1573:ARG:HG2 | 1.91 | 0.52 |
| 2:UB:860:ARG:HB3 | 27:CL:529:PRO:HG3 | 1.90 | 0.52 |
| 3:UC:597:GLN:HA | 3:UC:603:LYS:HD2 | 1.92 | 0.52 |
| 6:UG:109:THR:OG1 | 6:UG:385:TYR:O | 2.23 | 0.52 |
| 9:UL:76:SER:OG | 9:UL:79:ASP:O | 2.24 | 0.52 |
| 9:UL:899:LEU:HA | 9:UL:902:VAL:HG22 | 1.92 | 0.52 |
| 10:UM:738:LEU:HA | 10:UM:741:GLN:HE21 | 1.75 | 0.52 |
| 15:UU:141:ILE:HD11 | 15:UU:153:ALA:HB1 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:CG:352:ARG:HA | 22:CG:398:MET:HG2 | 1.92 | 0.52 |
| 24:CI:1006:ASN:HD22 | 24:CI:1007:LEU:HD23 | 1.75 | 0.52 |
| 25:CJ:125:GLN:NE2 | 44:C1:416:U:O2' | 2.34 | 0.52 |
| 26:CK:75:ASP:OD1 | 26:CK:206:LYS:NZ | 2.39 | 0.52 |
| 28:CM:236:THR:HG22 | 28:CM:444:LYS:HA | 1.92 | 0.52 |
| 32:CR:28:VAL:HG21 | 32:CR:193:LEU:HD21 | 1.91 | 0.52 |
| 44:C1:6:G:N1 | 44:C1:30:U:N3 | 2.58 | 0.52 |
| 44:C1:1479:U:H2' | 44:C1:1480:G:H8 | 1.73 | 0.52 |
| 46:UV:336:GLY:HA3 | 46:UV:384:ALA:HB3 | 1.91 | 0.52 |
| 46:UV:364:LEU:HA | 46:UV:369:PHE:HB2 | 1.91 | 0.52 |
| 48:UH:736:LEU:HA | 48:UH:739:LEU:HG | 1.92 | 0.52 |
| 4:UD:832:PHE:HB2 | 4:UD:835:ILE:HD11 | 1.92 | 0.52 |
| 5:UF:279:PRO:HA | 5:UF:282:VAL:HG22 | 1.92 | 0.52 |
| 7:UJ:821:LYS:O | 7:UJ:824:THR:OG1 | 2.23 | 0.52 |
| 12:UO:551:MET:HE1 | 49:UE:236:ILE:HB | 1.92 | 0.52 |
| 18:CA:214:MET:HA | 18:CA:217:ARG:HD3 | 1.90 | 0.52 |
| 19:CC:325:LEU:HD22 | 19:CC:394:ASN:HD21 | 1.75 | 0.52 |
| 20:CD:234:GLU:HA | 20:CD:237:VAL:HG22 | 1.90 | 0.52 |
| 21:CF:119:ARG:HA | 21:CF:122:VAL:HG12 | 1.92 | 0.52 |
| 22:CG:414:ASP:N | 22:CG:414:ASP:OD2 | 2.43 | 0.52 |
| 29:CO:115:GLN:HE22 | 29:CO:117:ALA:HA | 1.75 | 0.52 |
| 34:Cc:57:ILE:HG13 | 34:Cc:59:HIS:H | 1.74 | 0.52 |
| 35:Ce:172:VAL:HG12 | 35:Ce:176:LEU:HG | 1.92 | 0.52 |
| 44:C1:1509:A:H4' | 54:Cz:1646:VAL:HG12 | 1.92 | 0.52 |
| 46:UV:821:THR:HG23 | 46:UV:827:LEU:HD21 | 1.91 | 0.52 |
| 4:UD:278:ASP:N | 4:UD:278:ASP:OD1 | 2.40 | 0.52 |
| 9:UL:198:ILE:HD11 | 9:UL:212:HIS:HB2 | 1.91 | 0.52 |
| 9:UL:525:SER:OG | 9:UL:535:TRP:NE1 | 2.40 | 0.52 |
| 10:UM:248:LEU:HD21 | 10:UM:258:LEU:HD13 | 1.92 | 0.52 |
| 12:UO:294:ASP:O | 12:UO:312:LYS:NZ | 2.42 | 0.52 |
| 15:UU:103:ARG:HG2 | 15:UU:123:GLN:HB2 | 1.90 | 0.52 |
| 23:CH:61:THR:HG22 | 23:CH:82:ILE:HD13 | 1.90 | 0.52 |
| 25:CJ:115:MET:HB2 | 25:CJ:120:MET:HG3 | 1.91 | 0.52 |
| 32:CS:424:LEU:HD22 | 32:CS:549:TYR:HA | 1.92 | 0.52 |
| 39:Cj:29:ILE:HG12 | 39:Cj:65:ILE:HD12 | 1.91 | 0.52 |
| 44:C1:1483:A:N1 | 44:C1:1496:U:O2' | 2.34 | 0.52 |
| 46:UV:174:ALA:HA | 46:UV:177:GLN:HG2 | 1.92 | 0.52 |
| 48:UH:816:GLN:HA | 48:UH:819:ILE:HB | 1.92 | 0.52 |
| 1:UA:191:LEU:HD21 | 1:UA:210:ILE:HD11 | 1.92 | 0.52 |
| 4:UD:568:GLY:HA2 | 4:UD:630:PRO:HD3 | 1.91 | 0.52 |
| 8:UK:12:ALA:HB2 | 44:C1:1137:G:H21 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:UL:195:ASP:OD1 | 9:UL:195:ASP:N | 2.43 | 0.52 |
| 10:UM:678:TRP:HB3 | 10:UM:685:THR:HA | 1.92 | 0.52 |
| 14:UR:402:ASN:O | 14:UR:406:MET:N | 2.43 | 0.52 |
| 15:UU:113:ASN:OD1 | 15:UU:113:ASN:N | 2.40 | 0.52 |
| 16:UX:62:THR:OG1 | 16:UX:63:ASN:N | 2.41 | 0.52 |
| 22:CG:163:TYR:HB3 | 22:CG:604:PHE:HB3 | 1.91 | 0.52 |
| 36:Cg:89:MET:N | 36:Cg:89:MET:SD | 2.83 | 0.52 |
| 44:C1:373:C:H2' | 44:C1:374:G:C8 | 2.45 | 0.52 |
| 44:C1:2356:C:H2' | 44:C1:2357:G:C8 | 2.45 | 0.52 |
| 46:UV:204:PRO:HG2 | 46:UV:215:LYS:HD2 | 1.90 | 0.52 |
| 50:US:135:ALA:HB3 | 50:US:181:LEU:HD21 | 1.90 | 0.52 |
| 52:CX:301:GLY:O | 52:CX:305:GLY:N | 2.42 | 0.52 |
| 1:UA:16:CYS:SG | 1:UA:34:GLY:N | 2.72 | 0.52 |
| 1:UA:216:ASP:OD1 | 1:UA:216:ASP:N | 2.32 | 0.52 |
| 5:UF:166:ARG:NH2 | 11:UN:358:GLN:O | 2.43 | 0.52 |
| 6:UG:304:ARG:N | 6:UG:318:THR:O | 2.40 | 0.52 |
| 7:UJ:656:ILE:HD12 | 7:UJ:660:LEU:HB3 | 1.92 | 0.52 |
| 9:UL:606:HIS:N | 9:UL:632:ARG:HH12 | 2.08 | 0.52 |
| 9:UL:711:LEU:HG | 9:UL:723:TRP:HB2 | 1.92 | 0.52 |
| 13:UQ:155:TYR:CE1 | 13:UQ:169:ASN:HB3 | 2.44 | 0.52 |
| 13:UQ:632:ASP:OD2 | 13:UQ:633:GLY:N | 2.43 | 0.52 |
| 15:UU:674:HIS:ND1 | 15:UU:675:PRO:O | 2.43 | 0.52 |
| 16:UX:64:PHE:HB2 | 16:UX:148:THR:HA | 1.91 | 0.52 |
| 23:CH:92:SER:OG | 23:CH:96:ASP:OD2 | 2.21 | 0.52 |
| 23:CH:124:SER:H | 23:CH:199:GLN:NE2 | 2.07 | 0.52 |
| 32:CR:424:LEU:HD22 | 32:CR:549:TYR:HA | 1.92 | 0.52 |
| 32:CR:838:HIS:HD2 | 32:CR:841:LEU:HD22 | 1.74 | 0.52 |
| 40:Cm:11:LEU:HD22 | 40:Cm:72:CYS:HB3 | 1.92 | 0.52 |
| 44:C1:207:U:OP1 | 44:C1:208:A:N6 | 2.43 | 0.52 |
| 44:C1:609:A:H2' | 44:C1:610:G:C8 | 2.45 | 0.52 |
| 47:CV:58:VAL:HG22 | 47:CV:89:GLN:HG2 | 1.92 | 0.52 |
| 49:UI:236:ILE:HA | 49:UI:239:LEU:HD12 | 1.90 | 0.52 |
| 53:UP:318:THR:OG1 | 53:UP:319:ALA:N | 2.43 | 0.52 |
| 1:UA:385:VAL:HG22 | 1:UA:401:SER:HB3 | 1.92 | 0.51 |
| 1:UA:559:ARG:NH2 | 1:UA:672:GLU:OE2 | 2.43 | 0.51 |
| 3:UC:605:ARG:NH1 | 44:C1:1062:C:OP1 | 2.43 | 0.51 |
| 4:UD:870:ASP:O | 53:UP:356:ARG:NH2 | 2.43 | 0.51 |
| 9:UL:111:SER:O | 9:UL:129:SER:OG | 2.27 | 0.51 |
| 11:UN:896:GLN:O | 11:UN:900:SER:HB3 | 2.09 | 0.51 |
| 19:CC:387:SER:O | 19:CC:390:SER:OG | 2.21 | 0.51 |
| 20:CD:438:ARG:NH2 | 44:C1:273:G:OP2 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:CG:272:VAL:HG21 | 22:CG:317:LEU:HD11 | 1.93 | 0.51 |
| 24:CI:135:ILE:HD12 | 24:CI:165:ASN:HB2 | 1.92 | 0.51 |
| 24:CI:944:ILE:O | 24:CI:947:PHE:N | 2.42 | 0.51 |
| 24:CI:1138:LYS:HD2 | 24:CI:1142:TRP:HD1 | 1.74 | 0.51 |
| 30:CP:98:LEU:HD11 | 30:CP:115:LEU:HD21 | 1.92 | 0.51 |
| 32:CR:138:ARG:O | 32:CR:142:THR:OG1 | 2.27 | 0.51 |
| 46:UV:1003:LYS:HZ1 | 46:UV:1018:MET:HE2 | 1.75 | 0.51 |
| 48:UH:566:ARG:HA | 48:UH:612:GLN:HE22 | 1.73 | 0.51 |
| 50:US:425:LYS:HD2 | 50:US:428:ARG:HD2 | 1.92 | 0.51 |
| 52:CX:364:ASN:HD21 | 52:CX:410:PHE:HB2 | 1.74 | 0.51 |
| 1:UA:448:PHE:HB2 | 26:CK:135:ARG:NH1 | 2.22 | 0.51 |
| 4:UD:447:THR:O | 4:UD:481:ALA:N | 2.41 | 0.51 |
| 4:UD:484:VAL:HG23 | 4:UD:493:ILE:HD11 | 1.92 | 0.51 |
| 5:UF:354:PRO:HA | 5:UF:357:LEU:HB2 | 1.91 | 0.51 |
| 13:UQ:783:ASN:ND2 | 13:UQ:786:SER:H | 2.08 | 0.51 |
| 14:UR:383:ARG:O | 14:UR:403:VAL:HG12 | 2.10 | 0.51 |
| 14:UR:555:LEU:HB2 | 14:UR:571:LEU:HD11 | 1.92 | 0.51 |
| 15:UU:136:ASP:OD1 | 15:UU:136:ASP:N | 2.37 | 0.51 |
| 17:UZ:67:THR:O | 17:UZ:279:ARG:HB3 | 2.10 | 0.51 |
| 17:UZ:275:TRP:HA | 17:UZ:278:VAL:HB | 1.91 | 0.51 |
| 19:CC:271:LEU:HA | 19:CC:274:VAL:HG12 | 1.93 | 0.51 |
| 24:CI:817:ILE:HD11 | 24:CI:901:ALA:HB1 | 1.91 | 0.51 |
| 26:CK:91:THR:HG22 | 26:CK:117:LEU:HB3 | 1.91 | 0.51 |
| 28:CM:109:HIS:NE2 | 28:CM:126:SER:OG | 2.39 | 0.51 |
| 29:CN:40:VAL:HG22 | 29:CN:113:TYR:HB2 | 1.90 | 0.51 |
| 32:CS:87:ARG:HD2 | 32:CS:91:GLN:HB3 | 1.92 | 0.51 |
| 32:CS:843:SER:HB2 | 32:CS:848:LEU:HD23 | 1.93 | 0.51 |
| 36:Cg:33:GLY:H | 36:Cg:120:ILE:HD12 | 1.76 | 0.51 |
| 44:C1:600:U:H2' | 44:C1:601:C:H6 | 1.76 | 0.51 |
| 44:C1:1702:G:H2' | 44:C1:1703:G:C8 | 2.45 | 0.51 |
| 46:UV:381:PRO:HD3 | 46:UV:395:ASP:HA | 1.92 | 0.51 |
| 46:UV:840:VAL:HG21 | 46:UV:984:PHE:HA | 1.91 | 0.51 |
| 48:UH:575:SER:HA | 48:UH:578:ILE:HG22 | 1.91 | 0.51 |
| 48:UH:830:VAL:HG11 | 49:UE:257:LEU:HD22 | 1.91 | 0.51 |
| 2:UB:726:LEU:HD22 | 2:UB:773:LEU:HD13 | 1.93 | 0.51 |
| 3:UC:592:ASN:N | 3:UC:592:ASN:OD1 | 2.44 | 0.51 |
| 4:UD:75:ARG:HD3 | 53:UP:332:ALA:HB3 | 1.92 | 0.51 |
| 4:UD:223:MET:HE2 | 4:UD:266:TYR:HB3 | 1.92 | 0.51 |
| 4:UD:432:THR:OG1 | 4:UD:446:SER:OG | 2.25 | 0.51 |
| 7:UJ:297:VAL:HG21 | 7:UJ:328:VAL:HG12 | 1.93 | 0.51 |
| 9:UL:202:ASP:OD1 | 9:UL:204:SER:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:UM:281:GLY:H | 10:UM:290:TYR:HB3 | 1.75 | 0.51 |
| 10:UM:392:ALA:HB2 | 10:UM:439:LEU:HD21 | 1.91 | 0.51 |
| 10:UM:798:LEU:HD13 | 10:UM:833:LEU:HD22 | 1.93 | 0.51 |
| 12:UO:140:TRP:HH2 | 12:UO:174:LEU:HD23 | 1.76 | 0.51 |
| 14:UR:261:ILE:HG12 | 14:UR:263:ILE:HG13 | 1.91 | 0.51 |
| 15:UU:214:SER:OG | 15:UU:215:THR:N | 2.41 | 0.51 |
| 24:CI:105:THR:HB | 24:CI:335:TRP:HB3 | 1.92 | 0.51 |
| 32:CR:289:ARG:HA | 32:CR:477:PRO:HA | 1.92 | 0.51 |
| 32:CR:843:SER:HB2 | 32:CR:848:LEU:HD23 | 1.93 | 0.51 |
| 32:CS:289:ARG:HA | 32:CS:477:PRO:HA | 1.92 | 0.51 |
| 32:CS:591:GLU:OE1 | 32:CS:612:ASP:N | 2.43 | 0.51 |
| 44:C1:108:C:H2' | 44:C1:109:G:C8 | 2.46 | 0.51 |
| 44:C1:225:C:H2' | 44:C1:226:C:H6 | 1.75 | 0.51 |
| 44:C1:1696:G:H2' | 44:C1:1697:A:H8 | 1.74 | 0.51 |
| 46:UV:312:PHE:HA | 46:UV:318:LYS:HG3 | 1.93 | 0.51 |
| 1:UA:83:ASN:HB2 | 1:UA:90:LEU:HD11 | 1.92 | 0.51 |
| 1:UA:136:LEU:HD12 | 15:UU:777:THR:HG21 | 1.92 | 0.51 |
| 6:UG:59:ASP:O | 6:UG:62:SER:OG | 2.28 | 0.51 |
| 7:UJ:266:GLY:HA2 | 7:UJ:269:ILE:HD12 | 1.92 | 0.51 |
| 7:UJ:649:LYS:HD2 | 7:UJ:652:LEU:HD21 | 1.91 | 0.51 |
| 18:CB:285:PHE:N | 18:CB:305:VAL:O | 2.41 | 0.51 |
| 19:CC:321:HIS:CD2 | 19:CC:339:LEU:HD22 | 2.45 | 0.51 |
| 20:CD:292:LEU:HB3 | 20:CD:293:ILE:HG23 | 1.92 | 0.51 |
| 23:CH:318:LEU:HA | 23:CH:321:ILE:HD12 | 1.93 | 0.51 |
| 31:CQ:98:ASN:N | 31:CQ:98:ASN:OD1 | 2.42 | 0.51 |
| 32:CS:138:ARG:O | 32:CS:142:THR:OG1 | 2.27 | 0.51 |
| 44:C1:123:U:H2' | 44:C1:124:C:H6 | 1.76 | 0.51 |
| 44:C1:246:G:H2' | 44:C1:247:C:C6 | 2.46 | 0.51 |
| 44:C1:381:G:H21 | 44:C1:385:A:H62 | 1.57 | 0.51 |
| 44:C1:2236:C:H2' | 44:C1:2237:G:C8 | 2.45 | 0.51 |
| 45:C2:94:A:H61 | 45:C2:260:G:H22 | 1.58 | 0.51 |
| 52:CX:227:ILE:HG21 | 52:CX:233:ILE:HD12 | 1.93 | 0.51 |
| 54:Cz:1629:LYS:H | 54:Cz:1629:LYS:HD2 | 1.76 | 0.51 |
| 1:UA:615:ASN:OD1 | 1:UA:616:LEU:N | 2.42 | 0.51 |
| 6:UG:125:VAL:O | 6:UG:128:LYS:N | 2.43 | 0.51 |
| 7:UJ:75:SER:O | 7:UJ:78:SER:OG | 2.24 | 0.51 |
| 10:UM:11:PHE:HB2 | 10:UM:689:LEU:HD21 | 1.93 | 0.51 |
| 18:CA:109:ILE:HG13 | 18:CA:129:ILE:HD11 | 1.91 | 0.51 |
| 19:CC:6:PHE:HA | 19:CC:18:PHE:O | 2.11 | 0.51 |
| 19:CC:414:ARG:NH2 | 19:CC:418:TYR:OH | 2.42 | 0.51 |
| 22:CG:273:TYR:HE2 | 22:CG:278:LEU:HD12 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:CI:355:ARG:HH21 | 24:CI:359:PHE:HA | 1.74 | 0.51 |
| 26:CK:202:GLN:HA | 26:CK:205:VAL:HG12 | 1.93 | 0.51 |
| 28:CM:287:MET:H | 28:CM:302:SER:HA | 1.75 | 0.51 |
| 32:CR:541:VAL:O | 32:CR:545:VAL:HG12 | 2.11 | 0.51 |
| 34:Cc:203:GLU:HA | 34:Cc:206:ARG:NE | 2.24 | 0.51 |
| 44:C1:373:C:H2' | 44:C1:374:G:H8 | 1.75 | 0.51 |
| 1:UA:453:TRP:HE1 | 1:UA:460:LEU:HD12 | 1.75 | 0.51 |
| 2:UB:63:ASN:OD1 | 2:UB:64:ALA:N | 2.43 | 0.51 |
| 2:UB:342:ARG:O | 2:UB:606:HIS:N | 2.36 | 0.51 |
| 6:UG:466:ILE:HG23 | 11:UN:882:TYR:HB3 | 1.93 | 0.51 |
| 11:UN:338:HIS:HA | 11:UN:922:ARG:O | 2.09 | 0.51 |
| 12:UO:258:LEU:HG | 12:UO:265:PRO:HA | 1.92 | 0.51 |
| 12:UO:324:THR:HA | 12:UO:331:ASP:HA | 1.93 | 0.51 |
| 14:UR:262:ASP:CB | 14:UR:617:ARG:O | 2.58 | 0.51 |
| 15:UU:190:ILE:HD12 | 15:UU:237:PRO:HD3 | 1.91 | 0.51 |
| 15:UU:195:PHE:HZ | 15:UU:259:LEU:HD23 | 1.75 | 0.51 |
| 18:CA:128:ARG:HH22 | 18:CA:169:HIS:HA | 1.75 | 0.51 |
| 19:CC:309:ILE:HA | 19:CC:408:ARG:HD3 | 1.93 | 0.51 |
| 28:CM:437:ARG:NE | 44:C1:586:G:O6 | 2.30 | 0.51 |
| 32:CR:258:THR:HG21 | 32:CR:476:GLU:HG3 | 1.93 | 0.51 |
| 32:CS:28:VAL:HG21 | 32:CS:193:LEU:HD21 | 1.91 | 0.51 |
| 32:CS:541:VAL:O | 32:CS:545:VAL:HG12 | 2.11 | 0.51 |
| 32:CS:864:LEU:HD23 | 32:CS:870:LEU:HD12 | 1.93 | 0.51 |
| 44:C1:456:A:H62 | 44:C1:476:G:N2 | 2.09 | 0.51 |
| 45:C2:43:C:H2' | 45:C2:44:U:C6 | 2.45 | 0.51 |
| 46:UV:642:ASN:HA | 46:UV:646:LYS:HG2 | 1.93 | 0.51 |
| 50:US:191:LYS:NZ | 50:US:231:GLU:H | 2.07 | 0.51 |
| 50:US:497:TYR:HA | 50:US:500:LEU:HD12 | 1.91 | 0.51 |
| 6:UG:214:ARG:NH1 | 44:C1:292:G:OP2 | 2.43 | 0.51 |
| 7:UJ:729:SER:O | 7:UJ:732:GLN:NE2 | 2.44 | 0.51 |
| 9:UL:72:ALA:HB1 | 9:UL:116:LEU:HG | 1.91 | 0.51 |
| 9:UL:375:ALA:HB3 | 9:UL:384:GLN:HB2 | 1.92 | 0.51 |
| 9:UL:576:ASP:OD1 | 9:UL:576:ASP:N | 2.43 | 0.51 |
| 9:UL:668:TYR:HB3 | 9:UL:680:TYR:HE1 | 1.75 | 0.51 |
| 10:UM:24:GLY:HA3 | 10:UM:38:THR:HG21 | 1.93 | 0.51 |
| 10:UM:328:LEU:O | 10:UM:330:GLU:N | 2.44 | 0.51 |
| 13:UQ:220:ALA:HB2 | 13:UQ:234:LEU:HD11 | 1.92 | 0.51 |
| 15:UU:159:ILE:HB | 15:UU:173:ILE:HB | 1.92 | 0.51 |
| 15:UU:421:SER:OG | 15:UU:423:ARG:N | 2.43 | 0.51 |
| 16:UX:61:ASP:OD1 | 16:UX:62:THR:N | 2.44 | 0.51 |
| 18:CB:213:PRO:HA | 18:CB:216:TYR:CZ | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:CM:310:TRP:NE1 | 28:CM:317:SER:HA | 2.26 | 0.51 |
| 28:CM:423:ARG:NH1 | 28:CM:431:GLU:O | 2.33 | 0.51 |
| 29:CN:150:ILE:O | 29:CN:159:LEU:N | 2.43 | 0.51 |
| 32:CR:87:ARG:HD2 | 32:CR:91:GLN:HB3 | 1.92 | 0.51 |
| 32:CR:204:ASP:O | 32:CR:207:ASN:ND2 | 2.44 | 0.51 |
| 32:CS:258:THR:HG21 | 32:CS:476:GLU:HG3 | 1.93 | 0.51 |
| 34:Cc:95:LEU:HD21 | 39:Cj:44:LEU:HD21 | 1.92 | 0.51 |
| 42:Cp:11:VAL:HG23 | 42:Cp:33:PHE:HD1 | 1.75 | 0.51 |
| 44:C1:2119:G:N2 | 44:C1:2121:U:H3 | 2.08 | 0.51 |
| 47:CV:171:THR:HA | 47:CV:174:TYR:HB2 | 1.93 | 0.51 |
| 50:US:333:ASN:N | 50:US:333:ASN:OD1 | 2.40 | 0.51 |
| 1:UA:213:VAL:HG12 | 1:UA:219:VAL:HB | 1.93 | 0.51 |
| 1:UA:576:ASN:H | 1:UA:591:GLY:HA3 | 1.75 | 0.51 |
| 2:UB:605:ASP:N | 2:UB:605:ASP:OD1 | 2.43 | 0.51 |
| 5:UF:285:VAL:HG11 | 11:UN:369:LEU:HD13 | 1.92 | 0.51 |
| 6:UG:360:TRP:NE1 | 6:UG:365:THR:OG1 | 2.33 | 0.51 |
| 8:UK:66:GLY:O | 8:UK:69:SER:C | 2.54 | 0.51 |
| 9:UL:614:ASP:OD2 | 9:UL:657:PHE:N | 2.35 | 0.51 |
| 12:UO:150:THR:HA | 12:UO:161:MET:O | 2.10 | 0.51 |
| 13:UQ:471:SER:OG | 13:UQ:474:ASN:O | 2.26 | 0.51 |
| 14:UR:453:GLY:HA3 | 14:UR:526:ILE:HG13 | 1.92 | 0.51 |
| 16:UX:13:ARG:HB3 | 25:CJ:19:ILE:HG13 | 1.92 | 0.51 |
| 22:CG:454:ASP:OD1 | 22:CG:454:ASP:N | 2.36 | 0.51 |
| 28:CM:224:LEU:O | 28:CM:233:VAL:N | 2.34 | 0.51 |
| 28:CM:310:TRP:HE1 | 28:CM:317:SER:HA | 1.75 | 0.51 |
| 42:Cp:63:GLU:O | 42:Cp:65:ARG:NH1 | 2.43 | 0.51 |
| 50:US:485:GLN:HG3 | 51:Cl:13:HIS:CG | 2.46 | 0.51 |
| 2:UB:792:ARG:HE | 2:UB:793:LEU:HD12 | 1.76 | 0.51 |
| 4:UD:377:ALA:O | 4:UD:381:ARG:N | 2.44 | 0.51 |
| 4:UD:877:PHE:C | 53:UP:351:ARG:HB2 | 2.36 | 0.51 |
| 7:UJ:496:SER:OG | 7:UJ:533:ARG:NH2 | 2.44 | 0.51 |
| 9:UL:153:ASP:OD1 | 9:UL:195:ASP:N | 2.43 | 0.51 |
| 9:UL:305:TRP:CE2 | 9:UL:359:GLN:HG2 | 2.46 | 0.51 |
| 12:UO:95:ILE:HD13 | 12:UO:126:PHE:HE2 | 1.76 | 0.51 |
| 12:UO:212:GLU:O | 12:UO:230:LYS:HA | 2.11 | 0.51 |
| 13:UQ:646:ASP:N | 13:UQ:646:ASP:OD1 | 2.42 | 0.51 |
| 15:UU:190:ILE:HD11 | 15:UU:244:LEU:HD11 | 1.93 | 0.51 |
| 20:CD:152:HIS:O | 20:CD:156:PHE:HB2 | 2.11 | 0.51 |
| 24:CI:854:ARG:HB2 | 41:Cn:61:ALA:O | 2.10 | 0.51 |
| 26:CK:146:ARG:NH1 | 44:C1:2049:G:N3 | 2.58 | 0.51 |
| 26:CK:191:LEU:HD21 | 26:CK:212:PHE:CD2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:CO:175:CYS:HA | 29:CO:201:SER:O | 2.11 | 0.51 |
| 45:C2:97:C:H2' | 45:C2:98:U:C6 | 2.46 | 0.51 |
| 46:UV:367:THR:OG1 | 46:UV:368:ASN:N | 2.44 | 0.51 |
| 9:UL:265:ASN:OD1 | 9:UL:265:ASN:N | 2.41 | 0.51 |
| 12:UO:45:SER:OG | 12:UO:76:THR:OG1 | 2.28 | 0.51 |
| 15:UU:931:GLY:O | 15:UU:934:LYS:C | 2.54 | 0.51 |
| 17:UZ:131:SER:OG | 17:UZ:132:HIS:N | 2.43 | 0.51 |
| 18:CB:96:ASN:ND2 | 18:CB:126:GLU:OE2 | 2.35 | 0.51 |
| 23:CH:42:THR:OG1 | 23:CH:43:ASN:N | 2.43 | 0.51 |
| 27:CL:611:LYS:NZ | 43:CU:195:ALA:O | 2.32 | 0.51 |
| 32:CR:200:LEU:HD11 | 32:CR:208:VAL:HG13 | 1.93 | 0.51 |
| 32:CR:390:GLU:H | 32:CR:411:ALA:HB3 | 1.75 | 0.51 |
| 32:CS:200:LEU:HD11 | 32:CS:208:VAL:HG13 | 1.93 | 0.51 |
| 34:Cc:187:ASN:HB3 | 34:Cc:195:SER:HB3 | 1.93 | 0.51 |
| 44:C1:483:U:H4' | 44:C1:484:G:H5" | 1.92 | 0.51 |
| 44:C1:1175:A:H2' | 44:C1:1176:A:C8 | 2.46 | 0.51 |
| 44:C1:1652:C:H2' | 44:C1:1653:G:C8 | 2.46 | 0.51 |
| 46:UV:927:HIS:O | 46:UV:951:ARG:NH2 | 2.38 | 0.51 |
| 50:US:166:PHE:HA | 50:US:169:ILE:HD12 | 1.92 | 0.51 |
| 53:UP:314:ARG:NH2 | 53:UP:316:GLY:O | 2.44 | 0.51 |
| 54:Cz:1627:HIS:HD2 | 54:Cz:1664:LEU:HG | 1.76 | 0.51 |
| 1:UA:817:ARG:HE | 15:UU:1045:ARG:HH21 | 1.57 | 0.50 |
| 2:UB:46:GLU:HA | 2:UB:49:LYS:HE2 | 1.93 | 0.50 |
| 2:UB:702:LEU:HD23 | 2:UB:728:THR:HG21 | 1.92 | 0.50 |
| 3:UC:648:LEU:HD13 | 18:CA:286:PRO:HB2 | 1.93 | 0.50 |
| 4:UD:64:TYR:CE1 | 4:UD:370:GLN:HG2 | 2.46 | 0.50 |
| 4:UD:115:ASP:HB2 | 4:UD:122:LYS:HB2 | 1.93 | 0.50 |
| 6:UG:279:ASN:OD1 | 6:UG:280:GLY:N | 2.44 | 0.50 |
| 7:UJ:199:TYR:HE2 | 7:UJ:213:LEU:HD11 | 1.76 | 0.50 |
| 7:UJ:393:LYS:HG2 | 7:UJ:441:ALA:HB2 | 1.91 | 0.50 |
| 7:UJ:793:PHE:O | 7:UJ:797:VAL:HG23 | 2.11 | 0.50 |
| 12:UO:492:PRO:HB3 | 12:UO:495:ARG:HH21 | 1.76 | 0.50 |
| 15:UU:506:THR:OG1 | 15:UU:507:GLY:N | 2.44 | 0.50 |
| 16:UX:67:ARG:HD3 | 16:UX:149:ASN:HD22 | 1.76 | 0.50 |
| 18:CB:130:TRP:HD1 | 18:CB:169:HIS:CG | 2.29 | 0.50 |
| 19:CC:3:VAL:HG13 | 19:CC:97:VAL:HG11 | 1.93 | 0.50 |
| 21:CF:106:ASN:O | 21:CF:112:ASN:ND2 | 2.44 | 0.50 |
| 24:CI:242:PRO:HG2 | 24:CI:802:GLY:HA3 | 1.93 | 0.50 |
| 24:CI:246:ILE:HB | 24:CI:798:ILE:HB | 1.92 | 0.50 |
| 27:CL:781:GLY:O | 27:CL:785:LEU:CB | 2.54 | 0.50 |
| 32:CS:41:LEU:HA | 32:CS:44:ILE:HD12 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:CS:423:SER:HA | 32:CS:426:LEU:HG | 1.93 | 0.50 |
| 44:C1:231:U:H2' | 44:C1:232:G:H8 | 1.76 | 0.50 |
| 44:C1:2107:A:H2' | 44:C1:2108:A:C8 | 2.46 | 0.50 |
| 46:UV:162:PHE:HD1 | 46:UV:165:ARG:HH21 | 1.58 | 0.50 |
| 46:UV:347:LEU:HD22 | 46:UV:356:LEU:HD12 | 1.93 | 0.50 |
| 46:UV:536:VAL:HG21 | 46:UV:603:MET:HE1 | 1.92 | 0.50 |
| 46:UV:855:PHE:HA | 46:UV:858:HIS:CD2 | 2.46 | 0.50 |
| 50:US:143:MET:HE2 | 50:US:189:PHE:CG | 2.47 | 0.50 |
| 1:UA:324:VAL:HG12 | 1:UA:333:ILE:HB | 1.93 | 0.50 |
| 4:UD:509:ALA:HB1 | 4:UD:516:ILE:HD11 | 1.92 | 0.50 |
| 14:UR:149:ALA:N | 14:UR:164:ASP:OD1 | 2.44 | 0.50 |
| 15:UU:313:LEU:HA | 15:UU:317:GLY:HA2 | 1.93 | 0.50 |
| 20:CD:438:ARG:HB3 | 44:C1:272:A:H5' | 1.93 | 0.50 |
| 24:CI:843:GLN:NE2 | 24:CI:1012:SER:OG | 2.44 | 0.50 |
| 25:CJ:62:SER:O | 43:CU:203:LYS:NZ | 2.43 | 0.50 |
| 28:CM:200:ILE:HA | 28:CM:217:ALA:HA | 1.93 | 0.50 |
| 28:CM:251:GLU:OE2 | 28:CM:312:ARG:NH1 | 2.44 | 0.50 |
| 32:CR:423:SER:HA | 32:CR:426:LEU:HG | 1.94 | 0.50 |
| 32:CR:591:GLU:OE1 | 32:CR:612:ASP:N | 2.44 | 0.50 |
| 32:CS:470:LYS:HZ2 | 32:CS:472:ILE:HD13 | 1.75 | 0.50 |
| 1:UA:825:LYS:O | 1:UA:829:GLU:CB | 2.58 | 0.50 |
| 3:UC:643:VAL:HG13 | 16:UX:36:GLU:HA | 1.93 | 0.50 |
| 4:UD:325:ASP:N | 4:UD:325:ASP:OD1 | 2.42 | 0.50 |
| 4:UD:632:VAL:HG12 | 4:UD:650:VAL:HB | 1.92 | 0.50 |
| 4:UD:698:ARG:HA | 4:UD:710:PHE:O | 2.11 | 0.50 |
| 7:UJ:210:TYR:CZ | 7:UJ:213:LEU:HB2 | 2.46 | 0.50 |
| 12:UO:492:PRO:HD3 | 49:UE:249:ARG:NH2 | 2.26 | 0.50 |
| 14:UR:232:SER:HA | 14:UR:235:ARG:HG2 | 1.93 | 0.50 |
| 19:CC:39:LYS:O | 19:CC:137:HIS:NE2 | 2.34 | 0.50 |
| 22:CG:300:THR:OG1 | 22:CG:301:ASN:N | 2.43 | 0.50 |
| 23:CH:323:GLN:HG3 | 23:CH:354:ARG:HB2 | 1.92 | 0.50 |
| 25:CJ:86:GLY:HA2 | 25:CJ:152:ARG:HE | 1.77 | 0.50 |
| 26:CK:88:VAL:O | 26:CK:114:ALA:HA | 2.10 | 0.50 |
| 31:CQ:198:LYS:O | 31:CQ:202:GLU:HG2 | 2.11 | 0.50 |
| 32:CS:191:LEU:O | 32:CS:195:SER:OG | 2.28 | 0.50 |
| 32:CS:387:VAL:HG23 | 32:CS:409:PHE:HD2 | 1.74 | 0.50 |
| 32:CS:421:GLY:HA2 | 32:CS:545:VAL:HG22 | 1.93 | 0.50 |
| 38:Ci:133:PRO:HB2 | 44:C1:1472:A:H5" | 1.92 | 0.50 |
| 40:Cm:114:GLU:OE2 | 40:Cm:117:ARG:NH2 | 2.42 | 0.50 |
| 44:C1:1662:C:H2' | 44:C1:1663:U:C6 | 2.46 | 0.50 |
| 46:UV:175:HIS:HA | 46:UV:178:LYS:HG2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:Cz:1517:ALA:HA | 54:Cz:1520:MET:HE3 | 1.93 | 0.50 |
| 4:UD:312:ARG:HH21 | 14:UR:449:ARG:HB3 | 1.75 | 0.50 |
| 4:UD:370:GLN:HE22 | 4:UD:690:LYS:HG2 | 1.77 | 0.50 |
| 7:UJ:85:GLN:NE2 | 28:CM:7:THR:OG1 | 2.44 | 0.50 |
| 7:UJ:256:SER:OG | 7:UJ:257:GLU:N | 2.44 | 0.50 |
| 9:UL:114:THR:H | 9:UL:129:SER:HA | 1.76 | 0.50 |
| 9:UL:615:ILE:HG22 | 9:UL:622:ILE:HG23 | 1.92 | 0.50 |
| 10:UM:236:GLN:HE21 | 10:UM:252:ARG:HA | 1.76 | 0.50 |
| 10:UM:808:GLN:HA | 10:UM:811:LEU:HG | 1.92 | 0.50 |
| 13:UQ:469:THR:OG1 | 13:UQ:470:ILE:N | 2.44 | 0.50 |
| 15:UU:82:LEU:O | 44:C1:259:U:O2' | 2.29 | 0.50 |
| 17:UZ:76:HIS:HA | 17:UZ:79:GLN:HG2 | 1.94 | 0.50 |
| 17:UZ:215:ARG:HB3 | 17:UZ:220:ILE:HD11 | 1.94 | 0.50 |
| 18:CA:145:LEU:HD23 | 18:CA:290:LEU:HD21 | 1.93 | 0.50 |
| 18:CB:272:PHE:HB3 | 18:CB:289:GLN:HE22 | 1.76 | 0.50 |
| 20:CD:179:LEU:HD22 | 20:CD:182:MET:HE3 | 1.93 | 0.50 |
| 20:CD:269:GLU:O | 20:CD:273:GLN:NE2 | 2.44 | 0.50 |
| 21:CF:11:LYS:HA | 21:CF:81:TYR:HB2 | 1.93 | 0.50 |
| 24:CI:155:ASN:O | 24:CI:159:ASN:ND2 | 2.34 | 0.50 |
| 30:CP:67:ILE:HG23 | 30:CP:82:THR:HA | 1.93 | 0.50 |
| 32:CS:174:ARG:HD3 | 32:CS:182:ILE:HG12 | 1.92 | 0.50 |
| 44:C1:2356:C:H2' | 44:C1:2357:G:H8 | 1.76 | 0.50 |
| 48:UH:581:VAL:HG13 | 48:UH:630:TYR:HB2 | 1.93 | 0.50 |
| 50:US:370:SER:HB3 | 50:US:373:LEU:HD11 | 1.94 | 0.50 |
| 4:UD:129:HIS:CD2 | 4:UD:164:VAL:HG11 | 2.47 | 0.50 |
| 4:UD:432:THR:HG1 | 4:UD:446:SER:HG | 1.59 | 0.50 |
| 5:UF:303:VAL:HA | 5:UF:306:LYS:HG2 | 1.93 | 0.50 |
| 6:UG:438:THR:OG1 | 6:UG:439:LYS:N | 2.45 | 0.50 |
| 7:UJ:862:THR:HG22 | 7:UJ:864:ASP:H | 1.75 | 0.50 |
| 9:UL:910:LEU:HD13 | 10:UM:878:VAL:HG22 | 1.94 | 0.50 |
| 10:UM:775:THR:O | 10:UM:779:THR:OG1 | 2.23 | 0.50 |
| 13:UQ:154:ASP:HA | 13:UQ:170:TRP:NE1 | 2.26 | 0.50 |
| 14:UR:156:LYS:HD3 | 44:C1:272:A:N3 | 2.26 | 0.50 |
| 18:CA:292:LEU:H | 18:CA:292:LEU:HD23 | 1.76 | 0.50 |
| 32:CS:58:TRP:HA | 32:CS:124:ILE:HG23 | 1.93 | 0.50 |
| 35:Ce:173:ASP:HA | 35:Ce:176:LEU:HD12 | 1.92 | 0.50 |
| 44:C1:6:G:C2 | 44:C1:30:U:O2 | 2.64 | 0.50 |
| 44:C1:438:C:H1' | 44:C1:441:A:N1 | 2.27 | 0.50 |
| 44:C1:495:G:OP2 | 44:C1:495:G:N2 | 2.44 | 0.50 |
| 44:C1:2044:C:H2' | 44:C1:2045:G:H8 | 1.75 | 0.50 |
| 46:UV:839:SER:O | 46:UV:842:LYS:NZ | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:US:184:HIS:O | 50:US:188:ASN:HB2 | 2.12 | 0.50 |
| 52:CX:377:LEU:HD12 | 52:CX:378:PRO:HD2 | 1.93 | 0.50 |
| 4:UD:90:MET:HE3 | 4:UD:96:ILE:HD11 | 1.93 | 0.50 |
| 5:UF:102:LYS:NZ | 44:C1:435:A:O2' | 2.32 | 0.50 |
| 8:UK:16:ARG:N | 44:C1:1140:A:OP1 | 2.34 | 0.50 |
| 10:UM:209:ILE:HD11 | 10:UM:247:LEU:HD22 | 1.93 | 0.50 |
| 10:UM:718:THR:OG1 | 10:UM:720:TRP:NE1 | 2.44 | 0.50 |
| 11:UN:311:MET:HB3 | 28:CM:231:MET:HE1 | 1.94 | 0.50 |
| 13:UQ:118:ASP:OD1 | 13:UQ:118:ASP:N | 2.40 | 0.50 |
| 13:UQ:707:PRO:O | 13:UQ:709:GLY:N | 2.45 | 0.50 |
| 15:UU:286:LEU:HD23 | 15:UU:293:ARG:HA | 1.93 | 0.50 |
| 15:UU:340:ILE:HA | 15:UU:356:GLY:HA2 | 1.93 | 0.50 |
| 15:UU:844:SER:OG | 15:UU:845:LEU:N | 2.45 | 0.50 |
| 21:CF:54:ILE:HG23 | 21:CF:80:VAL:HG13 | 1.94 | 0.50 |
| 23:CH:149:SER:OG | 23:CH:151:ASP:OD1 | 2.28 | 0.50 |
| 32:CR:174:ARG:HD3 | 32:CR:182:ILE:HG12 | 1.92 | 0.50 |
| 32:CR:421:GLY:HA2 | 32:CR:545:VAL:HG22 | 1.93 | 0.50 |
| 43:CU:230:ARG:HA | 43:CU:233:ILE:HG22 | 1.93 | 0.50 |
| 44:C1:196:G:H2' | 44:C1:197:G:H8 | 1.76 | 0.50 |
| 44:C1:301:U:C2 | 44:C1:341:G:N1 | 2.80 | 0.50 |
| 46:UV:89:LEU:HD23 | 46:UV:92:LYS:HE2 | 1.94 | 0.50 |
| 52:CX:213:LYS:O | 52:CX:245:ASN:ND2 | 2.41 | 0.50 |
| 1:UA:624:PHE:HE2 | 15:UU:477:GLY:HA3 | 1.76 | 0.50 |
| 4:UD:457:ASP:O | 4:UD:467:LEU:HA | 2.12 | 0.50 |
| 5:UF:332:PRO:HB2 | 5:UF:380:LYS:HE3 | 1.94 | 0.50 |
| 7:UJ:701:SER:O | 7:UJ:701:SER:OG | 2.29 | 0.50 |
| 8:UK:1:MET:H2 | 8:UK:4:LEU:HB2 | 1.77 | 0.50 |
| 9:UL:161:ILE:HB | 9:UL:188:PHE:HB2 | 1.93 | 0.50 |
| 9:UL:816:PRO:HA | 9:UL:819:VAL:HG22 | 1.94 | 0.50 |
| 13:UQ:194:ALA:HA | 13:UQ:202:ASP:O | 2.12 | 0.50 |
| 13:UQ:426:ALA:H | 13:UQ:428:MET:HE2 | 1.76 | 0.50 |
| 14:UR:390:SER:O | 14:UR:390:SER:OG | 2.22 | 0.50 |
| 14:UR:470:GLY:HA3 | 14:UR:481:ARG:HB3 | 1.92 | 0.50 |
| 20:CD:15:LEU:HB2 | 20:CD:47:GLU:HG2 | 1.94 | 0.50 |
| 20:CD:311:LEU:HD12 | 20:CD:314:ASN:HD22 | 1.77 | 0.50 |
| 23:CH:90:ASN:HD21 | 23:CH:98:ILE:HB | 1.75 | 0.50 |
| 26:CK:163:LEU:HD21 | 26:CK:265:PRO:HB3 | 1.94 | 0.50 |
| 28:CM:7:THR:OG1 | 28:CM:8:ARG:N | 2.44 | 0.50 |
| 30:CP:160:THR:OG1 | 30:CP:161:TYR:N | 2.45 | 0.50 |
| 32:CS:204:ASP:O | 32:CS:207:ASN:ND2 | 2.44 | 0.50 |
| 32:CS:390:GLU:H | 32:CS:411:ALA:HB3 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:Ce:50:VAL:HG11 | 35:Ce:69:PRO:HD3 | 1.93 | 0.50 |
| 44:C1:374:G:H2' | 44:C1:375:G:H8 | 1.75 | 0.50 |
| 44:C1:1173:C:H2' | 44:C1:1174:C:H6 | 1.77 | 0.50 |
| 44:C1:1486:G:OP1 | 44:C1:1501:U:O2' | 2.27 | 0.50 |
| 50:US:397:ILE:HA | 50:US:400:ILE:HD12 | 1.94 | 0.50 |
| 54:Cz:1633:PRO:HB2 | 54:Cz:1637:ARG:HH21 | 1.77 | 0.50 |
| 54:Cz:1643:ALA:HA | 54:Cz:1646:VAL:HG22 | 1.94 | 0.50 |
| 1:UA:495:TRP:CZ3 | 1:UA:504:SER:HB3 | 2.46 | 0.50 |
| 4:UD:477:THR:OG1 | 4:UD:478:GLY:N | 2.40 | 0.50 |
| 10:UM:593:ARG:HE | 10:UM:650:TRP:H | 1.58 | 0.50 |
| 12:UO:166:ASP:OD1 | 12:UO:168:THR:OG1 | 2.28 | 0.50 |
| 13:UQ:625:ARG:NH1 | 13:UQ:637:PHE:HB3 | 2.27 | 0.50 |
| 13:UQ:941:ILE:HA | 13:UQ:944:VAL:HG22 | 1.94 | 0.50 |
| 15:UU:698:ASN:OD1 | 15:UU:698:ASN:N | 2.42 | 0.50 |
| 22:CG:410:VAL:HG13 | 22:CG:469:LEU:HD21 | 1.94 | 0.50 |
| 22:CG:462:GLN:HE22 | 22:CG:483:TRP:HZ2 | 1.58 | 0.50 |
| 22:CG:590:ARG:NH2 | 45:C2:191:G:N7 | 2.59 | 0.50 |
| 23:CH:133:THR:HG22 | 23:CH:134:GLY:H | 1.77 | 0.50 |
| 24:CI:613:PRO:HA | 24:CI:616:ILE:HD12 | 1.94 | 0.50 |
| 24:CI:855:THR:OG1 | 24:CI:856:ARG:N | 2.44 | 0.50 |
| 24:CI:887:PHE:HD1 | 24:CI:899:ILE:HA | 1.77 | 0.50 |
| 24:CI:1000:PHE:CZ | 24:CI:1002:ASN:HB2 | 2.47 | 0.50 |
| 26:CK:155:SER:HA | 26:CK:162:THR:HG22 | 1.93 | 0.50 |
| 32:CR:58:TRP:HA | 32:CR:124:ILE:HG23 | 1.93 | 0.50 |
| 32:CS:10:ARG:NH1 | 32:CS:215:LYS:O | 2.43 | 0.50 |
| 44:C1:1485:A:C4 | 44:C1:1486:G:H8 | 2.30 | 0.50 |
| 46:UV:895:ILE:HG23 | 46:UV:934:THR:HB | 1.94 | 0.50 |
| 52:CX:374:ARG:HH11 | 52:CX:416:VAL:HG23 | 1.77 | 0.50 |
| 1:UA:27:THR:OG1 | 1:UA:28:HIS:ND1 | 2.41 | 0.50 |
| 2:UB:813:PRO:HA | 29:CN:152:GLY:HA2 | 1.93 | 0.50 |
| 4:UD:92:ASP:OD1 | 4:UD:92:ASP:N | 2.44 | 0.50 |
| 4:UD:277:GLN:HB3 | 4:UD:296:MET:HE2 | 1.94 | 0.50 |
| 4:UD:388:GLU:HB3 | 4:UD:430:HIS:CE1 | 2.47 | 0.50 |
| 4:UD:481:ALA:HA | 4:UD:497:GLU:HA | 1.92 | 0.50 |
| 4:UD:830:TYR:HB3 | 4:UD:833:ARG:HH12 | 1.76 | 0.50 |
| 6:UG:358:VAL:HG22 | 6:UG:360:TRP:HD1 | 1.76 | 0.50 |
| 7:UJ:541:SER:HB2 | 7:UJ:544:LYS:HD2 | 1.94 | 0.50 |
| 7:UJ:771:VAL:HG13 | 7:UJ:772:PRO:HD3 | 1.94 | 0.50 |
| 9:UL:138:ASP:HB2 | 9:UL:145:GLN:HE21 | 1.77 | 0.50 |
| 9:UL:697:GLY:H | 9:UL:717:ASP:HB2 | 1.77 | 0.50 |
| 13:UQ:299:ILE:O | 13:UQ:310:GLN:NE2 | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:UQ:804:LYS:HE2 | 44:C1:48:C:H5" | 1.94 | 0.50 |
| 14:UR:324:ASP:OD2 | 14:UR:326:ARG:NE | 2.34 | 0.50 |
| 14:UR:542:SER:HB2 | 14:UR:561:HIS:CE1 | 2.47 | 0.50 |
| 23:CH:343:SER:OG | 23:CH:344:GLU:N | 2.43 | 0.50 |
| 29:CO:88:ARG:HE | 29:CO:91:ILE:HG12 | 1.76 | 0.50 |
| 32:CR:824:LEU:HD22 | 32:CR:864:LEU:HD21 | 1.94 | 0.50 |
| 32:CR:864:LEU:HD23 | 32:CR:870:LEU:HD12 | 1.93 | 0.50 |
| 32:CR:865:TYR:HA | 32:CR:870:LEU:HB2 | 1.94 | 0.50 |
| 38:Ci:65:ARG:HD3 | 44:C1:1490:A:H4' | 1.94 | 0.50 |
| 44:C1:1141:G:H2' | 44:C1:1142:U:H6 | 1.75 | 0.50 |
| 44:C1:1506:U:H2' | 44:C1:1507:G:H8 | 1.76 | 0.50 |
| 44:C1:2086:A:H5" | 44:C1:2087:G:C8 | 2.46 | 0.50 |
| 45:C2:267:C:H2' | 45:C2:268:G:C8 | 2.47 | 0.50 |
| 46:UV:392:ILE:HG13 | 46:UV:401:ASN:HB3 | 1.93 | 0.50 |
| 46:UV:604:ARG:NH2 | 46:UV:616:LEU:HB3 | 2.26 | 0.50 |
| 49:UE:215:MET:SD | 49:UE:215:MET:N | 2.85 | 0.50 |
| 6:UG:41:ARG:NH2 | 6:UG:45:TYR:HB2 | 2.27 | 0.49 |
| 7:UJ:297:VAL:HA | 7:UJ:300:TRP:CZ3 | 2.47 | 0.49 |
| 9:UL:892:SER:OG | 9:UL:893:ARG:N | 2.45 | 0.49 |
| 12:UO:520:ALA:HB1 | 49:UE:270:LEU:HD11 | 1.92 | 0.49 |
| 14:UR:370:GLN:HE22 | 14:UR:387:LEU:HB3 | 1.76 | 0.49 |
| 17:UZ:27:CYS:HA | 17:UZ:30:LEU:HD12 | 1.93 | 0.49 |
| 19:CC:222:VAL:O | 19:CC:226:ILE:HB | 2.11 | 0.49 |
| 24:CI:759:GLU:HB2 | 24:CI:764:GLN:HE22 | 1.76 | 0.49 |
| 28:CM:72:MET:HG3 | 28:CM:333:MET:HE2 | 1.93 | 0.49 |
| 28:CM:337:ASP:O | 28:CM:339:LYS:NZ | 2.43 | 0.49 |
| 31:CQ:84:LYS:HZ3 | 31:CQ:121:ARG:HD2 | 1.76 | 0.49 |
| 32:CR:525:THR:O | 32:CR:528:SER:OG | 2.30 | 0.49 |
| 44:C1:1086:U:H2' | 44:C1:1087:G:C8 | 2.47 | 0.49 |
| 44:C1:1702:G:H2' | 44:C1:1703:G:H8 | 1.76 | 0.49 |
| 46:UV:485:ILE:HD13 | 46:UV:488:ARG:HE | 1.77 | 0.49 |
| 48:UH:756:LEU:H | 49:UI:210:ARG:NH2 | 2.10 | 0.49 |
| 1:UA:316:ALA:HB3 | 1:UA:321:GLN:HB3 | 1.94 | 0.49 |
| 4:UD:350:ILE:HG13 | 4:UD:364:THR:HA | 1.94 | 0.49 |
| 4:UD:653:LEU:HB2 | 4:UD:655:GLN:HG3 | 1.94 | 0.49 |
| 9:UL:226:SER:OG | 9:UL:230:THR:N | 2.40 | 0.49 |
| 9:UL:383:LEU:HB2 | 9:UL:399:ILE:HB | 1.92 | 0.49 |
| 11:UN:365:SER:O | 11:UN:371:GLN:NE2 | 2.45 | 0.49 |
| 13:UQ:202:ASP:OD1 | 13:UQ:202:ASP:N | 2.45 | 0.49 |
| 15:UU:1013:LEU:HA | 15:UU:1016:LEU:HB2 | 1.94 | 0.49 |
| 17:UZ:92:SER:HA | 17:UZ:95:ILE:HG12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:CB:138:ALA:HA | 18:CB:141:ILE:HB | 1.94 | 0.49 |
| 22:CG:351:ASP:N | 22:CG:351:ASP:OD1 | 2.44 | 0.49 |
| 29:CN:104:ILE:HG23 | 29:CN:110:LEU:HD22 | 1.94 | 0.49 |
| 30:CP:96:ARG:HG2 | 30:CP:100:LYS:HZ1 | 1.77 | 0.49 |
| 32:CS:543:LEU:HD23 | 32:CS:585:VAL:HG22 | 1.94 | 0.49 |
| 44:C1:104:U:H3' | 44:C1:105:A:C8 | 2.47 | 0.49 |
| 44:C1:107:C:H2' | 44:C1:108:C:C6 | 2.47 | 0.49 |
| 44:C1:265:G:O6 | 44:C1:274:A:C6 | 2.65 | 0.49 |
| 44:C1:345:U:H2' | 44:C1:346:C:C6 | 2.46 | 0.49 |
| 46:UV:1010:ILE:HD12 | 46:UV:1074:ARG:HG3 | 1.94 | 0.49 |
| 50:US:357:ARG:HA | 50:US:360:PHE:HB3 | 1.93 | 0.49 |
| 1:UA:367:TRP:CZ3 | 1:UA:374:CYS:HB3 | 2.48 | 0.49 |
| 1:UA:716:THR:N | 1:UA:719:SER:OG | 2.45 | 0.49 |
| 4:UD:700:TRP:HA | 4:UD:709:MET:HA | 1.93 | 0.49 |
| 6:UG:127:GLN:NE2 | 7:UJ:17:ARG:H | 2.10 | 0.49 |
| 6:UG:225:LEU:HD12 | 6:UG:230:LEU:HB3 | 1.94 | 0.49 |
| 9:UL:491:LEU:HG | 9:UL:500:LEU:HB2 | 1.93 | 0.49 |
| 10:UM:43:ALA:H | 10:UM:57:ILE:HG22 | 1.76 | 0.49 |
| 12:UO:97:ARG:HG2 | 12:UO:136:ILE:HD11 | 1.94 | 0.49 |
| 19:CC:284:MET:SD | 20:CD:267:ARG:NH2 | 2.84 | 0.49 |
| 27:CL:715:ARG:NH1 | 44:C1:2224:C:H5" | 2.27 | 0.49 |
| 28:CM:299:VAL:HG13 | 28:CM:334:TRP:CE2 | 2.47 | 0.49 |
| 32:CS:824:LEU:HD22 | 32:CS:864:LEU:HD21 | 1.94 | 0.49 |
| 36:Cg:45:LEU:O | 36:Cg:48:SER:OG | 2.26 | 0.49 |
| 44:C1:1759:U:O4 | 44:C1:2047:G:C6 | 2.65 | 0.49 |
| 44:C1:2059:C:H2' | 44:C1:2060:A:H8 | 1.76 | 0.49 |
| 45:C2:92:A:O2' | 45:C2:93:G:O4' | 2.26 | 0.49 |
| 46:UV:563:CYS:SG | 46:UV:564:GLU:N | 2.83 | 0.49 |
| 46:UV:1054:LEU:HD12 | 47:CV:90:GLU:HG3 | 1.94 | 0.49 |
| 47:CV:50:SER:OG | 47:CV:51:LEU:N | 2.45 | 0.49 |
| 50:US:522:HIS:ND1 | 50:US:531:GLU:OE1 | 2.44 | 0.49 |
| 49:UI:215:MET:N | 49:UI:215:MET:SD | 2.85 | 0.49 |
| 1:UA:65:PRO:HG2 | 1:UA:106:PRO:HA | 1.94 | 0.49 |
| 1:UA:659:SER:OG | 27:CL:633:LEU:O | 2.31 | 0.49 |
| 4:UD:835:ILE:HG12 | 4:UD:862:LEU:HD21 | 1.94 | 0.49 |
| 7:UJ:810:PHE:HB3 | 7:UJ:855:VAL:HG11 | 1.94 | 0.49 |
| 9:UL:119:ASP:HA | 9:UL:160:PHE:HD2 | 1.77 | 0.49 |
| 9:UL:432:VAL:HG23 | 9:UL:441:LEU:HD13 | 1.93 | 0.49 |
| 9:UL:814:ARG:NH2 | 9:UL:824:ILE:O | 2.33 | 0.49 |
| 10:UM:730:ALA:O | 10:UM:733:GLN:NE2 | 2.46 | 0.49 |
| 13:UQ:296:ARG:NH2 | 13:UQ:367:GLY:HA3 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:CC:63:LEU:HD12 | 19:CC:66:ILE:HD11 | 1.95 | 0.49 |
| 20:CD:119:PHE:HA | 20:CD:122:ILE:HG12 | 1.94 | 0.49 |
| 20:CD:363:ARG:NH2 | 45:C2:86:U:OP2 | 2.37 | 0.49 |
| 21:CF:18:VAL:HG23 | 21:CF:19:GLN:HE21 | 1.77 | 0.49 |
| 26:CK:190:HIS:HB2 | 26:CK:227:VAL:HG22 | 1.93 | 0.49 |
| 28:CM:296:GLU:HA | 28:CM:312:ARG:HB2 | 1.95 | 0.49 |
| 32:CR:41:LEU:HA | 32:CR:44:ILE:HD12 | 1.93 | 0.49 |
| 32:CR:543:LEU:HD23 | 32:CR:585:VAL:HG22 | 1.94 | 0.49 |
| 32:CS:113:ASP:OD1 | 32:CS:113:ASP:N | 2.37 | 0.49 |
| 32:CS:428:LEU:HA | 32:CS:431:GLN:HG3 | 1.93 | 0.49 |
| 44:C1:456:A:H62 | 44:C1:476:G:H21 | 1.59 | 0.49 |
| 44:C1:2208:C:H2' | 44:C1:2209:U:H6 | 1.78 | 0.49 |
| 44:C1:2218:A:H2' | 44:C1:2219:C:C6 | 2.48 | 0.49 |
| 44:C1:2331:G:H2' | 44:C1:2332:A:C8 | 2.47 | 0.49 |
| 45:C2:96:C:H2' | 45:C2:97:C:H6 | 1.77 | 0.49 |
| 45:C2:268:G:H2' | 45:C2:269:G:H8 | 1.78 | 0.49 |
| 50:US:444:GLU:HB3 | 50:US:450:THR:HG22 | 1.94 | 0.49 |
| 51:Cl:53:ASP:HB3 | 51:Cl:56:LYS:HG3 | 1.95 | 0.49 |
| 52:CX:242:TRP:O | 52:CX:273:ARG:NH2 | 2.37 | 0.49 |
| 1:UA:264:HIS:HB2 | 1:UA:305:ILE:HD13 | 1.95 | 0.49 |
| 2:UB:559:LEU:O | 2:UB:563:PHE:HB2 | 2.13 | 0.49 |
| 4:UD:488:PRO:HD2 | 4:UD:558:SER:HB3 | 1.93 | 0.49 |
| 5:UF:6:ASP:OD2 | 28:CM:367:ARG:NH1 | 2.46 | 0.49 |
| 5:UF:85:SER:OG | 5:UF:89:GLN:NE2 | 2.44 | 0.49 |
| 8:UK:35:ARG:NH2 | 44:C1:1150:C:OP2 | 2.44 | 0.49 |
| 9:UL:959:ALA:N | 27:CL:574:GLY:O | 2.45 | 0.49 |
| 10:UM:692:HIS:NE2 | 10:UM:714:ASP:OD1 | 2.46 | 0.49 |
| 13:UQ:89:MET:N | 13:UQ:418:ASN:OD1 | 2.29 | 0.49 |
| 15:UU:1010:GLU:O | 15:UU:1013:LEU:N | 2.46 | 0.49 |
| 16:UX:132:ASP:HA | 16:UX:135:VAL:HG12 | 1.94 | 0.49 |
| 18:CB:130:TRP:CZ2 | 18:CB:138:ALA:HB3 | 2.48 | 0.49 |
| 18:CB:216:TYR:HA | 18:CB:219:LEU:HD13 | 1.95 | 0.49 |
| 20:CD:178:GLU:HA | 20:CD:181:VAL:HG12 | 1.94 | 0.49 |
| 20:CD:187:LYS:HD3 | 20:CD:207:TYR:CZ | 2.47 | 0.49 |
| 22:CG:388:ASP:O | 22:CG:391:SER:OG | 2.27 | 0.49 |
| 24:CI:271:SER:HA | 24:CI:777:ALA:O | 2.12 | 0.49 |
| 24:CI:604:GLU:HA | 24:CI:607:LYS:HE2 | 1.94 | 0.49 |
| 28:CM:422:GLU:O | 28:CM:426:SER:CB | 2.60 | 0.49 |
| 32:CS:525:THR:O | 32:CS:528:SER:OG | 2.30 | 0.49 |
| 32:CS:801:LEU:O | 32:CS:805:ILE:HG13 | 2.12 | 0.49 |
| 40:Cm:83:LEU:HD22 | 40:Cm:122:ALA:HB2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:1455:C:H2' | 44:C1:1456:A:C8 | 2.48 | 0.49 |
| 44:C1:1696:G:H2' | 44:C1:1697:A:C8 | 2.48 | 0.49 |
| 45:C2:147:G:H2' | 45:C2:148:G:C8 | 2.47 | 0.49 |
| 46:UV:309:GLN:HG3 | 46:UV:310:ARG:HH11 | 1.77 | 0.49 |
| 49:UE:181:ILE:O | 49:UE:184:THR:OG1 | 2.25 | 0.49 |
| 52:CX:379:TRP:HA | 52:CX:382:ILE:HD12 | 1.95 | 0.49 |
| 7:UJ:42:SER:HA | 28:CM:17:GLY:HA2 | 1.95 | 0.49 |
| 8:UK:256:PHE:CE1 | 8:UK:262:ARG:HG2 | 2.48 | 0.49 |
| 9:UL:469:LEU:HD11 | 9:UL:510:ALA:HB1 | 1.93 | 0.49 |
| 12:UO:340:SER:O | 12:UO:340:SER:OG | 2.27 | 0.49 |
| 12:UO:535:GLU:HA | 12:UO:538:GLU:HG2 | 1.95 | 0.49 |
| 13:UQ:441:VAL:HG22 | 13:UQ:850:ALA:HB2 | 1.94 | 0.49 |
| 18:CA:151:LYS:O | 18:CA:154:SER:OG | 2.24 | 0.49 |
| 18:CB:128:ARG:NH2 | 18:CB:168:SER:OG | 2.45 | 0.49 |
| 22:CG:223:ARG:N | 45:C2:183:A:OP1 | 2.43 | 0.49 |
| 23:CH:208:LEU:HD21 | 23:CH:326:CYS:HB2 | 1.94 | 0.49 |
| 35:Ce:67:PHE:HE1 | 35:Ce:99:LEU:HD12 | 1.78 | 0.49 |
| 35:Ce:68:VAL:HG13 | 35:Ce:73:LEU:HD22 | 1.94 | 0.49 |
| 45:C2:13:U:H2' | 45:C2:14:C:C6 | 2.47 | 0.49 |
| 46:UV:548:ASP:HB2 | 46:UV:588:LEU:HB2 | 1.94 | 0.49 |
| 48:UH:777:ALA:O | 48:UH:781:SER:OG | 2.28 | 0.49 |
| 48:UH:817:ALA:O | 48:UH:820:SER:OG | 2.29 | 0.49 |
| 49:UI:181:ILE:O | 49:UI:184:THR:OG1 | 2.25 | 0.49 |
| 54:Cz:1620:TYR:HB2 | 54:Cz:1660:LYS:HE3 | 1.93 | 0.49 |
| 6:UG:67:LYS:HG3 | 44:C1:581:C:H6 | 1.77 | 0.49 |
| 9:UL:931:LEU:HD22 | 10:UM:856:LEU:HD22 | 1.95 | 0.49 |
| 10:UM:673:THR:OG1 | 10:UM:693:GLU:O | 2.19 | 0.49 |
| 12:UO:50:PRO:HB3 | 12:UO:107:ILE:HG13 | 1.94 | 0.49 |
| 12:UO:394:MET:HA | 12:UO:397:LEU:HD12 | 1.94 | 0.49 |
| 15:UU:78:ARG:NH2 | 44:C1:262:G:OP1 | 2.45 | 0.49 |
| 15:UU:571:GLN:HE22 | 39:Cj:99:GLU:H | 1.58 | 0.49 |
| 17:UZ:117:PRO:HA | 17:UZ:121:ARG:HB2 | 1.94 | 0.49 |
| 25:CJ:100:ASN:O | 25:CJ:102:THR:OG1 | 2.26 | 0.49 |
| 29:CO:77:MET:HG2 | 29:CO:84:ILE:HA | 1.94 | 0.49 |
| 32:CR:313:THR:HB | 32:CR:388:ILE:HG12 | 1.94 | 0.49 |
| 37:Ch:91:LEU:HA | 37:Ch:94:LYS:HE3 | 1.94 | 0.49 |
| 37:Ch:99:ARG:HH21 | 37:Ch:119:GLU:HG2 | 1.76 | 0.49 |
| 38:Ci:65:ARG:HH21 | 44:C1:1490:A:H4' | 1.78 | 0.49 |
| 44:C1:212:C:H2' | 44:C1:213:G:C8 | 2.47 | 0.49 |
| 44:C1:1479:U:H2' | 44:C1:1480:G:C8 | 2.47 | 0.49 |
| 46:UV:776:GLU:HG3 | 46:UV:803:PHE:HE2 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:1033:PRO:HG3 | 46:UV:1040:LEU:HD22 | 1.95 | 0.49 |
| 48:UH:644:SER:HA | 48:UH:647:LEU:HD12 | 1.94 | 0.49 |
| 1:UA:717:PRO:O | 1:UA:720:THR:OG1 | 2.27 | 0.49 |
| 9:UL:479:VAL:HA | 9:UL:493:ASP:HA | 1.94 | 0.49 |
| 9:UL:786:LEU:HA | 9:UL:860:PHE:HE2 | 1.77 | 0.49 |
| 9:UL:954:ARG:HB2 | 27:CL:652:ASP:HB2 | 1.94 | 0.49 |
| 10:UM:772:ASN:O | 10:UM:775:THR:OG1 | 2.27 | 0.49 |
| 10:UM:823:ALA:O | 10:UM:827:GLN:N | 2.46 | 0.49 |
| 13:UQ:89:MET:HE3 | 13:UQ:105:ILE:HG21 | 1.94 | 0.49 |
| 13:UQ:186:LYS:HD3 | 13:UQ:210:ARG:HD3 | 1.94 | 0.49 |
| 13:UQ:810:GLU:HA | 13:UQ:826:THR:HA | 1.94 | 0.49 |
| 14:UR:269:ILE:HB | 14:UR:611:VAL:HB | 1.95 | 0.49 |
| 23:CH:163:LEU:HB3 | 23:CH:206:LEU:HD11 | 1.95 | 0.49 |
| 24:CI:57:PRO:HB3 | 24:CI:743:LYS:HD3 | 1.95 | 0.49 |
| 24:CI:217:ARG:O | 24:CI:221:ASN:ND2 | 2.45 | 0.49 |
| 24:CI:1138:LYS:HZ3 | 24:CI:1142:TRP:CD1 | 2.31 | 0.49 |
| 29:CO:218:ASP:N | 29:CO:218:ASP:OD1 | 2.46 | 0.49 |
| 32:CR:164:THR:HA | 32:CR:167:MET:HE2 | 1.95 | 0.49 |
| 32:CS:849:LEU:HD23 | 32:CS:849:LEU:H | 1.78 | 0.49 |
| 42:Cp:11:VAL:HG23 | 42:Cp:33:PHE:HA | 1.95 | 0.49 |
| 44:C1:62:U:C2 | 48:UH:894:ARG:HG3 | 2.48 | 0.49 |
| 45:C2:153:G:C6 | 45:C2:176:U:O2 | 2.65 | 0.49 |
| 47:CV:42:ILE:HG21 | 47:CV:48:SER:HA | 1.94 | 0.49 |
| 49:UE:156:VAL:HG21 | 50:US:301:GLU:HB3 | 1.94 | 0.49 |
| 50:US:202:GLU:HA | 50:US:205:LYS:HG2 | 1.94 | 0.49 |
| 50:US:301:GLU:N | 50:US:301:GLU:OE1 | 2.46 | 0.49 |
| 4:UD:4:HIS:CD2 | 48:UH:909:ILE:HD12 | 2.48 | 0.49 |
| 8:UK:117:ASN:HD21 | 21:CE:47:ARG:HG2 | 1.77 | 0.49 |
| 12:UO:206:VAL:HG22 | 12:UO:216:VAL:HB | 1.93 | 0.49 |
| 12:UO:447:SER:O | 12:UO:447:SER:OG | 2.28 | 0.49 |
| 15:UU:550:SER:OG | 15:UU:552:CYS:N | 2.46 | 0.49 |
| 18:CB:228:ALA:HB3 | 18:CB:255:ILE:HG13 | 1.95 | 0.49 |
| 22:CG:430:HIS:HD2 | 22:CG:499:LEU:HB2 | 1.78 | 0.49 |
| 23:CH:132:PHE:HB2 | 23:CH:192:VAL:HG12 | 1.95 | 0.49 |
| 24:CI:854:ARG:NE | 41:Cn:61:ALA:O | 2.45 | 0.49 |
| 25:CJ:92:ALA:HB1 | 26:CK:62:ARG:NE | 2.27 | 0.49 |
| 26:CK:173:ARG:NH2 | 26:CK:182:GLY:H | 2.10 | 0.49 |
| 28:CM:297:GLU:HA | 28:CM:310:TRP:O | 2.12 | 0.49 |
| 32:CS:313:THR:HB | 32:CS:388:ILE:HG12 | 1.94 | 0.49 |
| 34:Cc:68:ARG:HB3 | 34:Cc:69:PHE:HD2 | 1.77 | 0.49 |
| 45:C2:137:U:O4 | 45:C2:150:G:O6 | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:US:488:ASN:N | 50:US:488:ASN:OD1 | 2.46 | 0.49 |
| 51:Cl:12:ASN:HA | 51:Cl:25:LYS:HD3 | 1.95 | 0.49 |
| 52:CX:370:LEU:HD12 | 52:CX:373:LYS:HB2 | 1.95 | 0.49 |
| 1:UA:508:GLN:NE2 | 1:UA:509:LEU:O | 2.30 | 0.49 |
| 2:UB:116:ILE:HG13 | 23:CH:58:GLU:HG3 | 1.95 | 0.49 |
| 6:UG:78:LYS:NZ | 11:UN:917:ASP:O | 2.29 | 0.49 |
| 7:UJ:237:ARG:HG3 | 14:UR:254:ARG:HH12 | 1.78 | 0.49 |
| 9:UL:695:HIS:CE1 | 9:UL:721:ARG:HH11 | 2.31 | 0.49 |
| 11:UN:893:SER:HB3 | 11:UN:896:GLN:HB2 | 1.94 | 0.49 |
| 12:UO:482:LEU:HD11 | 12:UO:526:LEU:HD22 | 1.95 | 0.49 |
| 13:UQ:326:TYR:HB3 | 13:UQ:329:LEU:HD21 | 1.94 | 0.49 |
| 13:UQ:765:TYR:OH | 13:UQ:819:GLU:O | 2.26 | 0.49 |
| 14:UR:345:ARG:NH1 | 44:C1:75:G:OP1 | 2.45 | 0.49 |
| 15:UU:287:GLY:N | 15:UU:294:LYS:O | 2.45 | 0.49 |
| 15:UU:1031:SER:HA | 15:UU:1034:VAL:HG12 | 1.95 | 0.49 |
| 18:CA:155:LYS:HB3 | 18:CA:223:VAL:HG12 | 1.94 | 0.49 |
| 18:CA:225:VAL:HA | 18:CA:252:GLY:O | 2.13 | 0.49 |
| 19:CC:212:ILE:HD13 | 19:CC:254:ILE:HD13 | 1.95 | 0.49 |
| 24:CI:278:ASN:ND2 | 24:CI:769:GLU:O | 2.40 | 0.49 |
| 24:CI:886:CYS:HB3 | 24:CI:901:ALA:HB3 | 1.94 | 0.49 |
| 24:CI:931:THR:HG22 | 24:CI:976:THR:HG23 | 1.94 | 0.49 |
| 28:CM:65:HIS:HE2 | 28:CM:84:SER:C | 2.20 | 0.49 |
| 29:CN:35:LYS:NZ | 29:CN:197:GLY:O | 2.44 | 0.49 |
| 29:CO:84:ILE:O | 29:CO:86:ASP:N | 2.40 | 0.49 |
| 32:CR:849:LEU:HD23 | 32:CR:849:LEU:H | 1.78 | 0.49 |
| 32:CS:164:THR:HA | 32:CS:167:MET:HE2 | 1.95 | 0.49 |
| 32:CS:865:TYR:HA | 32:CS:870:LEU:HB2 | 1.94 | 0.49 |
| 44:C1:1626:G:H2' | 44:C1:1627:G:H8 | 1.78 | 0.49 |
| 44:C1:2174:C:H2' | 44:C1:2175:A:H8 | 1.78 | 0.49 |
| 44:C1:2333:A:H2' | 44:C1:2334:G:H8 | 1.75 | 0.49 |
| 45:C2:105:C:H2' | 45:C2:200:U:C6 | 2.48 | 0.49 |
| 1:UA:720:THR:HG22 | 1:UA:736:MET:HE2 | 1.95 | 0.48 |
| 2:UB:13:LEU:HD11 | 2:UB:18:LEU:HB2 | 1.94 | 0.48 |
| 4:UD:758:ARG:HA | 4:UD:769:GLU:O | 2.13 | 0.48 |
| 7:UJ:828:THR:HA | 7:UJ:831:THR:HG22 | 1.95 | 0.48 |
| 9:UL:243:VAL:O | 9:UL:269:ASN:ND2 | 2.45 | 0.48 |
| 10:UM:114:VAL:HG11 | 10:UM:128:THR:HB | 1.95 | 0.48 |
| 10:UM:321:ALA:O | 10:UM:339:ALA:N | 2.44 | 0.48 |
| 11:UN:312:ARG:HD3 | 28:CM:232:PRO:HG2 | 1.95 | 0.48 |
| 12:UO:104:CYS:SG | 12:UO:150:THR:N | 2.71 | 0.48 |
| 13:UQ:127:LEU:HD12 | 13:UQ:128:PRO:HD2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:UR:372:THR:HG23 | 14:UR:374:GLU:H | 1.78 | 0.48 |
| 15:UU:81:ASN:OD1 | 15:UU:81:ASN:N | 2.44 | 0.48 |
| 26:CK:244:TYR:HB3 | 26:CK:254:LEU:HD23 | 1.95 | 0.48 |
| 31:CQ:85:ILE:HD12 | 31:CQ:86:PRO:HD2 | 1.95 | 0.48 |
| 35:Ce:143:VAL:HG13 | 35:Ce:165:ASP:HB2 | 1.95 | 0.48 |
| 44:C1:108:C:H2' | 44:C1:109:G:H8 | 1.78 | 0.48 |
| 44:C1:1169:A:HO2' | 44:C1:1170:G:H21 | 1.61 | 0.48 |
| 46:UV:729:LEU:HD11 | 46:UV:739:THR:HB | 1.94 | 0.48 |
| 48:UH:755:TYR:CE2 | 49:UI:204:MET:HA | 2.48 | 0.48 |
| 50:US:425:LYS:HA | 50:US:428:ARG:HD2 | 1.95 | 0.48 |
| 9:UL:576:ASP:O | 9:UL:578:ARG:N | 2.46 | 0.48 |
| 10:UM:591:THR:O | 10:UM:617:THR:HA | 2.12 | 0.48 |
| 15:UU:546:THR:OG1 | 15:UU:547:VAL:N | 2.45 | 0.48 |
| 15:UU:621:HIS:CD2 | 15:UU:641:SER:HB2 | 2.48 | 0.48 |
| 18:CA:132:PRO:HA | 18:CA:138:ALA:HB3 | 1.95 | 0.48 |
| 19:CC:157:LEU:HA | 19:CC:157:LEU:HD12 | 1.70 | 0.48 |
| 20:CD:169:VAL:HG21 | 20:CD:303:ALA:HB2 | 1.95 | 0.48 |
| 22:CG:427:LYS:HD2 | 22:CG:428:PRO:HD2 | 1.94 | 0.48 |
| 25:CJ:112:PRO:O | 25:CJ:115:MET:HG2 | 2.13 | 0.48 |
| 32:CR:428:LEU:HA | 32:CR:431:GLN:HG3 | 1.94 | 0.48 |
| 32:CR:428:LEU:HD22 | 32:CR:431:GLN:HE21 | 1.79 | 0.48 |
| 41:Cn:104:LEU:HD13 | 41:Cn:122:PHE:HB3 | 1.94 | 0.48 |
| 44:C1:67:G:H2' | 48:UH:894:ARG:HH12 | 1.78 | 0.48 |
| 44:C1:462:G:H2' | 44:C1:463:C:H6 | 1.78 | 0.48 |
| 44:C1:480:U:H2' | 44:C1:481:G:C8 | 2.48 | 0.48 |
| 50:US:222:ASN:HA | 50:US:225:ASN:HD22 | 1.79 | 0.48 |
| 50:US:266:GLN:O | 50:US:270:LEU:HG | 2.12 | 0.48 |
| 51:Cl:28:VAL:O | 51:Cl:32:LEU:HG | 2.14 | 0.48 |
| 1:UA:204:SER:OG | 1:UA:206:ASP:O | 2.27 | 0.48 |
| 2:UB:681:PRO:HB2 | 2:UB:683:HIS:CE1 | 2.48 | 0.48 |
| 3:UC:582:GLN:O | 3:UC:585:LYS:C | 2.56 | 0.48 |
| 4:UD:841:ILE:HG23 | 4:UD:859:GLU:HB2 | 1.95 | 0.48 |
| 7:UJ:236:ARG:NH1 | 44:C1:244:G:OP1 | 2.28 | 0.48 |
| 7:UJ:354:LEU:O | 7:UJ:358:LEU:HG | 2.12 | 0.48 |
| 9:UL:204:SER:O | 9:UL:206:ARG:NH1 | 2.45 | 0.48 |
| 10:UM:816:TRP:O | 10:UM:822:THR:OG1 | 2.32 | 0.48 |
| 12:UO:115:VAL:HG23 | 12:UO:125:VAL:HB | 1.94 | 0.48 |
| 13:UQ:401:ASN:HB3 | 13:UQ:414:HIS:HB3 | 1.95 | 0.48 |
| 13:UQ:535:GLU:HG3 | 13:UQ:536:PRO:HD2 | 1.95 | 0.48 |
| 14:UR:596:SER:OG | 14:UR:597:SER:N | 2.47 | 0.48 |
| 15:UU:224:PRO:CB | 15:UU:248:TYR:OH | 2.58 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:UU:766:ALA:HB2 | 15:UU:773:VAL:HG12 | 1.95 | 0.48 |
| 19:CC:180:GLY:O | 19:CC:183:THR:OG1 | 2.26 | 0.48 |
| 20:CD:105:ILE:HG23 | 20:CD:107:ILE:H | 1.78 | 0.48 |
| 20:CD:117:ASP:O | 20:CD:121:ALA:CB | 2.61 | 0.48 |
| 20:CD:194:PHE:CD2 | 20:CD:197:LEU:HB2 | 2.49 | 0.48 |
| 22:CG:235:ARG:HH12 | 45:C2:119:C:H3' | 1.77 | 0.48 |
| 22:CG:335:ASP:HB3 | 22:CG:401:VAL:HG12 | 1.95 | 0.48 |
| 23:CH:128:LEU:HD13 | 23:CH:128:LEU:HA | 1.68 | 0.48 |
| 26:CK:77:TYR:HE1 | 26:CK:156:HIS:CE1 | 2.31 | 0.48 |
| 28:CM:264:ILE:HG13 | 28:CM:310:TRP:CZ3 | 2.48 | 0.48 |
| 29:CN:40:VAL:HA | 29:CN:113:TYR:O | 2.14 | 0.48 |
| 33:CT:117:MET:HE2 | 33:CT:117:MET:HB3 | 1.77 | 0.48 |
| 44:C1:365:G:H2' | 44:C1:366:G:C8 | 2.48 | 0.48 |
| 44:C1:1075:C:O2' | 44:C1:1076:U:H5' | 2.14 | 0.48 |
| 44:C1:2238:A:C5 | 44:C1:2328:G:N2 | 2.74 | 0.48 |
| 54:Cz:1680:PHE:HB3 | 54:Cz:1697:LEU:HD22 | 1.95 | 0.48 |
| 4:UD:127:GLY:N | 4:UD:166:TYR:OH | 2.45 | 0.48 |
| 7:UJ:39:VAL:HG12 | 7:UJ:43:GLN:HE21 | 1.78 | 0.48 |
| 9:UL:50:TRP:HA | 9:UL:57:LEU:HA | 1.95 | 0.48 |
| 9:UL:940:VAL:HG21 | 31:CQ:241:PRO:HB2 | 1.95 | 0.48 |
| 12:UO:254:ALA:HB1 | 12:UO:268:LEU:HD21 | 1.95 | 0.48 |
| 12:UO:289:VAL:HG22 | 12:UO:299:VAL:HB | 1.95 | 0.48 |
| 12:UO:476:LEU:HA | 12:UO:479:ILE:HD12 | 1.94 | 0.48 |
| 13:UQ:422:VAL:HB | 13:UQ:432:MET:HB3 | 1.95 | 0.48 |
| 17:UZ:77:ARG:NH2 | 44:C1:373:C:O3' | 2.46 | 0.48 |
| 17:UZ:173:LYS:HD2 | 17:UZ:174:THR:HA | 1.94 | 0.48 |
| 17:UZ:275:TRP:HE3 | 17:UZ:278:VAL:HG11 | 1.78 | 0.48 |
| 18:CA:181:TYR:HD2 | 18:CA:220:VAL:HG13 | 1.78 | 0.48 |
| 22:CG:436:HIS:HA | 22:CG:488:ARG:HH22 | 1.78 | 0.48 |
| 23:CH:212:PRO:HB3 | 23:CH:290:VAL:HG21 | 1.94 | 0.48 |
| 31:CQ:151:ASP:O | 31:CQ:155:ALA:CB | 2.62 | 0.48 |
| 32:CR:58:TRP:HE1 | 32:CR:126:GLN:NE2 | 2.11 | 0.48 |
| 43:CU:113:LYS:NZ | 44:C1:1709:A:O3' | 2.46 | 0.48 |
| 44:C1:1648:G:H2' | 44:C1:1649:A:H8 | 1.77 | 0.48 |
| 44:C1:2044:C:H2' | 44:C1:2045:G:C8 | 2.48 | 0.48 |
| 48:UH:486:LEU:HD22 | 48:UH:552:LYS:HE3 | 1.94 | 0.48 |
| 50:US:151:GLN:HG3 | 50:US:152:HIS:CD2 | 2.48 | 0.48 |
| 54:Cz:1604:PHE:HB3 | 54:Cz:1622:TYR:CD1 | 2.48 | 0.48 |
| 1:UA:306:ASN:OD1 | 1:UA:307:LYS:N | 2.46 | 0.48 |
| 6:UG:145:SER:OG | 6:UG:146:ARG:N | 2.45 | 0.48 |
| 7:UJ:595:TYR:HE2 | 7:UJ:719:LEU:HD12 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:UK:28:LEU:HD21 | 24:CI:986:ILE:HD11 | 1.95 | 0.48 |
| 10:UM:568:VAL:HG11 | 10:UM:582:LEU:HD22 | 1.96 | 0.48 |
| 11:UN:361:THR:N | 11:UN:364:THR:OG1 | 2.43 | 0.48 |
| 12:UO:283:SER:OG | 12:UO:284:GLN:N | 2.46 | 0.48 |
| 20:CD:186:VAL:HA | 20:CD:189:TRP:HB3 | 1.96 | 0.48 |
| 23:CH:34:SER:HA | 23:CH:74:THR:HG22 | 1.94 | 0.48 |
| 24:CI:955:VAL:HG21 | 24:CI:986:ILE:HD12 | 1.95 | 0.48 |
| 26:CK:108:ARG:HG2 | 26:CK:114:ALA:HB3 | 1.96 | 0.48 |
| 26:CK:183:THR:HG22 | 44:C1:1743:C:C2 | 2.49 | 0.48 |
| 28:CM:304:ASP:N | 28:CM:304:ASP:OD1 | 2.44 | 0.48 |
| 32:CR:10:ARG:NH1 | 32:CR:215:LYS:O | 2.43 | 0.48 |
| 32:CR:618:VAL:HG23 | 32:CR:622:PHE:HD2 | 1.78 | 0.48 |
| 32:CS:497:ASP:OD1 | 32:CS:497:ASP:N | 2.47 | 0.48 |
| 36:Cg:122:HIS:ND1 | 44:C1:1062:C:O2' | 2.47 | 0.48 |
| 39:Cj:94:ALA:HB2 | 39:Cj:102:LYS:HD3 | 1.96 | 0.48 |
| 43:CU:229:MET:HG2 | 44:C1:298:A:C2 | 2.49 | 0.48 |
| 44:C1:61:G:H22 | 48:UH:901:SER:HB3 | 1.79 | 0.48 |
| 44:C1:176:G:H2' | 44:C1:177:G:C8 | 2.48 | 0.48 |
| 44:C1:391:C:H2' | 44:C1:392:C:C6 | 2.48 | 0.48 |
| 44:C1:1457:G:O6 | 44:C1:1540:A:N1 | 2.46 | 0.48 |
| 44:C1:2219:C:H2' | 44:C1:2220:C:C6 | 2.47 | 0.48 |
| 45:C2:113:G:H1' | 45:C2:195:A:N6 | 2.26 | 0.48 |
| 45:C2:267:C:H2' | 45:C2:268:G:H8 | 1.79 | 0.48 |
| 46:UV:245:GLY:H | 46:UV:260:GLN:HE22 | 1.62 | 0.48 |
| 46:UV:417:HIS:CE1 | 46:UV:439:LEU:HD21 | 2.49 | 0.48 |
| 52:CX:333:ILE:HG13 | 52:CX:375:TYR:HE2 | 1.79 | 0.48 |
| 2:UB:655:PRO:O | 2:UB:659:ASN:ND2 | 2.46 | 0.48 |
| 6:UG:425:GLU:OE2 | 6:UG:426:ALA:N | 2.47 | 0.48 |
| 7:UJ:248:LEU:HD11 | 14:UR:233:PHE:HE2 | 1.78 | 0.48 |
| 7:UJ:591:ALA:HB1 | 7:UJ:637:LEU:HD11 | 1.95 | 0.48 |
| 9:UL:716:HIS:O | 9:UL:718:LYS:NZ | 2.39 | 0.48 |
| 12:UO:147:VAL:HA | 12:UO:164:SER:HA | 1.95 | 0.48 |
| 13:UQ:640:PRO:HB3 | 13:UQ:661:TRP:CE2 | 2.49 | 0.48 |
| 14:UR:255:LYS:HE3 | 14:UR:553:GLN:HE21 | 1.78 | 0.48 |
| 14:UR:569:VAL:HG22 | 14:UR:576:VAL:HG22 | 1.95 | 0.48 |
| 15:UU:406:LYS:NZ | 44:C1:258:C:OP2 | 2.39 | 0.48 |
| 17:UZ:68:THR:OG1 | 17:UZ:69:LYS:N | 2.46 | 0.48 |
| 21:CF:90:ARG:HH12 | 22:CG:586:MET:HE3 | 1.78 | 0.48 |
| 23:CH:56:LEU:HD13 | 23:CH:100:HIS:CG | 2.48 | 0.48 |
| 24:CI:71:VAL:HA | 24:CI:135:ILE:O | 2.14 | 0.48 |
| 24:CI:761:ASP:OD2 | 24:CI:761:ASP:N | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:CI:1069:PRO:HB3 | 44:C1:364:C:H5" | 1.96 | 0.48 |
| 30:CP:176:LYS:HE2 | 44:C1:1489:G:H4' | 1.96 | 0.48 |
| 31:CQ:114:ARG:HD3 | 31:CQ:114:ARG:HA | 1.63 | 0.48 |
| 32:CS:428:LEU:HD22 | 32:CS:431:GLN:HE21 | 1.79 | 0.48 |
| 44:C1:60:A:H61 | 48:UH:859:MET:HE2 | 1.78 | 0.48 |
| 44:C1:2110:C:H2' | 44:C1:2111:U:H6 | 1.79 | 0.48 |
| 44:C1:2185:C:H2' | 44:C1:2186:U:H6 | 1.79 | 0.48 |
| 46:UV:740:HIS:ND1 | 47:CV:202:SER:O | 2.46 | 0.48 |
| 48:UH:599:VAL:HA | 48:UH:602:VAL:HG23 | 1.95 | 0.48 |
| 50:US:195:ASP:OD2 | 50:US:244:PHE:N | 2.46 | 0.48 |
| 1:UA:413:ARG:HH12 | 27:CL:678:ALA:HB2 | 1.78 | 0.48 |
| 2:UB:686:PRO:HD2 | 2:UB:689:ILE:HD12 | 1.95 | 0.48 |
| 4:UD:122:LYS:HG2 | 4:UD:123:LYS:HG3 | 1.96 | 0.48 |
| 4:UD:261:TRP:HA | 4:UD:267:THR:O | 2.13 | 0.48 |
| 5:UF:328:PHE:O | 5:UF:334:THR:OG1 | 2.31 | 0.48 |
| 6:UG:95:ASN:ND2 | 6:UG:426:ALA:O | 2.46 | 0.48 |
| 7:UJ:121:LEU:HB3 | 7:UJ:127:ILE:HG13 | 1.96 | 0.48 |
| 12:UO:491:ASP:HA | 49:UE:208:PRO:HG2 | 1.94 | 0.48 |
| 14:UR:466:MET:HE3 | 14:UR:466:MET:HB2 | 1.74 | 0.48 |
| 15:UU:889:SER:HB2 | 31:CQ:258:ARG:HG3 | 1.94 | 0.48 |
| 17:UZ:180:ILE:HD12 | 17:UZ:181:PRO:HD2 | 1.96 | 0.48 |
| 22:CG:149:TYR:OH | 22:CG:476:ASP:OD1 | 2.28 | 0.48 |
| 22:CG:430:HIS:CD2 | 22:CG:499:LEU:H | 2.32 | 0.48 |
| 24:CI:363:LYS:NZ | 24:CI:377:VAL:O | 2.47 | 0.48 |
| 35:Ce:75:GLY:HA2 | 35:Ce:78:ARG:HE | 1.79 | 0.48 |
| 44:C1:69:U:H3 | 48:UH:884:SER:HG | 1.54 | 0.48 |
| 45:C2:79:G:H2' | 45:C2:80:G:H8 | 1.79 | 0.48 |
| 50:US:462:GLN:O | 50:US:465:SER:OG | 2.26 | 0.48 |
| 52:CX:366:LEU:HA | 52:CX:369:VAL:HG12 | 1.94 | 0.48 |
| 54:Cz:1674:GLU:OE1 | 54:Cz:1677:ARG:NH1 | 2.45 | 0.48 |
| 1:UA:50:PHE:HZ | 1:UA:84:VAL:HG23 | 1.78 | 0.48 |
| 1:UA:626:ASN:N | 1:UA:626:ASN:OD1 | 2.46 | 0.48 |
| 4:UD:667:SER:O | 4:UD:670:SER:OG | 2.22 | 0.48 |
| 7:UJ:436:ASP:O | 7:UJ:440:THR:OG1 | 2.25 | 0.48 |
| 9:UL:515:GLN:HG3 | 9:UL:573:PHE:HD1 | 1.79 | 0.48 |
| 10:UM:87:ILE:HD12 | 10:UM:105:ARG:HB2 | 1.94 | 0.48 |
| 12:UO:321:SER:OG | 12:UO:322:VAL:O | 2.32 | 0.48 |
| 13:UQ:222:ASN:H | 13:UQ:225:MET:HB2 | 1.79 | 0.48 |
| 13:UQ:802:LYS:NZ | 13:UQ:803:LEU:O | 2.46 | 0.48 |
| 14:UR:380:PRO:HD3 | 14:UR:425:TRP:HB3 | 1.94 | 0.48 |
| 16:UX:96:MET:HE2 | 16:UX:96:MET:HB2 | 1.68 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:UZ:220:ILE:O | 17:UZ:224:ILE:HG12 | 2.14 | 0.48 |
| 17:UZ:280:ASN:OD1 | 17:UZ:280:ASN:N | 2.37 | 0.48 |
| 18:CA:165:THR:OG1 | 18:CA:166:SER:N | 2.46 | 0.48 |
| 22:CG:229:PHE:O | 45:C2:124:U:N3 | 2.46 | 0.48 |
| 32:CR:801:LEU:O | 32:CR:805:ILE:HG13 | 2.12 | 0.48 |
| 36:Cg:90:LYS:HB3 | 36:Cg:93:TYR:HD2 | 1.78 | 0.48 |
| 44:C1:225:C:H2' | 44:C1:226:C:C6 | 2.49 | 0.48 |
| 46:UV:154:LYS:HG3 | 46:UV:160:ARG:HH22 | 1.79 | 0.48 |
| 46:UV:288:GLN:HA | 46:UV:291:LYS:HE2 | 1.95 | 0.48 |
| 46:UV:600:GLU:O | 46:UV:604:ARG:HG2 | 2.14 | 0.48 |
| 48:UH:881:ARG:NH2 | 48:UH:895:GLN:OE1 | 2.46 | 0.48 |
| 5:UF:337:VAL:O | 5:UF:341:GLN:HB2 | 2.13 | 0.48 |
| 10:UM:696:LEU:HA | 10:UM:712:GLY:HA3 | 1.94 | 0.48 |
| 12:UO:485:ALA:O | 12:UO:489:VAL:HG13 | 2.13 | 0.48 |
| 13:UQ:364:SER:CB | 13:UQ:369:TYR:O | 2.61 | 0.48 |
| 13:UQ:518:ARG:HH11 | 13:UQ:536:PRO:HD3 | 1.79 | 0.48 |
| 13:UQ:727:SER:OG | 13:UQ:728:GLY:N | 2.45 | 0.48 |
| 15:UU:665:MET:HG2 | 15:UU:666:THR:HG23 | 1.96 | 0.48 |
| 16:UX:176:GLU:O | 36:Cg:21:ARG:NH2 | 2.47 | 0.48 |
| 17:UZ:263:ILE:HD13 | 17:UZ:266:LEU:HD21 | 1.95 | 0.48 |
| 23:CH:124:SER:OG | 23:CH:199:GLN:NE2 | 2.47 | 0.48 |
| 23:CH:124:SER:H | 23:CH:199:GLN:HE21 | 1.62 | 0.48 |
| 24:CI:362:ASP:OD1 | 24:CI:362:ASP:N | 2.46 | 0.48 |
| 24:CI:849:SER:OG | 24:CI:850:ILE:N | 2.46 | 0.48 |
| 24:CI:1046:ASN:ND2 | 44:C1:2072:U:OP2 | 2.42 | 0.48 |
| 32:CR:283:LEU:HD12 | 32:CR:472:ILE:HG13 | 1.96 | 0.48 |
| 32:CR:470:LYS:HZ2 | 32:CR:472:ILE:HD13 | 1.79 | 0.48 |
| 32:CS:58:TRP:HE1 | 32:CS:126:GLN:NE2 | 2.11 | 0.48 |
| 34:Cc:134:THR:O | 34:Cc:134:THR:OG1 | 2.32 | 0.48 |
| 35:Ce:42:ALA:HB3 | 35:Ce:79:VAL:HG11 | 1.96 | 0.48 |
| 44:C1:2231:A:H2' | 44:C1:2232:C:C6 | 2.49 | 0.48 |
| 45:C2:53:U:H2' | 45:C2:54:C:C6 | 2.49 | 0.48 |
| 46:UV:274:VAL:HG13 | 46:UV:400:LEU:HD13 | 1.95 | 0.48 |
| 49:UE:266:LEU:HA | 49:UE:269:GLN:NE2 | 2.29 | 0.48 |
| 52:CX:303:PHE:O | 52:CX:308:PHE:N | 2.39 | 0.48 |
| 1:UA:263:TYR:CZ | 1:UA:265:ALA:HA | 2.48 | 0.48 |
| 7:UJ:853:VAL:HA | 7:UJ:856:LEU:HG | 1.95 | 0.48 |
| 12:UO:488:TYR:HB3 | 12:UO:494:TYR:HE2 | 1.78 | 0.48 |
| 12:UO:527:LEU:HB2 | 49:UE:263:LEU:HD23 | 1.95 | 0.48 |
| 15:UU:680:ILE:HD11 | 15:UU:694:ILE:HD12 | 1.96 | 0.48 |
| 22:CG:173:VAL:HA | 22:CG:187:THR:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:CG:343:ARG:NH2 | 22:CG:356:TYR:OH | 2.44 | 0.48 |
| 27:CL:572:ARG:HH21 | 44:C1:2214:A:H4' | 1.79 | 0.48 |
| 32:CR:621:GLN:HB3 | 32:CR:785:ARG:HH12 | 1.79 | 0.48 |
| 32:CR:804:THR:HA | 32:CR:807:GLU:HG3 | 1.96 | 0.48 |
| 32:CS:618:VAL:HG23 | 32:CS:622:PHE:HD2 | 1.79 | 0.48 |
| 34:Cc:71:LYS:NZ | 44:C1:2197:A:OP2 | 2.44 | 0.48 |
| 34:Cc:162:LEU:HD22 | 34:Cc:185:LEU:HD12 | 1.96 | 0.48 |
| 36:Cg:45:LEU:O | 36:Cg:49:LYS:HG2 | 2.13 | 0.48 |
| 39:Cj:3:SER:OG | 39:Cj:4:VAL:N | 2.44 | 0.48 |
| 44:C1:374:G:H2' | 44:C1:375:G:C8 | 2.48 | 0.48 |
| 44:C1:600:U:H2' | 44:C1:601:C:C6 | 2.49 | 0.48 |
| 44:C1:2334:G:H2' | 44:C1:2335:U:C6 | 2.49 | 0.48 |
| 45:C2:257:G:H2' | 45:C2:258:A:H8 | 1.79 | 0.48 |
| 46:UV:185:THR:OG1 | 46:UV:186:LEU:N | 2.47 | 0.48 |
| 47:CV:77:ARG:HB2 | 47:CV:153:ALA:HB2 | 1.96 | 0.48 |
| 48:UH:571:LEU:O | 48:UH:574:SER:OG | 2.31 | 0.48 |
| 5:UF:91:ARG:O | 5:UF:95:ILE:HG12 | 2.14 | 0.47 |
| 5:UF:330:ASN:ND2 | 5:UF:371:THR:O | 2.36 | 0.47 |
| 6:UG:45:TYR:HD1 | 6:UG:84:LEU:HD21 | 1.79 | 0.47 |
| 6:UG:293:LEU:HD23 | 6:UG:461:LEU:HG | 1.95 | 0.47 |
| 6:UG:478:GLN:HG2 | 6:UG:481:ARG:HH22 | 1.79 | 0.47 |
| 7:UJ:234:SER:OG | 7:UJ:235:GLY:N | 2.46 | 0.47 |
| 9:UL:211:THR:HG23 | 10:UM:743:GLN:HG3 | 1.96 | 0.47 |
| 10:UM:819:ASN:OD1 | 10:UM:820:ALA:N | 2.47 | 0.47 |
| 12:UO:317:ILE:HG22 | 12:UO:338:MET:HG2 | 1.95 | 0.47 |
| 14:UR:481:ARG:O | 14:UR:497:ARG:HG3 | 2.14 | 0.47 |
| 15:UU:233:THR:N | 15:UU:247:ALA:O | 2.21 | 0.47 |
| 15:UU:436:ILE:HD11 | 15:UU:460:LEU:HB3 | 1.95 | 0.47 |
| 19:CC:8:LEU:HB2 | 19:CC:100:VAL:HG12 | 1.95 | 0.47 |
| 20:CD:368:LYS:NZ | 45:C2:84:G:OP1 | 2.28 | 0.47 |
| 23:CH:219:ARG:HD2 | 43:CU:111:MET:HE3 | 1.95 | 0.47 |
| 23:CH:307:GLU:O | 23:CH:311:GLU:HG2 | 2.14 | 0.47 |
| 24:CI:132:VAL:C | 24:CI:238:ARG:HH22 | 2.21 | 0.47 |
| 24:CI:301:GLU:HG2 | 24:CI:766:ARG:HH22 | 1.79 | 0.47 |
| 25:CJ:13:LEU:HB3 | 25:CJ:16:HIS:HB3 | 1.95 | 0.47 |
| 30:CP:79:THR:HB | 30:CP:81:LYS:HE2 | 1.95 | 0.47 |
| 32:CR:42:TYR:OH | 32:CR:102:ASN:ND2 | 2.47 | 0.47 |
| 32:CR:647:MET:SD | 32:CR:649:TYR:OH | 2.66 | 0.47 |
| 44:C1:99:A:H2' | 44:C1:100:C:C6 | 2.49 | 0.47 |
| 44:C1:273:G:H2' | 44:C1:274:A:C8 | 2.49 | 0.47 |
| 45:C2:97:C:H2' | 45:C2:98:U:H6 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:156:TYR:HE2 | 46:UV:239:LYS:HD2 | 1.79 | 0.47 |
| 46:UV:676:ARG:HH12 | 46:UV:810:LEU:HB3 | 1.78 | 0.47 |
| 46:UV:695:MET:O | 46:UV:767:ARG:N | 2.46 | 0.47 |
| 1:UA:323:LEU:HD22 | 1:UA:332:TYR:HE1 | 1.79 | 0.47 |
| 1:UA:682:PRO:HB3 | 1:UA:817:ARG:HH11 | 1.79 | 0.47 |
| 5:UF:339:ILE:HG12 | 5:UF:364:LEU:HA | 1.96 | 0.47 |
| 9:UL:191:THR:HG23 | 9:UL:199:LYS:HB3 | 1.96 | 0.47 |
| 9:UL:369:VAL:HA | 9:UL:389:GLY:HA2 | 1.96 | 0.47 |
| 12:UO:45:SER:OG | 12:UO:46:HIS:N | 2.47 | 0.47 |
| 13:UQ:186:LYS:HD2 | 44:C1:46:C:H4' | 1.96 | 0.47 |
| 13:UQ:243:SER:O | 13:UQ:255:ALA:HA | 2.15 | 0.47 |
| 13:UQ:525:ASN:O | 13:UQ:533:ILE:HG22 | 2.14 | 0.47 |
| 15:UU:382:SER:OG | 15:UU:383:GLY:N | 2.47 | 0.47 |
| 16:UX:60:VAL:HB | 16:UX:91:ILE:HG22 | 1.96 | 0.47 |
| 17:UZ:68:THR:OG1 | 17:UZ:277:ASN:O | 2.26 | 0.47 |
| 22:CG:420:LEU:O | 22:CG:429:LEU:N | 2.48 | 0.47 |
| 23:CH:32:HIS:HD1 | 23:CH:76:THR:HG1 | 1.56 | 0.47 |
| 28:CM:310:TRP:CD1 | 28:CM:317:SER:HA | 2.49 | 0.47 |
| 34:Cc:84:LEU:HD23 | 34:Cc:163:THR:HG23 | 1.94 | 0.47 |
| 35:Ce:151:ARG:HA | 40:Cm:51:GLU:HG3 | 1.95 | 0.47 |
| 36:Cg:38:ARG:NH1 | 44:C1:1179:G:OP1 | 2.47 | 0.47 |
| 44:C1:196:G:H2' | 44:C1:197:G:C8 | 2.49 | 0.47 |
| 46:UV:446:HIS:CG | 46:UV:448:TYR:HH | 2.29 | 0.47 |
| 1:UA:371:SER:O | 1:UA:373:PHE:N | 2.47 | 0.47 |
| 2:UB:622:LEU:HD11 | 2:UB:657:MET:HA | 1.96 | 0.47 |
| 4:UD:388:GLU:HB3 | 4:UD:430:HIS:NE2 | 2.28 | 0.47 |
| 4:UD:555:SER:OG | 4:UD:557:ASP:OD1 | 2.25 | 0.47 |
| 4:UD:840:PRO:HA | 4:UD:860:VAL:HG23 | 1.96 | 0.47 |
| 5:UF:142:SER:O | 5:UF:145:THR:OG1 | 2.31 | 0.47 |
| 10:UM:27:ALA:HB1 | 10:UM:69:ILE:HG13 | 1.96 | 0.47 |
| 10:UM:442:ASP:OD1 | 10:UM:442:ASP:N | 2.44 | 0.47 |
| 14:UR:256:LEU:HD23 | 14:UR:256:LEU:H | 1.79 | 0.47 |
| 14:UR:299:TYR:HE1 | 14:UR:317:SER:HB2 | 1.79 | 0.47 |
| 14:UR:568:LEU:HD12 | 14:UR:568:LEU:HA | 1.64 | 0.47 |
| 17:UZ:169:LYS:O | 17:UZ:173:LYS:HB3 | 2.15 | 0.47 |
| 20:CD:48:PHE:CG | 20:CD:133:MET:HB3 | 2.49 | 0.47 |
| 20:CD:189:TRP:NE1 | 20:CD:257:ILE:HG12 | 2.29 | 0.47 |
| 24:CI:143:ASN:OD1 | 24:CI:143:ASN:N | 2.45 | 0.47 |
| 24:CI:395:LEU:O | 24:CI:397:ALA:N | 2.47 | 0.47 |
| 24:CI:822:TRP:HB2 | 24:CI:897:PHE:CZ | 2.48 | 0.47 |
| 24:CI:833:LEU:HD12 | 24:CI:833:LEU:HA | 1.73 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:CK:146:ARG:NE | 44:C1:2048:C:O2 | 2.47 | 0.47 |
| 26:CK:229:THR:HG21 | 27:CL:545:ILE:HD11 | 1.95 | 0.47 |
| 28:CM:166:ASN:HB3 | 28:CM:182:LEU:HB2 | 1.96 | 0.47 |
| 30:CP:184:VAL:HG13 | 30:CP:197:LEU:HD22 | 1.95 | 0.47 |
| 32:CS:80:LYS:HA | 32:CS:83:LYS:HG2 | 1.97 | 0.47 |
| 34:Cc:92:GLY:O | 34:Cc:94:LYS:N | 2.46 | 0.47 |
| 38:Ci:136:SER:O | 38:Ci:136:SER:OG | 2.32 | 0.47 |
| 44:C1:384:C:H3' | 44:C1:385:A:C8 | 2.49 | 0.47 |
| 44:C1:1172:U:H2' | 44:C1:1173:C:C6 | 2.49 | 0.47 |
| 45:C2:101:G:N1 | 45:C2:251:U:N3 | 2.60 | 0.47 |
| 45:C2:135:U:H4' | 45:C2:136:C:H4' | 1.96 | 0.47 |
| 45:C2:256:G:H2' | 45:C2:257:G:C8 | 2.48 | 0.47 |
| 46:UV:393:LEU:O | 46:UV:401:ASN:HA | 2.15 | 0.47 |
| 47:CV:35:VAL:HG21 | 47:CV:165:ILE:HD13 | 1.96 | 0.47 |
| 54:Cz:1544:GLU:HA | 54:Cz:1547:LYS:HG2 | 1.97 | 0.47 |
| 7:UJ:234:SER:OG | 7:UJ:236:ARG:O | 2.32 | 0.47 |
| 9:UL:72:ALA:O | 9:UL:85:VAL:HA | 2.15 | 0.47 |
| 10:UM:575:LYS:HG3 | 10:UM:577:GLU:HB2 | 1.95 | 0.47 |
| 13:UQ:184:THR:OG1 | 13:UQ:185:LYS:N | 2.47 | 0.47 |
| 13:UQ:447:SER:OG | 13:UQ:448:LYS:N | 2.47 | 0.47 |
| 13:UQ:471:SER:HB2 | 13:UQ:543:PHE:CZ | 2.50 | 0.47 |
| 15:UU:780:THR:OG1 | 15:UU:781:LEU:N | 2.48 | 0.47 |
| 18:CA:131:ASN:HD21 | 18:CA:133:PHE:HB2 | 1.80 | 0.47 |
| 18:CB:230:VAL:H | 18:CB:235:GLN:HE21 | 1.62 | 0.47 |
| 19:CC:239:ASP:OD2 | 19:CC:239:ASP:N | 2.47 | 0.47 |
| 21:CE:18:VAL:HA | 21:CE:21:LEU:HD12 | 1.97 | 0.47 |
| 23:CH:56:LEU:HB2 | 23:CH:100:HIS:NE2 | 2.29 | 0.47 |
| 30:CP:40:MET:N | 30:CP:40:MET:SD | 2.88 | 0.47 |
| 30:CP:158:THR:HG23 | 30:CP:201:LEU:HD11 | 1.95 | 0.47 |
| 32:CS:42:TYR:OH | 32:CS:102:ASN:ND2 | 2.47 | 0.47 |
| 32:CS:51:ARG:HD3 | 32:CS:51:ARG:H | 1.80 | 0.47 |
| 32:CS:804:THR:HA | 32:CS:807:GLU:HG3 | 1.96 | 0.47 |
| 35:Ce:87:LEU:O | 35:Ce:91:PHE:CB | 2.63 | 0.47 |
| 46:UV:127:VAL:HG11 | 46:UV:283:LEU:HD11 | 1.96 | 0.47 |
| 49:UE:271:LYS:HA | 49:UE:274:LYS:HE2 | 1.96 | 0.47 |
| 50:US:310:CYS:O | 50:US:313:SER:OG | 2.26 | 0.47 |
| 1:UA:68:ASN:HA | 1:UA:84:VAL:HG12 | 1.95 | 0.47 |
| 6:UG:242:TYR:CE1 | 6:UG:287:PRO:HG3 | 2.50 | 0.47 |
| 9:UL:505:ALA:O | 9:UL:533:LYS:NZ | 2.32 | 0.47 |
| 9:UL:896:ARG:HH22 | 10:UM:892:ASP:HB2 | 1.80 | 0.47 |
| 10:UM:513:GLY:HA3 | 10:UM:550:LEU:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:UM:743:GLN:NE2 | 10:UM:747:ASN:OD1 | 2.48 | 0.47 |
| 10:UM:745:LEU:O | 10:UM:749:ILE:HG12 | 2.14 | 0.47 |
| 13:UQ:359:HIS:HA | 13:UQ:448:LYS:HD3 | 1.95 | 0.47 |
| 13:UQ:496:SER:O | 13:UQ:496:SER:OG | 2.23 | 0.47 |
| 13:UQ:754:TYR:OH | 13:UQ:759:ASP:OD1 | 2.30 | 0.47 |
| 15:UU:104:VAL:HG23 | 15:UU:122:PHE:HB2 | 1.97 | 0.47 |
| 19:CC:176:HIS:HA | 20:CD:189:TRP:CZ3 | 2.49 | 0.47 |
| 22:CG:402:ALA:HB1 | 22:CG:471:THR:HG22 | 1.96 | 0.47 |
| 23:CH:153:PHE:O | 23:CH:157:VAL:HG22 | 2.13 | 0.47 |
| 23:CH:225:THR:O | 23:CH:225:THR:OG1 | 2.30 | 0.47 |
| 24:CI:299:ILE:HB | 24:CI:771:TYR:CZ | 2.49 | 0.47 |
| 26:CK:81:SER:HB3 | 27:CL:560:ARG:NH2 | 2.30 | 0.47 |
| 27:CL:567:ASN:HD21 | 27:CL:571:VAL:HG12 | 1.79 | 0.47 |
| 28:CM:321:TYR:HB3 | 28:CM:353:TRP:CZ3 | 2.49 | 0.47 |
| 28:CM:356:ASN:HB3 | 28:CM:359:GLU:HB2 | 1.96 | 0.47 |
| 29:CN:34:THR:O | 29:CN:36:ARG:NE | 2.47 | 0.47 |
| 31:CQ:110:LYS:O | 31:CQ:130:THR:OG1 | 2.27 | 0.47 |
| 32:CS:571:THR:HG21 | 32:CS:580:PRO:HB2 | 1.96 | 0.47 |
| 38:Ci:48:GLY:O | 44:C1:1503:U:O2' | 2.27 | 0.47 |
| 44:C1:213:G:H2' | 44:C1:214:C:C6 | 2.50 | 0.47 |
| 44:C1:217:G:H2' | 44:C1:218:G:C8 | 2.50 | 0.47 |
| 44:C1:362:G:H2' | 44:C1:363:G:C8 | 2.48 | 0.47 |
| 44:C1:405:C:H2' | 44:C1:406:G:O4' | 2.15 | 0.47 |
| 44:C1:598:A:H2' | 44:C1:599:U:C6 | 2.50 | 0.47 |
| 44:C1:1647:U:H2' | 44:C1:1648:G:H8 | 1.79 | 0.47 |
| 44:C1:1747:A:H2' | 44:C1:1748:G:O4' | 2.14 | 0.47 |
| 45:C2:50:G:H2' | 45:C2:51:U:H6 | 1.80 | 0.47 |
| 46:UV:152:GLN:O | 46:UV:155:ASP:HB2 | 2.14 | 0.47 |
| 46:UV:573:LYS:HD2 | 46:UV:588:LEU:HD23 | 1.97 | 0.47 |
| 46:UV:1042:VAL:HG22 | 47:CV:195:LEU:HD21 | 1.96 | 0.47 |
| 50:US:338:GLU:O | 50:US:342:LYS:HB2 | 2.14 | 0.47 |
| 1:UA:487:SER:OG | 1:UA:488:TRP:N | 2.47 | 0.47 |
| 4:UD:487:SER:HB3 | 4:UD:492:TRP:HB2 | 1.96 | 0.47 |
| 7:UJ:527:SER:OG | 7:UJ:530:ASP:OD2 | 2.32 | 0.47 |
| 8:UK:256:PHE:HE1 | 8:UK:262:ARG:HG2 | 1.80 | 0.47 |
| 9:UL:51:ASP:HB2 | 9:UL:58:LEU:HD21 | 1.96 | 0.47 |
| 10:UM:670:GLY:O | 10:UM:696:LEU:HB3 | 2.15 | 0.47 |
| 12:UO:552:MET:HE1 | 49:UI:262:LYS:NZ | 2.29 | 0.47 |
| 13:UQ:328:ASN:O | 13:UQ:332:HIS:ND1 | 2.46 | 0.47 |
| 13:UQ:749:ASP:OD2 | 13:UQ:749:ASP:N | 2.46 | 0.47 |
| 21:CF:14:ASP:O | 21:CF:16:ALA:N | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:CH:93:LEU:H | 23:CH:96:ASP:HB2 | 1.79 | 0.47 |
| 26:CK:128:VAL:HG21 | 26:CK:274:GLU:HG2 | 1.95 | 0.47 |
| 30:CP:50:TYR:OH | 43:CU:251:ASN:O | 2.30 | 0.47 |
| 32:CR:562:ALA:HB3 | 32:CR:565:HIS:CD2 | 2.50 | 0.47 |
| 32:CS:621:GLN:HB3 | 32:CS:785:ARG:HH12 | 1.79 | 0.47 |
| 34:Cc:129:PRO:HB3 | 34:Cc:201:LYS:HG3 | 1.96 | 0.47 |
| 44:C1:244:G:H2' | 44:C1:245:G:C8 | 2.49 | 0.47 |
| 44:C1:1506:U:H2' | 44:C1:1507:G:C8 | 2.49 | 0.47 |
| 44:C1:1753:G:N1 | 44:C1:2158:G:OP2 | 2.48 | 0.47 |
| 44:C1:2169:A:H2' | 44:C1:2170:A:O4' | 2.15 | 0.47 |
| 49:UI:271:LYS:HA | 49:UI:274:LYS:HE2 | 1.96 | 0.47 |
| 2:UB:710:LYS:HE2 | 2:UB:710:LYS:HB2 | 1.82 | 0.47 |
| 4:UD:675:TYR:HA | 4:UD:678:LEU:HD23 | 1.97 | 0.47 |
| 5:UF:282:VAL:HA | 5:UF:285:VAL:HG12 | 1.97 | 0.47 |
| 7:UJ:664:LEU:O | 7:UJ:667:SER:OG | 2.27 | 0.47 |
| 8:UK:17:ALA:HB2 | 24:CI:1038:ILE:HD11 | 1.96 | 0.47 |
| 9:UL:660:HIS:ND1 | 9:UL:706:HIS:O | 2.47 | 0.47 |
| 10:UM:135:ILE:HD11 | 10:UM:159:LEU:HD21 | 1.95 | 0.47 |
| 10:UM:250:GLY:HA3 | 10:UM:277:LEU:HD22 | 1.96 | 0.47 |
| 13:UQ:113:VAL:HG12 | 13:UQ:123:ARG:HB2 | 1.97 | 0.47 |
| 13:UQ:311:ASP:HA | 13:UQ:330:LEU:HB2 | 1.95 | 0.47 |
| 13:UQ:544:SER:HB3 | 13:UQ:549:TRP:HB2 | 1.96 | 0.47 |
| 13:UQ:609:LYS:O | 49:UE:254:SER:OG | 2.24 | 0.47 |
| 14:UR:361:SER:O | 14:UR:361:SER:OG | 2.27 | 0.47 |
| 15:UU:109:GLY:HA3 | 15:UU:117:GLN:HA | 1.97 | 0.47 |
| 18:CB:189:SER:O | 18:CB:193:LEU:HB2 | 2.15 | 0.47 |
| 21:CF:118:LEU:HA | 21:CF:121:LYS:HE2 | 1.96 | 0.47 |
| 24:CI:45:ARG:O | 24:CI:49:ILE:HG12 | 2.15 | 0.47 |
| 29:CN:12:PRO:HA | 29:CN:13:PRO:HD3 | 1.82 | 0.47 |
| 29:CO:104:ILE:HD11 | 29:CO:246:GLU:HB2 | 1.96 | 0.47 |
| 31:CQ:132:SER:OG | 31:CQ:135:ALA:N | 2.42 | 0.47 |
| 32:CR:78:ILE:HA | 32:CR:81:GLU:HG2 | 1.97 | 0.47 |
| 35:Ce:82:ARG:HA | 35:Ce:85:ARG:HG2 | 1.96 | 0.47 |
| 42:Cp:13:VAL:HA | 42:Cp:31:VAL:HG12 | 1.96 | 0.47 |
| 44:C1:4:G:C6 | 44:C1:32:U:N3 | 2.82 | 0.47 |
| 44:C1:104:U:H3' | 44:C1:105:A:H8 | 1.79 | 0.47 |
| 44:C1:213:G:H2' | 44:C1:214:C:H6 | 1.80 | 0.47 |
| 44:C1:250:U:H2' | 44:C1:251:G:C8 | 2.47 | 0.47 |
| 44:C1:495:G:C8 | 44:C1:503:G:N2 | 2.74 | 0.47 |
| 44:C1:1509:A:H2' | 44:C1:1510:G:C8 | 2.49 | 0.47 |
| 50:US:201:PHE:HA | 50:US:204:ILE:HD12 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:US:250:LYS:HB2 | 50:US:253:HIS:HB2 | 1.96 | 0.47 |
| 1:UA:444:SER:OG | 1:UA:445:ILE:N | 2.45 | 0.47 |
| 4:UD:702:TYR:CZ | 4:UD:838:ILE:HB | 2.50 | 0.47 |
| 7:UJ:162:ILE:H | 7:UJ:162:ILE:HD12 | 1.79 | 0.47 |
| 7:UJ:236:ARG:NH2 | 15:UU:443:MET:HG2 | 2.30 | 0.47 |
| 9:UL:90:GLY:HA2 | 9:UL:113:ILE:HG12 | 1.97 | 0.47 |
| 9:UL:304:ILE:O | 9:UL:360:HIS:N | 2.47 | 0.47 |
| 10:UM:283:LEU:HB3 | 10:UM:286:GLY:HA3 | 1.96 | 0.47 |
| 10:UM:587:ARG:NH1 | 44:C1:1497:U:OP1 | 2.48 | 0.47 |
| 12:UO:333:HIS:HB3 | 12:UO:347:THR:HG23 | 1.95 | 0.47 |
| 12:UO:413:HIS:CE1 | 12:UO:417:ARG:HG2 | 2.50 | 0.47 |
| 14:UR:461:ILE:H | 14:UR:461:ILE:HD12 | 1.79 | 0.47 |
| 15:UU:59:THR:HA | 20:CD:434:VAL:HG11 | 1.96 | 0.47 |
| 15:UU:298:MET:HG3 | 15:UU:311:TRP:HD1 | 1.79 | 0.47 |
| 16:UX:145:ILE:HG23 | 16:UX:164:PRO:HB2 | 1.97 | 0.47 |
| 18:CB:131:ASN:ND2 | 18:CB:134:ARG:HH21 | 2.13 | 0.47 |
| 20:CD:155:LYS:HA | 20:CD:158:PRO:HA | 1.97 | 0.47 |
| 20:CD:261:ALA:HA | 20:CD:264:VAL:HG12 | 1.95 | 0.47 |
| 24:CI:190:LYS:HE3 | 24:CI:191:HIS:CE1 | 2.49 | 0.47 |
| 24:CI:844:THR:OG1 | 24:CI:845:LEU:N | 2.47 | 0.47 |
| 26:CK:192:ILE:HG23 | 27:CL:554:PHE:HD1 | 1.80 | 0.47 |
| 28:CM:60:GLN:OE1 | 45:C2:32:G:N2 | 2.42 | 0.47 |
| 32:CS:562:ALA:HB3 | 32:CS:565:HIS:CD2 | 2.50 | 0.47 |
| 32:CS:749:GLN:HG3 | 32:CS:794:PHE:HE1 | 1.80 | 0.47 |
| 44:C1:1448:A:C6 | 44:C1:1549:U:C4 | 3.03 | 0.47 |
| 46:UV:1045:HIS:NE2 | 46:UV:1047:VAL:HB | 2.30 | 0.47 |
| 49:UI:271:LYS:O | 49:UI:275:ALA:N | 2.46 | 0.47 |
| 1:UA:172:ASP:OD1 | 1:UA:174:THR:OG1 | 2.29 | 0.47 |
| 1:UA:593:SER:OG | 1:UA:595:TYR:N | 2.48 | 0.47 |
| 7:UJ:659:VAL:HG11 | 7:UJ:681:ALA:HB2 | 1.97 | 0.47 |
| 9:UL:269:ASN:ND2 | 9:UL:271:GLY:O | 2.44 | 0.47 |
| 9:UL:654:GLN:NE2 | 9:UL:700:TRP:O | 2.48 | 0.47 |
| 9:UL:887:LYS:HB3 | 9:UL:887:LYS:HE2 | 1.70 | 0.47 |
| 10:UM:278:GLU:N | 10:UM:292:ALA:O | 2.41 | 0.47 |
| 15:UU:424:ARG:HB3 | 15:UU:427:GLN:HE21 | 1.80 | 0.47 |
| 15:UU:565:ILE:HB | 15:UU:579:PHE:HB2 | 1.96 | 0.47 |
| 15:UU:861:LYS:NZ | 31:CQ:257:GLU:OE1 | 2.32 | 0.47 |
| 18:CB:195:ASN:O | 18:CB:198:THR:OG1 | 2.31 | 0.47 |
| 20:CD:13:TYR:HE2 | 20:CD:72:LYS:HB3 | 1.80 | 0.47 |
| 23:CH:32:HIS:ND1 | 23:CH:76:THR:OG1 | 2.32 | 0.47 |
| 24:CI:1094:MET:HE2 | 24:CI:1094:MET:HB2 | 1.74 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:CN:90:ASP:N | 29:CN:90:ASP:OD2 | 2.46 | 0.47 |
| 32:CR:625:ASP:HA | 32:CR:628:ALA:HB3 | 1.97 | 0.47 |
| 32:CS:386:VAL:HG12 | 32:CS:406:TYR:CE2 | 2.49 | 0.47 |
| 34:Cc:43:ILE:HA | 34:Cc:46:THR:HG23 | 1.97 | 0.47 |
| 40:Cm:97:ARG:HH22 | 40:Cm:117:ARG:HH12 | 1.62 | 0.47 |
| 44:C1:603:G:H2' | 44:C1:604:C:C2 | 2.50 | 0.47 |
| 45:C2:20:A:H2' | 45:C2:21:U:H6 | 1.80 | 0.47 |
| 46:UV:346:PRO:HB2 | 46:UV:359:ALA:HB2 | 1.96 | 0.47 |
| 1:UA:193:GLY:O | 1:UA:194:HIS:ND1 | 2.47 | 0.47 |
| 1:UA:276:ASN:OD1 | 1:UA:276:ASN:N | 2.44 | 0.47 |
| 1:UA:559:ARG:HD3 | 1:UA:672:GLU:HG3 | 1.96 | 0.47 |
| 4:UD:483:ARG:HB2 | 4:UD:496:ALA:HB3 | 1.97 | 0.47 |
| 9:UL:512:TRP:N | 9:UL:526:GLY:O | 2.48 | 0.47 |
| 10:UM:641:HIS:ND1 | 10:UM:672:ASP:OD2 | 2.42 | 0.47 |
| 12:UO:549:SER:HB2 | 49:UI:265:MET:SD | 2.56 | 0.47 |
| 12:UO:552:MET:HE1 | 49:UI:262:LYS:HZ2 | 1.79 | 0.47 |
| 13:UQ:370:LEU:HB3 | 13:UQ:382:TRP:HB2 | 1.97 | 0.47 |
| 13:UQ:802:LYS:HA | 13:UQ:802:LYS:HD2 | 1.76 | 0.47 |
| 14:UR:308:TYR:CD1 | 14:UR:309:PRO:HA | 2.50 | 0.47 |
| 18:CA:159:LEU:HD23 | 18:CA:159:LEU:HA | 1.69 | 0.47 |
| 20:CD:318:THR:OG1 | 45:C2:261:U:O2' | 2.31 | 0.47 |
| 23:CH:32:HIS:HB2 | 23:CH:76:THR:HG23 | 1.97 | 0.47 |
| 25:CJ:28:ARG:NH1 | 44:C1:348:U:OP2 | 2.37 | 0.47 |
| 25:CJ:93:LYS:HG2 | 25:CJ:96:ALA:H | 1.80 | 0.47 |
| 26:CK:97:SER:OG | 26:CK:98:SER:N | 2.48 | 0.47 |
| 29:CN:77:MET:HG2 | 29:CN:84:ILE:HA | 1.97 | 0.47 |
| 29:CO:89:PRO:O | 29:CO:92:THR:OG1 | 2.24 | 0.47 |
| 32:CR:62:LYS:HA | 32:CR:62:LYS:HD2 | 1.53 | 0.47 |
| 32:CR:153:LEU:HD13 | 32:CR:158:SER:HB3 | 1.97 | 0.47 |
| 32:CR:839:LYS:NZ | 32:CS:623:GLN:OE1 | 2.26 | 0.47 |
| 32:CS:826:LYS:HA | 32:CS:829:LEU:HB2 | 1.97 | 0.47 |
| 34:Cc:80:LEU:O | 34:Cc:83:SER:OG | 2.33 | 0.47 |
| 44:C1:176:G:H2' | 44:C1:177:G:H8 | 1.80 | 0.47 |
| 44:C1:246:G:H2' | 44:C1:247:C:H6 | 1.79 | 0.47 |
| 46:UV:874:THR:O | 46:UV:878:ARG:HG2 | 2.15 | 0.47 |
| 46:UV:893:LEU:HD11 | 46:UV:932:VAL:HA | 1.96 | 0.47 |
| 2:UB:320:THR:O | 2:UB:323:GLU:HG2 | 2.15 | 0.46 |
| 4:UD:480:GLY:N | 4:UD:497:GLU:OE2 | 2.48 | 0.46 |
| 5:UF:126:TRP:CH2 | 5:UF:150:ARG:HD3 | 2.50 | 0.46 |
| 6:UG:162:THR:O | 6:UG:171:GLY:N | 2.45 | 0.46 |
| 7:UJ:860:ASP:OD2 | 7:UJ:860:ASP:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:UL:575:PRO:HG2 | 9:UL:617:TYR:HA | 1.97 | 0.46 |
| 9:UL:606:HIS:HA | 9:UL:632:ARG:HH22 | 1.80 | 0.46 |
| 9:UL:631:ILE:HD11 | 9:UL:645:LEU:HD22 | 1.97 | 0.46 |
| 10:UM:436:VAL:HA | 10:UM:451:GLY:HA2 | 1.97 | 0.46 |
| 13:UQ:291:SER:OG | 13:UQ:319:ALA:N | 2.48 | 0.46 |
| 14:UR:266:THR:OG1 | 14:UR:613:LEU:HB2 | 2.14 | 0.46 |
| 15:UU:418:TRP:CZ2 | 15:UU:430:GLU:HB3 | 2.50 | 0.46 |
| 24:CI:136:VAL:HB | 24:CI:166:VAL:HG12 | 1.98 | 0.46 |
| 32:CR:530:HIS:HB2 | 32:CR:533:SER:HB3 | 1.97 | 0.46 |
| 32:CS:48:MET:HE3 | 32:CS:48:MET:HB3 | 1.74 | 0.46 |
| 40:Cm:41:MET:HB3 | 40:Cm:47:ILE:HD13 | 1.97 | 0.46 |
| 44:C1:82:C:H2' | 44:C1:83:A:C8 | 2.50 | 0.46 |
| 44:C1:100:C:H2' | 44:C1:101:G:C8 | 2.50 | 0.46 |
| 44:C1:285:A:H2' | 44:C1:286:G:H8 | 1.80 | 0.46 |
| 44:C1:1532:C:H2' | 44:C1:1533:G:C8 | 2.49 | 0.46 |
| 44:C1:2208:C:H2' | 44:C1:2209:U:C6 | 2.50 | 0.46 |
| 44:C1:2368:U:H2' | 44:C1:2369:G:C8 | 2.50 | 0.46 |
| 45:C2:160:U:H2' | 45:C2:161:G:C8 | 2.48 | 0.46 |
| 46:UV:671:ILE:HA | 46:UV:814:THR:HG21 | 1.96 | 0.46 |
| 46:UV:1057:VAL:HG11 | 47:CV:86:GLU:HG3 | 1.98 | 0.46 |
| 50:US:464:GLN:NE2 | 50:US:479:SER:OG | 2.48 | 0.46 |
| 2:UB:5:GLN:OE1 | 26:CK:255:SER:OG | 2.27 | 0.46 |
| 4:UD:107:TYR:CE2 | 53:UP:340:LEU:HD13 | 2.50 | 0.46 |
| 4:UD:207:SER:HB2 | 4:UD:236:ILE:HG22 | 1.98 | 0.46 |
| 4:UD:394:TRP:CD1 | 4:UD:419:PHE:HA | 2.50 | 0.46 |
| 6:UG:222:MET:HE2 | 6:UG:231:LEU:HD11 | 1.96 | 0.46 |
| 9:UL:21:ASN:OD1 | 9:UL:69:ARG:NH2 | 2.48 | 0.46 |
| 9:UL:633:ILE:HG22 | 9:UL:642:HIS:HB2 | 1.97 | 0.46 |
| 9:UL:924:LEU:HA | 9:UL:927:VAL:HG12 | 1.96 | 0.46 |
| 9:UL:939:TYR:HA | 44:C1:2350:G:H1 | 1.80 | 0.46 |
| 12:UO:94:THR:HG21 | 51:Cl:55:LYS:HE3 | 1.96 | 0.46 |
| 20:CD:13:TYR:CE2 | 20:CD:72:LYS:HB3 | 2.50 | 0.46 |
| 23:CH:28:GLY:HA3 | 24:CI:809:ARG:CZ | 2.45 | 0.46 |
| 23:CH:110:ILE:O | 23:CH:114:LEU:HG | 2.14 | 0.46 |
| 23:CH:152:THR:HG21 | 23:CH:295:ASP:HB2 | 1.97 | 0.46 |
| 29:CO:192:TYR:O | 29:CO:195:THR:OG1 | 2.25 | 0.46 |
| 31:CQ:170:ASP:OD1 | 31:CQ:173:ASP:N | 2.48 | 0.46 |
| 34:Cc:69:PHE:CZ | 42:Cp:50:ARG:HB2 | 2.50 | 0.46 |
| 44:C1:83:A:H2' | 44:C1:84:A:H8 | 1.79 | 0.46 |
| 44:C1:346:C:O2' | 44:C1:347:C:O5' | 2.28 | 0.46 |
| 44:C1:2067:G:O2' | 44:C1:2189:C:O2' | 2.29 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:2078:C:H2' | 44:C1:2079:U:H6 | 1.80 | 0.46 |
| 45:C2:50:G:H2' | 45:C2:51:U:C6 | 2.50 | 0.46 |
| 46:UV:142:MET:HE3 | 46:UV:226:ILE:HG13 | 1.97 | 0.46 |
| 46:UV:268:PHE:HB3 | 46:UV:474:ARG:CZ | 2.45 | 0.46 |
| 46:UV:719:ILE:HG12 | 46:UV:754:ALA:HB3 | 1.96 | 0.46 |
| 48:UH:486:LEU:HD13 | 48:UH:552:LYS:HZ1 | 1.80 | 0.46 |
| 48:UH:554:PHE:HB3 | 48:UH:567:LEU:HD12 | 1.97 | 0.46 |
| 49:UE:271:LYS:O | 49:UE:275:ALA:N | 2.46 | 0.46 |
| 49:UI:269:GLN:O | 49:UI:273:ARG:N | 2.28 | 0.46 |
| 54:Cz:1518:SER:HA | 54:Cz:1521:GLN:HG2 | 1.98 | 0.46 |
| 2:UB:49:LYS:HE2 | 2:UB:49:LYS:HB3 | 1.61 | 0.46 |
| 4:UD:390:GLU:HG3 | 4:UD:422:GLN:HE21 | 1.80 | 0.46 |
| 4:UD:830:TYR:CZ | 44:C1:63:C:H5" | 2.50 | 0.46 |
| 6:UG:137:LEU:HD13 | 6:UG:159:HIS:HB2 | 1.97 | 0.46 |
| 7:UJ:559:TRP:HZ2 | 7:UJ:575:VAL:HG21 | 1.79 | 0.46 |
| 11:UN:905:VAL:HA | 11:UN:910:MET:HE3 | 1.98 | 0.46 |
| 15:UU:43:LEU:HD21 | 15:UU:46:PRO:HG3 | 1.98 | 0.46 |
| 17:UZ:63:TRP:HA | 17:UZ:245:VAL:HG12 | 1.96 | 0.46 |
| 18:CA:82:PHE:HE1 | 33:CT:90:TRP:HB3 | 1.80 | 0.46 |
| 28:CM:291:PHE:HA | 28:CM:298:LEU:HD23 | 1.97 | 0.46 |
| 29:CN:167:ILE:O | 29:CN:171:LEU:HG | 2.16 | 0.46 |
| 31:CQ:145:ALA:HA | 31:CQ:148:MET:HG2 | 1.97 | 0.46 |
| 32:CR:80:LYS:HA | 32:CR:83:LYS:HG2 | 1.97 | 0.46 |
| 32:CR:720:LEU:O | 32:CR:767:GLN:NE2 | 2.49 | 0.46 |
| 32:CS:62:LYS:HA | 32:CS:62:LYS:HD2 | 1.53 | 0.46 |
| 32:CS:153:LEU:HD13 | 32:CS:158:SER:HB3 | 1.97 | 0.46 |
| 32:CS:283:LEU:HD12 | 32:CS:472:ILE:HG13 | 1.96 | 0.46 |
| 32:CS:537:LEU:O | 32:CS:541:VAL:HG22 | 2.16 | 0.46 |
| 36:Cg:131:HIS:NE2 | 44:C1:1096:A:O2' | 2.26 | 0.46 |
| 44:C1:23:G:H2' | 44:C1:24:G:C8 | 2.49 | 0.46 |
| 44:C1:98:A:H2' | 44:C1:99:A:C8 | 2.50 | 0.46 |
| 44:C1:354:G:H2' | 44:C1:355:G:C8 | 2.50 | 0.46 |
| 44:C1:474:A:O2' | 44:C1:475:C:H5" | 2.16 | 0.46 |
| 45:C2:252:C:H2' | 45:C2:253:G:C8 | 2.49 | 0.46 |
| 46:UV:329:LEU:HD11 | 46:UV:360:LEU:HD21 | 1.98 | 0.46 |
| 46:UV:1007:ARG:HH22 | 46:UV:1079:ALA:HB3 | 1.81 | 0.46 |
| 47:CV:174:TYR:HD2 | 47:CV:176:VAL:HG12 | 1.81 | 0.46 |
| 50:US:191:LYS:HZ3 | 50:US:231:GLU:H | 1.62 | 0.46 |
| 3:UC:586:ASN:OD1 | 3:UC:586:ASN:N | 2.44 | 0.46 |
| 6:UG:165:TRP:H | 6:UG:165:TRP:CD1 | 2.33 | 0.46 |
| 6:UG:315:MET:HB2 | 6:UG:329:ILE:HD11 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:UK:102:ARG:O | 8:UK:106:THR:OG1 | 2.30 | 0.46 |
| 9:UL:453:ASN:ND2 | 9:UL:456:THR:H | 2.12 | 0.46 |
| 12:UO:338:MET:HB2 | 12:UO:342:VAL:HG23 | 1.98 | 0.46 |
| 13:UQ:571:LYS:HZ2 | 13:UQ:575:ASP:HB3 | 1.81 | 0.46 |
| 13:UQ:783:ASN:ND2 | 13:UQ:841:SER:OG | 2.48 | 0.46 |
| 14:UR:487:SER:OG | 14:UR:489:SER:N | 2.49 | 0.46 |
| 15:UU:177:ALA:HB2 | 15:UU:203:ARG:HH12 | 1.80 | 0.46 |
| 15:UU:394:LEU:HD12 | 15:UU:394:LEU:HA | 1.78 | 0.46 |
| 20:CD:331:ALA:O | 20:CD:336:HIS:N | 2.42 | 0.46 |
| 24:CI:187:LYS:HE3 | 24:CI:187:LYS:HB3 | 1.76 | 0.46 |
| 28:CM:167:THR:HG22 | 28:CM:181:ASP:HA | 1.98 | 0.46 |
| 32:CR:826:LYS:HA | 32:CR:829:LEU:HB2 | 1.98 | 0.46 |
| 32:CS:172:ARG:NH1 | 32:CS:187:GLU:OE1 | 2.49 | 0.46 |
| 44:C1:1738:G:H2' | 44:C1:1739:G:H8 | 1.80 | 0.46 |
| 44:C1:2092:C:H2' | 44:C1:2093:C:C6 | 2.50 | 0.46 |
| 46:UV:139:GLY:HA3 | 46:UV:223:ARG:HB3 | 1.96 | 0.46 |
| 46:UV:245:GLY:H | 46:UV:260:GLN:NE2 | 2.14 | 0.46 |
| 46:UV:329:LEU:HB2 | 46:UV:369:PHE:HE2 | 1.80 | 0.46 |
| 46:UV:1051:LEU:HD13 | 46:UV:1054:LEU:HD23 | 1.97 | 0.46 |
| 48:UH:532:PRO:HG2 | 48:UH:538:TYR:HE1 | 1.81 | 0.46 |
| 48:UH:774:GLN:HB2 | 49:UI:255:SER:OG | 2.16 | 0.46 |
| 50:US:412:PRO:HA | 50:US:415:THR:HG23 | 1.98 | 0.46 |
| 1:UA:6:LYS:HD3 | 1:UA:6:LYS:HA | 1.52 | 0.46 |
| 1:UA:27:THR:OG1 | 1:UA:28:HIS:N | 2.48 | 0.46 |
| 7:UJ:228:MET:O | 7:UJ:232:MET:HG2 | 2.16 | 0.46 |
| 7:UJ:229:ILE:HD11 | 7:UJ:278:LEU:HD12 | 1.98 | 0.46 |
| 9:UL:202:ASP:OD1 | 9:UL:203:LEU:N | 2.49 | 0.46 |
| 10:UM:789:THR:HG23 | 10:UM:791:LEU:H | 1.80 | 0.46 |
| 11:UN:365:SER:HB3 | 11:UN:374:LEU:HD12 | 1.97 | 0.46 |
| 13:UQ:380:VAL:HA | 13:UQ:391:PHE:HB3 | 1.98 | 0.46 |
| 13:UQ:694:SER:OG | 13:UQ:697:GLY:N | 2.49 | 0.46 |
| 13:UQ:704:PHE:HD2 | 13:UQ:706:PRO:HD3 | 1.79 | 0.46 |
| 14:UR:445:SER:OG | 14:UR:446:MET:N | 2.47 | 0.46 |
| 15:UU:466:THR:N | 15:UU:514:ALA:O | 2.46 | 0.46 |
| 18:CB:212:LYS:HD3 | 18:CB:212:LYS:HA | 1.71 | 0.46 |
| 19:CC:388:ILE:O | 19:CC:391:ARG:HG2 | 2.16 | 0.46 |
| 23:CH:149:SER:O | 23:CH:152:THR:OG1 | 2.33 | 0.46 |
| 24:CI:1020:ARG:HD3 | 24:CI:1027:THR:HG22 | 1.97 | 0.46 |
| 28:CM:201:THR:OG1 | 28:CM:202:ASP:N | 2.48 | 0.46 |
| 29:CN:191:ASP:O | 29:CN:195:THR:OG1 | 2.28 | 0.46 |
| 31:CQ:194:ASP:H | 44:C1:2352:U:H5' | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:CR:172:ARG:NH1 | 32:CR:187:GLU:OE1 | 2.49 | 0.46 |
| 44:C1:452:G:H2' | 44:C1:453:G:H8 | 1.80 | 0.46 |
| 44:C1:1141:G:H2' | 44:C1:1142:U:C6 | 2.51 | 0.46 |
| 46:UV:1057:VAL:HG22 | 47:CV:96:LYS:NZ | 2.30 | 0.46 |
| 54:Cz:1658:LEU:HB2 | 54:Cz:1683:LEU:HD21 | 1.98 | 0.46 |
| 1:UA:206:ASP:O | 1:UA:208:GLU:N | 2.46 | 0.46 |
| 1:UA:398:PHE:CD2 | 1:UA:433:VAL:HG11 | 2.51 | 0.46 |
| 4:UD:116:LEU:HA | 4:UD:116:LEU:HD13 | 1.71 | 0.46 |
| 4:UD:395:HIS:CD2 | 4:UD:397:LEU:HG | 2.51 | 0.46 |
| 4:UD:695:GLN:HB3 | 4:UD:698:ARG:HB2 | 1.98 | 0.46 |
| 7:UJ:152:LEU:HG | 7:UJ:171:ILE:HG12 | 1.97 | 0.46 |
| 9:UL:138:ASP:OD1 | 9:UL:141:ALA:N | 2.32 | 0.46 |
| 9:UL:385:LEU:HA | 9:UL:385:LEU:HD13 | 1.77 | 0.46 |
| 10:UM:842:LEU:HD13 | 10:UM:845:LEU:HD11 | 1.96 | 0.46 |
| 13:UQ:417:ASP:HB3 | 13:UQ:485:GLY:HA2 | 1.98 | 0.46 |
| 15:UU:287:GLY:N | 15:UU:292:GLY:O | 2.48 | 0.46 |
| 15:UU:406:LYS:HZ1 | 44:C1:258:C:P | 2.38 | 0.46 |
| 19:CC:197:ARG:HG2 | 20:CD:171:LEU:HD12 | 1.97 | 0.46 |
| 20:CD:81:LYS:HG3 | 20:CD:82:ASP:H | 1.81 | 0.46 |
| 32:CR:791:SER:O | 32:CR:795:ARG:NH1 | 2.49 | 0.46 |
| 32:CS:625:ASP:HA | 32:CS:628:ALA:HB3 | 1.97 | 0.46 |
| 32:CS:851:TYR:O | 32:CS:855:LEU:HB2 | 2.15 | 0.46 |
| 34:Cc:145:GLN:HE21 | 42:Cp:62:ARG:HH12 | 1.62 | 0.46 |
| 43:CU:286:LEU:HD23 | 43:CU:288:ILE:HD11 | 1.98 | 0.46 |
| 44:C1:57:C:H2' | 44:C1:58:G:H8 | 1.78 | 0.46 |
| 44:C1:1129:A:H4' | 44:C1:1130:U:H5' | 1.98 | 0.46 |
| 44:C1:1508:A:H2' | 44:C1:1509:A:C8 | 2.51 | 0.46 |
| 44:C1:1532:C:H2' | 44:C1:1533:G:H8 | 1.80 | 0.46 |
| 44:C1:1759:U:H2' | 44:C1:1760:G:O4' | 2.16 | 0.46 |
| 46:UV:247:VAL:HB | 46:UV:249:LYS:HE2 | 1.97 | 0.46 |
| 46:UV:944:THR:O | 46:UV:951:ARG:NH1 | 2.43 | 0.46 |
| 46:UV:988:LEU:HD13 | 46:UV:994:LEU:HD21 | 1.97 | 0.46 |
| 47:CV:174:TYR:CD2 | 47:CV:176:VAL:HG12 | 2.51 | 0.46 |
| 48:UH:872:LYS:HA | 48:UH:872:LYS:HD2 | 1.66 | 0.46 |
| 50:US:289:MET:SD | 50:US:307:LEU:HD21 | 2.56 | 0.46 |
| 50:US:299:LYS:HE2 | 50:US:302:MET:HE1 | 1.98 | 0.46 |
| 50:US:468:HIS:HE1 | 50:US:470:ASN:HB2 | 1.81 | 0.46 |
| 1:UA:662:GLY:HA3 | 27:CL:636:TRP:CH2 | 2.51 | 0.46 |
| 4:UD:578:PRO:HB3 | 4:UD:611:GLY:HA3 | 1.98 | 0.46 |
| 5:UF:144:TRP:CD1 | 5:UF:177:LEU:HD11 | 2.51 | 0.46 |
| 7:UJ:278:LEU:HD23 | 7:UJ:292:PHE:HE2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:UJ:329:ALA:HA | 7:UJ:332:VAL:HG12 | 1.96 | 0.46 |
| 9:UL:598:LYS:HA | 9:UL:598:LYS:HD3 | 1.72 | 0.46 |
| 10:UM:447:TRP:CD1 | 10:UM:460:TRP:HB2 | 2.48 | 0.46 |
| 13:UQ:735:ARG:NH1 | 13:UQ:748:SER:O | 2.38 | 0.46 |
| 14:UR:418:HIS:HB2 | 14:UR:437:ARG:HD3 | 1.97 | 0.46 |
| 16:UX:65:LEU:HD21 | 16:UX:113:ALA:HB2 | 1.98 | 0.46 |
| 16:UX:125:HIS:HD1 | 16:UX:127:GLY:N | 2.12 | 0.46 |
| 17:UZ:82:LYS:HB3 | 17:UZ:180:ILE:HD11 | 1.98 | 0.46 |
| 17:UZ:167:LEU:HD13 | 17:UZ:171:PHE:CE2 | 2.50 | 0.46 |
| 20:CD:332:LEU:HD23 | 20:CD:332:LEU:HA | 1.72 | 0.46 |
| 21:CF:116:ARG:HA | 21:CF:119:ARG:HE | 1.80 | 0.46 |
| 22:CG:250:LEU:HG | 22:CG:265:GLY:HA2 | 1.96 | 0.46 |
| 23:CH:105:THR:HA | 23:CH:186:LYS:HD2 | 1.97 | 0.46 |
| 23:CH:288:GLU:OE1 | 23:CH:289:GLY:N | 2.48 | 0.46 |
| 24:CI:355:ARG:NE | 24:CI:358:GLY:O | 2.48 | 0.46 |
| 24:CI:369:ARG:HD3 | 24:CI:369:ARG:HA | 1.66 | 0.46 |
| 26:CK:127:LEU:HD12 | 26:CK:127:LEU:HA | 1.62 | 0.46 |
| 32:CR:497:ASP:N | 32:CR:497:ASP:OD1 | 2.47 | 0.46 |
| 32:CR:537:LEU:O | 32:CR:541:VAL:HG22 | 2.16 | 0.46 |
| 32:CS:569:VAL:HG23 | 32:CS:585:VAL:HG12 | 1.98 | 0.46 |
| 33:CT:171:VAL:HA | 33:CT:174:TYR:HD2 | 1.80 | 0.46 |
| 36:Cg:29:VAL:O | 36:Cg:33:GLY:HA2 | 2.15 | 0.46 |
| 39:Cj:18:ALA:HB2 | 39:Cj:80:ALA:HB1 | 1.98 | 0.46 |
| 44:C1:449:C:H2' | 44:C1:450:G:C8 | 2.51 | 0.46 |
| 44:C1:471:C:H2' | 44:C1:472:G:H8 | 1.79 | 0.46 |
| 45:C2:53:U:H2' | 45:C2:54:C:H6 | 1.81 | 0.46 |
| 45:C2:79:G:H2' | 45:C2:80:G:C8 | 2.51 | 0.46 |
| 48:UH:775:LEU:O | 48:UH:779:LEU:HG | 2.16 | 0.46 |
| 48:UH:842:TYR:CD1 | 48:UH:871:LEU:HB3 | 2.50 | 0.46 |
| 49:UE:165:ASP:OD1 | 49:UE:167:ASP:N | 2.49 | 0.46 |
| 54:Cz:1528:ALA:HA | 54:Cz:1531:ILE:HD12 | 1.98 | 0.46 |
| 1:UA:215:LYS:HZ1 | 1:UA:259:ARG:HD3 | 1.79 | 0.46 |
| 1:UA:476:PHE:HE1 | 1:UA:498:PHE:HZ | 1.64 | 0.46 |
| 2:UB:23:LYS:HB3 | 2:UB:27:GLN:HB2 | 1.97 | 0.46 |
| 2:UB:886:GLN:NE2 | 41:Cn:118:PRO:O | 2.34 | 0.46 |
| 4:UD:799:GLU:HA | 4:UD:802:ARG:HD2 | 1.97 | 0.46 |
| 6:UG:160:VAL:O | 6:UG:173:GLU:HA | 2.16 | 0.46 |
| 7:UJ:656:ILE:HG23 | 7:UJ:657:ARG:HG3 | 1.98 | 0.46 |
| 10:UM:394:ASN:HA | 10:UM:435:ILE:HG23 | 1.98 | 0.46 |
| 12:UO:474:ASP:O | 12:UO:477:SER:OG | 2.33 | 0.46 |
| 13:UQ:702:ALA:O | 13:UQ:712:VAL:HA | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:UQ:779:GLN:NE2 | 13:UQ:832:ILE:O | 2.49 | 0.46 |
| 14:UR:393:LYS:HD3 | 14:UR:393:LYS:HA | 1.70 | 0.46 |
| 15:UU:69:ARG:HD3 | 15:UU:69:ARG:HA | 1.60 | 0.46 |
| 15:UU:224:PRO:CB | 15:UU:248:TYR:CZ | 2.95 | 0.46 |
| 15:UU:890:SER:OG | 31:CQ:258:ARG:NH1 | 2.42 | 0.46 |
| 15:UU:1012:LEU:H | 15:UU:1012:LEU:HG | 1.55 | 0.46 |
| 16:UX:28:LYS:HD3 | 16:UX:28:LYS:HA | 1.80 | 0.46 |
| 16:UX:150:ASP:HB3 | 16:UX:153:LEU:HD12 | 1.98 | 0.46 |
| 17:UZ:63:TRP:HB3 | 17:UZ:244:LYS:HD2 | 1.98 | 0.46 |
| 17:UZ:130:ILE:HA | 17:UZ:133:LEU:HB2 | 1.98 | 0.46 |
| 21:CF:111:LEU:O | 21:CF:115:ILE:HG12 | 2.15 | 0.46 |
| 22:CG:354:ALA:HB3 | 22:CG:367:PHE:HB2 | 1.96 | 0.46 |
| 24:CI:107:VAL:HG21 | 24:CI:333:LYS:HE2 | 1.98 | 0.46 |
| 24:CI:1002:ASN:ND2 | 24:CI:1011:GLN:O | 2.48 | 0.46 |
| 25:CJ:37:MET:HE2 | 25:CJ:125:GLN:HA | 1.98 | 0.46 |
| 25:CJ:109:ARG:NH2 | 25:CJ:150:VAL:O | 2.48 | 0.46 |
| 28:CM:323:THR:HG22 | 28:CM:325:ARG:H | 1.80 | 0.46 |
| 32:CR:571:THR:HG21 | 32:CR:580:PRO:HB2 | 1.96 | 0.46 |
| 32:CR:749:GLN:HG3 | 32:CR:794:PHE:HE1 | 1.80 | 0.46 |
| 32:CR:791:SER:HA | 32:CR:795:ARG:HA | 1.97 | 0.46 |
| 32:CS:115:ILE:H | 32:CS:115:ILE:HG13 | 1.60 | 0.46 |
| 32:CS:647:MET:HE3 | 32:CS:647:MET:HB2 | 1.89 | 0.46 |
| 32:CS:791:SER:O | 32:CS:795:ARG:NH1 | 2.49 | 0.46 |
| 40:Cm:54:ASP:HA | 40:Cm:59:GLY:HA3 | 1.97 | 0.46 |
| 44:C1:384:C:H3' | 44:C1:385:A:H8 | 1.80 | 0.46 |
| 44:C1:1665:A:H1' | 44:C1:1666:C:C4 | 2.50 | 0.46 |
| 44:C1:2059:C:H2' | 44:C1:2060:A:C8 | 2.51 | 0.46 |
| 44:C1:2110:C:H2' | 44:C1:2111:U:C6 | 2.51 | 0.46 |
| 45:C2:19:A:H2' | 45:C2:20:A:C8 | 2.50 | 0.46 |
| 51:Cl:62:THR:O | 51:Cl:65:GLU:HG2 | 2.16 | 0.46 |
| 1:UA:136:LEU:HD11 | 15:UU:782:PHE:CE2 | 2.50 | 0.46 |
| 1:UA:558:ARG:HA | 1:UA:558:ARG:HD3 | 1.47 | 0.46 |
| 4:UD:109:THR:HA | 4:UD:132:ILE:HG13 | 1.98 | 0.46 |
| 4:UD:551:GLN:NE2 | 4:UD:631:VAL:O | 2.48 | 0.46 |
| 6:UG:370:LEU:HD12 | 6:UG:370:LEU:HA | 1.72 | 0.46 |
| 7:UJ:221:MET:HE2 | 7:UJ:274:VAL:HG21 | 1.98 | 0.46 |
| 7:UJ:820:MET:HB2 | 7:UJ:825:LYS:HD3 | 1.97 | 0.46 |
| 9:UL:293:PHE:CE1 | 9:UL:305:TRP:HB2 | 2.51 | 0.46 |
| 9:UL:560:ARG:HB2 | 43:CU:96:GLN:HB3 | 1.98 | 0.46 |
| 9:UL:580:LEU:HD11 | 9:UL:592:PHE:HB2 | 1.98 | 0.46 |
| 9:UL:788:LEU:O | 9:UL:791:THR:OG1 | 2.32 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:UM:70:THR:HG23 | 10:UM:123:SER:HA | 1.97 | 0.46 |
| 12:UO:47:ILE:HG22 | 12:UO:75:VAL:HG23 | 1.97 | 0.46 |
| 12:UO:146:PRO:O | 12:UO:165:ASP:N | 2.45 | 0.46 |
| 13:UQ:236:THR:O | 13:UQ:236:THR:OG1 | 2.34 | 0.46 |
| 13:UQ:402:ILE:HA | 13:UQ:412:ALA:O | 2.15 | 0.46 |
| 15:UU:179:LYS:HA | 15:UU:179:LYS:HD2 | 1.75 | 0.46 |
| 15:UU:376:ARG:NH1 | 44:C1:252:U:O2' | 2.43 | 0.46 |
| 15:UU:396:SER:OG | 15:UU:403:GLY:O | 2.28 | 0.46 |
| 17:UZ:241:THR:OG1 | 17:UZ:242:ALA:N | 2.49 | 0.46 |
| 21:CF:18:VAL:O | 21:CF:22:LEU:HG | 2.16 | 0.46 |
| 24:CI:308:THR:OG1 | 24:CI:311:MET:SD | 2.73 | 0.46 |
| 29:CN:22:GLU:N | 29:CN:22:GLU:OE2 | 2.49 | 0.46 |
| 29:CO:37:LEU:HB2 | 29:CO:110:LEU:HD12 | 1.97 | 0.46 |
| 32:CR:51:ARG:H | 32:CR:51:ARG:HD3 | 1.80 | 0.46 |
| 44:C1:101:G:H2' | 44:C1:102:G:C8 | 2.49 | 0.46 |
| 44:C1:154:C:H2' | 44:C1:155:G:C8 | 2.50 | 0.46 |
| 44:C1:364:C:H2' | 44:C1:365:G:H8 | 1.81 | 0.46 |
| 44:C1:471:C:H2' | 44:C1:472:G:C8 | 2.51 | 0.46 |
| 44:C1:1074:U:H2' | 44:C1:1075:C:C6 | 2.51 | 0.46 |
| 44:C1:1219:A:N7 | 44:C1:1448:A:N6 | 2.64 | 0.46 |
| 45:C2:95:U:H2' | 45:C2:96:C:H6 | 1.80 | 0.46 |
| 47:CV:201:LEU:HD12 | 47:CV:202:SER:HB3 | 1.97 | 0.46 |
| 50:US:224:PHE:CD2 | 50:US:281:GLN:HG2 | 2.50 | 0.46 |
| 52:CX:238:ARG:HH11 | 52:CX:241:LEU:HD23 | 1.81 | 0.46 |
| 52:CX:368:LYS:O | 52:CX:368:LYS:NZ | 2.49 | 0.46 |
| 49:UI:165:ASP:OD1 | 49:UI:167:ASP:N | 2.49 | 0.46 |
| 49:UI:185:ILE:HA | 49:UI:188:MET:HE3 | 1.98 | 0.46 |
| 49:UI:266:LEU:HA | 49:UI:269:GLN:NE2 | 2.29 | 0.46 |
| 4:UD:141:PRO:HG3 | 4:UD:197:HIS:CD2 | 2.51 | 0.46 |
| 4:UD:754:PRO:HG3 | 13:UQ:346:ILE:HD11 | 1.98 | 0.46 |
| 5:UF:36:LEU:HD13 | 5:UF:36:LEU:HA | 1.75 | 0.46 |
| 7:UJ:189:ARG:HA | 7:UJ:189:ARG:HH11 | 1.80 | 0.46 |
| 8:UK:10:ARG:NH1 | 44:C1:1136:G:N7 | 2.64 | 0.46 |
| 10:UM:782:ASN:OD1 | 10:UM:782:ASN:N | 2.48 | 0.46 |
| 11:UN:316:TYR:OH | 28:CM:270:ARG:O | 2.33 | 0.46 |
| 11:UN:374:LEU:HD23 | 11:UN:374:LEU:HA | 1.80 | 0.46 |
| 15:UU:241:LEU:HA | 15:UU:241:LEU:HD23 | 1.72 | 0.46 |
| 15:UU:928:LEU:HD23 | 15:UU:929:LEU:HD12 | 1.96 | 0.46 |
| 16:UX:12:GLU:HG2 | 45:C2:48:G:H1' | 1.98 | 0.46 |
| 18:CA:218:MET:HB2 | 18:CA:219:LEU:HD12 | 1.97 | 0.46 |
| 18:CA:306:TYR:CD1 | 18:CA:307:LEU:HD13 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:CC:195:ALA:HB1 | 19:CC:216:ASN:HB2 | 1.98 | 0.46 |
| 24:CI:336:ALA:H | 24:CI:341:ARG:NH2 | 2.14 | 0.46 |
| 28:CM:93:VAL:HB | 28:CM:104:TRP:HB3 | 1.98 | 0.46 |
| 28:CM:260:GLU:C | 28:CM:262:HIS:H | 2.23 | 0.46 |
| 32:CS:908:VAL:HA | 32:CS:911:ILE:HG22 | 1.98 | 0.46 |
| 34:Cc:16:LEU:HD23 | 34:Cc:16:LEU:HA | 1.74 | 0.46 |
| 34:Cc:206:ARG:HA | 34:Cc:209:LYS:HE2 | 1.98 | 0.46 |
| 36:Cg:24:SER:O | 36:Cg:28:LEU:HG | 2.16 | 0.46 |
| 36:Cg:90:LYS:HD3 | 36:Cg:91:LEU:H | 1.80 | 0.46 |
| 37:Ch:108:ASP:OD1 | 44:C1:1463:G:O2' | 2.34 | 0.46 |
| 41:Cn:103:LEU:N | 41:Cn:126:LYS:O | 2.47 | 0.46 |
| 50:US:364:LEU:HD12 | 50:US:364:LEU:HA | 1.76 | 0.46 |
| 1:UA:661:ARG:HG3 | 27:CL:636:TRP:CE3 | 2.51 | 0.45 |
| 4:UD:248:ASP:OD1 | 4:UD:248:ASP:N | 2.47 | 0.45 |
| 4:UD:446:SER:OG | 4:UD:446:SER:O | 2.34 | 0.45 |
| 4:UD:717:SER:O | 4:UD:717:SER:OG | 2.31 | 0.45 |
| 7:UJ:71:ALA:O | 7:UJ:75:SER:OG | 2.31 | 0.45 |
| 8:UK:35:ARG:O | 8:UK:39:ARG:HG2 | 2.15 | 0.45 |
| 9:UL:444:ALA:HB1 | 9:UL:468:ALA:HB1 | 1.98 | 0.45 |
| 13:UQ:189:ASP:OD2 | 13:UQ:190:MET:N | 2.49 | 0.45 |
| 13:UQ:947:GLN:O | 13:UQ:950:SER:OG | 2.31 | 0.45 |
| 17:UZ:75:SER:HA | 17:UZ:78:LEU:HB2 | 1.97 | 0.45 |
| 17:UZ:163:LEU:HD23 | 17:UZ:166:ALA:HB3 | 1.98 | 0.45 |
| 19:CC:184:LEU:HD21 | 19:CC:291:LEU:HB3 | 1.98 | 0.45 |
| 19:CC:199:ARG:HA | 19:CC:219:TYR:CE2 | 2.52 | 0.45 |
| 20:CD:240:ALA:O | 20:CD:244:SER:HB2 | 2.15 | 0.45 |
| 20:CD:301:LEU:HD22 | 20:CD:322:LEU:HD23 | 1.96 | 0.45 |
| 20:CD:345:TYR:HE1 | 20:CD:358:LYS:HD3 | 1.80 | 0.45 |
| 22:CG:243:GLN:HE21 | 22:CG:282:LYS:HA | 1.80 | 0.45 |
| 24:CI:172:HIS:HB3 | 24:CI:175:LEU:HD13 | 1.96 | 0.45 |
| 24:CI:384:LYS:HE3 | 24:CI:384:LYS:HB2 | 1.77 | 0.45 |
| 27:CL:716:ARG:HD2 | 44:C1:2222:C:N3 | 2.31 | 0.45 |
| 30:CP:62:LEU:HD21 | 30:CP:80:VAL:HG13 | 1.99 | 0.45 |
| 32:CR:569:VAL:HG23 | 32:CR:585:VAL:HG12 | 1.98 | 0.45 |
| 32:CR:897:LEU:HD22 | 32:CR:908:VAL:HG11 | 1.98 | 0.45 |
| 32:CS:78:ILE:HA | 32:CS:81:GLU:HG2 | 1.97 | 0.45 |
| 32:CS:530:HIS:HB2 | 32:CS:533:SER:HB3 | 1.97 | 0.45 |
| 34:Cc:44:SER:HA | 42:Cp:54:ILE:HB | 1.97 | 0.45 |
| 40:Cm:102:VAL:HG22 | 40:Cm:113:HIS:HD2 | 1.81 | 0.45 |
| 43:CU:115:GLU:HA | 43:CU:118:VAL:HG12 | 1.98 | 0.45 |
| 44:C1:2177:G:O2' | 44:C1:2183:A:N6 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:C2:149:U:H2' | 45:C2:150:G:C8 | 2.50 | 0.45 |
| 46:UV:409:TRP:CD1 | 46:UV:409:TRP:H | 2.33 | 0.45 |
| 49:UE:277:LYS:HD2 | 49:UE:277:LYS:HA | 1.81 | 0.45 |
| 54:Cz:1520:MET:O | 54:Cz:1523:ASN:ND2 | 2.49 | 0.45 |
| 1:UA:191:LEU:HD23 | 1:UA:222:TRP:CE3 | 2.51 | 0.45 |
| 1:UA:332:TYR:CE2 | 15:UU:866:PRO:HB3 | 2.51 | 0.45 |
| 2:UB:338:LYS:HD2 | 2:UB:338:LYS:HA | 1.67 | 0.45 |
| 2:UB:742:LYS:HB2 | 2:UB:743:LEU:HD12 | 1.98 | 0.45 |
| 7:UJ:25:LEU:O | 7:UJ:28:SER:OG | 2.27 | 0.45 |
| 7:UJ:286:ASP:HA | 7:UJ:289:LEU:HD12 | 1.97 | 0.45 |
| 7:UJ:355:ALA:HA | 7:UJ:358:LEU:HD12 | 1.97 | 0.45 |
| 8:UK:97:SER:OG | 44:C1:233:C:O2' | 2.15 | 0.45 |
| 11:UN:912:LYS:HZ1 | 28:CM:370:GLN:HE22 | 1.64 | 0.45 |
| 13:UQ:225:MET:SD | 13:UQ:274:TRP:NE1 | 2.86 | 0.45 |
| 13:UQ:364:SER:HB3 | 13:UQ:369:TYR:O | 2.15 | 0.45 |
| 13:UQ:694:SER:HB3 | 13:UQ:699:ILE:HG23 | 1.98 | 0.45 |
| 15:UU:734:TRP:HA | 15:UU:740:HIS:O | 2.17 | 0.45 |
| 15:UU:972:LEU:HD21 | 15:UU:976:ARG:HH22 | 1.81 | 0.45 |
| 18:CA:109:ILE:HG12 | 33:CT:140:ILE:HD13 | 1.98 | 0.45 |
| 19:CC:188:ASP:O | 19:CC:192:ASN:ND2 | 2.49 | 0.45 |
| 20:CD:415:LYS:HE2 | 20:CD:415:LYS:HB2 | 1.66 | 0.45 |
| 24:CI:59:VAL:HG12 | 24:CI:746:LEU:HD22 | 1.98 | 0.45 |
| 25:CJ:87:ILE:HD13 | 25:CJ:106:PHE:CE2 | 2.51 | 0.45 |
| 25:CJ:115:MET:HE1 | 25:CJ:136:VAL:HG21 | 1.98 | 0.45 |
| 29:CN:116:THR:O | 29:CN:119:GLY:N | 2.46 | 0.45 |
| 29:CN:145:LEU:HD23 | 29:CN:145:LEU:HA | 1.71 | 0.45 |
| 32:CS:647:MET:SD | 32:CS:649:TYR:OH | 2.66 | 0.45 |
| 32:CS:897:LEU:HD22 | 32:CS:908:VAL:HG11 | 1.98 | 0.45 |
| 37:Ch:107:LYS:NZ | 44:C1:1465:C:OP1 | 2.49 | 0.45 |
| 39:Cj:67:ILE:HD13 | 39:Cj:81:VAL:HG13 | 1.97 | 0.45 |
| 44:C1:26:C:N4 | 44:C1:27:A:H62 | 2.11 | 0.45 |
| 44:C1:287:C:H2' | 44:C1:288:C:C6 | 2.52 | 0.45 |
| 44:C1:399:G:H2' | 44:C1:400:C:H6 | 1.81 | 0.45 |
| 44:C1:1156:C:P | 44:C1:1157:C:H41 | 2.38 | 0.45 |
| 46:UV:1061:ALA:HB2 | 46:UV:1106:THR:HA | 1.99 | 0.45 |
| 48:UH:871:LEU:HG | 49:UE:265:MET:HE1 | 1.98 | 0.45 |
| 49:UE:244:ARG:HD3 | 49:UE:244:ARG:HA | 1.65 | 0.45 |
| 50:US:227:LEU:HB3 | 50:US:269:TRP:CZ2 | 2.51 | 0.45 |
| 54:Cz:1604:PHE:HB3 | 54:Cz:1622:TYR:HD1 | 1.82 | 0.45 |
| 2:UB:777:LEU:HA | 2:UB:780:LEU:HB2 | 1.99 | 0.45 |
| 4:UD:7:ARG:HD3 | 4:UD:866:PRO:HG3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:UD:252:GLY:HA3 | 4:UD:279:VAL:HG11 | 1.98 | 0.45 |
| 6:UG:270:ASN:HB2 | 6:UG:272:ILE:HG12 | 1.97 | 0.45 |
| 6:UG:403:PHE:HB3 | 28:CM:8:ARG:HH12 | 1.81 | 0.45 |
| 7:UJ:179:ARG:NH1 | 13:UQ:930:PHE:HB3 | 2.31 | 0.45 |
| 7:UJ:514:PHE:CZ | 7:UJ:557:ARG:HB3 | 2.51 | 0.45 |
| 10:UM:595:ALA:HB3 | 10:UM:614:VAL:HB | 1.97 | 0.45 |
| 14:UR:555:LEU:HB3 | 14:UR:569:VAL:HB | 1.98 | 0.45 |
| 15:UU:415:ARG:NH2 | 15:UU:458:GLU:O | 2.50 | 0.45 |
| 15:UU:976:ARG:O | 15:UU:979:THR:OG1 | 2.32 | 0.45 |
| 17:UZ:86:PRO:HG3 | 17:UZ:261:THR:HG21 | 1.99 | 0.45 |
| 18:CA:164:GLY:HA2 | 18:CA:167:VAL:HB | 1.98 | 0.45 |
| 19:CC:176:HIS:HD2 | 19:CC:177:ILE:HD13 | 1.80 | 0.45 |
| 19:CC:241:ALA:HA | 19:CC:246:GLN:HB2 | 1.98 | 0.45 |
| 20:CD:346:HIS:CE1 | 45:C2:90:C:H42 | 2.34 | 0.45 |
| 22:CG:358:LYS:HB2 | 22:CG:363:SER:HB3 | 1.97 | 0.45 |
| 22:CG:586:MET:N | 22:CG:586:MET:SD | 2.89 | 0.45 |
| 23:CH:167:PRO:HA | 23:CH:168:PRO:HD3 | 1.81 | 0.45 |
| 24:CI:960:GLY:HA2 | 26:CK:287:TYR:CE1 | 2.51 | 0.45 |
| 26:CK:117:LEU:HD11 | 39:Cj:126:PRO:HG2 | 1.98 | 0.45 |
| 26:CK:188:TYR:CD1 | 26:CK:213:PRO:HG3 | 2.51 | 0.45 |
| 28:CM:39:GLU:OE2 | 28:CM:382:TYR:OH | 2.31 | 0.45 |
| 28:CM:65:HIS:HB2 | 28:CM:69:VAL:HG22 | 1.97 | 0.45 |
| 28:CM:155:PRO:HB3 | 35:Ce:155:ASP:OD1 | 2.16 | 0.45 |
| 31:CQ:161:LEU:HB2 | 31:CQ:164:LEU:HD22 | 1.98 | 0.45 |
| 31:CQ:223:GLU:O | 31:CQ:227:MET:HG2 | 2.15 | 0.45 |
| 33:CT:152:LEU:HD13 | 33:CT:152:LEU:HA | 1.83 | 0.45 |
| 39:Cj:104:LEU:HD12 | 39:Cj:104:LEU:HA | 1.71 | 0.45 |
| 44:C1:381:G:H21 | 44:C1:385:A:N6 | 2.14 | 0.45 |
| 44:C1:2046:C:H2' | 44:C1:2047:G:C8 | 2.51 | 0.45 |
| 46:UV:727:ARG:HH21 | 46:UV:731:ARG:NH1 | 2.15 | 0.45 |
| 48:UH:860:THR:OG1 | 48:UH:930:ARG:NH2 | 2.47 | 0.45 |
| 50:US:220:ARG:HG2 | 50:US:281:GLN:HE22 | 1.80 | 0.45 |
| 50:US:342:LYS:HD2 | 50:US:342:LYS:HA | 1.72 | 0.45 |
| 50:US:385:LEU:HA | 50:US:385:LEU:HD13 | 1.76 | 0.45 |
| 54:Cz:1564:ASP:O | 54:Cz:1568:GLN:HG2 | 2.17 | 0.45 |
| 1:UA:278:ILE:HG13 | 1:UA:293:LEU:C | 2.41 | 0.45 |
| 1:UA:416:ASN:N | 1:UA:416:ASN:OD1 | 2.38 | 0.45 |
| 2:UB:13:LEU:HD12 | 2:UB:16:GLN:HB2 | 1.98 | 0.45 |
| 2:UB:106:GLU:O | 2:UB:109:ARG:N | 2.50 | 0.45 |
| 6:UG:342:ARG:NH1 | 44:C1:265:G:N3 | 2.63 | 0.45 |
| 7:UJ:251:ILE:HG22 | 7:UJ:255:LEU:HD22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:UJ:578:ARG:NH1 | 7:UJ:584:CYS:SG | 2.90 | 0.45 |
| 9:UL:260:LEU:N | 9:UL:262:GLN:OE1 | 2.50 | 0.45 |
| 11:UN:303:ALA:N | 11:UN:306:GLN:HE21 | 2.15 | 0.45 |
| 11:UN:329:THR:HG22 | 11:UN:938:TYR:H | 1.81 | 0.45 |
| 12:UO:271:ASN:O | 12:UO:298:LYS:NZ | 2.34 | 0.45 |
| 13:UQ:540:LYS:HA | 13:UQ:540:LYS:HD2 | 1.63 | 0.45 |
| 15:UU:217:LYS:HE2 | 15:UU:217:LYS:HB2 | 1.84 | 0.45 |
| 15:UU:927:LYS:HE3 | 15:UU:927:LYS:HB3 | 1.67 | 0.45 |
| 19:CC:232:LEU:HD12 | 19:CC:255:ILE:HA | 1.98 | 0.45 |
| 21:CF:110:ASP:O | 21:CF:113:SER:OG | 2.29 | 0.45 |
| 23:CH:123:PHE:HA | 23:CH:405:ASN:HB3 | 1.98 | 0.45 |
| 23:CH:150:ILE:HD12 | 23:CH:175:VAL:HG11 | 1.98 | 0.45 |
| 24:CI:128:ASP:O | 24:CI:132:VAL:HG23 | 2.17 | 0.45 |
| 24:CI:223:SER:HA | 24:CI:226:LEU:HG | 1.98 | 0.45 |
| 24:CI:1075:TYR:CZ | 24:CI:1079:ARG:HD2 | 2.52 | 0.45 |
| 25:CJ:68:ASN:OD1 | 25:CJ:69:GLU:N | 2.50 | 0.45 |
| 27:CL:653:VAL:HG12 | 27:CL:654:ALA:H | 1.80 | 0.45 |
| 28:CM:13:GLN:HG3 | 28:CM:14:GLN:HG3 | 1.98 | 0.45 |
| 32:CR:211:ILE:H | 32:CR:211:ILE:HG12 | 1.35 | 0.45 |
| 44:C1:2:G:H2' | 44:C1:3:G:C8 | 2.52 | 0.45 |
| 44:C1:64:C:H2' | 44:C1:65:C:O4' | 2.16 | 0.45 |
| 44:C1:493:G:H2' | 44:C1:494:G:C8 | 2.51 | 0.45 |
| 46:UV:715:GLN:NE2 | 46:UV:775:GLU:OE2 | 2.44 | 0.45 |
| 48:UH:723:VAL:HG13 | 48:UH:786:ALA:HA | 1.99 | 0.45 |
| 52:CX:275:ARG:O | 52:CX:279:HIS:ND1 | 2.38 | 0.45 |
| 52:CX:433:LEU:HD13 | 52:CX:436:LEU:HD23 | 1.99 | 0.45 |
| 1:UA:146:THR:O | 1:UA:147:HIS:ND1 | 2.49 | 0.45 |
| 1:UA:168:SER:OG | 1:UA:178:TRP:NE1 | 2.35 | 0.45 |
| 2:UB:758:GLN:HA | 2:UB:761:LEU:HB2 | 1.98 | 0.45 |
| 5:UF:398:ILE:O | 5:UF:402:LEU:HG | 2.17 | 0.45 |
| 7:UJ:533:ARG:HH12 | 7:UJ:537:THR:HG22 | 1.81 | 0.45 |
| 9:UL:119:ASP:HB3 | 9:UL:122:GLY:N | 2.32 | 0.45 |
| 9:UL:130:LYS:NZ | 44:C1:2332:A:O2' | 2.40 | 0.45 |
| 9:UL:152:LYS:HA | 27:CL:710:ARG:CZ | 2.45 | 0.45 |
| 9:UL:569:LEU:HD11 | 9:UL:585:LEU:HA | 1.99 | 0.45 |
| 13:UQ:849:ALA:O | 13:UQ:851:GLN:N | 2.50 | 0.45 |
| 13:UQ:935:ALA:HA | 13:UQ:938:MET:HE3 | 1.98 | 0.45 |
| 14:UR:457:ASP:O | 14:UR:459:GLY:N | 2.50 | 0.45 |
| 15:UU:637:VAL:HG22 | 15:UU:649:TRP:HB2 | 1.98 | 0.45 |
| 16:UX:139:GLN:HA | 16:UX:142:ARG:HH22 | 1.82 | 0.45 |
| 18:CA:157:LEU:HD23 | 18:CA:226:ILE:HG12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:CA:191:ARG:HH12 | 19:CC:168:PHE:HA | 1.79 | 0.45 |
| 18:CB:112:GLU:HB3 | 18:CB:123:THR:H | 1.81 | 0.45 |
| 19:CC:221:LYS:HA | 19:CC:224:LEU:HD12 | 1.98 | 0.45 |
| 19:CC:403:PHE:HZ | 22:CG:446:ASP:HA | 1.81 | 0.45 |
| 20:CD:147:HIS:HB3 | 20:CD:151:ARG:NH1 | 2.31 | 0.45 |
| 24:CI:548:ASP:OD2 | 24:CI:551:LEU:N | 2.49 | 0.45 |
| 24:CI:754:LYS:HB3 | 24:CI:754:LYS:HE3 | 1.69 | 0.45 |
| 29:CO:95:CYS:O | 29:CO:98:THR:OG1 | 2.31 | 0.45 |
| 32:CS:34:ALA:HB3 | 32:CS:154:LYS:NZ | 2.32 | 0.45 |
| 44:C1:7:A:H2' | 44:C1:8:U:C6 | 2.52 | 0.45 |
| 46:UV:299:ALA:HB2 | 46:UV:356:LEU:HD23 | 1.99 | 0.45 |
| 46:UV:445:THR:HG23 | 46:UV:446:HIS:CD2 | 2.51 | 0.45 |
| 46:UV:755:PHE:HE1 | 46:UV:769:ARG:HD3 | 1.82 | 0.45 |
| 48:UH:604:LYS:HD3 | 48:UH:604:LYS:HA | 1.76 | 0.45 |
| 54:Cz:1672:ASP:O | 54:Cz:1675:GLN:N | 2.49 | 0.45 |
| 5:UF:375:LYS:HD3 | 5:UF:375:LYS:HA | 1.74 | 0.45 |
| 5:UF:385:MET:HA | 5:UF:388:ILE:HB | 1.99 | 0.45 |
| 6:UG:189:ASN:OD1 | 6:UG:189:ASN:N | 2.50 | 0.45 |
| 9:UL:668:TYR:HB3 | 9:UL:680:TYR:CE1 | 2.51 | 0.45 |
| 11:UN:350:ARG:HH22 | 44:C1:453:G:P | 2.39 | 0.45 |
| 13:UQ:298:ILE:HB | 13:UQ:311:ASP:O | 2.16 | 0.45 |
| 15:UU:534:TRP:HB3 | 15:UU:536:PHE:CE1 | 2.52 | 0.45 |
| 23:CH:95:SER:O | 23:CH:95:SER:OG | 2.30 | 0.45 |
| 25:CJ:131:ILE:HD11 | 25:CJ:146:PRO:HB3 | 1.99 | 0.45 |
| 27:CL:561:ARG:HG2 | 27:CL:563:ASP:H | 1.82 | 0.45 |
| 27:CL:697:THR:OG1 | 27:CL:701:ILE:N | 2.49 | 0.45 |
| 32:CS:212:SER:O | 32:CS:215:LYS:NZ | 2.44 | 0.45 |
| 32:CS:485:ASN:HA | 32:CS:488:LYS:HG3 | 1.99 | 0.45 |
| 32:CS:791:SER:HA | 32:CS:795:ARG:HA | 1.97 | 0.45 |
| 36:Cg:141:VAL:HG22 | 36:Cg:143:SER:H | 1.81 | 0.45 |
| 44:C1:350:U:H5" | 44:C1:351:U:H5' | 1.97 | 0.45 |
| 44:C1:1078:U:H5" | 44:C1:1080:G:H1' | 1.97 | 0.45 |
| 44:C1:2230:U:H2' | 44:C1:2231:A:H8 | 1.81 | 0.45 |
| 45:C2:137:U:H2' | 45:C2:138:A:C8 | 2.52 | 0.45 |
| 45:C2:200:U:O4 | 45:C2:246:G:O6 | 2.34 | 0.45 |
| 46:UV:395:ASP:O | 46:UV:399:GLN:N | 2.49 | 0.45 |
| 46:UV:460:SER:C | 46:UV:612:ARG:HG3 | 2.42 | 0.45 |
| 46:UV:550:GLY:H | 46:UV:585:ARG:NH2 | 2.14 | 0.45 |
| 1:UA:306:ASN:OD1 | 1:UA:308:SER:N | 2.46 | 0.45 |
| 1:UA:629:LEU:HG | 1:UA:636:VAL:HG12 | 1.99 | 0.45 |
| 4:UD:872:LEU:O | 53:UP:356:ARG:NH2 | 2.39 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:UF:385:MET:SD | 5:UF:406:LYS:HB2 | 2.56 | 0.45 |
| 6:UG:256:THR:HG21 | 6:UG:277:GLN:NE2 | 2.30 | 0.45 |
| 6:UG:267:ASN:O | 6:UG:271:ALA:N | 2.50 | 0.45 |
| 7:UJ:309:LEU:O | 7:UJ:313:THR:HG23 | 2.16 | 0.45 |
| 7:UJ:711:CYS:HA | 7:UJ:714:VAL:HG22 | 1.99 | 0.45 |
| 8:UK:29:GLU:O | 24:CI:956:SER:OG | 2.23 | 0.45 |
| 8:UK:79:ARG:HB2 | 8:UK:83:PHE:HB2 | 1.99 | 0.45 |
| 8:UK:268:ARG:HG3 | 21:CE:93:GLY:C | 2.42 | 0.45 |
| 9:UL:675:ASP:OD1 | 9:UL:677:THR:OG1 | 2.25 | 0.45 |
| 10:UM:446:HIS:CE1 | 10:UM:487:LEU:HD22 | 2.52 | 0.45 |
| 10:UM:582:LEU:HD23 | 10:UM:627:TRP:CD2 | 2.52 | 0.45 |
| 12:UO:397:LEU:HB3 | 14:UR:297:ILE:HD11 | 1.99 | 0.45 |
| 13:UQ:291:SER:HB3 | 13:UQ:448:LYS:HE2 | 1.99 | 0.45 |
| 13:UQ:364:SER:OG | 13:UQ:369:TYR:O | 2.33 | 0.45 |
| 15:UU:72:GLN:HG2 | 15:UU:85:VAL:HG23 | 1.98 | 0.45 |
| 17:UZ:82:LYS:HG2 | 17:UZ:181:PRO:HG2 | 1.99 | 0.45 |
| 18:CB:76:HIS:CE1 | 18:CB:78:HIS:HD2 | 2.35 | 0.45 |
| 19:CC:189:LYS:HA | 19:CC:192:ASN:HD22 | 1.81 | 0.45 |
| 24:CI:248:ASN:HB2 | 24:CI:337:PRO:HB2 | 1.99 | 0.45 |
| 24:CI:1095:GLN:O | 24:CI:1099:THR:HG23 | 2.16 | 0.45 |
| 25:CJ:79:LEU:HD23 | 25:CJ:79:LEU:HA | 1.58 | 0.45 |
| 25:CJ:125:GLN:NE2 | 44:C1:416:U:O3’ | 2.50 | 0.45 |
| 32:CS:720:LEU:O | 32:CS:767:GLN:NE2 | 2.49 | 0.45 |
| 33:CT:87:LEU:H | 33:CT:92:ASN:HA | 1.81 | 0.45 |
| 43:CU:204:LYS:NZ | 43:CU:207:ASP:OD2 | 2.50 | 0.45 |
| 44:C1:494:G:H3’ | 44:C1:495:G:H21 | 1.81 | 0.45 |
| 44:C1:496:U:N3 | 44:C1:503:G:N1 | 2.65 | 0.45 |
| 44:C1:2328:G:H2’ | 44:C1:2329:A:C8 | 2.52 | 0.45 |
| 45:C2:87:G:C6 | 45:C2:263:U:O2 | 2.69 | 0.45 |
| 48:UH:719:ALA:O | 48:UH:722:THR:OG1 | 2.31 | 0.45 |
| 49:UE:272:TYR:HB2 | 49:UI:223:VAL:CG1 | 2.47 | 0.45 |
| 2:UB:621:TYR:CZ | 2:UB:625:LYS:HD3 | 2.51 | 0.45 |
| 7:UJ:156:PRO:HB2 | 7:UJ:159:ARG:HB2 | 1.99 | 0.45 |
| 7:UJ:558:VAL:HA | 7:UJ:563:TYR:HE2 | 1.82 | 0.45 |
| 11:UN:935:LYS:HG2 | 11:UN:936:PRO:HD2 | 1.99 | 0.45 |
| 14:UR:170:GLU:O | 14:UR:174:ARG:HG2 | 2.17 | 0.45 |
| 14:UR:542:SER:HB2 | 14:UR:561:HIS:HE1 | 1.82 | 0.45 |
| 18:CB:72:ILE:HG13 | 18:CB:85:ARG:HH22 | 1.82 | 0.45 |
| 19:CC:14:GLY:HA2 | 19:CC:56:TRP:CE2 | 2.52 | 0.45 |
| 19:CC:68:LEU:HD12 | 19:CC:75:PRO:HB3 | 1.99 | 0.45 |
| 22:CG:231:LYS:NZ | 45:C2:119:C:N3 | 2.62 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:CH:285:THR:HB | 23:CH:290:VAL:HB | 1.98 | 0.45 |
| 24:CI:391:LYS:HB2 | 32:CR:170:HIS:HE2 | 1.81 | 0.45 |
| 28:CM:374:TYR:O | 28:CM:378:LEU:HB2 | 2.16 | 0.45 |
| 28:CM:424:LYS:HD3 | 28:CM:429:LYS:HD3 | 1.98 | 0.45 |
| 29:CN:95:CYS:O | 29:CN:98:THR:OG1 | 2.35 | 0.45 |
| 31:CQ:128:LYS:HA | 31:CQ:128:LYS:HD3 | 1.76 | 0.45 |
| 32:CR:851:TYR:O | 32:CR:855:LEU:HB2 | 2.15 | 0.45 |
| 44:C1:447:C:H2' | 44:C1:448:C:C6 | 2.51 | 0.45 |
| 44:C1:1122:A:H5" | 44:C1:1127:C:H41 | 1.82 | 0.45 |
| 44:C1:2095:G:N1 | 44:C1:2096:G:C6 | 2.85 | 0.45 |
| 45:C2:64:C:H2' | 45:C2:65:C:C6 | 2.51 | 0.45 |
| 52:CX:262:VAL:HG12 | 52:CX:266:MET:HE3 | 1.99 | 0.45 |
| 52:CX:407:PRO:HB2 | 52:CX:409:ILE:HG22 | 1.98 | 0.45 |
| 1:UA:552:ARG:NH2 | 1:UA:552:ARG:O | 2.50 | 0.45 |
| 1:UA:582:MET:HG3 | 1:UA:682:PRO:HA | 1.99 | 0.45 |
| 1:UA:712:ASN:ND2 | 1:UA:714:GLU:OE2 | 2.49 | 0.45 |
| 2:UB:89:GLU:OE2 | 27:CL:535:GLU:HA | 2.17 | 0.45 |
| 2:UB:597:ILE:HG23 | 2:UB:601:PHE:HD2 | 1.82 | 0.45 |
| 4:UD:53:ILE:HG12 | 4:UD:69:ILE:HB | 1.99 | 0.45 |
| 6:UG:134:LEU:HD11 | 7:UJ:5:LEU:HD13 | 1.99 | 0.45 |
| 7:UJ:542:ARG:NE | 7:UJ:578:ARG:HE | 2.15 | 0.45 |
| 9:UL:287:HIS:CD2 | 9:UL:290:ARG:HB2 | 2.51 | 0.45 |
| 12:UO:76:THR:OG1 | 12:UO:76:THR:O | 2.34 | 0.45 |
| 12:UO:283:SER:OG | 12:UO:286:ARG:NH2 | 2.50 | 0.45 |
| 12:UO:490:ALA:O | 12:UO:495:ARG:NH2 | 2.48 | 0.45 |
| 13:UQ:849:ALA:O | 13:UQ:851:GLN:HG2 | 2.17 | 0.45 |
| 14:UR:307:ALA:HB3 | 14:UR:311:PRO:HA | 1.98 | 0.45 |
| 15:UU:679:LEU:HD23 | 15:UU:679:LEU:HA | 1.81 | 0.45 |
| 18:CB:171:ALA:HA | 18:CB:174:VAL:HG22 | 1.99 | 0.45 |
| 20:CD:335:LYS:NZ | 24:CI:1079:ARG:O | 2.41 | 0.45 |
| 24:CI:958:ILE:HG23 | 24:CI:978:GLU:HB3 | 1.98 | 0.45 |
| 26:CK:196:PHE:HZ | 26:CK:237:ILE:HD12 | 1.81 | 0.45 |
| 28:CM:26:ASN:OD1 | 28:CM:27:LEU:N | 2.49 | 0.45 |
| 28:CM:134:LEU:HB3 | 28:CM:148:ALA:HB3 | 1.99 | 0.45 |
| 32:CR:34:ALA:HB3 | 32:CR:154:LYS:NZ | 2.32 | 0.45 |
| 32:CR:485:ASN:HA | 32:CR:488:LYS:HG3 | 1.99 | 0.45 |
| 35:Ce:34:GLU:HA | 35:Ce:41:LYS:HE2 | 1.98 | 0.45 |
| 43:CU:245:ARG:HD3 | 43:CU:245:ARG:HA | 1.57 | 0.45 |
| 44:C1:97:C:H2' | 44:C1:98:A:O4' | 2.17 | 0.45 |
| 44:C1:401:C:H3' | 44:C1:402:U:H5" | 1.98 | 0.45 |
| 45:C2:87:G:C6 | 45:C2:263:U:N3 | 2.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:175:HIS:ND1 | 46:UV:178:LYS:HE3 | 2.32 | 0.45 |
| 48:UH:896:ILE:O | 48:UH:900:ILE:HG12 | 2.17 | 0.45 |
| 49:UE:185:ILE:HA | 49:UE:188:MET:HE3 | 1.98 | 0.45 |
| 50:US:189:PHE:O | 50:US:193:TYR:N | 2.41 | 0.45 |
| 50:US:335:ASP:OD1 | 50:US:335:ASP:N | 2.41 | 0.45 |
| 52:CX:413:CYS:HA | 52:CX:416:VAL:HG12 | 1.98 | 0.45 |
| 54:Cz:1672:ASP:HB3 | 54:Cz:1675:GLN:HG3 | 1.99 | 0.45 |
| 1:UA:116:LYS:O | 1:UA:153:ASP:HA | 2.17 | 0.45 |
| 4:UD:253:ASP:OD2 | 4:UD:257:GLN:HB2 | 2.17 | 0.45 |
| 4:UD:324:HIS:CE1 | 4:UD:875:ARG:HD2 | 2.52 | 0.45 |
| 4:UD:480:GLY:O | 4:UD:497:GLU:HG3 | 2.17 | 0.45 |
| 4:UD:804:ARG:HA | 4:UD:807:ASN:ND2 | 2.32 | 0.45 |
| 6:UG:80:LYS:HE2 | 6:UG:80:LYS:HB3 | 1.81 | 0.45 |
| 6:UG:247:THR:OG1 | 6:UG:249:GLN:HG2 | 2.17 | 0.45 |
| 7:UJ:124:ARG:NE | 7:UJ:124:ARG:O | 2.50 | 0.45 |
| 9:UL:517:HIS:CD2 | 9:UL:519:ASP:H | 2.34 | 0.45 |
| 10:UM:15:ASN:HB2 | 10:UM:719:PHE:CD2 | 2.52 | 0.45 |
| 10:UM:766:HIS:HB2 | 27:CL:707:GLU:CD | 2.42 | 0.45 |
| 12:UO:218:ASP:OD1 | 12:UO:219:ALA:N | 2.50 | 0.45 |
| 14:UR:241:LYS:HD3 | 14:UR:241:LYS:HA | 1.73 | 0.45 |
| 19:CC:233:THR:HG23 | 19:CC:236:SER:HB3 | 1.99 | 0.45 |
| 19:CC:299:MET:HG2 | 19:CC:307:GLN:HB2 | 1.99 | 0.45 |
| 20:CD:6:LEU:HB3 | 20:CD:90:VAL:HB | 1.99 | 0.45 |
| 24:CI:220:HIS:O | 24:CI:223:SER:OG | 2.31 | 0.45 |
| 24:CI:287:HIS:CE1 | 24:CI:289:ALA:HA | 2.52 | 0.45 |
| 24:CI:330:LYS:HD3 | 32:CR:100:SER:O | 2.16 | 0.45 |
| 28:CM:216:VAL:HG21 | 28:CM:242:CYS:HB3 | 1.97 | 0.45 |
| 29:CO:137:PHE:O | 29:CO:141:MET:HG2 | 2.17 | 0.45 |
| 30:CP:100:LYS:HE3 | 30:CP:100:LYS:HB3 | 1.79 | 0.45 |
| 32:CR:786:PHE:HA | 32:CR:789:LEU:HB2 | 1.99 | 0.45 |
| 32:CR:908:VAL:HA | 32:CR:911:ILE:HG22 | 1.98 | 0.45 |
| 35:Ce:139:LEU:HD13 | 35:Ce:183:TYR:HD2 | 1.81 | 0.45 |
| 44:C1:421:A:H2' | 44:C1:422:A:C8 | 2.52 | 0.45 |
| 44:C1:421:A:H2' | 44:C1:422:A:H8 | 1.81 | 0.45 |
| 44:C1:496:U:O4 | 44:C1:503:G:C6 | 2.70 | 0.45 |
| 44:C1:1508:A:H2' | 44:C1:1509:A:H8 | 1.81 | 0.45 |
| 1:UA:381:HIS:CE1 | 1:UA:407:ARG:HB2 | 2.53 | 0.44 |
| 2:UB:84:ILE:HG22 | 2:UB:86:GLY:H | 1.82 | 0.44 |
| 8:UK:8:ILE:HD12 | 8:UK:11:ARG:HD3 | 1.99 | 0.44 |
| 9:UL:50:TRP:HA | 9:UL:58:LEU:H | 1.82 | 0.44 |
| 10:UM:792:LYS:H | 10:UM:792:LYS:HG3 | 1.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:UO:286:ARG:HB3 | 12:UO:287:ARG:HH22 | 1.82 | 0.44 |
| 13:UQ:158:VAL:O | 13:UQ:165:ILE:HA | 2.17 | 0.44 |
| 14:UR:156:LYS:NZ | 44:C1:272:A:O3' | 2.50 | 0.44 |
| 14:UR:417:ARG:HE | 14:UR:417:ARG:HB3 | 1.55 | 0.44 |
| 15:UU:695:GLU:O | 15:UU:697:LYS:NZ | 2.35 | 0.44 |
| 15:UU:972:LEU:HD13 | 15:UU:1012:LEU:HA | 1.98 | 0.44 |
| 16:UX:27:ARG:NH2 | 45:C2:47:U:H4' | 2.32 | 0.44 |
| 16:UX:48:HIS:CE1 | 36:Cg:24:SER:HG | 2.33 | 0.44 |
| 17:UZ:267:VAL:HG11 | 17:UZ:275:TRP:CZ2 | 2.52 | 0.44 |
| 18:CA:191:ARG:NH1 | 19:CC:168:PHE:HA | 2.32 | 0.44 |
| 18:CB:221:PRO:HA | 20:CD:123:ARG:HD2 | 1.99 | 0.44 |
| 19:CC:310:LEU:HB2 | 19:CC:315:ALA:HB2 | 1.99 | 0.44 |
| 21:CF:106:ASN:OD1 | 21:CF:112:ASN:ND2 | 2.47 | 0.44 |
| 22:CG:393:ALA:O | 22:CG:415:ASN:ND2 | 2.44 | 0.44 |
| 23:CH:295:ASP:OD2 | 23:CH:296:GLU:N | 2.50 | 0.44 |
| 24:CI:194:TRP:NE1 | 24:CI:201:ALA:H | 2.14 | 0.44 |
| 25:CJ:109:ARG:HH11 | 25:CJ:117:ARG:HH22 | 1.65 | 0.44 |
| 26:CK:89:LEU:HD11 | 26:CK:139:ILE:HG13 | 1.99 | 0.44 |
| 29:CN:100:LEU:HA | 29:CN:105:ASN:HD22 | 1.81 | 0.44 |
| 29:CO:44:ALA:HB3 | 29:CO:116:THR:HA | 1.99 | 0.44 |
| 32:CR:4:GLN:HA | 32:CR:4:GLN:NE2 | 2.32 | 0.44 |
| 32:CS:618:VAL:HG11 | 32:CS:627:PHE:CD2 | 2.53 | 0.44 |
| 32:CS:840:ARG:NH1 | 32:CS:856:ASP:OD2 | 2.50 | 0.44 |
| 33:CT:106:LEU:HD23 | 33:CT:106:LEU:HA | 1.75 | 0.44 |
| 40:Cm:35:VAL:O | 40:Cm:39:GLN:HG2 | 2.18 | 0.44 |
| 43:CU:298:ARG:O | 43:CU:298:ARG:NH1 | 2.48 | 0.44 |
| 44:C1:78:G:H2' | 44:C1:79:C:C6 | 2.52 | 0.44 |
| 44:C1:397:U:H2' | 44:C1:398:C:C6 | 2.52 | 0.44 |
| 44:C1:1085:U:H2' | 44:C1:1086:U:C6 | 2.52 | 0.44 |
| 44:C1:1136:G:H2' | 44:C1:1137:G:H8 | 1.81 | 0.44 |
| 45:C2:128:C:H2' | 45:C2:129:U:C6 | 2.52 | 0.44 |
| 48:UH:585:HIS:O | 48:UH:587:SER:N | 2.50 | 0.44 |
| 52:CX:411:HIS:CG | 52:CX:442:HIS:HB2 | 2.51 | 0.44 |
| 53:UP:315:VAL:HG12 | 53:UP:318:THR:H | 1.80 | 0.44 |
| 1:UA:226:ALA:HA | 1:UA:241:MET:HA | 1.98 | 0.44 |
| 1:UA:546:SER:HB3 | 1:UA:604:MET:HE2 | 1.99 | 0.44 |
| 1:UA:794:ILE:HA | 1:UA:797:LEU:HD12 | 1.98 | 0.44 |
| 4:UD:163:LEU:HB3 | 4:UD:179:LEU:HD13 | 1.99 | 0.44 |
| 5:UF:7:LYS:NZ | 44:C1:438:C:OP2 | 2.48 | 0.44 |
| 5:UF:70:LEU:HD13 | 14:UR:55:LEU:HB2 | 1.98 | 0.44 |
| 6:UG:75:LEU:HA | 6:UG:75:LEU:HD12 | 1.77 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:UK:264:LYS:NZ | 44:C1:200:A:OP1 | 2.43 | 0.44 |
| 9:UL:282:ALA:H | 9:UL:297:GLY:HA2 | 1.82 | 0.44 |
| 9:UL:607:LYS:HD2 | 9:UL:607:LYS:HA | 1.85 | 0.44 |
| 10:UM:766:HIS:HA | 10:UM:767:PRO:HD3 | 1.78 | 0.44 |
| 12:UO:129:GLY:H | 12:UO:133:ARG:HB2 | 1.82 | 0.44 |
| 13:UQ:466:LEU:H | 13:UQ:832:ILE:HG13 | 1.83 | 0.44 |
| 14:UR:455:TRP:NE1 | 14:UR:500:LEU:HD21 | 2.32 | 0.44 |
| 15:UU:154:CYS:HB3 | 15:UU:185:LEU:HD21 | 1.99 | 0.44 |
| 15:UU:215:THR:HG23 | 15:UU:217:LYS:HB2 | 2.00 | 0.44 |
| 15:UU:779:ARG:HD3 | 15:UU:783:ARG:HH21 | 1.80 | 0.44 |
| 18:CA:181:TYR:HD1 | 18:CA:204:ILE:HG12 | 1.81 | 0.44 |
| 19:CC:295:LEU:HA | 19:CC:298:LYS:HG2 | 2.00 | 0.44 |
| 19:CC:309:ILE:HG13 | 19:CC:310:LEU:HD12 | 1.99 | 0.44 |
| 20:CD:253:ASP:O | 20:CD:257:ILE:HG13 | 2.17 | 0.44 |
| 20:CD:286:SER:O | 20:CD:286:SER:OG | 2.27 | 0.44 |
| 24:CI:68:PRO:HB2 | 24:CI:115:THR:HG23 | 1.99 | 0.44 |
| 24:CI:280:ALA:H | 24:CI:284:GLN:CD | 2.25 | 0.44 |
| 24:CI:393:VAL:HG13 | 32:CR:530:HIS:CE1 | 2.53 | 0.44 |
| 24:CI:917:LYS:NZ | 44:C1:1141:G:H4' | 2.32 | 0.44 |
| 26:CK:119:ARG:HH12 | 26:CK:124:LEU:HB2 | 1.82 | 0.44 |
| 26:CK:240:ARG:CZ | 26:CK:260:ARG:HB3 | 2.47 | 0.44 |
| 27:CL:626:ILE:HG23 | 27:CL:630:LEU:HD13 | 1.98 | 0.44 |
| 28:CM:171:SER:OG | 28:CM:200:ILE:O | 2.35 | 0.44 |
| 28:CM:305:ARG:HD2 | 28:CM:327:GLN:O | 2.17 | 0.44 |
| 32:CR:618:VAL:HG11 | 32:CR:627:PHE:CD2 | 2.53 | 0.44 |
| 32:CS:828:GLU:HA | 32:CS:831:GLN:HG3 | 2.00 | 0.44 |
| 32:CS:918:LYS:HA | 32:CS:921:GLN:NE2 | 2.32 | 0.44 |
| 39:Cj:72:GLY:H | 44:C1:2066:A:H4' | 1.82 | 0.44 |
| 44:C1:28:C:H2' | 44:C1:29:C:C6 | 2.52 | 0.44 |
| 44:C1:2162:C:H2' | 44:C1:2163:C:C6 | 2.53 | 0.44 |
| 46:UV:381:PRO:HG3 | 46:UV:396:SER:H | 1.82 | 0.44 |
| 46:UV:485:ILE:HD12 | 46:UV:569:PHE:HE1 | 1.82 | 0.44 |
| 46:UV:502:ARG:CZ | 46:UV:599:CYS:HB2 | 2.46 | 0.44 |
| 46:UV:947:ASP:OD1 | 46:UV:947:ASP:N | 2.50 | 0.44 |
| 48:UH:908:SER:OG | 48:UH:909:ILE:N | 2.50 | 0.44 |
| 50:US:208:LEU:HD11 | 50:US:271:ALA:HB1 | 1.98 | 0.44 |
| 2:UB:773:LEU:O | 2:UB:777:LEU:HG | 2.18 | 0.44 |
| 2:UB:828:ASN:OD1 | 2:UB:828:ASN:N | 2.36 | 0.44 |
| 4:UD:75:ARG:HG2 | 53:UP:334:LYS:HA | 1.99 | 0.44 |
| 4:UD:327:LYS:H | 4:UD:344:GLY:HA2 | 1.82 | 0.44 |
| 4:UD:680:GLU:HA | 4:UD:683:ARG:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:UJ:75:SER:N | 7:UJ:78:SER:OG | 2.50 | 0.44 |
| 8:UK:103:LEU:O | 8:UK:107:GLN:HG3 | 2.18 | 0.44 |
| 9:UL:393:LEU:HD21 | 9:UL:426:ARG:HE | 1.82 | 0.44 |
| 10:UM:198:LEU:HB3 | 10:UM:210:PHE:CE1 | 2.52 | 0.44 |
| 11:UN:308:ASP:HB3 | 11:UN:312:ARG:HH21 | 1.82 | 0.44 |
| 11:UN:916:GLN:HE22 | 44:C1:441:A:H62 | 1.64 | 0.44 |
| 12:UO:402:ASP:H | 14:UR:317:SER:HG | 1.65 | 0.44 |
| 12:UO:467:ARG:HD2 | 12:UO:467:ARG:HA | 1.81 | 0.44 |
| 12:UO:488:TYR:HB3 | 12:UO:494:TYR:CE2 | 2.52 | 0.44 |
| 15:UU:192:MET:CA | 15:UU:192:MET:CE | 2.85 | 0.44 |
| 15:UU:754:LEU:HD22 | 15:UU:763:LEU:HD21 | 1.99 | 0.44 |
| 16:UX:122:THR:O | 16:UX:137:ARG:NH1 | 2.49 | 0.44 |
| 19:CC:209:LEU:HD12 | 19:CC:209:LEU:HA | 1.81 | 0.44 |
| 19:CC:228:ASN:OD1 | 19:CC:229:LYS:N | 2.49 | 0.44 |
| 22:CG:328:GLY:H | 36:Cg:153:HIS:CE1 | 2.35 | 0.44 |
| 26:CK:20:LEU:HD23 | 26:CK:20:LEU:HA | 1.83 | 0.44 |
| 32:CR:76:ALA:O | 32:CR:80:LYS:HG2 | 2.17 | 0.44 |
| 32:CS:738:LYS:HD3 | 32:CS:738:LYS:HA | 1.73 | 0.44 |
| 33:CT:87:LEU:HD23 | 33:CT:87:LEU:HA | 1.72 | 0.44 |
| 33:CT:119:LYS:HA | 33:CT:119:LYS:HD3 | 1.68 | 0.44 |
| 34:Cc:110:LEU:HA | 34:Cc:110:LEU:HD23 | 1.79 | 0.44 |
| 44:C1:138:A:H2' | 44:C1:139:C:H6 | 1.83 | 0.44 |
| 44:C1:379:G:H2' | 44:C1:380:C:H6 | 1.82 | 0.44 |
| 44:C1:448:C:H2' | 44:C1:449:C:H6 | 1.83 | 0.44 |
| 44:C1:2054:A:O2' | 44:C1:2055:C:O5' | 2.35 | 0.44 |
| 45:C2:70:A:H2' | 45:C2:71:U:C6 | 2.52 | 0.44 |
| 46:UV:183:GLU:O | 46:UV:205:ASN:ND2 | 2.50 | 0.44 |
| 48:UH:557:GLU:CD | 48:UH:566:ARG:HB3 | 2.42 | 0.44 |
| 1:UA:217:GLY:HA2 | 1:UA:258:LEU:HD23 | 2.00 | 0.44 |
| 1:UA:329:SER:HA | 31:CQ:256:LYS:HE2 | 2.00 | 0.44 |
| 1:UA:332:TYR:HE2 | 15:UU:866:PRO:HB3 | 1.83 | 0.44 |
| 1:UA:519:ARG:HA | 1:UA:580:TYR:CD2 | 2.52 | 0.44 |
| 1:UA:579:ARG:HD3 | 1:UA:579:ARG:HA | 1.78 | 0.44 |
| 2:UB:780:LEU:O | 2:UB:784:LEU:HB2 | 2.17 | 0.44 |
| 2:UB:805:PRO:HD2 | 29:CO:229:ASN:HB3 | 2.00 | 0.44 |
| 4:UD:487:SER:OG | 4:UD:489:ASP:OD1 | 2.27 | 0.44 |
| 4:UD:546:ASP:HB2 | 4:UD:567:ALA:HB2 | 1.97 | 0.44 |
| 4:UD:700:TRP:CD2 | 4:UD:709:MET:HB3 | 2.51 | 0.44 |
| 8:UK:104:LEU:HA | 8:UK:104:LEU:HD23 | 1.74 | 0.44 |
| 9:UL:868:GLU:OE1 | 9:UL:868:GLU:N | 2.49 | 0.44 |
| 10:UM:155:LEU:HB3 | 10:UM:203:GLN:HG3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:UQ:113:VAL:HG13 | 13:UQ:122:VAL:HG13 | 1.99 | 0.44 |
| 13:UQ:162:ASP:OD2 | 13:UQ:164:ARG:NE | 2.51 | 0.44 |
| 15:UU:127:LYS:HD2 | 15:UU:130:GLU:HG2 | 1.97 | 0.44 |
| 15:UU:628:ILE:HA | 15:UU:638:VAL:O | 2.17 | 0.44 |
| 19:CC:245:ASN:HD21 | 19:CC:248:GLN:HE22 | 1.64 | 0.44 |
| 20:CD:419:LEU:HA | 20:CD:419:LEU:HD13 | 1.83 | 0.44 |
| 23:CH:285:THR:HG22 | 23:CH:287:ALA:H | 1.83 | 0.44 |
| 23:CH:350:ARG:NE | 23:CH:393:ASP:OD2 | 2.49 | 0.44 |
| 24:CI:241:HIS:HB3 | 24:CI:839:TRP:HZ2 | 1.83 | 0.44 |
| 24:CI:250:ARG:NH1 | 24:CI:252:ILE:HG13 | 2.32 | 0.44 |
| 24:CI:301:GLU:HB3 | 24:CI:771:TYR:HD1 | 1.82 | 0.44 |
| 24:CI:993:TYR:HD1 | 27:CL:521:MET:HG2 | 1.83 | 0.44 |
| 26:CK:132:GLN:NE2 | 26:CK:158:PRO:O | 2.40 | 0.44 |
| 29:CN:114:ILE:HB | 29:CN:122:ILE:HB | 2.00 | 0.44 |
| 32:CR:212:SER:O | 32:CR:215:LYS:NZ | 2.44 | 0.44 |
| 32:CR:386:VAL:HG12 | 32:CR:406:TYR:CE2 | 2.49 | 0.44 |
| 32:CR:425:SER:O | 32:CR:429:ILE:HG12 | 2.17 | 0.44 |
| 32:CR:840:ARG:NH1 | 32:CR:856:ASP:OD2 | 2.50 | 0.44 |
| 36:Cg:174:LYS:HE2 | 44:C1:1095:A:P | 2.58 | 0.44 |
| 39:Cj:106:LYS:HG2 | 39:Cj:117:LEU:HD11 | 1.99 | 0.44 |
| 41:Cn:126:LYS:HD2 | 44:C1:617:G:H5' | 1.99 | 0.44 |
| 44:C1:354:G:H2' | 44:C1:355:G:H8 | 1.81 | 0.44 |
| 44:C1:614:U:H2' | 44:C1:615:A:H8 | 1.83 | 0.44 |
| 44:C1:1209:C:O2' | 44:C1:1524:A:N3 | 2.39 | 0.44 |
| 44:C1:2174:C:H2' | 44:C1:2175:A:C8 | 2.52 | 0.44 |
| 50:US:220:ARG:HG3 | 50:US:272:PHE:HE1 | 1.83 | 0.44 |
| 49:UI:153:LEU:HB2 | 49:UI:184:THR:HG21 | 2.00 | 0.44 |
| 1:UA:686:SER:HA | 1:UA:699:SER:HA | 2.00 | 0.44 |
| 2:UB:329:ALA:HA | 2:UB:332:LEU:HD12 | 1.99 | 0.44 |
| 4:UD:80:LEU:HD23 | 4:UD:80:LEU:HA | 1.80 | 0.44 |
| 4:UD:505:SER:HB2 | 4:UD:523:PRO:HA | 1.99 | 0.44 |
| 4:UD:528:ARG:HH22 | 4:UD:547:ARG:HB3 | 1.82 | 0.44 |
| 4:UD:868:SER:OG | 4:UD:871:ASP:N | 2.51 | 0.44 |
| 6:UG:358:VAL:HG22 | 6:UG:360:TRP:CD1 | 2.52 | 0.44 |
| 7:UJ:255:LEU:HD21 | 7:UJ:275:VAL:HG12 | 1.99 | 0.44 |
| 7:UJ:285:ASN:O | 7:UJ:289:LEU:HG | 2.18 | 0.44 |
| 9:UL:12:LYS:NZ | 9:UL:454:ILE:O | 2.37 | 0.44 |
| 9:UL:912:ARG:HE | 10:UM:828:ARG:NH1 | 2.15 | 0.44 |
| 11:UN:912:LYS:NZ | 28:CM:370:GLN:HE22 | 2.16 | 0.44 |
| 12:UO:42:TRP:O | 12:UO:341:GLY:HA2 | 2.18 | 0.44 |
| 13:UQ:186:LYS:HB3 | 13:UQ:210:ARG:HG2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:UU:239:PRO:HG3 | 15:UU:283:THR:HG22 | 1.98 | 0.44 |
| 15:UU:668:ILE:HA | 15:UU:684:CYS:HA | 2.00 | 0.44 |
| 15:UU:686:ASP:OD2 | 15:UU:686:ASP:N | 2.50 | 0.44 |
| 17:UZ:35:LYS:HA | 17:UZ:35:LYS:HD2 | 1.66 | 0.44 |
| 18:CA:181:TYR:CD2 | 18:CA:220:VAL:HG13 | 2.53 | 0.44 |
| 18:CB:106:GLU:OE2 | 18:CB:128:ARG:NH1 | 2.49 | 0.44 |
| 19:CC:84:MET:HE3 | 19:CC:84:MET:HB3 | 1.86 | 0.44 |
| 20:CD:194:PHE:CE2 | 20:CD:197:LEU:HB2 | 2.52 | 0.44 |
| 24:CI:218:GLU:HA | 24:CI:221:ASN:HD21 | 1.82 | 0.44 |
| 24:CI:274:LEU:HD21 | 24:CI:278:ASN:HA | 1.98 | 0.44 |
| 25:CJ:85:MET:HE2 | 25:CJ:87:ILE:HD11 | 1.99 | 0.44 |
| 26:CK:87:ARG:O | 26:CK:137:SER:OG | 2.28 | 0.44 |
| 29:CO:80:MET:SD | 29:CO:82:ARG:NH2 | 2.70 | 0.44 |
| 29:CO:161:LYS:HG3 | 29:CO:163:ILE:HG23 | 2.00 | 0.44 |
| 32:CR:119:THR:HA | 32:CR:479:ARG:NH2 | 2.33 | 0.44 |
| 32:CR:296:GLY:HA3 | 32:CR:326:PHE:HB2 | 1.99 | 0.44 |
| 32:CS:27:PHE:CZ | 32:CS:200:LEU:HD23 | 2.52 | 0.44 |
| 32:CS:76:ALA:O | 32:CS:80:LYS:HG2 | 2.17 | 0.44 |
| 34:Cc:130:ARG:O | 34:Cc:149:VAL:HG12 | 2.18 | 0.44 |
| 36:Cg:107:LEU:HA | 36:Cg:110:LEU:HD12 | 1.99 | 0.44 |
| 44:C1:145:C:H2' | 44:C1:146:C:H6 | 1.82 | 0.44 |
| 44:C1:1172:U:H2' | 44:C1:1173:C:H6 | 1.83 | 0.44 |
| 45:C2:128:C:H2' | 45:C2:129:U:H6 | 1.82 | 0.44 |
| 45:C2:240:C:H2' | 45:C2:241:G:H8 | 1.83 | 0.44 |
| 52:CX:324:ILE:HA | 52:CX:327:VAL:HG12 | 1.99 | 0.44 |
| 49:UI:272:TYR:O | 49:UI:276:LEU:N | 2.51 | 0.44 |
| 4:UD:120:ARG:HD3 | 53:UP:330:ARG:CZ | 2.48 | 0.44 |
| 4:UD:368:LEU:HD11 | 4:UD:865:ARG:HB3 | 1.99 | 0.44 |
| 4:UD:453:VAL:HB | 4:UD:472:VAL:HB | 2.00 | 0.44 |
| 6:UG:147:ASN:OD1 | 6:UG:147:ASN:N | 2.48 | 0.44 |
| 6:UG:195:ALA:HB2 | 6:UG:222:MET:SD | 2.58 | 0.44 |
| 7:UJ:345:ILE:O | 7:UJ:349:HIS:HB2 | 2.18 | 0.44 |
| 14:UR:488:ASN:OD1 | 14:UR:489:SER:N | 2.51 | 0.44 |
| 15:UU:633:LEU:HB3 | 15:UU:635:ARG:HG2 | 1.99 | 0.44 |
| 18:CA:183:VAL:HG11 | 18:CA:210:ALA:HB2 | 2.00 | 0.44 |
| 18:CA:245:LEU:HD12 | 18:CA:245:LEU:HA | 1.82 | 0.44 |
| 20:CD:174:GLU:O | 20:CD:178:GLU:HG2 | 2.18 | 0.44 |
| 21:CE:18:VAL:O | 21:CE:22:LEU:HG | 2.17 | 0.44 |
| 21:CE:60:GLN:HB3 | 21:CE:61:PRO:HD3 | 1.97 | 0.44 |
| 23:CH:169:ALA:O | 43:CU:123:ARG:NH1 | 2.49 | 0.44 |
| 23:CH:344:GLU:HB2 | 24:CI:61:ARG:HH22 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:CH:393:ASP:OD1 | 23:CH:393:ASP:N | 2.49 | 0.44 |
| 24:CI:893:SER:O | 24:CI:893:SER:OG | 2.35 | 0.44 |
| 31:CQ:96:LYS:HD2 | 31:CQ:96:LYS:HA | 1.85 | 0.44 |
| 32:CR:27:PHE:CZ | 32:CR:200:LEU:HD23 | 2.52 | 0.44 |
| 34:Cc:45:LEU:HD12 | 34:Cc:125:VAL:HG22 | 2.00 | 0.44 |
| 34:Cc:59:HIS:CD2 | 34:Cc:94:LYS:HG2 | 2.52 | 0.44 |
| 36:Cg:35:ARG:NH2 | 44:C1:1060:U:O4 | 2.39 | 0.44 |
| 38:Ci:73:ALA:HB2 | 38:Ci:110:GLY:HA2 | 2.00 | 0.44 |
| 44:C1:67:G:H2' | 48:UH:894:ARG:HH22 | 1.83 | 0.44 |
| 44:C1:100:C:H2' | 44:C1:101:G:H8 | 1.80 | 0.44 |
| 44:C1:105:A:H2' | 44:C1:106:A:C8 | 2.53 | 0.44 |
| 44:C1:1139:A:C6 | 44:C1:1141:G:C5 | 3.06 | 0.44 |
| 44:C1:2173:G:H2' | 44:C1:2174:C:C6 | 2.53 | 0.44 |
| 46:UV:720:ALA:O | 46:UV:724:MET:HG3 | 2.18 | 0.44 |
| 46:UV:1051:LEU:HA | 46:UV:1054:LEU:HB3 | 2.00 | 0.44 |
| 50:US:468:HIS:CE1 | 50:US:470:ASN:HB2 | 2.52 | 0.44 |
| 52:CX:358:GLU:OE1 | 52:CX:391:ARG:NH1 | 2.47 | 0.44 |
| 2:UB:343:MET:HE2 | 2:UB:343:MET:HB2 | 1.88 | 0.44 |
| 2:UB:672:ARG:HD3 | 2:UB:673:ALA:N | 2.33 | 0.44 |
| 4:UD:9:VAL:HG12 | 4:UD:394:TRP:CH2 | 2.53 | 0.44 |
| 4:UD:647:LEU:HD13 | 4:UD:647:LEU:HA | 1.83 | 0.44 |
| 5:UF:46:LEU:HD12 | 5:UF:46:LEU:HA | 1.76 | 0.44 |
| 6:UG:213:LEU:HD22 | 6:UG:243:GLN:HE22 | 1.83 | 0.44 |
| 7:UJ:337:ASP:O | 7:UJ:341:SER:OG | 2.22 | 0.44 |
| 9:UL:604:TYR:HB3 | 44:C1:1712:C:C2 | 2.53 | 0.44 |
| 10:UM:57:ILE:HD11 | 10:UM:88:TYR:CZ | 2.52 | 0.44 |
| 12:UO:166:ASP:OD1 | 12:UO:167:LYS:N | 2.48 | 0.44 |
| 13:UQ:316:VAL:HG22 | 13:UQ:324:TYR:HB2 | 2.00 | 0.44 |
| 13:UQ:740:LEU:HD21 | 13:UQ:787:ARG:HB3 | 1.99 | 0.44 |
| 14:UR:273:HIS:CG | 14:UR:293:SER:HG | 2.25 | 0.44 |
| 14:UR:528:LYS:HE3 | 14:UR:528:LYS:HB3 | 1.71 | 0.44 |
| 15:UU:100:TRP:CG | 15:UU:101:LYS:H | 2.35 | 0.44 |
| 15:UU:473:ASN:HD21 | 15:UU:474:ARG:NH1 | 2.14 | 0.44 |
| 15:UU:1010:GLU:HG3 | 15:UU:1013:LEU:HD12 | 1.99 | 0.44 |
| 16:UX:5:ARG:HD3 | 16:UX:5:ARG:HA | 1.72 | 0.44 |
| 16:UX:154:LYS:HE3 | 16:UX:165:ILE:HG21 | 1.98 | 0.44 |
| 18:CA:218:MET:HB2 | 18:CA:218:MET:HE3 | 1.86 | 0.44 |
| 18:CB:246:PHE:HA | 20:CD:123:ARG:NH2 | 2.31 | 0.44 |
| 20:CD:5:ILE:HD11 | 20:CD:118:LEU:HD21 | 1.98 | 0.44 |
| 22:CG:354:ALA:O | 22:CG:367:PHE:HB2 | 2.18 | 0.44 |
| 24:CI:849:SER:OG | 24:CI:850:ILE:O | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:CI:966:LEU:H | 24:CI:973:PHE:HA | 1.83 | 0.44 |
| 26:CK:81:SER:HB3 | 27:CL:560:ARG:CZ | 2.47 | 0.44 |
| 30:CP:101:LEU:HB3 | 30:CP:106:VAL:HB | 1.99 | 0.44 |
| 30:CP:218:TRP:HB3 | 30:CP:221:TYR:HD2 | 1.83 | 0.44 |
| 32:CR:559:MET:HE3 | 32:CR:559:MET:HB3 | 1.70 | 0.44 |
| 32:CS:586:ILE:HG22 | 32:CS:638:ILE:HG23 | 2.00 | 0.44 |
| 34:Cc:150:SER:O | 34:Cc:154:ARG:HG3 | 2.18 | 0.44 |
| 37:Ch:99:ARG:HG3 | 37:Ch:115:LEU:HD11 | 2.00 | 0.44 |
| 44:C1:351:U:O4 | 44:C1:353:G:N1 | 2.51 | 0.44 |
| 44:C1:1164:A:H2' | 44:C1:1165:U:O4' | 2.16 | 0.44 |
| 44:C1:1173:C:H2' | 44:C1:1174:C:C6 | 2.53 | 0.44 |
| 44:C1:1494:U:H2' | 44:C1:1495:C:C6 | 2.53 | 0.44 |
| 44:C1:2217:C:H3' | 44:C1:2218:A:H8 | 1.82 | 0.44 |
| 46:UV:566:PHE:HB3 | 46:UV:567:ARG:H | 1.73 | 0.44 |
| 46:UV:721:PHE:HA | 46:UV:724:MET:HE2 | 1.99 | 0.44 |
| 48:UH:836:ILE:HD12 | 48:UH:839:ALA:HB3 | 1.99 | 0.44 |
| 48:UH:916:MET:HE2 | 48:UH:916:MET:HB3 | 1.75 | 0.44 |
| 50:US:146:LEU:HD11 | 50:US:169:ILE:HD13 | 2.00 | 0.44 |
| 50:US:522:HIS:HB3 | 50:US:525:THR:HB | 2.00 | 0.44 |
| 52:CX:298:LYS:HD3 | 52:CX:299:PRO:HD2 | 1.99 | 0.44 |
| 54:Cz:1744:GLN:O | 54:Cz:1748:LYS:HG3 | 2.17 | 0.44 |
| 2:UB:527:SER:O | 2:UB:531:ILE:HG12 | 2.17 | 0.44 |
| 4:UD:196:SER:HB2 | 4:UD:199:ILE:HD12 | 1.99 | 0.44 |
| 4:UD:650:VAL:HA | 4:UD:655:GLN:O | 2.17 | 0.44 |
| 5:UF:93:PHE:HB3 | 5:UF:125:ARG:HH22 | 1.82 | 0.44 |
| 10:UM:570:ILE:HG21 | 10:UM:632:TYR:CZ | 2.53 | 0.44 |
| 12:UO:128:VAL:HA | 12:UO:133:ARG:HB2 | 2.00 | 0.44 |
| 13:UQ:472:PRO:O | 13:UQ:473:GLN:HG3 | 2.17 | 0.44 |
| 13:UQ:699:ILE:HD12 | 13:UQ:715:ILE:C | 2.43 | 0.44 |
| 15:UU:928:LEU:HD21 | 15:UU:973:HIS:HB2 | 1.99 | 0.44 |
| 17:UZ:77:ARG:NH2 | 17:UZ:272:PRO:HB3 | 2.33 | 0.44 |
| 20:CD:165:ILE:HD11 | 20:CD:281:ARG:HG3 | 2.00 | 0.44 |
| 23:CH:45:GLY:HA2 | 23:CH:73:THR:HA | 1.99 | 0.44 |
| 23:CH:219:ARG:HH12 | 23:CH:249:ASP:C | 2.25 | 0.44 |
| 26:CK:83:ILE:HG22 | 26:CK:84:VAL:HG13 | 2.00 | 0.44 |
| 26:CK:146:ARG:HD3 | 44:C1:1759:U:O2 | 2.18 | 0.44 |
| 28:CM:61:LEU:HD22 | 28:CM:99:ARG:HB3 | 2.00 | 0.44 |
| 28:CM:82:ILE:HD12 | 28:CM:333:MET:HE3 | 1.99 | 0.44 |
| 28:CM:399:LYS:O | 28:CM:403:LYS:HG2 | 2.18 | 0.44 |
| 29:CO:175:CYS:SG | 29:CO:176:ARG:N | 2.91 | 0.44 |
| 32:CS:786:PHE:HA | 32:CS:789:LEU:HB2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:449:C:H2' | 44:C1:450:G:H8 | 1.83 | 0.44 |
| 44:C1:614:U:H2' | 44:C1:615:A:C8 | 2.52 | 0.44 |
| 45:C2:123:A:C2 | 45:C2:124:U:H2' | 2.52 | 0.44 |
| 46:UV:611:LEU:HD12 | 46:UV:611:LEU:HA | 1.86 | 0.44 |
| 46:UV:783:THR:HG21 | 46:UV:800:LEU:HB2 | 2.00 | 0.44 |
| 46:UV:837:TRP:HB2 | 46:UV:876:PHE:HE1 | 1.83 | 0.44 |
| 50:US:85:CYS:SG | 50:US:141:LEU:HB3 | 2.58 | 0.44 |
| 50:US:388:LEU:HD13 | 50:US:388:LEU:HA | 1.76 | 0.44 |
| 1:UA:354:ARG:HA | 1:UA:369:VAL:HG23 | 2.00 | 0.44 |
| 1:UA:684:GLY:O | 1:UA:686:SER:N | 2.51 | 0.44 |
| 3:UC:576:LYS:HD2 | 24:CI:144:TYR:CZ | 2.53 | 0.44 |
| 4:UD:181:ARG:NH2 | 21:CE:124:ARG:O | 2.40 | 0.44 |
| 5:UF:188:TRP:CE3 | 5:UF:189:LEU:HD22 | 2.53 | 0.44 |
| 6:UG:137:LEU:HD23 | 6:UG:137:LEU:HA | 1.63 | 0.44 |
| 6:UG:450:LEU:HD23 | 6:UG:450:LEU:HA | 1.67 | 0.44 |
| 7:UJ:590:GLN:HB2 | 7:UJ:647:LEU:HD21 | 1.99 | 0.44 |
| 9:UL:148:LEU:HD13 | 9:UL:201:TRP:CD2 | 2.52 | 0.44 |
| 9:UL:196:SER:HA | 9:UL:220:CYS:H | 1.82 | 0.44 |
| 12:UO:95:ILE:HD13 | 12:UO:126:PHE:CE2 | 2.53 | 0.44 |
| 12:UO:215:ARG:HB2 | 12:UO:217:TRP:CH2 | 2.53 | 0.44 |
| 14:UR:481:ARG:NH1 | 14:UR:498:ASN:HD22 | 2.15 | 0.44 |
| 15:UU:177:ALA:HB2 | 15:UU:203:ARG:NH1 | 2.33 | 0.44 |
| 15:UU:723:VAL:HG22 | 15:UU:733:VAL:HG13 | 2.00 | 0.44 |
| 20:CD:146:ALA:O | 20:CD:150:SER:OG | 2.26 | 0.44 |
| 23:CH:218:ILE:O | 23:CH:250:VAL:HA | 2.18 | 0.44 |
| 24:CI:1043:ARG:HH22 | 44:C1:2073:A:P | 2.40 | 0.44 |
| 25:CJ:108:ARG:HA | 25:CJ:113:VAL:HG11 | 1.98 | 0.44 |
| 27:CL:696:VAL:HG22 | 27:CL:700:GLY:HA2 | 2.00 | 0.44 |
| 28:CM:264:ILE:HG13 | 28:CM:310:TRP:HZ3 | 1.83 | 0.44 |
| 29:CO:37:LEU:HD11 | 29:CO:245:CYS:SG | 2.58 | 0.44 |
| 30:CP:51:LEU:HD23 | 30:CP:51:LEU:HA | 1.83 | 0.44 |
| 31:CQ:186:ALA:O | 31:CQ:190:ILE:HG13 | 2.17 | 0.44 |
| 32:CR:286:ALA:HB3 | 32:CR:289:ARG:NE | 2.33 | 0.44 |
| 32:CR:742:PHE:HB3 | 32:CR:762:MET:HB3 | 2.00 | 0.44 |
| 32:CR:803:LEU:HD22 | 32:CR:881:GLN:HG2 | 2.00 | 0.44 |
| 32:CS:425:SER:O | 32:CS:429:ILE:HG12 | 2.17 | 0.44 |
| 34:Cc:162:LEU:HD23 | 34:Cc:162:LEU:HA | 1.83 | 0.44 |
| 34:Cc:212:ARG:HD3 | 42:Cp:62:ARG:HH21 | 1.82 | 0.44 |
| 38:Ci:109:PRO:O | 38:Ci:113:SER:OG | 2.24 | 0.44 |
| 41:Cn:89:ASN:OD1 | 41:Cn:90:ASP:N | 2.51 | 0.44 |
| 44:C1:20:C:H2' | 44:C1:21:C:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:186:C:H2' | 44:C1:187:G:C8 | 2.51 | 0.44 |
| 44:C1:452:G:H1 | 44:C1:480:U:H3 | 1.66 | 0.44 |
| 44:C1:599:U:H2' | 44:C1:600:U:H6 | 1.83 | 0.44 |
| 44:C1:1051:G:O2' | 44:C1:1053:C:OP1 | 2.36 | 0.44 |
| 44:C1:1056:U:H2' | 44:C1:1057:A:H8 | 1.82 | 0.44 |
| 44:C1:2108:A:H2' | 44:C1:2109:A:O4' | 2.17 | 0.44 |
| 44:C1:2210:U:O2 | 44:C1:2223:C:N4 | 2.48 | 0.44 |
| 50:US:75:LYS:HA | 50:US:78:LEU:HD12 | 1.99 | 0.44 |
| 50:US:320:LEU:O | 50:US:323:SER:OG | 2.35 | 0.44 |
| 52:CX:338:SER:HB2 | 52:CX:370:LEU:HD11 | 2.00 | 0.44 |
| 49:UI:169:LEU:HD13 | 49:UI:169:LEU:HA | 1.77 | 0.44 |
| 54:Cz:1657:LEU:HA | 54:Cz:1657:LEU:HD23 | 1.85 | 0.44 |
| 4:UD:370:GLN:NE2 | 4:UD:690:LYS:HG2 | 2.33 | 0.43 |
| 4:UD:391:ILE:HB | 4:UD:423:VAL:HG12 | 2.00 | 0.43 |
| 4:UD:401:GLN:HA | 4:UD:404:LEU:HB2 | 1.99 | 0.43 |
| 4:UD:804:ARG:HA | 4:UD:804:ARG:HD3 | 1.79 | 0.43 |
| 5:UF:140:ASN:OD1 | 5:UF:142:SER:OG | 2.24 | 0.43 |
| 5:UF:330:ASN:HA | 5:UF:335:TRP:HE1 | 1.83 | 0.43 |
| 6:UG:127:GLN:HE22 | 7:UJ:18:SER:H | 1.65 | 0.43 |
| 8:UK:114:THR:OG1 | 8:UK:115:MET:N | 2.50 | 0.43 |
| 10:UM:705:THR:HG23 | 10:UM:707:ILE:HG12 | 2.00 | 0.43 |
| 10:UM:791:LEU:HD23 | 10:UM:794:VAL:HG23 | 2.00 | 0.43 |
| 13:UQ:922:ALA:O | 13:UQ:925:ARG:N | 2.48 | 0.43 |
| 14:UR:554:LEU:HD23 | 14:UR:554:LEU:HA | 1.66 | 0.43 |
| 17:UZ:115:GLU:HG3 | 17:UZ:120:LEU:HD12 | 2.00 | 0.43 |
| 17:UZ:251:GLU:O | 17:UZ:255:LEU:HG | 2.18 | 0.43 |
| 18:CA:247:LEU:HA | 18:CA:247:LEU:HD12 | 1.60 | 0.43 |
| 19:CC:140:LYS:HZ3 | 44:C1:435:A:P | 2.41 | 0.43 |
| 20:CD:322:LEU:HD12 | 20:CD:322:LEU:HA | 1.67 | 0.43 |
| 20:CD:385:ALA:HB3 | 20:CD:390:ARG:NH2 | 2.33 | 0.43 |
| 22:CG:266:ALA:HA | 22:CG:290:ALA:HB1 | 1.99 | 0.43 |
| 23:CH:164:PHE:CZ | 23:CH:338:LEU:HB2 | 2.53 | 0.43 |
| 24:CI:123:LEU:HD13 | 24:CI:898:ARG:HH11 | 1.83 | 0.43 |
| 24:CI:340:ASP:OD1 | 24:CI:340:ASP:N | 2.42 | 0.43 |
| 24:CI:537:TRP:HB2 | 24:CI:560:TRP:CE2 | 2.53 | 0.43 |
| 24:CI:959:ARG:NH1 | 44:C1:1149:C:OP1 | 2.51 | 0.43 |
| 27:CL:548:ARG:O | 27:CL:551:ALA:C | 2.61 | 0.43 |
| 32:CR:34:ALA:HB3 | 32:CR:154:LYS:HZ2 | 1.83 | 0.43 |
| 32:CR:48:MET:HE3 | 32:CR:48:MET:HB3 | 1.74 | 0.43 |
| 32:CR:918:LYS:HA | 32:CR:921:GLN:NE2 | 2.32 | 0.43 |
| 32:CS:380:LEU:HB3 | 32:CS:406:TYR:OH | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:Cc:48:TYR:HE1 | 34:Cc:152:LEU:HD22 | 1.82 | 0.43 |
| 34:Cc:109:HIS:CE1 | 34:Cc:113:ASP:HA | 2.53 | 0.43 |
| 37:Ch:104:ARG:HH22 | 44:C1:1464:G:H21 | 1.65 | 0.43 |
| 44:C1:83:A:H2' | 44:C1:84:A:C8 | 2.53 | 0.43 |
| 44:C1:448:C:H2' | 44:C1:449:C:C6 | 2.53 | 0.43 |
| 44:C1:1705:C:H2' | 44:C1:1706:G:C8 | 2.53 | 0.43 |
| 44:C1:1744:A:H2' | 44:C1:1745:C:C6 | 2.51 | 0.43 |
| 45:C2:183:A:H2' | 45:C2:184:G:H8 | 1.83 | 0.43 |
| 46:UV:476:TRP:CH2 | 46:UV:510:PRO:HG3 | 2.53 | 0.43 |
| 49:UE:211:ALA:HB1 | 49:UE:215:MET:HG2 | 2.00 | 0.43 |
| 1:UA:169:ALA:HB1 | 1:UA:198:VAL:HG13 | 2.00 | 0.43 |
| 2:UB:792:ARG:NH1 | 50:US:435:GLY:O | 2.44 | 0.43 |
| 4:UD:442:LEU:HD21 | 4:UD:518:TYR:CE2 | 2.52 | 0.43 |
| 7:UJ:40:ALA:HA | 7:UJ:43:GLN:CD | 2.43 | 0.43 |
| 7:UJ:45:PHE:HD1 | 7:UJ:48:ILE:HD12 | 1.83 | 0.43 |
| 7:UJ:207:LYS:HE2 | 7:UJ:207:LYS:HB2 | 1.73 | 0.43 |
| 7:UJ:237:ARG:HE | 14:UR:254:ARG:NH2 | 2.15 | 0.43 |
| 7:UJ:255:LEU:HA | 7:UJ:255:LEU:HD12 | 1.77 | 0.43 |
| 7:UJ:257:GLU:HA | 7:UJ:260:VAL:HG12 | 2.00 | 0.43 |
| 7:UJ:700:HIS:HA | 7:UJ:701:SER:HA | 1.62 | 0.43 |
| 9:UL:796:ILE:HD13 | 9:UL:796:ILE:HA | 1.86 | 0.43 |
| 11:UN:337:GLU:O | 11:UN:338:HIS:ND1 | 2.51 | 0.43 |
| 13:UQ:142:HIS:ND1 | 13:UQ:161:SER:OG | 2.51 | 0.43 |
| 15:UU:142:LYS:HD3 | 15:UU:143:GLN:HB3 | 2.01 | 0.43 |
| 15:UU:478:MET:HE3 | 15:UU:478:MET:HB2 | 1.64 | 0.43 |
| 17:UZ:105:GLN:HG3 | 17:UZ:129:ASP:N | 2.33 | 0.43 |
| 17:UZ:105:GLN:HE21 | 17:UZ:127:VAL:HG23 | 1.83 | 0.43 |
| 18:CA:249:GLN:HB3 | 19:CC:39:LYS:NZ | 2.33 | 0.43 |
| 18:CB:82:PHE:HB2 | 18:CB:93:CYS:SG | 2.58 | 0.43 |
| 18:CB:297:ARG:O | 18:CB:299:HIS:HD2 | 2.02 | 0.43 |
| 24:CI:81:LYS:O | 24:CI:85:LEU:HG | 2.17 | 0.43 |
| 24:CI:142:GLY:HA2 | 24:CI:170:LEU:HD11 | 2.00 | 0.43 |
| 24:CI:279:PHE:HB2 | 24:CI:771:TYR:HB2 | 1.99 | 0.43 |
| 24:CI:934:ILE:HB | 24:CI:973:PHE:CZ | 2.53 | 0.43 |
| 24:CI:1090:LEU:HD23 | 24:CI:1090:LEU:HA | 1.70 | 0.43 |
| 26:CK:164:MET:HB2 | 26:CK:267:SER:HB3 | 2.01 | 0.43 |
| 28:CM:50:GLU:OE1 | 28:CM:51:ARG:NE | 2.42 | 0.43 |
| 28:CM:137:PRO:HG2 | 28:CM:138:TYR:CD2 | 2.52 | 0.43 |
| 30:CP:193:HIS:HB3 | 30:CP:196:TYR:HD2 | 1.83 | 0.43 |
| 32:CR:134:ASN:HB3 | 32:CR:553:PRO:HG2 | 2.00 | 0.43 |
| 32:CS:803:LEU:HD22 | 32:CS:881:GLN:HG2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:222:U:O4' | 44:C1:224:C:N4 | 2.52 | 0.43 |
| 46:UV:100:PRO:HA | 46:UV:101:SER:HA | 1.68 | 0.43 |
| 46:UV:419:ARG:O | 46:UV:422:ARG:HG3 | 2.18 | 0.43 |
| 46:UV:419:ARG:HG2 | 46:UV:423:LYS:NZ | 2.33 | 0.43 |
| 46:UV:486:LEU:HB3 | 46:UV:506:LEU:HD21 | 2.00 | 0.43 |
| 1:UA:509:LEU:HD13 | 1:UA:529:THR:HG21 | 2.00 | 0.43 |
| 1:UA:633:ALA:HB2 | 6:UG:137:LEU:HD11 | 2.01 | 0.43 |
| 2:UB:22:GLN:HE22 | 44:C1:2228:G:H4' | 1.83 | 0.43 |
| 4:UD:184:SER:OG | 4:UD:187:THR:OG1 | 2.35 | 0.43 |
| 4:UD:474:MET:HE1 | 4:UD:520:VAL:HG21 | 1.99 | 0.43 |
| 4:UD:533:ILE:HD12 | 4:UD:534:PRO:HD2 | 1.99 | 0.43 |
| 4:UD:773:MET:HB3 | 4:UD:773:MET:HE2 | 1.73 | 0.43 |
| 5:UF:361:LEU:HD23 | 5:UF:364:LEU:HD23 | 2.01 | 0.43 |
| 6:UG:172:CYS:SG | 6:UG:207:GLY:HA3 | 2.58 | 0.43 |
| 7:UJ:277:ILE:HG23 | 13:UQ:952:PHE:CE1 | 2.52 | 0.43 |
| 7:UJ:608:ARG:NH1 | 7:UJ:668:VAL:O | 2.52 | 0.43 |
| 7:UJ:652:LEU:O | 7:UJ:656:ILE:HG22 | 2.18 | 0.43 |
| 9:UL:481:ILE:HG23 | 9:UL:489:LEU:HD11 | 2.00 | 0.43 |
| 9:UL:924:LEU:HD13 | 10:UM:860:LEU:HD12 | 2.00 | 0.43 |
| 10:UM:593:ARG:NH1 | 10:UM:594:PHE:O | 2.51 | 0.43 |
| 12:UO:390:SER:OG | 12:UO:391:ASN:N | 2.49 | 0.43 |
| 12:UO:482:LEU:HD12 | 12:UO:482:LEU:HA | 1.78 | 0.43 |
| 13:UQ:154:ASP:HA | 13:UQ:170:TRP:HE1 | 1.83 | 0.43 |
| 13:UQ:159:ALA:HB2 | 13:UQ:165:ILE:HG12 | 2.00 | 0.43 |
| 13:UQ:395:LEU:HG | 13:UQ:399:ILE:HD11 | 1.99 | 0.43 |
| 13:UQ:571:LYS:HD2 | 13:UQ:575:ASP:HB2 | 1.98 | 0.43 |
| 13:UQ:921:VAL:HG21 | 13:UQ:952:PHE:CZ | 2.53 | 0.43 |
| 14:UR:417:ARG:NH1 | 21:CE:19:GLN:HB3 | 2.33 | 0.43 |
| 16:UX:17:GLU:HA | 16:UX:20:LYS:HB2 | 2.01 | 0.43 |
| 16:UX:80:MET:HE3 | 16:UX:80:MET:HB3 | 1.91 | 0.43 |
| 16:UX:83:LEU:HB3 | 16:UX:85:ALA:HB3 | 1.99 | 0.43 |
| 16:UX:135:VAL:HG11 | 16:UX:156:ARG:HH11 | 1.83 | 0.43 |
| 18:CA:68:GLY:N | 33:CT:140:ILE:HB | 2.31 | 0.43 |
| 19:CC:206:PHE:CD2 | 19:CC:209:LEU:HB2 | 2.53 | 0.43 |
| 19:CC:414:ARG:HD2 | 19:CC:414:ARG:HA | 1.66 | 0.43 |
| 23:CH:334:THR:O | 23:CH:337:THR:OG1 | 2.31 | 0.43 |
| 28:CM:342:LEU:HD23 | 28:CM:352:LEU:HA | 2.00 | 0.43 |
| 30:CP:62:LEU:HG | 30:CP:67:ILE:HB | 2.00 | 0.43 |
| 31:CQ:207:THR:OG1 | 31:CQ:208:ARG:N | 2.51 | 0.43 |
| 32:CR:380:LEU:HB3 | 32:CR:406:TYR:OH | 2.18 | 0.43 |
| 34:Cc:203:GLU:O | 34:Cc:206:ARG:HG2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:Ce:15:SER:HB2 | 35:Ce:48:GLN:HE21 | 1.83 | 0.43 |
| 35:Ce:55:ILE:HG21 | 35:Ce:185:ARG:NE | 2.32 | 0.43 |
| 38:Ci:63:ALA:O | 38:Ci:67:GLU:N | 2.51 | 0.43 |
| 38:Ci:84:CYS:HA | 38:Ci:87:LEU:HG | 2.00 | 0.43 |
| 40:Cm:106:THR:OG1 | 40:Cm:111:MET:SD | 2.70 | 0.43 |
| 44:C1:391:C:H2' | 44:C1:392:C:H6 | 1.81 | 0.43 |
| 44:C1:1472:A:H2 | 44:C1:1510:G:N1 | 2.08 | 0.43 |
| 44:C1:1480:G:N2 | 44:C1:1502:U:O2 | 2.46 | 0.43 |
| 44:C1:1512:C:H2' | 44:C1:1513:U:C6 | 2.53 | 0.43 |
| 44:C1:2095:G:N2 | 44:C1:2096:G:C2 | 2.86 | 0.43 |
| 45:C2:19:A:H2' | 45:C2:20:A:H8 | 1.83 | 0.43 |
| 46:UV:100:PRO:HA | 46:UV:102:PRO:HD3 | 1.98 | 0.43 |
| 46:UV:918:TRP:HB3 | 46:UV:919:ARG:HH21 | 1.82 | 0.43 |
| 46:UV:1098:ARG:NH1 | 46:UV:1104:LEU:HB2 | 2.33 | 0.43 |
| 52:CX:288:LEU:O | 52:CX:292:LEU:HG | 2.19 | 0.43 |
| 52:CX:299:PRO:HG3 | 52:CX:334:PRO:HG2 | 2.01 | 0.43 |
| 49:UI:165:ASP:CG | 49:UI:168:LEU:HB2 | 2.43 | 0.43 |
| 1:UA:2:LYS:HB2 | 1:UA:2:LYS:HE2 | 1.89 | 0.43 |
| 1:UA:11:LEU:HD13 | 1:UA:697:VAL:HG21 | 2.00 | 0.43 |
| 1:UA:306:ASN:HD21 | 1:UA:308:SER:HB3 | 1.83 | 0.43 |
| 1:UA:798:ILE:HG13 | 1:UA:799:ASP:N | 2.34 | 0.43 |
| 2:UB:878:PHE:O | 2:UB:882:ILE:HG23 | 2.19 | 0.43 |
| 4:UD:237:ILE:O | 4:UD:254:SER:OG | 2.30 | 0.43 |
| 5:UF:88:SER:O | 5:UF:92:THR:OG1 | 2.25 | 0.43 |
| 7:UJ:180:ALA:HA | 7:UJ:183:VAL:HG12 | 1.99 | 0.43 |
| 9:UL:595:ASP:OD1 | 9:UL:595:ASP:N | 2.49 | 0.43 |
| 9:UL:957:ALA:HB3 | 27:CL:576:VAL:H | 1.82 | 0.43 |
| 10:UM:63:PRO:O | 10:UM:81:ARG:N | 2.50 | 0.43 |
| 10:UM:738:LEU:HA | 10:UM:741:GLN:NE2 | 2.32 | 0.43 |
| 12:UO:162:SER:OG | 12:UO:172:TRP:NE1 | 2.48 | 0.43 |
| 12:UO:215:ARG:HB3 | 12:UO:225:ALA:HB2 | 2.01 | 0.43 |
| 12:UO:524:GLN:O | 12:UO:528:ALA:N | 2.45 | 0.43 |
| 13:UQ:457:ARG:NH1 | 44:C1:39:C:OP1 | 2.50 | 0.43 |
| 14:UR:366:HIS:O | 14:UR:369:GLU:N | 2.50 | 0.43 |
| 15:UU:233:THR:OG1 | 15:UU:247:ALA:O | 2.36 | 0.43 |
| 15:UU:1022:HIS:CD2 | 15:UU:1025:ARG:HH21 | 2.35 | 0.43 |
| 18:CB:130:TRP:CZ2 | 18:CB:135:SER:HB3 | 2.53 | 0.43 |
| 18:CB:138:ALA:HA | 18:CB:141:ILE:HD12 | 1.98 | 0.43 |
| 21:CF:62:LEU:HD12 | 21:CF:66:LEU:HB2 | 2.00 | 0.43 |
| 23:CH:305:VAL:HB | 23:CH:308:ASP:OD1 | 2.18 | 0.43 |
| 23:CH:353:ARG:HD3 | 24:CI:537:TRP:CD1 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:CI:813:VAL:O | 24:CI:872:THR:HA | 2.17 | 0.43 |
| 24:CI:1011:GLN:HB2 | 27:CL:480:GLN:NE2 | 2.33 | 0.43 |
| 26:CK:208:LEU:HD23 | 26:CK:208:LEU:HA | 1.81 | 0.43 |
| 27:CL:535:GLU:O | 27:CL:538:SER:OG | 2.29 | 0.43 |
| 32:CR:15:ILE:O | 32:CR:19:LEU:HG | 2.19 | 0.43 |
| 44:C1:81:G:C6 | 44:C1:128:G:C6 | 3.05 | 0.43 |
| 46:UV:633:ILE:HA | 46:UV:634:LYS:HA | 1.69 | 0.43 |
| 46:UV:664:ARG:HG3 | 46:UV:666:ARG:HH22 | 1.83 | 0.43 |
| 46:UV:929:VAL:HG12 | 46:UV:951:ARG:HE | 1.84 | 0.43 |
| 54:Cz:1591:TYR:HB3 | 54:Cz:1600:ALA:HB2 | 1.99 | 0.43 |
| 54:Cz:1726:LYS:HA | 54:Cz:1726:LYS:HD3 | 1.82 | 0.43 |
| 1:UA:708:PRO:HB3 | 1:UA:711:LEU:HD22 | 1.99 | 0.43 |
| 4:UD:297:ASP:OD1 | 4:UD:297:ASP:N | 2.51 | 0.43 |
| 5:UF:177:LEU:HD23 | 5:UF:177:LEU:HA | 1.74 | 0.43 |
| 5:UF:317:ILE:HD13 | 5:UF:317:ILE:HA | 1.86 | 0.43 |
| 7:UJ:65:ARG:H | 7:UJ:65:ARG:HG2 | 1.51 | 0.43 |
| 7:UJ:236:ARG:NH1 | 44:C1:243:U:H3' | 2.33 | 0.43 |
| 7:UJ:725:ARG:HD3 | 7:UJ:728:ARG:NH1 | 2.33 | 0.43 |
| 9:UL:150:GLY:O | 27:CL:710:ARG:NH2 | 2.52 | 0.43 |
| 9:UL:282:ALA:N | 9:UL:297:GLY:HA2 | 2.34 | 0.43 |
| 11:UN:348:HIS:HB2 | 19:CC:95:LYS:NZ | 2.34 | 0.43 |
| 12:UO:297:VAL:HG23 | 12:UO:311:ALA:H | 1.83 | 0.43 |
| 12:UO:499:VAL:HG23 | 49:UE:259:LEU:HD22 | 2.00 | 0.43 |
| 15:UU:651:PHE:O | 15:UU:654:GLY:N | 2.52 | 0.43 |
| 15:UU:681:ALA:HB2 | 15:UU:715:PHE:CZ | 2.52 | 0.43 |
| 16:UX:139:GLN:HA | 16:UX:142:ARG:NH2 | 2.34 | 0.43 |
| 18:CA:130:TRP:CE3 | 18:CA:138:ALA:HB2 | 2.52 | 0.43 |
| 18:CA:149:TYR:HB3 | 18:CA:311:PHE:CE1 | 2.53 | 0.43 |
| 20:CD:96:SER:O | 20:CD:100:THR:HG23 | 2.18 | 0.43 |
| 22:CG:358:LYS:HB3 | 22:CG:361:GLU:CD | 2.44 | 0.43 |
| 22:CG:595:LYS:HA | 22:CG:595:LYS:HD2 | 1.76 | 0.43 |
| 24:CI:1113:GLU:O | 24:CI:1117:GLU:HG2 | 2.19 | 0.43 |
| 25:CJ:125:GLN:NE2 | 44:C1:417:G:H5' | 2.34 | 0.43 |
| 26:CK:289:ARG:NH2 | 44:C1:1144:U:O5' | 2.51 | 0.43 |
| 27:CL:710:ARG:NH1 | 44:C1:2335:U:OP1 | 2.43 | 0.43 |
| 28:CM:172:SER:OG | 28:CM:173:GLY:N | 2.51 | 0.43 |
| 32:CR:781:ASP:OD1 | 32:CR:784:LYS:NZ | 2.32 | 0.43 |
| 32:CR:880:GLN:NE2 | 32:CR:915:ILE:HG12 | 2.26 | 0.43 |
| 34:Cc:69:PHE:CE1 | 42:Cp:50:ARG:HB2 | 2.53 | 0.43 |
| 40:Cm:71:LYS:HB3 | 40:Cm:130:TYR:CZ | 2.53 | 0.43 |
| 44:C1:279:C:H2' | 44:C1:280:U:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:1485:A:C5 | 44:C1:1486:G:H8 | 2.35 | 0.43 |
| 45:C2:11:C:H2' | 45:C2:12:U:C6 | 2.53 | 0.43 |
| 45:C2:127:A:O2' | 45:C2:128:C:O5' | 2.36 | 0.43 |
| 46:UV:999:THR:HB | 46:UV:1001:VAL:HG13 | 2.00 | 0.43 |
| 48:UH:742:LEU:HB3 | 48:UH:776:ILE:HD11 | 2.01 | 0.43 |
| 48:UH:833:LYS:HA | 49:UI:246:LEU:HB3 | 1.99 | 0.43 |
| 49:UE:153:LEU:HB2 | 49:UE:184:THR:HG21 | 2.00 | 0.43 |
| 49:UE:272:TYR:O | 49:UE:276:LEU:N | 2.51 | 0.43 |
| 50:US:496:SER:O | 50:US:500:LEU:HG | 2.18 | 0.43 |
| 54:Cz:1608:VAL:HB | 54:Cz:1619:TRP:CH2 | 2.54 | 0.43 |
| 1:UA:43:VAL:HG13 | 1:UA:44:GLU:H | 1.84 | 0.43 |
| 4:UD:310:SER:O | 14:UR:450:ARG:NH2 | 2.49 | 0.43 |
| 4:UD:764:ASP:OD1 | 4:UD:764:ASP:N | 2.50 | 0.43 |
| 8:UK:110:GLY:O | 8:UK:114:THR:HG23 | 2.18 | 0.43 |
| 8:UK:252:THR:HG23 | 8:UK:269:LYS:HE2 | 2.01 | 0.43 |
| 9:UL:675:ASP:OD1 | 9:UL:675:ASP:N | 2.42 | 0.43 |
| 10:UM:753:ALA:O | 10:UM:757:ALA:CB | 2.66 | 0.43 |
| 10:UM:870:HIS:CG | 10:UM:873:ARG:HH22 | 2.36 | 0.43 |
| 13:UQ:402:ILE:HG22 | 13:UQ:413:LEU:HD22 | 2.00 | 0.43 |
| 13:UQ:552:SER:OG | 13:UQ:553:ILE:N | 2.50 | 0.43 |
| 15:UU:136:ASP:CG | 15:UU:158:ARG:HH22 | 2.26 | 0.43 |
| 15:UU:528:ARG:HH11 | 45:C2:65:C:P | 2.41 | 0.43 |
| 18:CA:85:ARG:HD3 | 33:CT:112:ARG:HH22 | 1.82 | 0.43 |
| 28:CM:266:ILE:O | 28:CM:276:LEU:N | 2.47 | 0.43 |
| 30:CP:109:PRO:HA | 30:CP:112:LEU:HG | 2.00 | 0.43 |
| 31:CQ:215:LYS:HD3 | 31:CQ:217:HIS:CE1 | 2.53 | 0.43 |
| 32:CS:61:LYS:HE3 | 32:CS:130:ALA:HB3 | 2.01 | 0.43 |
| 32:CS:211:ILE:H | 32:CS:211:ILE:HG12 | 1.35 | 0.43 |
| 34:Cc:84:LEU:HD23 | 34:Cc:84:LEU:HA | 1.80 | 0.43 |
| 37:Ch:105:ASN:ND2 | 44:C1:1464:G:O2' | 2.50 | 0.43 |
| 43:CU:245:ARG:HH22 | 43:CU:258:GLU:HG2 | 1.83 | 0.43 |
| 44:C1:1487:G:H1' | 44:C1:1492:A:H62 | 1.84 | 0.43 |
| 45:C2:3:C:H2' | 45:C2:4:G:C8 | 2.53 | 0.43 |
| 45:C2:127:A:O2' | 45:C2:128:C:H6 | 2.02 | 0.43 |
| 46:UV:161:TYR:HA | 46:UV:164:LYS:HG2 | 2.01 | 0.43 |
| 46:UV:485:ILE:HD12 | 46:UV:569:PHE:CE1 | 2.54 | 0.43 |
| 46:UV:639:ALA:O | 46:UV:643:VAL:HG12 | 2.18 | 0.43 |
| 46:UV:641:PHE:HA | 46:UV:645:ARG:HG3 | 2.01 | 0.43 |
| 46:UV:673:PRO:HA | 46:UV:676:ARG:HG2 | 2.00 | 0.43 |
| 46:UV:686:GLY:HA2 | 46:UV:763:GLY:HA3 | 2.01 | 0.43 |
| 46:UV:722:LEU:HG | 46:UV:756:LEU:HG | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:Cz:1714:PRO:HA | 54:Cz:1717:ILE:HB | 2.01 | 0.43 |
| 1:UA:431:MET:HE2 | 1:UA:431:MET:HB2 | 1.81 | 0.43 |
| 2:UB:653:TYR:HA | 2:UB:740:TRP:CZ2 | 2.54 | 0.43 |
| 2:UB:852:LEU:HD23 | 2:UB:852:LEU:HA | 1.77 | 0.43 |
| 4:UD:759:ALA:HB3 | 4:UD:769:GLU:HB2 | 2.01 | 0.43 |
| 4:UD:799:GLU:HA | 4:UD:802:ARG:HB2 | 2.00 | 0.43 |
| 7:UJ:152:LEU:HD12 | 7:UJ:152:LEU:HA | 1.72 | 0.43 |
| 9:UL:700:TRP:HE1 | 9:UL:716:HIS:HB2 | 1.84 | 0.43 |
| 9:UL:782:ILE:HD11 | 9:UL:849:LEU:HD11 | 2.00 | 0.43 |
| 10:UM:383:LEU:HD13 | 10:UM:441:VAL:HG21 | 2.00 | 0.43 |
| 10:UM:514:SER:OG | 10:UM:518:PHE:N | 2.36 | 0.43 |
| 15:UU:42:GLY:HA2 | 15:UU:420:TRP:CH2 | 2.53 | 0.43 |
| 15:UU:113:ASN:O | 15:UU:115:GLU:N | 2.47 | 0.43 |
| 15:UU:528:ARG:HB2 | 15:UU:530:ARG:HG2 | 2.00 | 0.43 |
| 17:UZ:67:THR:HB | 17:UZ:280:ASN:OD1 | 2.19 | 0.43 |
| 20:CD:212:LEU:HA | 20:CD:212:LEU:HD23 | 1.72 | 0.43 |
| 23:CH:405:ASN:OD1 | 23:CH:405:ASN:N | 2.52 | 0.43 |
| 24:CI:214:TYR:HD1 | 24:CI:214:TYR:HA | 1.62 | 0.43 |
| 24:CI:271:SER:HB2 | 24:CI:776:TYR:CE2 | 2.51 | 0.43 |
| 24:CI:391:LYS:HB2 | 32:CR:170:HIS:NE2 | 2.34 | 0.43 |
| 24:CI:1100:ILE:HG13 | 33:CT:114:VAL:HG21 | 2.01 | 0.43 |
| 24:CI:1138:LYS:HD2 | 24:CI:1142:TRP:CD1 | 2.52 | 0.43 |
| 25:CJ:125:GLN:HE22 | 44:C1:417:G:H5' | 1.83 | 0.43 |
| 27:CL:785:LEU:HD13 | 44:C1:2239:U:H5" | 1.99 | 0.43 |
| 29:CN:77:MET:HE3 | 29:CN:80:MET:HB2 | 2.00 | 0.43 |
| 29:CN:243:HIS:HD2 | 29:CN:246:GLU:OE1 | 2.02 | 0.43 |
| 32:CS:94:PRO:HA | 32:CS:97:LEU:HD12 | 2.00 | 0.43 |
| 32:CS:110:LYS:HD3 | 32:CS:110:LYS:N | 2.34 | 0.43 |
| 33:CT:109:LEU:HD23 | 33:CT:109:LEU:HA | 1.79 | 0.43 |
| 37:Ch:121:ARG:NH1 | 44:C1:1452:G:O3' | 2.51 | 0.43 |
| 44:C1:172:C:H2' | 44:C1:173:G:C8 | 2.53 | 0.43 |
| 44:C1:609:A:H2' | 44:C1:610:G:H8 | 1.82 | 0.43 |
| 46:UV:368:ASN:C | 46:UV:373:PRO:HD3 | 2.44 | 0.43 |
| 46:UV:970:VAL:HG22 | 46:UV:974:GLN:HE21 | 1.82 | 0.43 |
| 46:UV:977:ASP:OD2 | 46:UV:977:ASP:N | 2.52 | 0.43 |
| 49:UE:268:ALA:O | 49:UE:272:TYR:N | 2.51 | 0.43 |
| 1:UA:173:LEU:HG | 1:UA:197:GLY:H | 1.84 | 0.43 |
| 2:UB:22:GLN:O | 44:C1:2227:C:O2' | 2.37 | 0.43 |
| 4:UD:647:LEU:HB2 | 4:UD:659:PHE:HB2 | 1.99 | 0.43 |
| 4:UD:701:PHE:HB2 | 4:UD:708:PHE:HB2 | 2.01 | 0.43 |
| 6:UG:228:HIS:HB3 | 6:UG:230:LEU:HD13 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:UG:267:ASN:HB2 | 6:UG:274:HIS:NE2 | 2.34 | 0.43 |
| 7:UJ:201:LEU:HA | 7:UJ:204:CYS:SG | 2.59 | 0.43 |
| 7:UJ:306:ARG:O | 7:UJ:310:VAL:HG23 | 2.19 | 0.43 |
| 9:UL:352:GLU:O | 9:UL:356:VAL:HG23 | 2.19 | 0.43 |
| 10:UM:520:GLN:NE2 | 10:UM:522:ARG:HH21 | 2.17 | 0.43 |
| 12:UO:76:THR:HG21 | 12:UO:105:GLY:N | 2.34 | 0.43 |
| 12:UO:104:CYS:O | 12:UO:116:ALA:HA | 2.19 | 0.43 |
| 13:UQ:506:SER:OG | 13:UQ:507:SER:N | 2.50 | 0.43 |
| 13:UQ:598:LEU:HD23 | 13:UQ:598:LEU:HA | 1.72 | 0.43 |
| 13:UQ:648:LEU:HD23 | 13:UQ:648:LEU:HA | 1.69 | 0.43 |
| 15:UU:34:ILE:HG23 | 15:UU:780:THR:HG23 | 2.01 | 0.43 |
| 16:UX:66:SER:OG | 16:UX:67:ARG:N | 2.52 | 0.43 |
| 18:CA:85:ARG:HB2 | 33:CT:112:ARG:HH22 | 1.82 | 0.43 |
| 18:CB:202:ASN:OD1 | 18:CB:202:ASN:N | 2.43 | 0.43 |
| 19:CC:11:SER:OG | 19:CC:12:ALA:N | 2.50 | 0.43 |
| 21:CF:10:PRO:HG2 | 21:CF:81:TYR:HD2 | 1.83 | 0.43 |
| 22:CG:304:TYR:HD1 | 22:CG:314:VAL:HG22 | 1.83 | 0.43 |
| 22:CG:329:HIS:HA | 22:CG:355:ARG:NH1 | 2.34 | 0.43 |
| 24:CI:287:HIS:HA | 24:CI:293:ASP:HA | 2.00 | 0.43 |
| 24:CI:1013:MET:HE1 | 27:CL:490:LEU:HB2 | 1.99 | 0.43 |
| 24:CI:1054:LEU:HD12 | 24:CI:1054:LEU:HA | 1.77 | 0.43 |
| 25:CJ:178:ASP:OD1 | 25:CJ:180:PHE:N | 2.49 | 0.43 |
| 26:CK:192:ILE:HG13 | 26:CK:229:THR:HA | 2.01 | 0.43 |
| 27:CL:568:PRO:HG2 | 27:CL:569:HIS:CD2 | 2.54 | 0.43 |
| 28:CM:366:THR:HG21 | 44:C1:438:C:C5 | 2.54 | 0.43 |
| 29:CN:233:SER:N | 29:CO:101:ASP:OD1 | 2.51 | 0.43 |
| 32:CR:763:ILE:HG22 | 32:CR:765:PRO:HD3 | 2.00 | 0.43 |
| 32:CS:15:ILE:O | 32:CS:19:LEU:HG | 2.19 | 0.43 |
| 32:CS:134:ASN:HB3 | 32:CS:553:PRO:HG2 | 2.00 | 0.43 |
| 32:CS:296:GLY:HA3 | 32:CS:326:PHE:HB2 | 1.99 | 0.43 |
| 32:CS:559:MET:HB3 | 32:CS:559:MET:HE3 | 1.70 | 0.43 |
| 36:Cg:56:ILE:HD12 | 36:Cg:56:ILE:HA | 1.93 | 0.43 |
| 44:C1:217:G:H2' | 44:C1:218:G:H8 | 1.82 | 0.43 |
| 45:C2:74:C:H2' | 45:C2:75:A:C8 | 2.50 | 0.43 |
| 45:C2:129:U:H2' | 45:C2:130:C:H6 | 1.84 | 0.43 |
| 46:UV:1094:THR:HG23 | 46:UV:1095:LEU:HD12 | 2.00 | 0.43 |
| 48:UH:730:PHE:HD1 | 48:UH:730:PHE:HA | 1.65 | 0.43 |
| 49:UE:165:ASP:CG | 49:UE:168:LEU:HB2 | 2.43 | 0.43 |
| 50:US:420:ARG:CZ | 50:US:454:ASP:HA | 2.49 | 0.43 |
| 50:US:483:THR:OG1 | 50:US:484:LYS:N | 2.50 | 0.43 |
| 52:CX:426:THR:OG1 | 52:CX:428:ASP:OD2 | 2.28 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:UI:227:GLY:O | 49:UI:231:THR:HG23 | 2.19 | 0.43 |
| 4:UD:66:GLU:HG2 | 4:UD:566:LEU:HD21 | 1.99 | 0.43 |
| 4:UD:534:PRO:HB2 | 4:UD:537:ILE:HG13 | 2.00 | 0.43 |
| 9:UL:450:LYS:HB3 | 9:UL:459:CYS:SG | 2.58 | 0.43 |
| 9:UL:562:LEU:HD21 | 9:UL:597:LEU:HG | 2.01 | 0.43 |
| 9:UL:645:LEU:HD21 | 9:UL:681:TRP:CH2 | 2.53 | 0.43 |
| 10:UM:340:ASP:O | 10:UM:373:HIS:ND1 | 2.52 | 0.43 |
| 10:UM:702:HIS:HB2 | 10:UM:707:ILE:HB | 1.99 | 0.43 |
| 10:UM:870:HIS:HA | 10:UM:873:ARG:NH1 | 2.34 | 0.43 |
| 12:UO:167:LYS:HG2 | 12:UO:186:HIS:O | 2.18 | 0.43 |
| 12:UO:272:HIS:CE1 | 12:UO:298:LYS:HD2 | 2.53 | 0.43 |
| 13:UQ:771:SER:OG | 13:UQ:772:GLU:OE1 | 2.37 | 0.43 |
| 14:UR:163:GLU:CD | 14:UR:174:ARG:HH22 | 2.27 | 0.43 |
| 14:UR:278:SER:OG | 14:UR:326:ARG:O | 2.27 | 0.43 |
| 14:UR:550:PRO:HD2 | 14:UR:599:SER:HB2 | 1.99 | 0.43 |
| 15:UU:377:ILE:HD11 | 15:UU:380:GLN:HB3 | 2.00 | 0.43 |
| 16:UX:17:GLU:O | 16:UX:21:LYS:NZ | 2.50 | 0.43 |
| 16:UX:154:LYS:O | 16:UX:158:ARG:HB2 | 2.18 | 0.43 |
| 18:CA:127:TYR:OH | 33:CT:136:GLN:OE1 | 2.27 | 0.43 |
| 19:CC:9:PHE:O | 19:CC:15:PHE:HA | 2.19 | 0.43 |
| 20:CD:154:LEU:HD13 | 20:CD:154:LEU:HA | 1.94 | 0.43 |
| 23:CH:334:THR:O | 23:CH:338:LEU:HG | 2.18 | 0.43 |
| 24:CI:76:PRO:HG2 | 24:CI:79:VAL:HB | 2.00 | 0.43 |
| 25:CJ:28:ARG:HD3 | 25:CJ:28:ARG:HA | 1.73 | 0.43 |
| 29:CN:88:ARG:NH1 | 29:CO:132:ARG:HB2 | 2.33 | 0.43 |
| 32:CS:4:GLN:HA | 32:CS:4:GLN:NE2 | 2.32 | 0.43 |
| 32:CS:742:PHE:HB3 | 32:CS:762:MET:HB3 | 2.00 | 0.43 |
| 33:CT:175:LYS:HE3 | 33:CT:175:LYS:HB2 | 1.80 | 0.43 |
| 34:Cc:95:LEU:HA | 34:Cc:95:LEU:HD23 | 1.62 | 0.43 |
| 36:Cg:36:ASN:ND2 | 44:C1:1178:A:OP1 | 2.52 | 0.43 |
| 40:Cm:36:LYS:HG3 | 40:Cm:110:ILE:HD13 | 1.99 | 0.43 |
| 43:CU:113:LYS:HZ1 | 44:C1:1710:G:P | 2.42 | 0.43 |
| 44:C1:39:C:H3' | 44:C1:40:A:H8 | 1.84 | 0.43 |
| 44:C1:1056:U:H2' | 44:C1:1057:A:C8 | 2.54 | 0.43 |
| 44:C1:1509:A:H4' | 54:Cz:1646:VAL:HA | 2.00 | 0.43 |
| 44:C1:2211:U:H2' | 44:C1:2212:G:C8 | 2.54 | 0.43 |
| 46:UV:650:SER:HA | 46:UV:651:PHE:HA | 1.57 | 0.43 |
| 46:UV:693:ARG:HD2 | 46:UV:693:ARG:HA | 1.78 | 0.43 |
| 46:UV:769:ARG:HA | 46:UV:769:ARG:HD2 | 1.70 | 0.43 |
| 47:CV:87:SER:OG | 47:CV:146:SER:N | 2.52 | 0.43 |
| 48:UH:646:LYS:HB2 | 48:UH:730:PHE:HE1 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:UE:227:GLY:O | 49:UE:231:THR:HG23 | 2.19 | 0.43 |
| 50:US:459:GLU:OE2 | 50:US:459:GLU:N | 2.45 | 0.43 |
| 49:UI:161:LEU:HA | 49:UI:161:LEU:HD13 | 1.78 | 0.43 |
| 49:UI:244:ARG:HA | 49:UI:244:ARG:HD3 | 1.65 | 0.43 |
| 2:UB:734:LYS:HA | 2:UB:734:LYS:HD2 | 1.80 | 0.43 |
| 9:UL:652:ILE:HA | 9:UL:673:SER:HA | 1.99 | 0.43 |
| 9:UL:844:ASP:O | 9:UL:847:LEU:HB3 | 2.19 | 0.43 |
| 10:UM:676:LYS:HB3 | 10:UM:678:TRP:HZ3 | 1.84 | 0.43 |
| 10:UM:855:SER:HB2 | 10:UM:858:GLU:OE2 | 2.19 | 0.43 |
| 13:UQ:108:ASN:OD1 | 13:UQ:108:ASN:N | 2.51 | 0.43 |
| 15:UU:674:HIS:HB2 | 15:UU:715:PHE:CD1 | 2.54 | 0.43 |
| 18:CA:71:VAL:HG12 | 18:CA:86:GLY:HA3 | 2.00 | 0.43 |
| 18:CA:233:PRO:HA | 18:CA:262:ILE:HD13 | 2.00 | 0.43 |
| 18:CB:108:ARG:HA | 18:CB:127:TYR:O | 2.18 | 0.43 |
| 20:CD:99:ILE:HG13 | 20:CD:109:PRO:HG3 | 2.00 | 0.43 |
| 20:CD:254:TYR:HA | 20:CD:257:ILE:HD12 | 2.00 | 0.43 |
| 21:CF:122:VAL:HG23 | 21:CF:125:LEU:HD23 | 1.99 | 0.43 |
| 24:CI:309:PRO:HA | 24:CI:312:GLU:HB2 | 2.01 | 0.43 |
| 24:CI:1095:GLN:HE22 | 44:C1:400:C:H1' | 1.84 | 0.43 |
| 27:CL:507:THR:HG23 | 27:CL:509:ALA:H | 1.84 | 0.43 |
| 28:CM:299:VAL:HG13 | 28:CM:334:TRP:CZ2 | 2.54 | 0.43 |
| 32:CR:61:LYS:HE3 | 32:CR:130:ALA:HB3 | 2.01 | 0.43 |
| 32:CR:127:ASP:N | 32:CR:127:ASP:OD1 | 2.52 | 0.43 |
| 32:CS:286:ALA:HB3 | 32:CS:289:ARG:NE | 2.33 | 0.43 |
| 39:Cj:90:VAL:HG21 | 39:Cj:106:LYS:HG3 | 2.00 | 0.43 |
| 44:C1:399:G:H2' | 44:C1:400:C:C6 | 2.53 | 0.43 |
| 44:C1:581:C:H4' | 44:C1:582:G:H2' | 2.01 | 0.43 |
| 46:UV:131:MET:HE2 | 46:UV:131:MET:HA | 2.00 | 0.43 |
| 46:UV:842:LYS:O | 46:UV:959:ARG:NH1 | 2.51 | 0.43 |
| 48:UH:726:LEU:O | 48:UH:730:PHE:HB2 | 2.19 | 0.43 |
| 2:UB:9:LEU:HA | 2:UB:9:LEU:HD23 | 1.66 | 0.42 |
| 4:UD:831:GLN:HB2 | 44:C1:61:G:C8 | 2.54 | 0.42 |
| 6:UG:110:TYR:HA | 6:UG:386:MET:HA | 2.01 | 0.42 |
| 6:UG:470:ASP:HB3 | 11:UN:885:THR:HA | 2.00 | 0.42 |
| 7:UJ:293:MET:HE2 | 7:UJ:312:LEU:HD23 | 2.00 | 0.42 |
| 7:UJ:809:ILE:O | 7:UJ:813:ILE:HG12 | 2.19 | 0.42 |
| 9:UL:937:ARG:HG2 | 9:UL:944:TRP:CH2 | 2.54 | 0.42 |
| 10:UM:376:ILE:HA | 10:UM:393:THR:HG22 | 2.00 | 0.42 |
| 10:UM:858:GLU:OE1 | 10:UM:858:GLU:N | 2.40 | 0.42 |
| 13:UQ:94:PRO:HB3 | 13:UQ:105:ILE:HG23 | 2.01 | 0.42 |
| 13:UQ:629:ILE:HB | 13:UQ:635:VAL:HG22 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:UR:402:ASN:OD1 | 14:UR:404:GLY:N | 2.33 | 0.42 |
| 15:UU:337:ARG:NH2 | 15:UU:769:GLY:O | 2.52 | 0.42 |
| 19:CC:74:MET:HE3 | 19:CC:74:MET:HB2 | 1.66 | 0.42 |
| 20:CD:9:THR:OG1 | 20:CD:10:SER:N | 2.50 | 0.42 |
| 20:CD:329:PHE:HB3 | 20:CD:333:LYS:HE2 | 2.00 | 0.42 |
| 24:CI:206:LEU:HD13 | 24:CI:206:LEU:HA | 1.85 | 0.42 |
| 24:CI:284:GLN:H | 24:CI:296:ILE:HG22 | 1.83 | 0.42 |
| 24:CI:751:ASP:O | 24:CI:755:ALA:HB2 | 2.19 | 0.42 |
| 26:CK:145:HIS:ND1 | 44:C1:2182:C:H4' | 2.34 | 0.42 |
| 28:CM:278:ILE:HB | 44:C1:586:G:N1 | 2.34 | 0.42 |
| 32:CR:278:ARG:O | 32:CR:278:ARG:NE | 2.46 | 0.42 |
| 32:CR:828:GLU:HA | 32:CR:831:GLN:HG3 | 2.00 | 0.42 |
| 32:CS:278:ARG:O | 32:CS:278:ARG:NE | 2.46 | 0.42 |
| 43:CU:248:ALA:HB1 | 43:CU:253:ILE:HB | 2.01 | 0.42 |
| 44:C1:82:C:H2' | 44:C1:83:A:H8 | 1.84 | 0.42 |
| 44:C1:394:U:H2' | 44:C1:395:C:C6 | 2.54 | 0.42 |
| 44:C1:1221:C:N3 | 44:C1:1222:C:N4 | 2.67 | 0.42 |
| 44:C1:2162:C:H2' | 44:C1:2163:C:H6 | 1.84 | 0.42 |
| 44:C1:2198:C:H4' | 44:C1:2199:G:C8 | 2.53 | 0.42 |
| 48:UH:755:TYR:CD2 | 49:UI:214:LEU:HD13 | 2.54 | 0.42 |
| 48:UH:859:MET:HE1 | 48:UH:876:LYS:HB3 | 2.01 | 0.42 |
| 50:US:515:ILE:HD11 | 50:US:517:PHE:HE1 | 1.84 | 0.42 |
| 49:UI:229:LEU:HD13 | 49:UI:229:LEU:HA | 1.89 | 0.42 |
| 1:UA:304:THR:HG22 | 1:UA:305:ILE:H | 1.83 | 0.42 |
| 1:UA:516:VAL:HG13 | 1:UA:527:ILE:HG22 | 2.00 | 0.42 |
| 1:UA:616:LEU:HA | 1:UA:616:LEU:HD12 | 1.79 | 0.42 |
| 1:UA:667:ARG:O | 1:UA:669:LYS:N | 2.52 | 0.42 |
| 4:UD:298:ARG:NH1 | 4:UD:320:ARG:HD2 | 2.33 | 0.42 |
| 5:UF:136:LEU:HA | 5:UF:136:LEU:HD23 | 1.71 | 0.42 |
| 6:UG:199:TYR:CG | 6:UG:214:ARG:HG2 | 2.54 | 0.42 |
| 6:UG:215:LYS:HD3 | 6:UG:215:LYS:HA | 1.83 | 0.42 |
| 6:UG:222:MET:HE2 | 6:UG:222:MET:HB3 | 1.83 | 0.42 |
| 7:UJ:657:ARG:HE | 7:UJ:657:ARG:HB2 | 1.63 | 0.42 |
| 8:UK:6:HIS:HB2 | 8:UK:9:GLN:HG2 | 2.00 | 0.42 |
| 9:UL:138:ASP:H | 9:UL:145:GLN:HG3 | 1.84 | 0.42 |
| 9:UL:441:LEU:O | 9:UL:451:ILE:HA | 2.19 | 0.42 |
| 9:UL:806:ASN:OD1 | 9:UL:806:ASN:N | 2.51 | 0.42 |
| 9:UL:895:MET:HB3 | 9:UL:899:LEU:HD13 | 2.00 | 0.42 |
| 10:UM:41:GLU:HA | 10:UM:63:PRO:HA | 2.00 | 0.42 |
| 10:UM:376:ILE:HG23 | 10:UM:391:ILE:HG23 | 2.01 | 0.42 |
| 12:UO:145:GLN:NE2 | 12:UO:146:PRO:HD2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:UQ:699:ILE:HD11 | 13:UQ:714:ALA:HB1 | 2.02 | 0.42 |
| 13:UQ:779:GLN:OE1 | 13:UQ:779:GLN:N | 2.52 | 0.42 |
| 14:UR:421:ALA:HB2 | 14:UR:437:ARG:HG2 | 2.00 | 0.42 |
| 15:UU:150:TRP:CD1 | 15:UU:163:LYS:HA | 2.54 | 0.42 |
| 15:UU:163:LYS:HD2 | 15:UU:166:THR:OG1 | 2.19 | 0.42 |
| 15:UU:391:LEU:HD23 | 15:UU:391:LEU:HA | 1.82 | 0.42 |
| 16:UX:92:THR:OG1 | 16:UX:95:VAL:HG23 | 2.19 | 0.42 |
| 16:UX:114:ARG:NH2 | 28:CM:348:GLY:O | 2.47 | 0.42 |
| 19:CC:175:ASN:HA | 19:CC:178:ILE:HG12 | 2.02 | 0.42 |
| 24:CI:914:ILE:O | 24:CI:994:PRO:HA | 2.19 | 0.42 |
| 25:CJ:166:ILE:HD13 | 25:CJ:166:ILE:HA | 1.79 | 0.42 |
| 27:CL:639:LYS:H | 27:CL:639:LYS:HG3 | 1.57 | 0.42 |
| 28:CM:27:LEU:HD23 | 28:CM:27:LEU:HA | 1.84 | 0.42 |
| 28:CM:44:LEU:HA | 28:CM:388:ILE:HD12 | 2.01 | 0.42 |
| 28:CM:158:SER:OG | 28:CM:201:THR:O | 2.35 | 0.42 |
| 28:CM:197:VAL:HB | 35:Ce:161:LYS:HE3 | 2.01 | 0.42 |
| 32:CR:37:ALA:O | 32:CR:41:LEU:HG | 2.19 | 0.42 |
| 32:CR:586:ILE:HG22 | 32:CR:638:ILE:HG23 | 2.00 | 0.42 |
| 32:CR:647:MET:HE3 | 32:CR:647:MET:HB2 | 1.89 | 0.42 |
| 32:CS:37:ALA:O | 32:CS:41:LEU:HG | 2.19 | 0.42 |
| 32:CS:400:LYS:NZ | 32:CS:431:GLN:OE1 | 2.52 | 0.42 |
| 36:Cg:90:LYS:HD3 | 36:Cg:91:LEU:HD12 | 2.01 | 0.42 |
| 37:Ch:91:LEU:HD11 | 37:Ch:125:LEU:HD12 | 2.01 | 0.42 |
| 44:C1:178:G:H2' | 44:C1:179:G:C8 | 2.54 | 0.42 |
| 44:C1:270:C:H4' | 44:C1:273:G:C4 | 2.55 | 0.42 |
| 44:C1:461:G:H2' | 44:C1:462:G:C8 | 2.54 | 0.42 |
| 44:C1:1703:G:H2' | 44:C1:1704:U:C6 | 2.55 | 0.42 |
| 44:C1:2058:A:H2' | 44:C1:2059:C:C6 | 2.54 | 0.42 |
| 45:C2:162:C:O2' | 45:C2:164:U:OP2 | 2.31 | 0.42 |
| 46:UV:740:HIS:CE1 | 46:UV:757:ASP:HB2 | 2.53 | 0.42 |
| 48:UH:811:PHE:HA | 48:UH:814:GLN:NE2 | 2.35 | 0.42 |
| 49:UE:179:LEU:HB2 | 49:UE:180:ILE:H | 1.63 | 0.42 |
| 50:US:279:LYS:O | 50:US:283:LYS:HE3 | 2.20 | 0.42 |
| 50:US:331:GLU:CD | 50:US:332:ARG:HB2 | 2.44 | 0.42 |
| 50:US:384:ARG:HH22 | 50:US:443:ASN:H | 1.67 | 0.42 |
| 52:CX:374:ARG:HG2 | 52:CX:420:ARG:HG2 | 2.01 | 0.42 |
| 1:UA:558:ARG:NH2 | 45:C2:62:A:N7 | 2.68 | 0.42 |
| 2:UB:64:ALA:HA | 26:CK:177:PRO:HG3 | 2.01 | 0.42 |
| 4:UD:709:MET:O | 4:UD:826:TRP:HA | 2.18 | 0.42 |
| 5:UF:102:LYS:HA | 44:C1:437:G:O6 | 2.19 | 0.42 |
| 6:UG:469:LEU:HD11 | 6:UG:474:GLU:HB2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:UJ:295:GLN:HA | 14:UR:229:PRO:HG2 | 2.01 | 0.42 |
| 7:UJ:606:LYS:HA | 7:UJ:609:ARG:HE | 1.85 | 0.42 |
| 7:UJ:654:ALA:O | 7:UJ:658:SER:HB3 | 2.20 | 0.42 |
| 9:UL:621:LEU:N | 9:UL:636:LEU:HD12 | 2.34 | 0.42 |
| 12:UO:313:TYR:HA | 12:UO:314:PRO:HD3 | 1.91 | 0.42 |
| 12:UO:443:THR:HA | 12:UO:448:TYR:CD1 | 2.54 | 0.42 |
| 16:UX:167:SER:O | 16:UX:174:ALA:HB3 | 2.19 | 0.42 |
| 17:UZ:267:VAL:HG21 | 17:UZ:275:TRP:CE2 | 2.54 | 0.42 |
| 18:CA:97:LEU:HD13 | 18:CA:97:LEU:HA | 1.83 | 0.42 |
| 18:CA:97:LEU:HD23 | 18:CA:172:ASP:HA | 2.01 | 0.42 |
| 18:CA:183:VAL:HA | 18:CA:206:ILE:O | 2.19 | 0.42 |
| 18:CA:253:LEU:HD22 | 18:CA:284:PHE:CE1 | 2.54 | 0.42 |
| 21:CF:80:VAL:HB | 21:CF:122:VAL:HG21 | 2.01 | 0.42 |
| 22:CG:402:ALA:HB3 | 22:CG:410:VAL:HG12 | 2.00 | 0.42 |
| 23:CH:107:THR:HG22 | 23:CH:185:GLY:C | 2.43 | 0.42 |
| 24:CI:918:LEU:HD12 | 24:CI:918:LEU:HA | 1.77 | 0.42 |
| 24:CI:1101:ARG:HD2 | 33:CT:111:MET:HG2 | 2.00 | 0.42 |
| 26:CK:122:LEU:HA | 26:CK:122:LEU:HD12 | 1.66 | 0.42 |
| 27:CL:561:ARG:HH21 | 27:CL:564:MET:HA | 1.84 | 0.42 |
| 28:CM:378:LEU:HA | 28:CM:378:LEU:HD12 | 1.63 | 0.42 |
| 32:CR:110:LYS:N | 32:CR:110:LYS:HD3 | 2.34 | 0.42 |
| 32:CR:400:LYS:NZ | 32:CR:431:GLN:OE1 | 2.52 | 0.42 |
| 32:CS:195:SER:H | 32:CS:195:SER:HG | 1.59 | 0.42 |
| 32:CS:196:CYS:O | 32:CS:213:GLY:HA2 | 2.20 | 0.42 |
| 32:CS:735:LYS:HA | 32:CS:735:LYS:HD3 | 1.84 | 0.42 |
| 35:Ce:143:VAL:HG11 | 35:Ce:164:LEU:HB3 | 2.01 | 0.42 |
| 44:C1:351:U:O2' | 44:C1:352:G:H5' | 2.19 | 0.42 |
| 44:C1:379:G:H2' | 44:C1:380:C:C6 | 2.55 | 0.42 |
| 44:C1:381:G:H1 | 44:C1:384:C:P | 2.41 | 0.42 |
| 44:C1:455:G:H21 | 44:C1:477:A:H62 | 1.67 | 0.42 |
| 44:C1:580:A:H2' | 44:C1:581:C:H5" | 1.99 | 0.42 |
| 44:C1:2082:G:H2' | 44:C1:2083:C:C6 | 2.55 | 0.42 |
| 44:C1:2231:A:H2' | 44:C1:2232:C:H6 | 1.84 | 0.42 |
| 45:C2:90:C:H1' | 45:C2:91:G:H5' | 2.00 | 0.42 |
| 45:C2:91:G:H21 | 45:C2:91:G:P | 2.40 | 0.42 |
| 46:UV:41:GLU:HA | 46:UV:44:GLU:HG3 | 2.00 | 0.42 |
| 46:UV:670:PRO:HG2 | 46:UV:675:LEU:HD22 | 2.00 | 0.42 |
| 46:UV:676:ARG:HH21 | 46:UV:813:HIS:HD2 | 1.66 | 0.42 |
| 46:UV:707:TRP:HB2 | 46:UV:774:LEU:HD11 | 2.01 | 0.42 |
| 50:US:173:VAL:HG13 | 50:US:174:LEU:HD22 | 2.00 | 0.42 |
| 1:UA:73:ILE:HG21 | 1:UA:99:VAL:HG21 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:215:LYS:NZ | 1:UA:259:ARG:HD3 | 2.35 | 0.42 |
| 2:UB:65:ARG:HA | 2:UB:65:ARG:HD3 | 1.85 | 0.42 |
| 5:UF:14:ARG:HA | 5:UF:14:ARG:HD2 | 1.68 | 0.42 |
| 6:UG:61:LYS:HD3 | 6:UG:61:LYS:HA | 1.79 | 0.42 |
| 6:UG:321:ASP:O | 6:UG:323:LYS:N | 2.52 | 0.42 |
| 7:UJ:121:LEU:HD23 | 7:UJ:121:LEU:HA | 1.83 | 0.42 |
| 7:UJ:544:LYS:O | 7:UJ:547:SER:OG | 2.24 | 0.42 |
| 8:UK:18:GLN:O | 24:CI:1036:ARG:NH2 | 2.52 | 0.42 |
| 9:UL:270:ARG:HE | 9:UL:270:ARG:HB2 | 1.54 | 0.42 |
| 9:UL:293:PHE:CZ | 9:UL:305:TRP:HB2 | 2.54 | 0.42 |
| 9:UL:592:PHE:HD1 | 9:UL:599:LEU:HA | 1.84 | 0.42 |
| 9:UL:699:ILE:HA | 9:UL:715:SER:HA | 2.01 | 0.42 |
| 9:UL:934:LYS:HD3 | 9:UL:934:LYS:HA | 1.85 | 0.42 |
| 10:UM:869:ARG:CZ | 27:CL:679:PRO:HG2 | 2.49 | 0.42 |
| 12:UO:159:THR:HA | 12:UO:172:TRP:O | 2.20 | 0.42 |
| 12:UO:521:THR:OG1 | 12:UO:522:GLN:N | 2.52 | 0.42 |
| 13:UQ:369:TYR:CE1 | 13:UQ:383:GLN:HA | 2.54 | 0.42 |
| 13:UQ:560:GLU:OE2 | 13:UQ:574:SER:N | 2.52 | 0.42 |
| 14:UR:180:LEU:HD23 | 14:UR:180:LEU:HA | 1.87 | 0.42 |
| 14:UR:286:TYR:HB2 | 14:UR:288:ILE:HD12 | 2.01 | 0.42 |
| 15:UU:579:PHE:HD1 | 15:UU:649:TRP:CD2 | 2.37 | 0.42 |
| 16:UX:112:ILE:HD13 | 16:UX:112:ILE:HA | 1.84 | 0.42 |
| 19:CC:104:LYS:HE3 | 19:CC:104:LYS:HB3 | 1.78 | 0.42 |
| 20:CD:277:TYR:CD2 | 20:CD:278:LEU:HD23 | 2.54 | 0.42 |
| 22:CG:292:THR:HG23 | 22:CG:308:LYS:HD2 | 2.01 | 0.42 |
| 22:CG:443:LYS:HB2 | 22:CG:446:ASP:OD1 | 2.19 | 0.42 |
| 23:CH:296:GLU:HG3 | 23:CH:309:ILE:HG23 | 2.02 | 0.42 |
| 26:CK:43:ASP:HA | 26:CK:44:PRO:HD3 | 1.90 | 0.42 |
| 26:CK:190:HIS:HB3 | 27:CL:554:PHE:CG | 2.54 | 0.42 |
| 30:CP:41:THR:OG1 | 30:CP:42:LEU:N | 2.52 | 0.42 |
| 31:CQ:187:ILE:HD11 | 44:C1:2351:G:C6 | 2.54 | 0.42 |
| 32:CR:132:THR:HB | 32:CR:135:ILE:HG12 | 2.01 | 0.42 |
| 32:CR:488:LYS:HE3 | 32:CR:488:LYS:HB3 | 1.92 | 0.42 |
| 32:CS:46:SER:H | 32:CS:46:SER:HG | 1.53 | 0.42 |
| 32:CS:127:ASP:OD1 | 32:CS:127:ASP:N | 2.52 | 0.42 |
| 35:Ce:30:LEU:HB2 | 35:Ce:44:LEU:HD11 | 2.02 | 0.42 |
| 44:C1:99:A:H2' | 44:C1:100:C:H6 | 1.85 | 0.42 |
| 44:C1:1738:G:H2' | 44:C1:1739:G:C8 | 2.53 | 0.42 |
| 53:UP:343:LYS:HE2 | 53:UP:343:LYS:HB2 | 1.71 | 0.42 |
| 54:Cz:1526:SER:HA | 54:Cz:1529:ARG:HD2 | 2.00 | 0.42 |
| 54:Cz:1725:THR:OG1 | 54:Cz:1726:LYS:NZ | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:611:THR:H | 1:UA:611:THR:HG22 | 1.60 | 0.42 |
| 5:UF:188:TRP:HE3 | 5:UF:189:LEU:HD22 | 1.85 | 0.42 |
| 6:UG:304:ARG:HD2 | 6:UG:304:ARG:HA | 1.74 | 0.42 |
| 6:UG:309:ASP:OD2 | 6:UG:310:ARG:N | 2.52 | 0.42 |
| 7:UJ:273:MET:HE1 | 13:UQ:944:VAL:HG23 | 2.02 | 0.42 |
| 8:UK:66:GLY:O | 8:UK:69:SER:N | 2.52 | 0.42 |
| 9:UL:242:THR:OG1 | 9:UL:244:TRP:NE1 | 2.40 | 0.42 |
| 9:UL:574:SER:HG | 9:UL:578:ARG:H | 1.66 | 0.42 |
| 9:UL:825:PRO:O | 9:UL:828:THR:OG1 | 2.24 | 0.42 |
| 10:UM:626:LEU:HG | 10:UM:635:ILE:HD12 | 2.02 | 0.42 |
| 11:UN:887:LEU:HD23 | 11:UN:887:LEU:HA | 1.86 | 0.42 |
| 12:UO:317:ILE:HA | 12:UO:338:MET:HA | 2.01 | 0.42 |
| 13:UQ:543:PHE:CE2 | 13:UQ:547:GLY:HA2 | 2.55 | 0.42 |
| 13:UQ:748:SER:OG | 13:UQ:749:ASP:N | 2.52 | 0.42 |
| 16:UX:40:MET:HE3 | 16:UX:40:MET:HB2 | 1.71 | 0.42 |
| 18:CB:106:GLU:H | 18:CB:106:GLU:HG2 | 1.62 | 0.42 |
| 20:CD:117:ASP:O | 20:CD:121:ALA:HB3 | 2.20 | 0.42 |
| 21:CE:68:ILE:HA | 21:CE:71:ILE:HD12 | 2.01 | 0.42 |
| 22:CG:579:VAL:HG23 | 22:CG:603:ILE:HG13 | 2.01 | 0.42 |
| 24:CI:394:LYS:HA | 24:CI:401:GLN:HA | 2.00 | 0.42 |
| 26:CK:156:HIS:O | 26:CK:160:GLY:N | 2.50 | 0.42 |
| 26:CK:269:THR:O | 26:CK:271:GLY:N | 2.53 | 0.42 |
| 27:CL:564:MET:HE2 | 27:CL:564:MET:HB2 | 1.89 | 0.42 |
| 28:CM:304:ASP:O | 28:CM:306:THR:N | 2.50 | 0.42 |
| 28:CM:376:ASN:HA | 28:CM:379:LEU:HD12 | 2.00 | 0.42 |
| 32:CR:11:ILE:HG23 | 32:CR:27:PHE:CZ | 2.55 | 0.42 |
| 32:CR:196:CYS:O | 32:CR:213:GLY:HA2 | 2.20 | 0.42 |
| 32:CR:284:THR:HG23 | 32:CR:412:SER:HB2 | 2.01 | 0.42 |
| 32:CR:735:LYS:NZ | 32:CR:804:THR:HG21 | 2.34 | 0.42 |
| 35:Ce:29:ALA:O | 35:Ce:33:LEU:HG | 2.19 | 0.42 |
| 40:Cm:101:TYR:HB2 | 40:Cm:129:PHE:CZ | 2.55 | 0.42 |
| 44:C1:1463:G:H2' | 44:C1:1464:G:C8 | 2.55 | 0.42 |
| 44:C1:2054:A:H8 | 44:C1:2054:A:OP1 | 2.02 | 0.42 |
| 45:C2:45:C:H2' | 45:C2:46:U:O4' | 2.19 | 0.42 |
| 50:US:111:ILE:HD12 | 50:US:111:ILE:H | 1.84 | 0.42 |
| 50:US:233:VAL:HG22 | 50:US:296:TRP:CE2 | 2.55 | 0.42 |
| 50:US:389:ALA:HA | 50:US:392:ALA:HB2 | 2.00 | 0.42 |
| 52:CX:303:PHE:HA | 52:CX:307:LEU:HB3 | 2.02 | 0.42 |
| 52:CX:318:LEU:O | 52:CX:322:GLN:HG2 | 2.20 | 0.42 |
| 52:CX:342:ILE:HD13 | 52:CX:370:LEU:HD23 | 2.01 | 0.42 |
| 1:UA:131:ASN:OD1 | 1:UA:134:GLY:HA3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:247:ASN:N | 1:UA:247:ASN:OD1 | 2.52 | 0.42 |
| 1:UA:466:GLY:O | 1:UA:493:ARG:NH2 | 2.53 | 0.42 |
| 2:UB:650:ALA:O | 2:UB:652:ARG:N | 2.50 | 0.42 |
| 3:UC:599:ASN:HB3 | 3:UC:602:VAL:HG12 | 2.02 | 0.42 |
| 4:UD:424:LEU:H | 4:UD:424:LEU:HD23 | 1.84 | 0.42 |
| 5:UF:117:ALA:O | 5:UF:120:VAL:O | 2.37 | 0.42 |
| 6:UG:229:PHE:O | 6:UG:245:THR:OG1 | 2.24 | 0.42 |
| 6:UG:310:ARG:HD2 | 6:UG:352:ASP:HA | 2.00 | 0.42 |
| 6:UG:393:GLN:HB3 | 6:UG:411:HIS:HB2 | 2.01 | 0.42 |
| 7:UJ:128:HIS:CE1 | 7:UJ:129:GLU:HG3 | 2.55 | 0.42 |
| 7:UJ:140:LEU:O | 7:UJ:143:HIS:HB3 | 2.19 | 0.42 |
| 7:UJ:237:ARG:HE | 14:UR:254:ARG:HH22 | 1.68 | 0.42 |
| 9:UL:391:ASN:N | 9:UL:391:ASN:OD1 | 2.40 | 0.42 |
| 10:UM:236:GLN:HE21 | 10:UM:252:ARG:HD3 | 1.84 | 0.42 |
| 10:UM:591:THR:HG22 | 10:UM:618:GLY:HA3 | 2.01 | 0.42 |
| 10:UM:807:PHE:HA | 10:UM:810:LEU:HG | 2.01 | 0.42 |
| 13:UQ:640:PRO:HA | 13:UQ:661:TRP:HA | 2.00 | 0.42 |
| 13:UQ:920:VAL:HG21 | 14:UR:575:THR:HG21 | 2.00 | 0.42 |
| 17:UZ:92:SER:C | 17:UZ:123:LYS:HZ1 | 2.27 | 0.42 |
| 19:CC:8:LEU:HD13 | 19:CC:8:LEU:HA | 1.88 | 0.42 |
| 20:CD:187:LYS:HA | 20:CD:207:TYR:CE2 | 2.54 | 0.42 |
| 21:CF:26:GLN:NE2 | 21:CF:91:ALA:O | 2.53 | 0.42 |
| 22:CG:236:LYS:HE2 | 22:CG:236:LYS:HB3 | 1.89 | 0.42 |
| 23:CH:157:VAL:HG12 | 23:CH:331:SER:HB2 | 2.02 | 0.42 |
| 24:CI:537:TRP:HB2 | 24:CI:560:TRP:CD2 | 2.54 | 0.42 |
| 24:CI:740:GLU:OE1 | 24:CI:740:GLU:N | 2.45 | 0.42 |
| 25:CJ:59:HIS:CD2 | 44:C1:294:G:H4' | 2.54 | 0.42 |
| 27:CL:477:GLU:HG2 | 27:CL:478:ARG:HD2 | 2.00 | 0.42 |
| 27:CL:678:ALA:HB3 | 27:CL:681:GLU:OE1 | 2.19 | 0.42 |
| 28:CM:336:MET:N | 28:CM:336:MET:SD | 2.92 | 0.42 |
| 29:CN:94:GLN:HG2 | 29:CO:94:GLN:CD | 2.45 | 0.42 |
| 32:CR:24:ARG:HB2 | 32:CR:486:VAL:HG21 | 2.02 | 0.42 |
| 32:CR:737:TRP:HA | 32:CR:740:ALA:HB3 | 2.01 | 0.42 |
| 32:CS:160:LYS:O | 32:CS:164:THR:HG22 | 2.20 | 0.42 |
| 32:CS:724:GLY:HA3 | 32:CS:763:ILE:HD13 | 2.02 | 0.42 |
| 36:Cg:58:LEU:HA | 36:Cg:67:ARG:NH2 | 2.33 | 0.42 |
| 39:Cj:40:ALA:HB3 | 39:Cj:45:ARG:HE | 1.85 | 0.42 |
| 39:Cj:48:LEU:HD23 | 39:Cj:48:LEU:HA | 1.66 | 0.42 |
| 43:CU:102:ASN:OD1 | 43:CU:102:ASN:N | 2.53 | 0.42 |
| 43:CU:253:ILE:HG21 | 43:CU:253:ILE:HD13 | 1.79 | 0.42 |
| 44:C1:30:U:H2' | 44:C1:31:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:141:C:H2' | 44:C1:142:C:C6 | 2.55 | 0.42 |
| 44:C1:2066:A:C5 | 44:C1:2107:A:C5 | 3.07 | 0.42 |
| 45:C2:35:G:O2' | 45:C2:36:U:OP1 | 2.28 | 0.42 |
| 45:C2:247:G:H2' | 45:C2:248:G:C8 | 2.55 | 0.42 |
| 46:UV:96:LYS:HG3 | 46:UV:98:PRO:HD3 | 2.01 | 0.42 |
| 46:UV:379:ALA:HA | 46:UV:385:GLY:O | 2.20 | 0.42 |
| 46:UV:566:PHE:HA | 46:UV:570:TRP:CD1 | 2.54 | 0.42 |
| 48:UH:774:GLN:O | 48:UH:777:ALA:HB3 | 2.20 | 0.42 |
| 50:US:236:SER:OG | 50:US:238:ASP:OD1 | 2.34 | 0.42 |
| 50:US:425:LYS:HE3 | 50:US:425:LYS:HB3 | 1.67 | 0.42 |
| 52:CX:312:ALA:HB1 | 52:CX:350:ALA:HB2 | 2.00 | 0.42 |
| 1:UA:707:ASP:O | 1:UA:741:ASN:HB3 | 2.20 | 0.42 |
| 1:UA:791:LEU:HA | 1:UA:794:ILE:HG22 | 2.01 | 0.42 |
| 3:UC:598:ARG:HG3 | 44:C1:1129:A:H2' | 2.01 | 0.42 |
| 4:UD:329:MET:HB3 | 4:UD:342:SER:HA | 2.02 | 0.42 |
| 4:UD:389:ASN:ND2 | 4:UD:425:ILE:HB | 2.35 | 0.42 |
| 5:UF:93:PHE:O | 5:UF:97:GLU:HG2 | 2.19 | 0.42 |
| 5:UF:102:LYS:NZ | 44:C1:437:G:N7 | 2.67 | 0.42 |
| 5:UF:166:ARG:HG2 | 5:UF:169:ARG:NH2 | 2.34 | 0.42 |
| 5:UF:287:ARG:HA | 5:UF:292:TRP:CE2 | 2.55 | 0.42 |
| 6:UG:239:GLN:HA | 6:UG:254:ILE:O | 2.20 | 0.42 |
| 7:UJ:157:VAL:HA | 7:UJ:160:ILE:HD12 | 2.02 | 0.42 |
| 7:UJ:295:GLN:HG3 | 14:UR:229:PRO:HD2 | 2.01 | 0.42 |
| 9:UL:496:SER:OG | 9:UL:498:SER:OG | 2.29 | 0.42 |
| 9:UL:955:LYS:HD3 | 27:CL:649:VAL:HG21 | 2.01 | 0.42 |
| 10:UM:623:THR:HG1 | 10:UM:637:THR:HG1 | 1.60 | 0.42 |
| 11:UN:317:LYS:HE3 | 11:UN:317:LYS:HB3 | 1.88 | 0.42 |
| 11:UN:325:ARG:NH1 | 28:CM:209:GLU:OE1 | 2.52 | 0.42 |
| 13:UQ:184:THR:OG1 | 13:UQ:186:LYS:N | 2.53 | 0.42 |
| 13:UQ:395:LEU:HD12 | 13:UQ:415:LEU:HD11 | 2.00 | 0.42 |
| 14:UR:140:ASP:O | 14:UR:144:LEU:HG | 2.20 | 0.42 |
| 15:UU:80:LEU:HD23 | 15:UU:80:LEU:HA | 1.89 | 0.42 |
| 15:UU:121:VAL:HB | 15:UU:129:ALA:HB3 | 2.02 | 0.42 |
| 16:UX:114:ARG:HH22 | 28:CM:64:GLY:HA3 | 1.85 | 0.42 |
| 18:CA:77:ARG:HH21 | 18:CA:78:HIS:CE1 | 2.37 | 0.42 |
| 18:CA:103:VAL:HG13 | 18:CA:196:MET:HE3 | 2.01 | 0.42 |
| 19:CC:18:PHE:CD1 | 19:CC:50:LEU:HA | 2.55 | 0.42 |
| 21:CF:69:PRO:HA | 21:CF:72:CYS:HB2 | 2.02 | 0.42 |
| 23:CH:110:ILE:HG13 | 23:CH:114:LEU:HD11 | 2.02 | 0.42 |
| 23:CH:220:GLY:O | 23:CH:252:ILE:HA | 2.19 | 0.42 |
| 24:CI:216:ASP:HA | 24:CI:219:ILE:HG12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:CI:243:TYR:CZ | 24:CI:275:ARG:HB3 | 2.55 | 0.42 |
| 24:CI:826:ILE:HD12 | 24:CI:826:ILE:HA | 1.73 | 0.42 |
| 24:CI:860:LEU:HA | 24:CI:860:LEU:HD23 | 1.77 | 0.42 |
| 24:CI:959:ARG:NE | 26:CK:287:TYR:O | 2.52 | 0.42 |
| 26:CK:90:VAL:HG13 | 26:CK:116:ARG:HA | 2.01 | 0.42 |
| 26:CK:117:LEU:HD12 | 26:CK:117:LEU:HA | 1.77 | 0.42 |
| 27:CL:573:ARG:HG2 | 44:C1:2214:A:OP2 | 2.20 | 0.42 |
| 28:CM:104:TRP:CE2 | 28:CM:137:PRO:HA | 2.55 | 0.42 |
| 28:CM:253:MET:O | 28:CM:268:ASP:HA | 2.20 | 0.42 |
| 29:CO:67:LEU:HG | 29:CO:142:VAL:HG23 | 2.01 | 0.42 |
| 29:CO:114:ILE:O | 29:CO:121:LEU:HA | 2.19 | 0.42 |
| 29:CO:174:ASN:OD1 | 29:CO:174:ASN:N | 2.43 | 0.42 |
| 32:CR:285:ALA:HB2 | 32:CR:474:LEU:HB3 | 2.02 | 0.42 |
| 32:CS:781:ASP:HA | 32:CS:784:LYS:HE3 | 2.02 | 0.42 |
| 36:Cg:69:PHE:HA | 36:Cg:72:ASN:HD21 | 1.85 | 0.42 |
| 44:C1:129:G:H2' | 44:C1:130:C:C6 | 2.55 | 0.42 |
| 44:C1:1453:G:H2' | 44:C1:1454:A:C8 | 2.54 | 0.42 |
| 44:C1:1647:U:H2' | 44:C1:1648:G:C8 | 2.54 | 0.42 |
| 44:C1:2177:G:N3 | 44:C1:2183:A:N6 | 2.68 | 0.42 |
| 46:UV:186:LEU:HD12 | 46:UV:187:SER:H | 1.84 | 0.42 |
| 46:UV:489:ALA:HB2 | 46:UV:606:ILE:HG12 | 2.01 | 0.42 |
| 46:UV:503:LEU:HD21 | 46:UV:506:LEU:HD22 | 2.01 | 0.42 |
| 46:UV:508:VAL:HG13 | 46:UV:532:ILE:HG23 | 2.02 | 0.42 |
| 46:UV:542:ASN:ND2 | 46:UV:545:ARG:HH21 | 2.17 | 0.42 |
| 46:UV:618:ASP:OD1 | 46:UV:620:ILE:HG22 | 2.20 | 0.42 |
| 48:UH:717:CYS:O | 48:UH:782:ARG:NH1 | 2.41 | 0.42 |
| 48:UH:860:THR:HA | 48:UH:927:GLN:NE2 | 2.33 | 0.42 |
| 50:US:470:ASN:O | 50:US:473:THR:OG1 | 2.27 | 0.42 |
| 52:CX:313:SER:OG | 52:CX:315:THR:OG1 | 2.36 | 0.42 |
| 54:Cz:1595:GLY:HA2 | 54:Cz:1597:TYR:CZ | 2.54 | 0.42 |
| 1:UA:410:ASP:OD1 | 1:UA:411:LEU:N | 2.53 | 0.42 |
| 1:UA:477:ALA:O | 1:UA:480:GLY:N | 2.47 | 0.42 |
| 2:UB:332:LEU:O | 2:UB:335:LEU:HG | 2.19 | 0.42 |
| 2:UB:542:GLN:HB2 | 2:UB:545:TRP:CE2 | 2.55 | 0.42 |
| 4:UD:285:SER:OG | 4:UD:290:LYS:N | 2.42 | 0.42 |
| 5:UF:34:ARG:NH2 | 6:UG:96:GLN:HG2 | 2.35 | 0.42 |
| 7:UJ:542:ARG:HE | 7:UJ:578:ARG:NE | 2.18 | 0.42 |
| 7:UJ:664:LEU:HD12 | 7:UJ:664:LEU:HA | 1.79 | 0.42 |
| 9:UL:242:THR:HA | 9:UL:272:THR:HA | 2.02 | 0.42 |
| 9:UL:864:PHE:O | 9:UL:867:ARG:C | 2.63 | 0.42 |
| 11:UN:324:ASP:O | 11:UN:327:ILE:HG22 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:UN:367:THR:O | 11:UN:371:GLN:HG2 | 2.19 | 0.42 |
| 12:UO:2:ALA:HB2 | 13:UQ:392:LEU:HD11 | 2.01 | 0.42 |
| 13:UQ:157:TRP:CD1 | 13:UQ:192:VAL:HG11 | 2.54 | 0.42 |
| 13:UQ:268:THR:OG1 | 13:UQ:269:LYS:N | 2.53 | 0.42 |
| 13:UQ:777:LEU:HD12 | 13:UQ:777:LEU:HA | 1.74 | 0.42 |
| 15:UU:151:ILE:CG1 | 15:UU:162:TRP:HB2 | 2.50 | 0.42 |
| 15:UU:861:LYS:HD3 | 15:UU:861:LYS:HA | 1.72 | 0.42 |
| 17:UZ:154:LEU:HA | 17:UZ:180:ILE:HG22 | 2.02 | 0.42 |
| 19:CC:280:ASN:O | 19:CC:283:SER:OG | 2.32 | 0.42 |
| 20:CD:292:LEU:HD23 | 20:CD:292:LEU:HA | 1.79 | 0.42 |
| 21:CF:66:LEU:C | 21:CF:69:PRO:HD2 | 2.44 | 0.42 |
| 22:CG:165:GLN:HA | 22:CG:602:VAL:HG22 | 2.00 | 0.42 |
| 23:CH:151:ASP:O | 23:CH:155:THR:HG22 | 2.20 | 0.42 |
| 23:CH:379:ASP:HA | 23:CH:394:LEU:HD13 | 2.02 | 0.42 |
| 31:CQ:215:LYS:HD3 | 31:CQ:217:HIS:NE2 | 2.35 | 0.42 |
| 31:CQ:221:ALA:O | 31:CQ:225:ILE:HG12 | 2.20 | 0.42 |
| 32:CR:24:ARG:NH2 | 32:CR:487:GLU:HB2 | 2.35 | 0.42 |
| 32:CR:724:GLY:HA3 | 32:CR:763:ILE:HD13 | 2.02 | 0.42 |
| 32:CS:285:ALA:HB2 | 32:CS:474:LEU:HB3 | 2.02 | 0.42 |
| 32:CS:763:ILE:HG22 | 32:CS:765:PRO:HD3 | 2.01 | 0.42 |
| 33:CT:107:GLN:O | 33:CT:110:ARG:HG2 | 2.20 | 0.42 |
| 36:Cg:105:ARG:HH21 | 36:Cg:145:MET:HA | 1.85 | 0.42 |
| 44:C1:1623:U:H5” | 44:C1:1624:A:H2’ | 2.02 | 0.42 |
| 44:C1:1625:G:H1 | 44:C1:1663:U:H3 | 1.66 | 0.42 |
| 44:C1:1734:G:H2’ | 44:C1:1735:A:C8 | 2.50 | 0.42 |
| 44:C1:2232:C:H2’ | 44:C1:2233:U:C6 | 2.55 | 0.42 |
| 46:UV:154:LYS:HE2 | 46:UV:248:ARG:HH12 | 1.85 | 0.42 |
| 46:UV:485:ILE:HD13 | 46:UV:488:ARG:HH11 | 1.84 | 0.42 |
| 46:UV:824:PHE:O | 46:UV:827:LEU:HD22 | 2.20 | 0.42 |
| 48:UH:722:THR:O | 48:UH:725:SER:OG | 2.36 | 0.42 |
| 49:UE:269:GLN:O | 49:UE:273:ARG:N | 2.28 | 0.42 |
| 50:US:501:LEU:HD23 | 50:US:501:LEU:HA | 1.88 | 0.42 |
| 54:Cz:1690:ARG:HG3 | 54:Cz:1693:LEU:H | 1.83 | 0.42 |
| 1:UA:298:ASN:OD1 | 1:UA:318:LYS:HD3 | 2.20 | 0.42 |
| 2:UB:13:LEU:HD12 | 2:UB:13:LEU:HA | 1.75 | 0.42 |
| 2:UB:52:ARG:NH2 | 26:CK:253:GLU:OE2 | 2.50 | 0.42 |
| 2:UB:551:GLN:NE2 | 2:UB:554:ARG:HD3 | 2.33 | 0.42 |
| 2:UB:557:HIS:O | 2:UB:561:LYS:HG3 | 2.20 | 0.42 |
| 4:UD:702:TYR:CE1 | 4:UD:838:ILE:HB | 2.55 | 0.42 |
| 7:UJ:193:LEU:HA | 7:UJ:193:LEU:HD12 | 1.86 | 0.42 |
| 7:UJ:424:LEU:HD23 | 7:UJ:424:LEU:HA | 1.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:UJ:442:ILE:HA | 7:UJ:445:VAL:HG12 | 2.02 | 0.42 |
| 7:UJ:606:LYS:HA | 7:UJ:609:ARG:NE | 2.34 | 0.42 |
| 8:UK:18:GLN:HE21 | 8:UK:28:LEU:HB2 | 1.85 | 0.42 |
| 12:UO:391:ASN:ND2 | 44:C1:133:G:O6 | 2.39 | 0.42 |
| 13:UQ:421:MET:HA | 13:UQ:432:MET:O | 2.20 | 0.42 |
| 13:UQ:507:SER:O | 13:UQ:509:GLN:N | 2.51 | 0.42 |
| 13:UQ:837:VAL:HG22 | 13:UQ:840:SER:H | 1.84 | 0.42 |
| 14:UR:375:ARG:H | 14:UR:375:ARG:HG2 | 1.47 | 0.42 |
| 15:UU:286:LEU:HB3 | 15:UU:292:GLY:O | 2.20 | 0.42 |
| 15:UU:301:ALA:HB2 | 15:UU:343:ILE:HD12 | 2.00 | 0.42 |
| 15:UU:344:GLU:O | 15:UU:352:ILE:HG13 | 2.19 | 0.42 |
| 15:UU:533:ARG:H | 15:UU:533:ARG:HG2 | 1.64 | 0.42 |
| 15:UU:865:LYS:HD3 | 15:UU:865:LYS:HA | 1.80 | 0.42 |
| 15:UU:975:ILE:HG21 | 15:UU:1016:LEU:HD22 | 2.02 | 0.42 |
| 19:CC:155:LEU:C | 19:CC:159:HIS:HD1 | 2.22 | 0.42 |
| 19:CC:306:LEU:HD21 | 19:CC:390:SER:HA | 2.01 | 0.42 |
| 21:CE:115:ILE:HD13 | 21:CE:115:ILE:HA | 1.74 | 0.42 |
| 22:CG:181:PRO:HB2 | 22:CG:196:LYS:HE2 | 2.00 | 0.42 |
| 22:CG:237:ALA:HA | 22:CG:246:LEU:HD22 | 2.01 | 0.42 |
| 22:CG:421:TRP:CZ2 | 22:CG:428:PRO:HG3 | 2.54 | 0.42 |
| 24:CI:81:LYS:HE2 | 24:CI:81:LYS:HB2 | 1.90 | 0.42 |
| 24:CI:170:LEU:HG | 24:CI:173:LEU:HD11 | 2.02 | 0.42 |
| 24:CI:190:LYS:HE2 | 24:CI:190:LYS:HB3 | 1.64 | 0.42 |
| 24:CI:754:LYS:O | 24:CI:758:ALA:CB | 2.65 | 0.42 |
| 24:CI:914:ILE:HA | 24:CI:914:ILE:HD13 | 1.79 | 0.42 |
| 26:CK:142:LEU:HD23 | 26:CK:152:ILE:HG22 | 2.01 | 0.42 |
| 26:CK:289:ARG:HB3 | 44:C1:1146:G:N7 | 2.34 | 0.42 |
| 27:CL:567:ASN:HD21 | 27:CL:571:VAL:H | 1.67 | 0.42 |
| 27:CL:573:ARG:HD2 | 44:C1:2214:A:N7 | 2.35 | 0.42 |
| 27:CL:726:LYS:HD3 | 27:CL:726:LYS:HA | 1.80 | 0.42 |
| 28:CM:86:SER:OG | 28:CM:88:ASP:N | 2.51 | 0.42 |
| 28:CM:436:GLU:HA | 28:CM:439:LYS:HB2 | 2.01 | 0.42 |
| 29:CN:39:VAL:HG23 | 29:CN:204:VAL:HG13 | 2.02 | 0.42 |
| 29:CO:140:LEU:O | 29:CO:143:GLN:HG2 | 2.19 | 0.42 |
| 32:CS:735:LYS:NZ | 32:CS:804:THR:HG21 | 2.34 | 0.42 |
| 36:Cg:31:GLU:HG3 | 36:Cg:32:TYR:CE2 | 2.55 | 0.42 |
| 36:Cg:131:HIS:HE2 | 44:C1:1096:A:HO2' | 1.56 | 0.42 |
| 44:C1:107:C:OP1 | 50:US:163:ARG:NH1 | 2.53 | 0.42 |
| 44:C1:184:G:H2' | 44:C1:185:G:H8 | 1.85 | 0.42 |
| 44:C1:197:G:H2' | 44:C1:198:G:C8 | 2.49 | 0.42 |
| 44:C1:368:G:H2' | 44:C1:369:U:O4' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:800:LEU:HD11 | 46:UV:804:ARG:HH11 | 1.84 | 0.42 |
| 46:UV:802:SER:HA | 46:UV:805:ARG:HD2 | 2.02 | 0.42 |
| 48:UH:732:PRO:O | 48:UH:736:LEU:HG | 2.20 | 0.42 |
| 49:UE:223:VAL:HG13 | 49:UI:272:TYR:HB2 | 2.01 | 0.42 |
| 50:US:176:SER:HA | 50:US:177:PRO:HD3 | 1.94 | 0.42 |
| 50:US:178:ILE:HB | 50:US:181:LEU:HB2 | 2.02 | 0.42 |
| 50:US:363:LEU:O | 50:US:366:THR:OG1 | 2.28 | 0.42 |
| 49:UI:166:SER:OG | 49:UI:167:ASP:N | 2.52 | 0.42 |
| 49:UI:211:ALA:HB1 | 49:UI:215:MET:HG2 | 2.00 | 0.42 |
| 1:UA:122:TRP:CE2 | 1:UA:143:ARG:HG3 | 2.54 | 0.42 |
| 1:UA:558:ARG:HH21 | 1:UA:558:ARG:HD2 | 1.63 | 0.42 |
| 1:UA:732:LYS:HG2 | 1:UA:736:MET:SD | 2.60 | 0.42 |
| 6:UG:213:LEU:H | 6:UG:213:LEU:HG | 1.63 | 0.42 |
| 7:UJ:155:LEU:HD12 | 7:UJ:155:LEU:HA | 1.65 | 0.42 |
| 7:UJ:293:MET:HE1 | 7:UJ:316:ALA:HB2 | 2.01 | 0.42 |
| 8:UK:64:TYR:HD2 | 24:CI:1060:PHE:CD2 | 2.36 | 0.42 |
| 9:UL:705:SER:HB2 | 9:UL:708:GLY:N | 2.35 | 0.42 |
| 10:UM:294:THR:HA | 10:UM:321:ALA:HA | 2.02 | 0.42 |
| 11:UN:308:ASP:CG | 11:UN:312:ARG:HE | 2.28 | 0.42 |
| 11:UN:380:SER:O | 11:UN:380:SER:OG | 2.38 | 0.42 |
| 12:UO:297:VAL:O | 12:UO:310:GLY:HA3 | 2.19 | 0.42 |
| 13:UQ:611:THR:CG2 | 49:UE:251:ARG:HH12 | 2.33 | 0.42 |
| 16:UX:142:ARG:NH1 | 16:UX:142:ARG:HB2 | 2.35 | 0.42 |
| 18:CA:103:VAL:HA | 18:CA:196:MET:HE3 | 2.02 | 0.42 |
| 18:CA:149:TYR:HB3 | 18:CA:311:PHE:CZ | 2.54 | 0.42 |
| 18:CB:247:LEU:O | 20:CD:120:ARG:NH2 | 2.53 | 0.42 |
| 19:CC:96:VAL:O | 19:CC:116:VAL:HA | 2.19 | 0.42 |
| 20:CD:164:MET:H | 20:CD:164:MET:HG2 | 1.57 | 0.42 |
| 25:CJ:152:ARG:NH1 | 26:CK:11:ASP:OD2 | 2.53 | 0.42 |
| 26:CK:173:ARG:HA | 26:CK:173:ARG:HD2 | 1.76 | 0.42 |
| 27:CL:528:LYS:HE2 | 27:CL:528:LYS:HB2 | 1.85 | 0.42 |
| 27:CL:568:PRO:HG2 | 27:CL:569:HIS:HD2 | 1.85 | 0.42 |
| 28:CM:179:ILE:HD13 | 28:CM:227:LEU:HD11 | 2.00 | 0.42 |
| 29:CO:39:VAL:HG13 | 29:CO:112:ILE:HA | 2.02 | 0.42 |
| 32:CR:544:TYR:O | 32:CR:547:SER:OG | 2.37 | 0.42 |
| 32:CS:32:ASP:OD1 | 32:CS:32:ASP:N | 2.53 | 0.42 |
| 32:CS:34:ALA:HB3 | 32:CS:154:LYS:HZ2 | 1.84 | 0.42 |
| 35:Ce:74:GLN:O | 35:Ce:78:ARG:HG3 | 2.20 | 0.42 |
| 44:C1:90:A:H2' | 44:C1:91:G:O4' | 2.19 | 0.42 |
| 44:C1:111:U:H2' | 44:C1:112:C:H6 | 1.84 | 0.42 |
| 44:C1:364:C:H2' | 44:C1:365:G:C8 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:457:G:H2' | 44:C1:458:A:C8 | 2.55 | 0.42 |
| 44:C1:480:U:H2' | 44:C1:481:G:H8 | 1.84 | 0.42 |
| 44:C1:1143:C:H2' | 44:C1:1144:U:H6 | 1.85 | 0.42 |
| 44:C1:1630:C:H2' | 44:C1:1631:G:C8 | 2.52 | 0.42 |
| 46:UV:52:ASP:HB2 | 46:UV:55:GLU:HB3 | 2.02 | 0.42 |
| 46:UV:699:ILE:O | 46:UV:770:ILE:HA | 2.20 | 0.42 |
| 46:UV:713:ALA:HA | 46:UV:716:ARG:HG3 | 2.01 | 0.42 |
| 48:UH:557:GLU:H | 48:UH:566:ARG:H | 1.66 | 0.42 |
| 50:US:88:PHE:HD1 | 50:US:91:LEU:HD21 | 1.85 | 0.42 |
| 50:US:484:LYS:HD2 | 50:US:484:LYS:HA | 1.82 | 0.42 |
| 52:CX:201:VAL:O | 52:CX:204:LYS:HG3 | 2.19 | 0.42 |
| 1:UA:476:PHE:CE2 | 1:UA:483:LEU:HD13 | 2.55 | 0.41 |
| 2:UB:550:GLU:OE2 | 50:US:523:ILE:N | 2.53 | 0.41 |
| 2:UB:880:ARG:HH21 | 44:C1:1703:G:H5' | 1.84 | 0.41 |
| 3:UC:601:ARG:HH12 | 44:C1:1061:A:H4' | 1.84 | 0.41 |
| 4:UD:690:LYS:HE2 | 4:UD:690:LYS:HB3 | 1.74 | 0.41 |
| 6:UG:168:GLY:HA3 | 7:UJ:13:ALA:HB2 | 2.02 | 0.41 |
| 6:UG:221:HIS:HB3 | 6:UG:264:LEU:HD23 | 2.02 | 0.41 |
| 6:UG:234:LEU:HA | 6:UG:234:LEU:HD23 | 1.71 | 0.41 |
| 7:UJ:47:GLU:H | 7:UJ:47:GLU:CD | 2.27 | 0.41 |
| 9:UL:396:LEU:HB3 | 9:UL:418:LEU:HB2 | 2.02 | 0.41 |
| 9:UL:431:SER:HB3 | 9:UL:444:ALA:HB3 | 2.02 | 0.41 |
| 12:UO:203:ASN:HD21 | 12:UO:220:ARG:HG3 | 1.85 | 0.41 |
| 12:UO:324:THR:HA | 12:UO:332:ARG:H | 1.85 | 0.41 |
| 13:UQ:141:THR:HG22 | 13:UQ:161:SER:HB2 | 2.02 | 0.41 |
| 14:UR:132:ASP:N | 14:UR:132:ASP:OD1 | 2.51 | 0.41 |
| 15:UU:854:LEU:O | 15:UU:857:ILE:HG22 | 2.20 | 0.41 |
| 18:CA:130:TRP:CD1 | 18:CA:169:HIS:CE1 | 3.08 | 0.41 |
| 19:CC:89:THR:OG1 | 19:CC:90:SER:N | 2.53 | 0.41 |
| 19:CC:103:LYS:HB3 | 19:CC:103:LYS:HE2 | 1.57 | 0.41 |
| 19:CC:250:LYS:O | 19:CC:254:ILE:HG12 | 2.20 | 0.41 |
| 19:CC:276:ASP:O | 19:CC:279:SER:OG | 2.37 | 0.41 |
| 22:CG:586:MET:HE2 | 22:CG:586:MET:HB2 | 1.92 | 0.41 |
| 23:CH:125:LYS:HG3 | 23:CH:408:ARG:HA | 2.02 | 0.41 |
| 23:CH:196:PHE:HD1 | 23:CH:196:PHE:HA | 1.66 | 0.41 |
| 24:CI:109:SER:OG | 24:CI:110:LYS:N | 2.52 | 0.41 |
| 24:CI:237:TRP:CH2 | 24:CI:838:GLY:HA2 | 2.56 | 0.41 |
| 24:CI:242:PRO:HA | 24:CI:276:GLY:HA3 | 2.01 | 0.41 |
| 24:CI:1102:LYS:HA | 24:CI:1102:LYS:HD2 | 1.78 | 0.41 |
| 28:CM:262:HIS:HD2 | 28:CM:284:ALA:C | 2.28 | 0.41 |
| 29:CO:192:TYR:CZ | 29:CO:196:LEU:HD21 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:CP:163:LEU:O | 30:CP:170:SER:N | 2.49 | 0.41 |
| 32:CR:94:PRO:HA | 32:CR:97:LEU:HD12 | 2.00 | 0.41 |
| 40:Cm:75:ILE:HD13 | 40:Cm:125:ILE:HG22 | 2.02 | 0.41 |
| 44:C1:264:C:C4 | 44:C1:266:C:N3 | 2.88 | 0.41 |
| 44:C1:1066:U:H2' | 44:C1:1067:A:H8 | 1.84 | 0.41 |
| 44:C1:1754:G:C2 | 44:C1:1755:A:C8 | 3.08 | 0.41 |
| 45:C2:78:C:H2' | 45:C2:79:G:H8 | 1.85 | 0.41 |
| 45:C2:248:G:H2' | 45:C2:249:U:O4' | 2.20 | 0.41 |
| 46:UV:451:VAL:HG22 | 46:UV:615:GLN:HG3 | 2.01 | 0.41 |
| 48:UH:494:TRP:O | 48:UH:498:MET:HG2 | 2.20 | 0.41 |
| 48:UH:918:LEU:HD12 | 48:UH:918:LEU:HA | 1.91 | 0.41 |
| 49:UE:204:MET:HE2 | 49:UE:204:MET:HB2 | 1.84 | 0.41 |
| 49:UE:257:LEU:H | 49:UE:257:LEU:HG | 1.45 | 0.41 |
| 50:US:350:ASP:HA | 50:US:353:HIS:ND1 | 2.35 | 0.41 |
| 50:US:446:ASP:CG | 50:US:449:GLU:HB2 | 2.45 | 0.41 |
| 52:CX:250:ALA:HA | 52:CX:253:ILE:HG22 | 2.03 | 0.41 |
| 49:UI:219:GLN:O | 49:UI:223:VAL:HG23 | 2.20 | 0.41 |
| 2:UB:688:GLY:HA2 | 2:UB:690:ARG:NH1 | 2.34 | 0.41 |
| 4:UD:162:ASN:HA | 4:UD:181:ARG:HA | 2.02 | 0.41 |
| 4:UD:432:THR:OG1 | 4:UD:433:SER:N | 2.53 | 0.41 |
| 4:UD:798:SER:O | 4:UD:801:GLN:HG2 | 2.20 | 0.41 |
| 5:UF:406:LYS:HE2 | 5:UF:406:LYS:HB3 | 1.94 | 0.41 |
| 6:UG:163:MET:HB3 | 6:UG:163:MET:HE2 | 1.83 | 0.41 |
| 7:UJ:59:LEU:HD11 | 7:UJ:108:ARG:HD3 | 2.02 | 0.41 |
| 7:UJ:165:ARG:HD2 | 7:UJ:165:ARG:HA | 1.73 | 0.41 |
| 7:UJ:817:TRP:CG | 7:UJ:859:VAL:HG21 | 2.56 | 0.41 |
| 8:UK:67:MET:HG2 | 25:CJ:173:TYR:CD2 | 2.55 | 0.41 |
| 9:UL:800:GLU:HA | 9:UL:803:ARG:HG2 | 2.02 | 0.41 |
| 11:UN:329:THR:HG22 | 11:UN:938:TYR:N | 2.35 | 0.41 |
| 12:UO:30:PHE:CD1 | 12:UO:348:ARG:HB3 | 2.55 | 0.41 |
| 12:UO:205:LEU:O | 12:UO:216:VAL:HA | 2.20 | 0.41 |
| 13:UQ:256:ALA:HB2 | 13:UQ:293:PHE:CE1 | 2.55 | 0.41 |
| 14:UR:280:LEU:HD23 | 14:UR:291:SER:HA | 2.02 | 0.41 |
| 14:UR:437:ARG:NH2 | 44:C1:202:A:OP1 | 2.53 | 0.41 |
| 15:UU:150:TRP:HD1 | 15:UU:163:LYS:HA | 1.85 | 0.41 |
| 16:UX:116:GLU:O | 16:UX:118:TRP:N | 2.54 | 0.41 |
| 18:CA:188:ARG:NE | 21:CF:66:LEU:HD11 | 2.35 | 0.41 |
| 18:CB:97:LEU:HD23 | 18:CB:200:ARG:HG2 | 2.02 | 0.41 |
| 18:CB:169:HIS:O | 18:CB:173:ILE:HG12 | 2.20 | 0.41 |
| 19:CC:167:LYS:HE2 | 19:CC:167:LYS:HB2 | 1.88 | 0.41 |
| 19:CC:205:HIS:NE2 | 19:CC:229:LYS:HE3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:CD:160:LYS:HD3 | 20:CD:160:LYS:HA | 1.60 | 0.41 |
| 21:CE:118:LEU:HA | 21:CE:118:LEU:HD12 | 1.79 | 0.41 |
| 21:CF:86:VAL:O | 21:CF:90:ARG:HG3 | 2.20 | 0.41 |
| 22:CG:289:ASP:HB2 | 22:CG:308:LYS:HB2 | 2.02 | 0.41 |
| 23:CH:69:SER:OG | 23:CH:72:GLY:N | 2.53 | 0.41 |
| 23:CH:114:LEU:O | 23:CH:118:ALA:N | 2.34 | 0.41 |
| 23:CH:232:ASN:O | 23:CH:236:ILE:HG13 | 2.20 | 0.41 |
| 29:CN:90:ASP:OD2 | 29:CN:91:ILE:N | 2.51 | 0.41 |
| 29:CN:116:THR:HG22 | 29:CN:120:VAL:HB | 2.01 | 0.41 |
| 32:CR:32:ASP:OD1 | 32:CR:32:ASP:N | 2.53 | 0.41 |
| 32:CR:790:LEU:HD12 | 32:CR:791:SER:H | 1.86 | 0.41 |
| 32:CS:132:THR:HB | 32:CS:135:ILE:HG12 | 2.02 | 0.41 |
| 32:CS:389:ASP:HA | 32:CS:411:ALA:HB3 | 2.02 | 0.41 |
| 44:C1:237:G:H5” | 44:C1:238:G:OP2 | 2.20 | 0.41 |
| 44:C1:467:C:H4’ | 44:C1:468:C:H5’ | 2.03 | 0.41 |
| 44:C1:1472:A:H2’ | 44:C1:1473:U:C6 | 2.54 | 0.41 |
| 45:C2:93:G:H2’ | 45:C2:94:A:H4’ | 2.01 | 0.41 |
| 46:UV:120:PHE:CE1 | 46:UV:142:MET:HB2 | 2.53 | 0.41 |
| 46:UV:229:CYS:HB2 | 46:UV:276:GLU:O | 2.20 | 0.41 |
| 46:UV:883:LEU:HD11 | 46:UV:960:MET:HG2 | 2.02 | 0.41 |
| 46:UV:944:THR:C | 46:UV:951:ARG:HH12 | 2.27 | 0.41 |
| 2:UB:341:LYS:HD3 | 2:UB:344:ARG:HH21 | 1.84 | 0.41 |
| 2:UB:661:LEU:O | 2:UB:664:THR:OG1 | 2.34 | 0.41 |
| 2:UB:892:ALA:HA | 2:UB:895:GLU:OE1 | 2.20 | 0.41 |
| 6:UG:79:TYR:CE2 | 11:UN:903:LEU:HD13 | 2.55 | 0.41 |
| 6:UG:347:SER:HB3 | 6:UG:398:VAL:HG12 | 2.02 | 0.41 |
| 6:UG:348:VAL:HA | 6:UG:357:ALA:O | 2.20 | 0.41 |
| 7:UJ:556:LEU:HA | 7:UJ:556:LEU:HD23 | 1.82 | 0.41 |
| 7:UJ:675:VAL:HG23 | 7:UJ:729:SER:HA | 2.02 | 0.41 |
| 9:UL:159:TYR:HB3 | 9:UL:190:LEU:HG | 2.02 | 0.41 |
| 9:UL:460:ILE:HG13 | 9:UL:461:ARG:HG2 | 2.03 | 0.41 |
| 9:UL:566:ASP:HB3 | 9:UL:584:LEU:HG | 2.02 | 0.41 |
| 9:UL:711:LEU:O | 9:UL:722:VAL:HA | 2.20 | 0.41 |
| 10:UM:628:ASN:HB2 | 10:UM:635:ILE:HD11 | 2.01 | 0.41 |
| 10:UM:881:SER:O | 10:UM:884:VAL:HG12 | 2.20 | 0.41 |
| 11:UN:304:LYS:HD2 | 11:UN:304:LYS:HA | 1.87 | 0.41 |
| 12:UO:131:GLY:O | 12:UO:133:ARG:N | 2.52 | 0.41 |
| 12:UO:470:LEU:HA | 12:UO:470:LEU:HD12 | 1.63 | 0.41 |
| 14:UR:280:LEU:HD23 | 14:UR:280:LEU:HA | 1.88 | 0.41 |
| 14:UR:289:LEU:HA | 14:UR:289:LEU:HD12 | 1.86 | 0.41 |
| 15:UU:195:PHE:C | 15:UU:196:LEU:HD22 | 2.45 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:UU:460:LEU:HD12 | 15:UU:460:LEU:HA | 1.87 | 0.41 |
| 16:UX:11:ASP:OD1 | 16:UX:12:GLU:N | 2.54 | 0.41 |
| 16:UX:53:VAL:HG13 | 36:Cg:98:LYS:HE2 | 2.02 | 0.41 |
| 18:CB:165:THR:O | 18:CB:168:SER:OG | 2.30 | 0.41 |
| 19:CC:134:ILE:HD13 | 19:CC:134:ILE:HA | 1.86 | 0.41 |
| 20:CD:97:ASN:O | 20:CD:101:LYS:HG2 | 2.20 | 0.41 |
| 20:CD:330:ARG:O | 20:CD:334:THR:HG22 | 2.19 | 0.41 |
| 20:CD:345:TYR:CE1 | 20:CD:358:LYS:HD3 | 2.54 | 0.41 |
| 22:CG:235:ARG:HH22 | 45:C2:119:C:H2' | 1.85 | 0.41 |
| 24:CI:113:ARG:HH21 | 24:CI:308:THR:HG21 | 1.85 | 0.41 |
| 24:CI:904:THR:OG1 | 24:CI:905:VAL:N | 2.54 | 0.41 |
| 26:CK:161:PRO:HG2 | 26:CK:207:ILE:HG12 | 2.02 | 0.41 |
| 26:CK:171:VAL:HG12 | 26:CK:260:ARG:H | 1.85 | 0.41 |
| 26:CK:282:TRP:NE1 | 26:CK:283:HIS:O | 2.54 | 0.41 |
| 27:CL:558:LEU:HA | 27:CL:558:LEU:HD13 | 1.84 | 0.41 |
| 27:CL:618:GLU:HG3 | 27:CL:622:MET:HE3 | 2.03 | 0.41 |
| 27:CL:634:SER:O | 27:CL:635:SER:OG | 2.31 | 0.41 |
| 28:CM:189:GLN:HG2 | 28:CM:191:ILE:HG13 | 2.03 | 0.41 |
| 32:CR:494:LEU:HD12 | 32:CR:496:LEU:HD11 | 2.02 | 0.41 |
| 32:CS:24:ARG:NH2 | 32:CS:487:GLU:HB2 | 2.35 | 0.41 |
| 34:Cc:63:ARG:HG2 | 39:Cj:122:ARG:NH1 | 2.34 | 0.41 |
| 44:C1:2067:G:H1 | 44:C1:2174:C:H1' | 1.85 | 0.41 |
| 44:C1:2206:C:H2' | 44:C1:2207:C:C6 | 2.56 | 0.41 |
| 48:UH:842:TYR:CE2 | 48:UH:871:LEU:HD22 | 2.54 | 0.41 |
| 48:UH:915:GLU:HB3 | 48:UH:920:ALA:HB3 | 2.02 | 0.41 |
| 49:UE:166:SER:OG | 49:UE:167:ASP:N | 2.52 | 0.41 |
| 49:UE:238:ARG:HA | 49:UE:238:ARG:HD3 | 1.35 | 0.41 |
| 51:Cl:65:GLU:HA | 51:Cl:68:ARG:HB3 | 2.01 | 0.41 |
| 54:Cz:1673:ARG:HD3 | 54:Cz:1706:SER:HA | 2.01 | 0.41 |
| 4:UD:251:SER:O | 4:UD:251:SER:OG | 2.34 | 0.41 |
| 5:UF:280:ILE:HG23 | 5:UF:319:HIS:NE2 | 2.35 | 0.41 |
| 5:UF:367:ALA:HB1 | 5:UF:377:LEU:HD21 | 2.02 | 0.41 |
| 8:UK:109:LEU:HD13 | 8:UK:240:LEU:HB2 | 2.01 | 0.41 |
| 9:UL:12:LYS:HB2 | 9:UL:722:VAL:HB | 2.01 | 0.41 |
| 9:UL:287:HIS:CE1 | 9:UL:290:ARG:H | 2.38 | 0.41 |
| 9:UL:611:LEU:N | 9:UL:625:SER:O | 2.52 | 0.41 |
| 9:UL:661:ASN:OD1 | 9:UL:665:ASN:N | 2.53 | 0.41 |
| 9:UL:936:VAL:HG23 | 9:UL:937:ARG:H | 1.85 | 0.41 |
| 11:UN:345:GLN:H | 11:UN:345:GLN:HG2 | 1.54 | 0.41 |
| 13:UQ:267:LYS:HA | 13:UQ:267:LYS:HD3 | 1.71 | 0.41 |
| 13:UQ:654:ASP:N | 13:UQ:654:ASP:OD1 | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:UR:264:GLN:O | 14:UR:614:TRP:HA | 2.20 | 0.41 |
| 14:UR:370:GLN:HE21 | 14:UR:388:VAL:C | 2.28 | 0.41 |
| 14:UR:473:GLY:HA2 | 14:UR:498:ASN:HD21 | 1.84 | 0.41 |
| 15:UU:196:LEU:HA | 15:UU:196:LEU:HD13 | 1.74 | 0.41 |
| 15:UU:565:ILE:HG12 | 15:UU:625:VAL:HG11 | 2.03 | 0.41 |
| 16:UX:14:ARG:NH1 | 25:CJ:27:HIS:HB2 | 2.36 | 0.41 |
| 16:UX:169:GLN:HG3 | 16:UX:172:LYS:O | 2.21 | 0.41 |
| 18:CB:142:LEU:HA | 18:CB:142:LEU:HD13 | 1.83 | 0.41 |
| 18:CB:161:ALA:N | 18:CB:184:GLU:OE1 | 2.54 | 0.41 |
| 18:CB:184:GLU:O | 18:CB:207:VAL:HA | 2.20 | 0.41 |
| 20:CD:134:GLU:O | 20:CD:136:SER:N | 2.54 | 0.41 |
| 22:CG:467:THR:HG23 | 22:CG:482:SER:HA | 2.02 | 0.41 |
| 24:CI:162:MET:HE1 | 24:CI:166:VAL:HG13 | 2.02 | 0.41 |
| 24:CI:176:PHE:CG | 24:CI:182:LEU:HD13 | 2.55 | 0.41 |
| 24:CI:542:LEU:HD13 | 24:CI:560:TRP:CG | 2.56 | 0.41 |
| 28:CM:135:TRP:CE2 | 28:CM:146:PRO:HB3 | 2.55 | 0.41 |
| 28:CM:332:THR:O | 28:CM:332:THR:OG1 | 2.35 | 0.41 |
| 29:CN:41:LEU:HD23 | 29:CN:206:VAL:HG23 | 2.01 | 0.41 |
| 29:CN:186:LEU:HA | 29:CN:186:LEU:HD13 | 1.78 | 0.41 |
| 32:CR:782:PHE:HA | 32:CR:785:ARG:HB2 | 2.03 | 0.41 |
| 32:CS:16:ARG:O | 32:CS:20:GLN:HG3 | 2.20 | 0.41 |
| 32:CS:119:THR:HA | 32:CS:479:ARG:NH2 | 2.33 | 0.41 |
| 32:CS:484:ASP:HB3 | 32:CS:487:GLU:HB3 | 2.03 | 0.41 |
| 32:CS:737:TRP:HA | 32:CS:740:ALA:HB3 | 2.01 | 0.41 |
| 32:CS:844:TYR:OH | 32:CS:913:MET:HE1 | 2.21 | 0.41 |
| 32:CS:911:ILE:O | 32:CS:915:ILE:HG13 | 2.20 | 0.41 |
| 40:Cm:82:ARG:HA | 40:Cm:122:ALA:HB1 | 2.02 | 0.41 |
| 41:Cn:54:LEU:HD23 | 41:Cn:54:LEU:HA | 1.86 | 0.41 |
| 44:C1:1180:C:H2' | 44:C1:1181:G:C8 | 2.49 | 0.41 |
| 46:UV:230:ALA:HB3 | 46:UV:277:SER:HA | 2.01 | 0.41 |
| 46:UV:405:LYS:HE2 | 46:UV:405:LYS:HB2 | 1.88 | 0.41 |
| 46:UV:549:ARG:HG2 | 46:UV:585:ARG:HH12 | 1.85 | 0.41 |
| 46:UV:1097:LYS:HD2 | 46:UV:1097:LYS:HA | 1.77 | 0.41 |
| 48:UH:534:SER:OG | 48:UH:537:ASP:O | 2.37 | 0.41 |
| 48:UH:789:LEU:HD21 | 49:UI:269:GLN:HG2 | 2.03 | 0.41 |
| 48:UH:863:MET:O | 49:UI:231:THR:HG22 | 2.21 | 0.41 |
| 48:UH:866:GLU:C | 49:UI:227:GLY:HA3 | 2.46 | 0.41 |
| 50:US:360:PHE:CZ | 50:US:364:LEU:HD22 | 2.55 | 0.41 |
| 52:CX:205:ILE:HD13 | 52:CX:205:ILE:HA | 1.96 | 0.41 |
| 49:UI:238:ARG:HD3 | 49:UI:238:ARG:HA | 1.35 | 0.41 |
| 1:UA:122:TRP:CD2 | 1:UA:143:ARG:HG3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:UB:572:ARG:NH1 | 2:UB:609:GLN:OE1 | 2.43 | 0.41 |
| 3:UC:579:ILE:HA | 24:CI:148:MET:SD | 2.60 | 0.41 |
| 4:UD:3:ILE:HD13 | 48:UH:912:ILE:HG12 | 2.02 | 0.41 |
| 4:UD:43:ARG:HA | 4:UD:43:ARG:HD3 | 1.84 | 0.41 |
| 4:UD:120:ARG:NH2 | 53:UP:330:ARG:HB3 | 2.36 | 0.41 |
| 4:UD:632:VAL:HG21 | 4:UD:692:ILE:HG23 | 2.01 | 0.41 |
| 5:UF:78:LEU:HD13 | 5:UF:78:LEU:HA | 1.87 | 0.41 |
| 5:UF:97:GLU:OE2 | 5:UF:113:TYR:OH | 2.26 | 0.41 |
| 5:UF:117:ALA:O | 5:UF:120:VAL:C | 2.63 | 0.41 |
| 7:UJ:87:THR:OG1 | 7:UJ:89:GLU:OE1 | 2.28 | 0.41 |
| 7:UJ:572:LEU:HD12 | 7:UJ:610:ALA:HB3 | 2.01 | 0.41 |
| 10:UM:805:GLN:HA | 10:UM:808:GLN:HE21 | 1.85 | 0.41 |
| 12:UO:76:THR:HG21 | 12:UO:105:GLY:H | 1.86 | 0.41 |
| 12:UO:108:ARG:HB2 | 12:UO:113:VAL:HB | 2.03 | 0.41 |
| 13:UQ:538:ALA:HA | 13:UQ:553:ILE:O | 2.20 | 0.41 |
| 13:UQ:608:THR:OG1 | 13:UQ:609:LYS:N | 2.53 | 0.41 |
| 14:UR:63:LYS:HD3 | 14:UR:63:LYS:HA | 1.83 | 0.41 |
| 14:UR:338:ILE:HG13 | 14:UR:352:LEU:HD11 | 2.01 | 0.41 |
| 14:UR:351:ASN:O | 14:UR:355:GLY:HA2 | 2.21 | 0.41 |
| 15:UU:425:ASP:N | 44:C1:259:U:O2 | 2.35 | 0.41 |
| 15:UU:576:ARG:NH2 | 39:Cj:101:SER:OG | 2.54 | 0.41 |
| 17:UZ:77:ARG:HH21 | 17:UZ:272:PRO:HB3 | 1.85 | 0.41 |
| 18:CA:112:GLU:HA | 18:CA:123:THR:N | 2.35 | 0.41 |
| 21:CE:111:LEU:HD12 | 21:CE:111:LEU:HA | 1.81 | 0.41 |
| 22:CG:388:ASP:OD2 | 22:CG:391:SER:N | 2.53 | 0.41 |
| 22:CG:464:ARG:HA | 22:CG:483:TRP:CZ2 | 2.55 | 0.41 |
| 24:CI:137:LEU:HD12 | 24:CI:169:ILE:HD11 | 2.03 | 0.41 |
| 25:CJ:176:LYS:O | 25:CJ:178:ASP:N | 2.53 | 0.41 |
| 27:CL:647:LEU:HD23 | 27:CL:647:LEU:H | 1.85 | 0.41 |
| 28:CM:158:SER:HB2 | 28:CM:203:VAL:HG12 | 2.03 | 0.41 |
| 29:CN:121:LEU:HB3 | 29:CN:163:ILE:HG13 | 2.02 | 0.41 |
| 30:CP:97:ASP:HA | 30:CP:100:LYS:HG2 | 2.02 | 0.41 |
| 32:CR:160:LYS:HD2 | 32:CR:160:LYS:HA | 1.78 | 0.41 |
| 32:CR:426:LEU:HA | 32:CR:429:ILE:HG12 | 2.01 | 0.41 |
| 32:CR:523:ARG:HA | 32:CR:526:LEU:HB3 | 2.01 | 0.41 |
| 32:CR:844:TYR:OH | 32:CR:913:MET:HE1 | 2.21 | 0.41 |
| 32:CS:426:LEU:HA | 32:CS:429:ILE:HG12 | 2.01 | 0.41 |
| 32:CS:494:LEU:HD12 | 32:CS:496:LEU:HD11 | 2.02 | 0.41 |
| 32:CS:880:GLN:NE2 | 32:CS:915:ILE:HG12 | 2.26 | 0.41 |
| 33:CT:177:LYS:HA | 33:CT:177:LYS:HD2 | 1.92 | 0.41 |
| 34:Cc:67:LYS:HE3 | 34:Cc:67:LYS:HB2 | 1.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:Cg:31:GLU:HG3 | 36:Cg:32:TYR:CD2 | 2.56 | 0.41 |
| 44:C1:6:G:C6 | 44:C1:30:U:N3 | 2.89 | 0.41 |
| 44:C1:42:C:H2' | 44:C1:43:C:H6 | 1.84 | 0.41 |
| 44:C1:51:G:H2' | 44:C1:52:C:C6 | 2.55 | 0.41 |
| 44:C1:608:U:H2' | 44:C1:609:A:C8 | 2.56 | 0.41 |
| 44:C1:1459:C:H2' | 44:C1:1460:G:C8 | 2.56 | 0.41 |
| 46:UV:667:HIS:CD2 | 46:UV:700:SER:HB2 | 2.55 | 0.41 |
| 46:UV:854:LEU:HA | 46:UV:857:LEU:HB2 | 2.03 | 0.41 |
| 50:US:505:MET:HE3 | 50:US:505:MET:HB3 | 1.90 | 0.41 |
| 49:UI:246:LEU:HD12 | 49:UI:246:LEU:HA | 1.89 | 0.41 |
| 1:UA:607:LEU:HD23 | 1:UA:607:LEU:HA | 1.84 | 0.41 |
| 6:UG:79:TYR:CD1 | 11:UN:903:LEU:HD22 | 2.55 | 0.41 |
| 6:UG:267:ASN:HD22 | 6:UG:272:ILE:HD11 | 1.85 | 0.41 |
| 8:UK:171:ARG:CZ | 53:UP:313:LYS:HG3 | 2.50 | 0.41 |
| 9:UL:597:LEU:HD13 | 9:UL:597:LEU:HA | 1.79 | 0.41 |
| 9:UL:655:VAL:HA | 9:UL:670:PHE:O | 2.20 | 0.41 |
| 10:UM:715:SER:O | 10:UM:715:SER:OG | 2.38 | 0.41 |
| 12:UO:322:VAL:HA | 12:UO:334:LEU:HA | 2.02 | 0.41 |
| 13:UQ:320:ARG:HA | 13:UQ:320:ARG:HD3 | 1.84 | 0.41 |
| 16:UX:166:MET:SD | 16:UX:173:TYR:HB3 | 2.60 | 0.41 |
| 16:UX:168:VAL:HA | 16:UX:173:TYR:HA | 2.01 | 0.41 |
| 17:UZ:98:CYS:HB2 | 17:UZ:150:HIS:CG | 2.55 | 0.41 |
| 19:CC:69:ILE:HD13 | 19:CC:69:ILE:HA | 1.85 | 0.41 |
| 19:CC:140:LYS:NZ | 44:C1:436:A:H62 | 2.19 | 0.41 |
| 21:CE:53:VAL:O | 21:CE:79:TYR:HA | 2.20 | 0.41 |
| 21:CE:55:LEU:O | 21:CE:82:VAL:HG22 | 2.20 | 0.41 |
| 23:CH:21:LEU:O | 23:CH:25:THR:HG23 | 2.20 | 0.41 |
| 23:CH:167:PRO:O | 23:CH:171:ILE:HG12 | 2.20 | 0.41 |
| 23:CH:394:LEU:HD11 | 24:CI:539:ALA:HB2 | 2.02 | 0.41 |
| 25:CJ:94:LEU:HA | 25:CJ:97:VAL:HG23 | 2.02 | 0.41 |
| 25:CJ:109:ARG:HD2 | 25:CJ:109:ARG:HA | 1.81 | 0.41 |
| 26:CK:36:LEU:H | 26:CK:36:LEU:HG | 1.71 | 0.41 |
| 26:CK:73:ILE:HG13 | 26:CK:74:ASP:OD1 | 2.20 | 0.41 |
| 27:CL:620:LYS:HA | 27:CL:620:LYS:HD3 | 1.76 | 0.41 |
| 29:CO:99:LEU:HB2 | 29:CO:110:LEU:HD21 | 2.03 | 0.41 |
| 32:CS:291:LYS:HD3 | 32:CS:291:LYS:HA | 1.97 | 0.41 |
| 32:CS:903:LEU:HD11 | 32:CS:908:VAL:HG22 | 2.02 | 0.41 |
| 44:C1:378:C:H2' | 44:C1:379:G:O4' | 2.21 | 0.41 |
| 44:C1:1098:G:O2' | 44:C1:1099:A:H8 | 2.04 | 0.41 |
| 44:C1:1213:U:H2' | 44:C1:1214:A:H8 | 1.86 | 0.41 |
| 44:C1:1456:A:H2' | 44:C1:1457:G:H8 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:C1:1467:U:H2' | 44:C1:1468:C:C6 | 2.56 | 0.41 |
| 46:UV:382:ASP:HA | 46:UV:383:LEU:HA | 1.86 | 0.41 |
| 46:UV:1104:LEU:HD12 | 46:UV:1105:PRO:HA | 2.03 | 0.41 |
| 48:UH:478:LYS:HD3 | 48:UH:545:TRP:HZ2 | 1.85 | 0.41 |
| 48:UH:717:CYS:C | 48:UH:782:ARG:HH12 | 2.25 | 0.41 |
| 50:US:352:LEU:O | 50:US:357:ARG:HD3 | 2.20 | 0.41 |
| 52:CX:283:LYS:HE2 | 52:CX:283:LYS:HB2 | 1.92 | 0.41 |
| 1:UA:580:TYR:HE1 | 1:UA:587:LEU:HG | 1.86 | 0.41 |
| 1:UA:696:LEU:HA | 1:UA:696:LEU:HD23 | 1.83 | 0.41 |
| 1:UA:838:VAL:HA | 1:UA:841:VAL:HG12 | 2.02 | 0.41 |
| 5:UF:105:GLY:HA3 | 19:CC:145:LEU:HB3 | 2.02 | 0.41 |
| 5:UF:324:MET:HG3 | 5:UF:334:THR:HG23 | 2.02 | 0.41 |
| 7:UJ:423:ALA:O | 7:UJ:427:LEU:HG | 2.20 | 0.41 |
| 9:UL:98:LYS:H | 9:UL:98:LYS:HG3 | 1.66 | 0.41 |
| 11:UN:361:THR:N | 11:UN:364:THR:HG1 | 2.18 | 0.41 |
| 11:UN:866:LEU:HG | 11:UN:867:LYS:HG3 | 2.03 | 0.41 |
| 13:UQ:166:TRP:CE2 | 13:UQ:179:PRO:HB3 | 2.55 | 0.41 |
| 13:UQ:393:PRO:HG3 | 44:C1:73:A:C8 | 2.56 | 0.41 |
| 13:UQ:670:PRO:HG2 | 13:UQ:713:VAL:HG21 | 2.03 | 0.41 |
| 14:UR:72:ARG:HD3 | 14:UR:72:ARG:HA | 1.68 | 0.41 |
| 15:UU:100:TRP:CD1 | 15:UU:146:ILE:HG21 | 2.56 | 0.41 |
| 15:UU:151:ILE:HG13 | 15:UU:162:TRP:HB2 | 2.03 | 0.41 |
| 16:UX:9:LYS:HB3 | 16:UX:9:LYS:HE2 | 1.88 | 0.41 |
| 18:CA:157:LEU:HB3 | 18:CA:226:ILE:HG12 | 2.03 | 0.41 |
| 18:CB:258:LYS:HE2 | 18:CB:261:CYS:HB2 | 2.02 | 0.41 |
| 23:CH:137:VAL:O | 23:CH:179:SER:OG | 2.34 | 0.41 |
| 23:CH:173:LEU:HD12 | 23:CH:194:MET:SD | 2.60 | 0.41 |
| 23:CH:281:LEU:O | 23:CH:293:ALA:HA | 2.21 | 0.41 |
| 24:CI:233:ARG:HA | 24:CI:234:PRO:HD3 | 1.94 | 0.41 |
| 24:CI:906:LEU:HD23 | 24:CI:906:LEU:HA | 1.64 | 0.41 |
| 24:CI:939:ASN:OD1 | 24:CI:939:ASN:N | 2.52 | 0.41 |
| 24:CI:1096:LYS:HG2 | 33:CT:178:TYR:CD2 | 2.56 | 0.41 |
| 26:CK:56:PHE:CE1 | 26:CK:60:VAL:HG22 | 2.56 | 0.41 |
| 26:CK:168:HIS:CG | 27:CL:530:VAL:HG11 | 2.55 | 0.41 |
| 26:CK:189:PRO:HB3 | 26:CK:226:ARG:HG2 | 2.03 | 0.41 |
| 27:CL:575:LEU:HD13 | 27:CL:575:LEU:HA | 1.92 | 0.41 |
| 28:CM:28:ALA:HB3 | 28:CM:31:LEU:HB2 | 2.03 | 0.41 |
| 28:CM:89:GLY:O | 28:CM:108:ALA:N | 2.54 | 0.41 |
| 29:CO:178:VAL:HG23 | 29:CO:204:VAL:HA | 2.01 | 0.41 |
| 32:CR:160:LYS:O | 32:CR:164:THR:HG22 | 2.20 | 0.41 |
| 32:CR:903:LEU:HD11 | 32:CR:908:VAL:HG22 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:CT:162:VAL:HA | 33:CT:165:VAL:HG12 | 2.03 | 0.41 |
| 34:Cc:114:GLN:HG2 | 34:Cc:115:ASN:H | 1.86 | 0.41 |
| 35:Ce:180:SER:O | 35:Ce:184:ARG:HD3 | 2.21 | 0.41 |
| 43:CU:219:ILE:HD13 | 43:CU:219:ILE:HA | 1.86 | 0.41 |
| 44:C1:78:G:H2' | 44:C1:79:C:H6 | 1.85 | 0.41 |
| 44:C1:351:U:C4 | 44:C1:353:G:N1 | 2.88 | 0.41 |
| 44:C1:372:U:H3 | 44:C1:394:U:H3 | 1.67 | 0.41 |
| 44:C1:581:C:H5' | 44:C1:582:G:C8 | 2.56 | 0.41 |
| 44:C1:1213:U:C2 | 44:C1:1555:A:N7 | 2.88 | 0.41 |
| 46:UV:57:PHE:HA | 46:UV:58:ASP:HA | 1.92 | 0.41 |
| 46:UV:189:GLU:OE1 | 46:UV:201:SER:OG | 2.37 | 0.41 |
| 46:UV:676:ARG:HB2 | 46:UV:817:ILE:HB | 2.02 | 0.41 |
| 48:UH:782:ARG:HA | 49:UI:262:LYS:NZ | 2.36 | 0.41 |
| 50:US:122:ASP:O | 50:US:126:LEU:HG | 2.21 | 0.41 |
| 4:UD:198:ASN:O | 4:UD:214:VAL:HG22 | 2.21 | 0.41 |
| 4:UD:283:SER:OG | 4:UD:329:MET:HG3 | 2.19 | 0.41 |
| 4:UD:640:ARG:HD3 | 4:UD:644:ASP:HB3 | 2.03 | 0.41 |
| 5:UF:391:ILE:HD12 | 5:UF:391:ILE:HA | 1.86 | 0.41 |
| 7:UJ:251:ILE:HA | 7:UJ:251:ILE:HD13 | 1.75 | 0.41 |
| 7:UJ:821:LYS:O | 7:UJ:825:LYS:HG2 | 2.21 | 0.41 |
| 8:UK:63:PHE:HB2 | 25:CJ:170:ILE:HD11 | 2.03 | 0.41 |
| 9:UL:625:SER:HA | 9:UL:631:ILE:HG22 | 2.03 | 0.41 |
| 9:UL:854:ILE:HD13 | 9:UL:854:ILE:HA | 1.91 | 0.41 |
| 9:UL:856:SER:O | 9:UL:859:THR:OG1 | 2.32 | 0.41 |
| 10:UM:236:GLN:NE2 | 10:UM:252:ARG:HD3 | 2.36 | 0.41 |
| 10:UM:774:PHE:HA | 10:UM:777:VAL:HG12 | 2.03 | 0.41 |
| 10:UM:882:TYR:OH | 15:UU:1032:GLU:HA | 2.20 | 0.41 |
| 12:UO:32:LYS:O | 12:UO:346:ARG:HA | 2.21 | 0.41 |
| 13:UQ:107:TYR:N | 13:UQ:110:SER:O | 2.52 | 0.41 |
| 13:UQ:217:GLN:HA | 13:UQ:236:THR:HA | 2.02 | 0.41 |
| 13:UQ:438:GLN:HE22 | 13:UQ:513:LYS:NZ | 2.19 | 0.41 |
| 13:UQ:471:SER:OG | 13:UQ:471:SER:O | 2.39 | 0.41 |
| 13:UQ:854:SER:OG | 13:UQ:855:ILE:N | 2.53 | 0.41 |
| 15:UU:711:ASN:HD21 | 15:UU:727:GLN:HA | 1.85 | 0.41 |
| 15:UU:1016:LEU:HD13 | 15:UU:1016:LEU:HA | 1.92 | 0.41 |
| 17:UZ:19:ASP:O | 17:UZ:23:THR:HG23 | 2.21 | 0.41 |
| 17:UZ:267:VAL:O | 17:UZ:274:LYS:HG3 | 2.20 | 0.41 |
| 18:CA:272:PHE:O | 18:CA:276:VAL:HG23 | 2.20 | 0.41 |
| 19:CC:74:MET:HB2 | 19:CC:78:LEU:HD23 | 2.03 | 0.41 |
| 23:CH:231:HIS:O | 23:CH:235:MET:HG3 | 2.21 | 0.41 |
| 24:CI:367:VAL:HG23 | 24:CI:369:ARG:HH12 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:CI:837:LEU:HD13 | 24:CI:884:PHE:HB3 | 2.03 | 0.41 |
| 25:CJ:35:ARG:HA | 25:CJ:35:ARG:HD3 | 1.95 | 0.41 |
| 26:CK:99:ARG:NE | 26:CK:147:GLY:O | 2.54 | 0.41 |
| 29:CN:176:ARG:NE | 29:CN:192:TYR:OH | 2.32 | 0.41 |
| 29:CN:188:ARG:HB2 | 29:CN:191:ASP:OD2 | 2.20 | 0.41 |
| 29:CO:68:LEU:HD23 | 29:CO:68:LEU:HA | 1.89 | 0.41 |
| 30:CP:176:LYS:HA | 30:CP:179:LYS:HE2 | 2.03 | 0.41 |
| 30:CP:180:GLU:O | 30:CP:184:VAL:HG23 | 2.21 | 0.41 |
| 32:CR:11:ILE:O | 32:CR:15:ILE:HG13 | 2.21 | 0.41 |
| 32:CR:389:ASP:HA | 32:CR:411:ALA:HB3 | 2.02 | 0.41 |
| 32:CR:781:ASP:HA | 32:CR:784:LYS:HE3 | 2.02 | 0.41 |
| 32:CS:11:ILE:O | 32:CS:15:ILE:HG13 | 2.21 | 0.41 |
| 32:CS:284:THR:HG23 | 32:CS:412:SER:HB2 | 2.01 | 0.41 |
| 32:CS:523:ARG:HA | 32:CS:526:LEU:HB3 | 2.01 | 0.41 |
| 32:CS:782:PHE:HA | 32:CS:785:ARG:HB2 | 2.02 | 0.41 |
| 35:Ce:64:ILE:HD11 | 35:Ce:96:VAL:HG22 | 2.01 | 0.41 |
| 41:Cn:92:CYS:HG | 41:Cn:136:TRP:CD1 | 2.38 | 0.41 |
| 44:C1:10:U:C2 | 44:C1:25:G:N1 | 2.89 | 0.41 |
| 44:C1:116:C:H2' | 44:C1:117:A:O4' | 2.21 | 0.41 |
| 44:C1:134:C:H3' | 44:C1:135:A:H2' | 2.02 | 0.41 |
| 44:C1:2156:A:H5' | 44:C1:2157:G:C2 | 2.56 | 0.41 |
| 46:UV:119:GLN:NE2 | 46:UV:145:VAL:HB | 2.36 | 0.41 |
| 46:UV:495:MET:HE2 | 46:UV:579:PHE:HD2 | 1.86 | 0.41 |
| 46:UV:578:ARG:HH11 | 46:UV:584:ILE:HG13 | 1.86 | 0.41 |
| 46:UV:598:LEU:O | 46:UV:602:ILE:HG13 | 2.20 | 0.41 |
| 46:UV:871:SER:HA | 46:UV:872:PRO:HD3 | 1.96 | 0.41 |
| 47:CV:82:THR:HG23 | 47:CV:149:VAL:HB | 2.01 | 0.41 |
| 48:UH:586:LEU:HB2 | 48:UH:630:TYR:HE1 | 1.86 | 0.41 |
| 49:UE:181:ILE:HD13 | 49:UE:216:ARG:HH11 | 1.85 | 0.41 |
| 52:CX:377:LEU:HD11 | 52:CX:381:CYS:HB2 | 2.02 | 0.41 |
| 49:UI:181:ILE:HD13 | 49:UI:216:ARG:HH11 | 1.85 | 0.41 |
| 1:UA:63:LEU:HA | 1:UA:63:LEU:HD12 | 1.84 | 0.41 |
| 1:UA:409:TRP:HA | 1:UA:416:ASN:HA | 2.02 | 0.41 |
| 1:UA:453:TRP:CD1 | 1:UA:460:LEU:HA | 2.50 | 0.41 |
| 1:UA:493:ARG:HD3 | 1:UA:506:PRO:HA | 2.02 | 0.41 |
| 1:UA:707:ASP:HA | 15:UU:677:ASN:ND2 | 2.33 | 0.41 |
| 2:UB:631:SER:OG | 2:UB:708:LEU:O | 2.38 | 0.41 |
| 4:UD:420:LEU:HD12 | 4:UD:420:LEU:HA | 1.73 | 0.41 |
| 6:UG:225:LEU:HB2 | 6:UG:230:LEU:HB2 | 2.03 | 0.41 |
| 6:UG:243:GLN:HA | 6:UG:250:ILE:HA | 2.02 | 0.41 |
| 6:UG:323:LYS:HA | 6:UG:339:TYR:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:UG:326:ILE:O | 6:UG:334:GLU:HG3 | 2.21 | 0.41 |
| 6:UG:366:ILE:O | 6:UG:385:TYR:N | 2.47 | 0.41 |
| 7:UJ:333:ILE:HD13 | 7:UJ:333:ILE:HA | 1.88 | 0.41 |
| 7:UJ:862:THR:HB | 7:UJ:865:ILE:HG12 | 2.03 | 0.41 |
| 8:UK:25:LEU:HD13 | 24:CI:983:LEU:O | 2.21 | 0.41 |
| 8:UK:64:TYR:OH | 25:CJ:119:ARG:NH1 | 2.53 | 0.41 |
| 8:UK:177:LYS:HA | 8:UK:177:LYS:HD3 | 1.89 | 0.41 |
| 9:UL:43:ALA:HB3 | 9:UL:46:GLU:HG3 | 2.02 | 0.41 |
| 9:UL:514:LEU:HD23 | 9:UL:514:LEU:HA | 1.80 | 0.41 |
| 9:UL:588:THR:OG1 | 9:UL:589:VAL:N | 2.54 | 0.41 |
| 9:UL:861:LEU:HD23 | 9:UL:861:LEU:HA | 1.78 | 0.41 |
| 10:UM:568:VAL:HB | 10:UM:582:LEU:HB2 | 2.02 | 0.41 |
| 12:UO:32:LYS:NZ | 12:UO:34:LYS:HB2 | 2.36 | 0.41 |
| 12:UO:545:GLY:O | 12:UO:549:SER:OG | 2.22 | 0.41 |
| 13:UQ:295:ILE:H | 13:UQ:295:ILE:HG12 | 1.69 | 0.41 |
| 13:UQ:955:LYS:HA | 13:UQ:956:PRO:HD3 | 1.81 | 0.41 |
| 14:UR:349:CYS:SG | 14:UR:350:TRP:N | 2.92 | 0.41 |
| 18:CA:148:ILE:H | 18:CA:148:ILE:HG12 | 1.68 | 0.41 |
| 18:CB:131:ASN:HD22 | 18:CB:134:ARG:HD2 | 1.84 | 0.41 |
| 18:CB:161:ALA:HB2 | 18:CB:182:ALA:HB1 | 2.02 | 0.41 |
| 19:CC:39:LYS:HD3 | 19:CC:39:LYS:HA | 1.84 | 0.41 |
| 19:CC:90:SER:O | 19:CC:92:LYS:N | 2.52 | 0.41 |
| 19:CC:206:PHE:HE2 | 19:CC:209:LEU:HD13 | 1.85 | 0.41 |
| 20:CD:196:GLU:O | 20:CD:200:ILE:HG12 | 2.20 | 0.41 |
| 22:CG:343:ARG:CZ | 22:CG:358:LYS:HG3 | 2.51 | 0.41 |
| 23:CH:62:ASN:ND2 | 23:CH:89:MET:SD | 2.94 | 0.41 |
| 23:CH:164:PHE:CE2 | 23:CH:335:VAL:HG23 | 2.55 | 0.41 |
| 24:CI:54:LEU:HD23 | 24:CI:54:LEU:HA | 1.93 | 0.41 |
| 24:CI:66:PRO:O | 24:CI:113:ARG:NH1 | 2.53 | 0.41 |
| 24:CI:68:PRO:HD3 | 24:CI:113:ARG:HH11 | 1.86 | 0.41 |
| 24:CI:302:LEU:HD21 | 24:CI:776:TYR:HD2 | 1.86 | 0.41 |
| 24:CI:402:LEU:HA | 24:CI:402:LEU:HD13 | 1.87 | 0.41 |
| 24:CI:546:MET:HG3 | 24:CI:547:TYR:CD2 | 2.56 | 0.41 |
| 24:CI:940:SER:OG | 24:CI:942:LEU:N | 2.47 | 0.41 |
| 24:CI:974:ARG:HD2 | 44:C1:2183:A:C2 | 2.50 | 0.41 |
| 26:CK:76:GLU:CD | 26:CK:161:PRO:HD3 | 2.45 | 0.41 |
| 26:CK:220:ASN:OD1 | 26:CK:220:ASN:N | 2.51 | 0.41 |
| 26:CK:248:ASN:N | 26:CK:251:SER:O | 2.49 | 0.41 |
| 27:CL:698:LYS:NZ | 44:C1:2211:U:OP2 | 2.41 | 0.41 |
| 28:CM:422:GLU:O | 28:CM:426:SER:HB3 | 2.21 | 0.41 |
| 31:CQ:232:ILE:HD12 | 31:CQ:232:ILE:HA | 1.77 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:CR:16:ARG:O | 32:CR:20:GLN:HG3 | 2.20 | 0.41 |
| 32:CR:314:SER:O | 32:CR:374:PRO:HD3 | 2.21 | 0.41 |
| 32:CS:11:ILE:HG23 | 32:CS:27:PHE:CZ | 2.55 | 0.41 |
| 33:CT:176:ARG:HH22 | 33:CT:177:LYS:HD3 | 1.86 | 0.41 |
| 35:Ce:15:SER:OG | 35:Ce:16:ARG:N | 2.53 | 0.41 |
| 35:Ce:87:LEU:O | 35:Ce:91:PHE:HB3 | 2.21 | 0.41 |
| 36:Cg:173:LYS:HA | 36:Cg:173:LYS:HD3 | 1.81 | 0.41 |
| 38:Ci:83:ARG:HD2 | 38:Ci:83:ARG:HA | 1.69 | 0.41 |
| 39:Cj:13:LYS:HA | 39:Cj:13:LYS:HD3 | 1.81 | 0.41 |
| 40:Cm:52:GLU:HA | 40:Cm:61:ILE:HG13 | 2.02 | 0.41 |
| 40:Cm:61:ILE:HG22 | 40:Cm:63:VAL:HG22 | 2.02 | 0.41 |
| 41:Cn:71:CYS:HB3 | 41:Cn:86:PHE:HE1 | 1.85 | 0.41 |
| 43:CU:121:SER:OG | 43:CU:122:SER:N | 2.54 | 0.41 |
| 44:C1:147:C:H2' | 44:C1:148:C:C6 | 2.55 | 0.41 |
| 44:C1:293:G:O6 | 44:C1:347:C:N4 | 2.53 | 0.41 |
| 44:C1:442:U:N3 | 44:C1:483:U:O2 | 2.53 | 0.41 |
| 44:C1:504:C:H2' | 44:C1:505:C:C6 | 2.55 | 0.41 |
| 44:C1:1169:A:HO2' | 44:C1:1170:G:N2 | 2.16 | 0.41 |
| 44:C1:1622:U:H2' | 44:C1:1623:U:C6 | 2.56 | 0.41 |
| 44:C1:2169:A:C4 | 44:C1:2194:A:N6 | 2.89 | 0.41 |
| 44:C1:2232:C:H2' | 44:C1:2233:U:H6 | 1.86 | 0.41 |
| 46:UV:283:LEU:O | 46:UV:287:ARG:HG2 | 2.21 | 0.41 |
| 46:UV:627:LEU:HB3 | 46:UV:633:ILE:HD11 | 2.03 | 0.41 |
| 46:UV:784:LYS:HD2 | 46:UV:784:LYS:HA | 1.76 | 0.41 |
| 48:UH:569:CYS:SG | 48:UH:572:PRO:HB3 | 2.61 | 0.41 |
| 49:UE:182:GLN:OE1 | 49:UE:182:GLN:N | 2.54 | 0.41 |
| 50:US:177:PRO:HA | 50:US:182:ARG:NH2 | 2.35 | 0.41 |
| 50:US:458:TRP:HA | 50:US:461:VAL:HG12 | 2.03 | 0.41 |
| 53:UP:314:ARG:HH21 | 53:UP:317:SER:C | 2.29 | 0.41 |
| 54:Cz:1498:PHE:HD1 | 54:Cz:1501:LEU:HD11 | 1.86 | 0.41 |
| 54:Cz:1754:SER:O | 54:Cz:1758:VAL:HG23 | 2.20 | 0.41 |
| 1:UA:774:LEU:HD23 | 1:UA:774:LEU:HA | 1.88 | 0.41 |
| 3:UC:636:SER:O | 3:UC:636:SER:OG | 2.37 | 0.41 |
| 4:UD:82:TRP:CZ2 | 4:UD:102:LEU:HD22 | 2.55 | 0.41 |
| 4:UD:257:GLN:HE22 | 4:UD:271:ARG:HH21 | 1.68 | 0.41 |
| 4:UD:281:CYS:SG | 4:UD:329:MET:HG2 | 2.61 | 0.41 |
| 5:UF:157:MET:HE3 | 5:UF:188:TRP:CD1 | 2.56 | 0.41 |
| 7:UJ:102:LEU:HA | 7:UJ:105:VAL:HG12 | 2.03 | 0.41 |
| 9:UL:133:ASP:N | 9:UL:133:ASP:OD1 | 2.54 | 0.41 |
| 10:UM:42:ASN:ND2 | 10:UM:57:ILE:O | 2.43 | 0.41 |
| 10:UM:322:ILE:HG13 | 10:UM:338:GLN:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:UO:467:ARG:HH21 | 12:UO:508:LEU:HD21 | 1.85 | 0.41 |
| 13:UQ:481:CYS:HA | 13:UQ:499:LEU:O | 2.21 | 0.41 |
| 13:UQ:779:GLN:HE21 | 13:UQ:833:SER:HA | 1.86 | 0.41 |
| 14:UR:417:ARG:HH11 | 21:CE:19:GLN:HB3 | 1.86 | 0.41 |
| 15:UU:267:LEU:HD23 | 15:UU:267:LEU:HA | 1.85 | 0.41 |
| 15:UU:701:ARG:HD2 | 15:UU:739:ALA:HB2 | 2.02 | 0.41 |
| 16:UX:72:LYS:HD3 | 40:Cm:95:PRO:HA | 2.03 | 0.41 |
| 18:CA:75:PRO:HG3 | 33:CT:93:ILE:HD12 | 2.03 | 0.41 |
| 23:CH:36:ILE:H | 23:CH:73:THR:HG22 | 1.86 | 0.41 |
| 23:CH:323:GLN:HE21 | 23:CH:355:VAL:HA | 1.85 | 0.41 |
| 24:CI:58:LEU:HA | 24:CI:58:LEU:HD13 | 1.88 | 0.41 |
| 24:CI:192:ARG:HA | 24:CI:192:ARG:HD2 | 1.73 | 0.41 |
| 24:CI:250:ARG:CZ | 32:CR:16:ARG:HH12 | 2.33 | 0.41 |
| 24:CI:749:GLN:O | 24:CI:753:ASN:ND2 | 2.54 | 0.41 |
| 24:CI:985:ASP:OD1 | 24:CI:985:ASP:N | 2.53 | 0.41 |
| 28:CM:28:ALA:O | 28:CM:31:LEU:N | 2.52 | 0.41 |
| 29:CN:172:PRO:HA | 29:CN:173:PRO:HD3 | 1.91 | 0.41 |
| 32:CS:24:ARG:HB2 | 32:CS:486:VAL:HG21 | 2.02 | 0.41 |
| 32:CS:80:LYS:HG2 | 32:CS:80:LYS:H | 1.68 | 0.41 |
| 32:CS:421:GLY:HA3 | 32:CS:424:LEU:HD13 | 2.03 | 0.41 |
| 32:CS:790:LEU:HD12 | 32:CS:791:SER:H | 1.86 | 0.41 |
| 32:CS:903:LEU:HD13 | 32:CS:907:GLN:HB2 | 2.03 | 0.41 |
| 34:Cc:151:PRO:HA | 34:Cc:154:ARG:HD3 | 2.03 | 0.41 |
| 44:C1:1625:G:H2' | 44:C1:1626:G:H8 | 1.82 | 0.41 |
| 45:C2:148:G:H2' | 45:C2:149:U:C6 | 2.56 | 0.41 |
| 46:UV:506:LEU:HD12 | 46:UV:506:LEU:HA | 1.88 | 0.41 |
| 46:UV:733:LYS:HG3 | 46:UV:734:PRO:HD3 | 2.02 | 0.41 |
| 47:CV:88:LYS:HB2 | 47:CV:89:GLN:HE21 | 1.84 | 0.41 |
| 49:UE:165:ASP:OD1 | 49:UE:166:SER:N | 2.54 | 0.41 |
| 50:US:429:GLU:HB2 | 50:US:430:LYS:NZ | 2.35 | 0.41 |
| 52:CX:212:TYR:O | 52:CX:243:THR:HG21 | 2.20 | 0.41 |
| 1:UA:138:PHE:CE1 | 15:UU:39:ARG:HD2 | 2.55 | 0.40 |
| 4:UD:830:TYR:HB3 | 4:UD:833:ARG:NH1 | 2.35 | 0.40 |
| 6:UG:87:LYS:HD3 | 6:UG:87:LYS:HA | 1.89 | 0.40 |
| 6:UG:274:HIS:CG | 6:UG:284:LEU:HD21 | 2.56 | 0.40 |
| 6:UG:364:THR:HG21 | 6:UG:409:ILE:HD13 | 2.03 | 0.40 |
| 6:UG:386:MET:HE2 | 6:UG:386:MET:HB3 | 1.97 | 0.40 |
| 7:UJ:9:LEU:HD23 | 7:UJ:9:LEU:HA | 1.83 | 0.40 |
| 7:UJ:288:ILE:HG12 | 14:UR:233:PHE:HZ | 1.86 | 0.40 |
| 7:UJ:612:ALA:HA | 7:UJ:615:VAL:HG12 | 2.03 | 0.40 |
| 9:UL:16:VAL:HG23 | 9:UL:392:ASN:HD21 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:UM:21:TYR:OH | 10:UM:24:GLY:O | 2.34 | 0.40 |
| 10:UM:120:ASP:O | 10:UM:123:SER:N | 2.54 | 0.40 |
| 12:UO:81:VAL:HG23 | 12:UO:95:ILE:HD12 | 2.03 | 0.40 |
| 12:UO:313:TYR:HB3 | 12:UO:338:MET:SD | 2.61 | 0.40 |
| 13:UQ:79:TRP:HA | 13:UQ:857:GLU:HA | 2.03 | 0.40 |
| 13:UQ:269:LYS:HB3 | 13:UQ:269:LYS:HE3 | 1.86 | 0.40 |
| 13:UQ:444:ASP:OD1 | 13:UQ:805:ARG:NH2 | 2.50 | 0.40 |
| 15:UU:179:LYS:HZ3 | 15:UU:180:LYS:N | 2.19 | 0.40 |
| 16:UX:28:LYS:NZ | 16:UX:31:LYS:HE3 | 2.36 | 0.40 |
| 17:UZ:31:LEU:HA | 17:UZ:34:ILE:HD12 | 2.03 | 0.40 |
| 18:CA:148:ILE:O | 18:CA:150:MET:HG2 | 2.20 | 0.40 |
| 18:CA:262:ILE:HD13 | 18:CA:262:ILE:HA | 1.94 | 0.40 |
| 20:CD:171:LEU:O | 20:CD:175:LEU:HB2 | 2.21 | 0.40 |
| 20:CD:205:LEU:HD13 | 20:CD:205:LEU:HA | 1.88 | 0.40 |
| 22:CG:339:LEU:HD13 | 22:CG:474:TYR:CZ | 2.55 | 0.40 |
| 23:CH:238:ALA:O | 23:CH:242:VAL:HG23 | 2.21 | 0.40 |
| 24:CI:963:LYS:NZ | 44:C1:2180:A:OP1 | 2.53 | 0.40 |
| 28:CM:67:GLN:HE21 | 40:Cm:99:PHE:HE1 | 1.69 | 0.40 |
| 29:CO:35:LYS:HE3 | 29:CO:35:LYS:HB3 | 1.84 | 0.40 |
| 29:CO:94:GLN:O | 29:CO:98:THR:HG23 | 2.21 | 0.40 |
| 32:CR:829:LEU:HD21 | 32:CR:923:PHE:CE1 | 2.56 | 0.40 |
| 34:Cc:177:ILE:H | 34:Cc:177:ILE:HG13 | 1.62 | 0.40 |
| 36:Cg:90:LYS:O | 36:Cg:94:VAL:HG23 | 2.21 | 0.40 |
| 36:Cg:171:ARG:HA | 36:Cg:174:LYS:HE3 | 2.03 | 0.40 |
| 42:Cp:33:PHE:HE2 | 42:Cp:39:ARG:HH11 | 1.69 | 0.40 |
| 44:C1:452:G:H2' | 44:C1:453:G:C8 | 2.56 | 0.40 |
| 44:C1:2161:U:H2' | 44:C1:2162:C:C6 | 2.56 | 0.40 |
| 44:C1:2206:C:H2' | 44:C1:2207:C:H6 | 1.86 | 0.40 |
| 46:UV:278:SER:O | 46:UV:278:SER:OG | 2.32 | 0.40 |
| 46:UV:305:ILE:HG13 | 46:UV:306:TRP:N | 2.36 | 0.40 |
| 46:UV:721:PHE:O | 46:UV:725:ILE:HG12 | 2.21 | 0.40 |
| 46:UV:859:THR:OG1 | 46:UV:878:ARG:HD3 | 2.21 | 0.40 |
| 48:UH:714:LEU:HA | 48:UH:714:LEU:HD23 | 1.79 | 0.40 |
| 50:US:143:MET:HA | 50:US:146:LEU:HD12 | 2.03 | 0.40 |
| 50:US:191:LYS:NZ | 50:US:232:ASP:OD1 | 2.42 | 0.40 |
| 50:US:398:VAL:HG22 | 50:US:492:PHE:HD1 | 1.86 | 0.40 |
| 50:US:418:MET:HE2 | 50:US:418:MET:HB3 | 1.83 | 0.40 |
| 49:UI:165:ASP:OD1 | 49:UI:166:SER:N | 2.54 | 0.40 |
| 49:UI:169:LEU:O | 49:UI:173:LEU:HB2 | 2.21 | 0.40 |
| 49:UI:269:GLN:CD | 49:UI:269:GLN:H | 2.29 | 0.40 |
| 1:UA:1:MET:O | 1:UA:3:THR:HG23 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:UA:155:ARG:NH2 | 1:UA:171:LYS:HG3 | 2.36 | 0.40 |
| 1:UA:794:ILE:HA | 1:UA:794:ILE:HD12 | 1.88 | 0.40 |
| 4:UD:373:THR:HB | 4:UD:836:MET:HE2 | 2.04 | 0.40 |
| 5:UF:43:PHE:HD1 | 5:UF:43:PHE:HA | 1.75 | 0.40 |
| 6:UG:148:GLY:O | 6:UG:165:TRP:NE1 | 2.37 | 0.40 |
| 6:UG:221:HIS:O | 6:UG:233:THR:HA | 2.21 | 0.40 |
| 6:UG:358:VAL:HG13 | 6:UG:365:THR:OG1 | 2.20 | 0.40 |
| 7:UJ:748:LEU:HD23 | 7:UJ:748:LEU:HA | 1.84 | 0.40 |
| 7:UJ:825:LYS:HG2 | 7:UJ:825:LYS:H | 1.73 | 0.40 |
| 9:UL:847:LEU:HD21 | 42:Cp:15:ARG:HE | 1.86 | 0.40 |
| 10:UM:817:ASN:ND2 | 10:UM:867:THR:HG23 | 2.35 | 0.40 |
| 13:UQ:632:ASP:CG | 13:UQ:634:MET:HE2 | 2.46 | 0.40 |
| 15:UU:503:SER:OG | 15:UU:504:GLY:N | 2.54 | 0.40 |
| 15:UU:615:ALA:HA | 15:UU:616:PRO:HD3 | 1.96 | 0.40 |
| 15:UU:674:HIS:HB3 | 15:UU:679:LEU:HB2 | 2.03 | 0.40 |
| 15:UU:761:GLU:HG3 | 15:UU:762:TYR:CD1 | 2.57 | 0.40 |
| 15:UU:941:ILE:HD13 | 15:UU:941:ILE:HA | 1.86 | 0.40 |
| 16:UX:21:LYS:HE3 | 16:UX:21:LYS:HB3 | 1.85 | 0.40 |
| 18:CA:128:ARG:NH2 | 18:CA:169:HIS:HA | 2.36 | 0.40 |
| 18:CB:209:ASP:OD2 | 18:CB:211:ARG:HB2 | 2.21 | 0.40 |
| 19:CC:90:SER:HA | 19:CC:114:PRO:HG2 | 2.04 | 0.40 |
| 19:CC:105:LEU:O | 19:CC:109:ILE:HG12 | 2.21 | 0.40 |
| 19:CC:141:LEU:HD23 | 19:CC:141:LEU:HA | 1.87 | 0.40 |
| 20:CD:114:MET:H | 20:CD:114:MET:HE2 | 1.86 | 0.40 |
| 20:CD:153:LYS:HA | 20:CD:153:LYS:HD2 | 1.89 | 0.40 |
| 20:CD:233:ILE:O | 20:CD:237:VAL:HG13 | 2.21 | 0.40 |
| 21:CF:22:LEU:HB2 | 22:CG:350:ARG:NH2 | 2.36 | 0.40 |
| 23:CH:344:GLU:CD | 23:CH:402:GLY:HA3 | 2.46 | 0.40 |
| 32:CR:198:SER:O | 32:CR:198:SER:OG | 2.40 | 0.40 |
| 32:CR:903:LEU:HD13 | 32:CR:907:GLN:HB2 | 2.03 | 0.40 |
| 32:CR:911:ILE:O | 32:CR:915:ILE:HG13 | 2.20 | 0.40 |
| 32:CS:520:HIS:HB3 | 32:CS:710:SER:HB2 | 2.02 | 0.40 |
| 36:Cg:166:ARG:HH22 | 44:C1:1118:A:H5" | 1.85 | 0.40 |
| 40:Cm:38:LEU:HB3 | 40:Cm:50:PHE:CZ | 2.57 | 0.40 |
| 41:Cn:61:ALA:HB3 | 41:Cn:69:ARG:HD3 | 2.04 | 0.40 |
| 41:Cn:131:GLY:O | 41:Cn:135:LEU:HG | 2.21 | 0.40 |
| 43:CU:199:GLY:O | 43:CU:203:LYS:HG2 | 2.21 | 0.40 |
| 44:C1:61:G:N2 | 48:UH:901:SER:HB3 | 2.35 | 0.40 |
| 44:C1:1476:A:H2' | 44:C1:1477:A:C8 | 2.56 | 0.40 |
| 46:UV:395:ASP:O | 46:UV:399:GLN:HA | 2.21 | 0.40 |
| 46:UV:644:ALA:O | 46:UV:648:PHE:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:755:PHE:CD2 | 46:UV:767:ARG:HG3 | 2.56 | 0.40 |
| 46:UV:1057:VAL:HG22 | 47:CV:96:LYS:HZ1 | 1.84 | 0.40 |
| 47:CV:78:PHE:HZ | 47:CV:150:VAL:HB | 1.86 | 0.40 |
| 49:UE:214:LEU:O | 49:UE:218:ILE:HG12 | 2.21 | 0.40 |
| 50:US:248:PRO:HD2 | 50:US:256:LEU:HD21 | 2.02 | 0.40 |
| 49:UI:232:GLN:HG2 | 49:UI:234:ASP:OD1 | 2.21 | 0.40 |
| 1:UA:724:LEU:HA | 1:UA:724:LEU:HD12 | 1.84 | 0.40 |
| 4:UD:384:LEU:HD11 | 4:UD:436:ILE:HD11 | 2.04 | 0.40 |
| 4:UD:483:ARG:HD3 | 4:UD:483:ARG:HA | 1.90 | 0.40 |
| 4:UD:838:ILE:HA | 4:UD:861:ALA:O | 2.21 | 0.40 |
| 5:UF:117:ALA:HB3 | 5:UF:126:TRP:HD1 | 1.87 | 0.40 |
| 6:UG:200:VAL:HG12 | 6:UG:219:VAL:HG11 | 2.04 | 0.40 |
| 7:UJ:40:ALA:HB1 | 7:UJ:123:ARG:NH1 | 2.37 | 0.40 |
| 7:UJ:673:HIS:HA | 7:UJ:676:ALA:HB3 | 2.03 | 0.40 |
| 7:UJ:726:LEU:O | 7:UJ:729:SER:OG | 2.25 | 0.40 |
| 8:UK:163:VAL:HB | 53:UP:320:TYR:CD1 | 2.55 | 0.40 |
| 8:UK:242:LEU:HD13 | 8:UK:255:GLY:HA2 | 2.02 | 0.40 |
| 9:UL:94:LEU:HB3 | 9:UL:104:VAL:HG22 | 2.02 | 0.40 |
| 9:UL:296:HIS:HB3 | 9:UL:302:VAL:HG23 | 2.02 | 0.40 |
| 9:UL:492:TYR:CZ | 9:UL:499:LEU:HD12 | 2.56 | 0.40 |
| 9:UL:530:LYS:HE3 | 9:UL:566:ASP:HA | 2.03 | 0.40 |
| 9:UL:592:PHE:CD1 | 9:UL:599:LEU:HA | 2.56 | 0.40 |
| 10:UM:65:SER:OG | 10:UM:79:CYS:O | 2.30 | 0.40 |
| 10:UM:244:GLN:HB3 | 10:UM:287:LYS:NZ | 2.34 | 0.40 |
| 12:UO:304:SER:OG | 12:UO:306:ASN:ND2 | 2.54 | 0.40 |
| 13:UQ:625:ARG:HD3 | 13:UQ:637:PHE:HD1 | 1.85 | 0.40 |
| 14:UR:331:VAL:HB | 14:UR:337:GLU:HB2 | 2.02 | 0.40 |
| 14:UR:549:SER:HA | 14:UR:550:PRO:HD3 | 1.93 | 0.40 |
| 16:UX:88:ASN:OD1 | 16:UX:88:ASN:N | 2.51 | 0.40 |
| 16:UX:90:ILE:HD13 | 16:UX:121:LEU:HD13 | 2.03 | 0.40 |
| 16:UX:93:SER:HB2 | 16:UX:123:CYS:SG | 2.61 | 0.40 |
| 20:CD:63:GLY:HA2 | 20:CD:68:LYS:HG2 | 2.03 | 0.40 |
| 20:CD:66:GLU:HB2 | 20:CD:68:LYS:NZ | 2.37 | 0.40 |
| 20:CD:283:LYS:HE3 | 20:CD:283:LYS:HB3 | 1.75 | 0.40 |
| 21:CE:39:ASN:HB2 | 45:C2:84:G:O6 | 2.21 | 0.40 |
| 22:CG:234:ALA:HA | 22:CG:237:ALA:HB2 | 2.02 | 0.40 |
| 22:CG:559:ILE:HG13 | 22:CG:594:MET:HE2 | 2.03 | 0.40 |
| 25:CJ:12:LEU:HA | 25:CJ:12:LEU:HD23 | 1.83 | 0.40 |
| 26:CK:124:LEU:HD21 | 26:CK:273:LEU:HD21 | 2.02 | 0.40 |
| 26:CK:243:VAL:HG13 | 26:CK:255:SER:HB3 | 2.02 | 0.40 |
| 28:CM:277:ASN:ND2 | 28:CM:279:GLN:HE22 | 2.19 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:CN:31:ASP:OD2 | 29:CN:33:ASP:N | 2.53 | 0.40 |
| 29:CO:27:ILE:HG21 | 29:CO:36:ARG:NE | 2.36 | 0.40 |
| 30:CP:126:ILE:HA | 30:CP:129:MET:HG2 | 2.02 | 0.40 |
| 31:CQ:88:PRO:HD3 | 31:CQ:147:ALA:HB1 | 2.03 | 0.40 |
| 32:CR:79:LYS:HD3 | 32:CR:79:LYS:HA | 1.77 | 0.40 |
| 32:CS:53:ASN:HD22 | 32:CS:121:GLY:N | 2.19 | 0.40 |
| 35:Ce:65:VAL:HG12 | 35:Ce:97:LEU:HB2 | 2.03 | 0.40 |
| 35:Ce:73:LEU:HD21 | 35:Ce:100:ALA:HB2 | 2.01 | 0.40 |
| 36:Cg:166:ARG:NH1 | 44:C1:1119:A:OP2 | 2.54 | 0.40 |
| 42:Cp:28:GLN:HG2 | 42:Cp:44:ASN:OD1 | 2.21 | 0.40 |
| 44:C1:166:A:C6 | 44:C1:171:G:O6 | 2.75 | 0.40 |
| 44:C1:273:G:H2' | 44:C1:274:A:H8 | 1.85 | 0.40 |
| 44:C1:481:G:H2' | 44:C1:482:C:C6 | 2.57 | 0.40 |
| 44:C1:484:G:N1 | 44:C1:485:G:C6 | 2.89 | 0.40 |
| 44:C1:1703:G:H2' | 44:C1:1704:U:H6 | 1.86 | 0.40 |
| 44:C1:2218:A:H8 | 44:C1:2218:A:O5' | 2.05 | 0.40 |
| 45:C2:12:U:H2' | 45:C2:13:U:C6 | 2.56 | 0.40 |
| 46:UV:204:PRO:HG3 | 46:UV:214:LYS:HG3 | 2.02 | 0.40 |
| 46:UV:237:ARG:HD3 | 46:UV:240:LEU:HD23 | 2.04 | 0.40 |
| 49:UE:219:GLN:O | 49:UE:223:VAL:HG23 | 2.21 | 0.40 |
| 52:CX:244:PRO:HB2 | 52:CX:287:HIS:HB2 | 2.02 | 0.40 |
| 49:UI:274:LYS:O | 49:UI:277:LYS:HB2 | 2.22 | 0.40 |
| 54:Cz:1627:HIS:CD2 | 54:Cz:1664:LEU:HG | 2.56 | 0.40 |
| 54:Cz:1713:ASP:HA | 54:Cz:1714:PRO:HD3 | 1.96 | 0.40 |
| 1:UA:355:ILE:HG21 | 1:UA:355:ILE:HD13 | 1.83 | 0.40 |
| 2:UB:701:GLN:NE2 | 50:US:540:SER:O | 2.55 | 0.40 |
| 4:UD:644:ASP:CG | 4:UD:662:LEU:HB3 | 2.46 | 0.40 |
| 5:UF:336:SER:C | 5:UF:340:ARG:HE | 2.28 | 0.40 |
| 6:UG:458:MET:HE3 | 6:UG:458:MET:HB2 | 1.83 | 0.40 |
| 7:UJ:201:LEU:HA | 7:UJ:201:LEU:HD23 | 1.82 | 0.40 |
| 7:UJ:828:THR:O | 7:UJ:832:LEU:HG | 2.21 | 0.40 |
| 8:UK:22:ARG:HE | 8:UK:25:LEU:HD12 | 1.87 | 0.40 |
| 9:UL:304:ILE:C | 9:UL:305:TRP:HD1 | 2.30 | 0.40 |
| 9:UL:956:ARG:HA | 9:UL:956:ARG:HD3 | 1.77 | 0.40 |
| 10:UM:199:ALA:HB2 | 10:UM:209:ILE:HG12 | 2.03 | 0.40 |
| 10:UM:234:ASN:HB3 | 10:UM:252:ARG:HG3 | 2.04 | 0.40 |
| 10:UM:254:LYS:HB2 | 46:UV:555:PRO:HB2 | 2.03 | 0.40 |
| 10:UM:566:LYS:HE2 | 10:UM:566:LYS:HB2 | 1.99 | 0.40 |
| 10:UM:869:ARG:NH2 | 27:CL:679:PRO:HG2 | 2.36 | 0.40 |
| 11:UN:916:GLN:NE2 | 44:C1:441:A:H62 | 2.20 | 0.40 |
| 12:UO:473:ARG:HD3 | 12:UO:473:ARG:HA | 1.78 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:UQ:159:ALA:HB1 | 13:UQ:187:LEU:HD21 | 2.04 | 0.40 |
| 13:UQ:369:TYR:OH | 13:UQ:383:GLN:NE2 | 2.55 | 0.40 |
| 13:UQ:457:ARG:HA | 13:UQ:458:PRO:HD3 | 1.98 | 0.40 |
| 14:UR:563:LYS:HE3 | 14:UR:563:LYS:HB2 | 1.91 | 0.40 |
| 15:UU:579:PHE:HA | 15:UU:580:PRO:HA | 1.97 | 0.40 |
| 15:UU:947:LEU:HD23 | 15:UU:947:LEU:HA | 1.75 | 0.40 |
| 17:UZ:233:VAL:HG21 | 17:UZ:270:PHE:HE2 | 1.86 | 0.40 |
| 17:UZ:263:ILE:O | 17:UZ:267:VAL:HG12 | 2.21 | 0.40 |
| 18:CA:79:LYS:HA | 33:CT:90:TRP:NE1 | 2.37 | 0.40 |
| 18:CB:96:ASN:ND2 | 18:CB:98:VAL:O | 2.54 | 0.40 |
| 20:CD:318:THR:OG1 | 45:C2:262:C:OP2 | 2.39 | 0.40 |
| 20:CD:403:ASN:HA | 20:CD:406:ARG:HE | 1.87 | 0.40 |
| 22:CG:429:LEU:HD12 | 22:CG:429:LEU:HA | 1.90 | 0.40 |
| 24:CI:834:ILE:HG13 | 24:CI:843:GLN:HG3 | 2.03 | 0.40 |
| 28:CM:292:SER:OG | 28:CM:295:GLY:N | 2.53 | 0.40 |
| 28:CM:345:SER:OG | 28:CM:348:GLY:N | 2.54 | 0.40 |
| 29:CO:168:THR:HG22 | 29:CO:171:LEU:HD12 | 2.02 | 0.40 |
| 32:CR:41:LEU:HG | 32:CR:41:LEU:H | 1.78 | 0.40 |
| 32:CR:421:GLY:HA3 | 32:CR:424:LEU:HD13 | 2.03 | 0.40 |
| 34:Cc:81:THR:HG21 | 34:Cc:98:VAL:HG12 | 2.02 | 0.40 |
| 39:Cj:44:LEU:O | 39:Cj:47:LYS:N | 2.54 | 0.40 |
| 44:C1:253:G:C2 | 44:C1:254:G:C5 | 3.09 | 0.40 |
| 44:C1:269:G:C2 | 44:C1:270:C:C2 | 3.10 | 0.40 |
| 44:C1:411:C:H2' | 44:C1:412:G:C8 | 2.52 | 0.40 |
| 45:C2:13:U:H2' | 45:C2:14:C:H6 | 1.87 | 0.40 |
| 45:C2:123:A:H2 | 45:C2:124:U:H2' | 1.85 | 0.40 |
| 45:C2:269:G:C2 | 45:C2:270:C:C2 | 3.09 | 0.40 |
| 48:UH:613:LEU:HD13 | 48:UH:613:LEU:HA | 1.90 | 0.40 |
| 48:UH:904:ARG:HA | 48:UH:904:ARG:HD3 | 1.89 | 0.40 |
| 49:UE:274:LYS:O | 49:UE:277:LYS:HB2 | 2.22 | 0.40 |
| 50:US:304:MET:HB2 | 50:US:328:LEU:HD13 | 2.03 | 0.40 |
| 52:CX:406:LEU:HA | 52:CX:407:PRO:HD3 | 1.78 | 0.40 |
| 54:Cz:1564:ASP:HA | 54:Cz:1567:VAL:HG22 | 2.03 | 0.40 |
| 54:Cz:1582:GLU:O | 54:Cz:1586:ARG:HG2 | 2.21 | 0.40 |
| 54:Cz:1744:GLN:HA | 54:Cz:1747:GLU:OE1 | 2.21 | 0.40 |
| 1:UA:288:ASN:OD1 | 1:UA:289:LEU:N | 2.54 | 0.40 |
| 2:UB:714:SER:O | 2:UB:718:THR:HG23 | 2.20 | 0.40 |
| 4:UD:491:ARG:O | 4:UD:506:ARG:HD2 | 2.22 | 0.40 |
| 4:UD:686:ARG:NH1 | 4:UD:744:GLY:HA2 | 2.36 | 0.40 |
| 5:UF:19:LEU:H | 5:UF:19:LEU:HG | 1.57 | 0.40 |
| 6:UG:175:GLN:O | 6:UG:177:GLY:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:UG:274:HIS:CD2 | 6:UG:284:LEU:HD21 | 2.57 | 0.40 |
| 7:UJ:350:GLN:N | 13:UQ:955:LYS:HD2 | 2.36 | 0.40 |
| 7:UJ:415:ASN:O | 7:UJ:419:GLN:HG2 | 2.22 | 0.40 |
| 7:UJ:492:PHE:O | 7:UJ:496:SER:OG | 2.35 | 0.40 |
| 9:UL:21:ASN:HA | 9:UL:370:ARG:HH21 | 1.86 | 0.40 |
| 9:UL:202:ASP:HB3 | 9:UL:205:SER:O | 2.22 | 0.40 |
| 9:UL:275:ARG:HH12 | 9:UL:279:GLU:HG3 | 1.86 | 0.40 |
| 9:UL:430:ARG:HD3 | 9:UL:430:ARG:HA | 1.76 | 0.40 |
| 10:UM:818:THR:HA | 10:UM:866:TYR:CE1 | 2.56 | 0.40 |
| 11:UN:334:ARG:HH11 | 44:C1:582:G:P | 2.43 | 0.40 |
| 13:UQ:358:VAL:HG21 | 13:UQ:361:VAL:HG23 | 2.04 | 0.40 |
| 13:UQ:729:MET:HE1 | 48:UH:543:ARG:HD2 | 2.04 | 0.40 |
| 16:UX:35:ARG:CZ | 44:C1:1081:G:H4' | 2.52 | 0.40 |
| 18:CA:188:ARG:CZ | 21:CF:66:LEU:HD11 | 2.51 | 0.40 |
| 18:CA:199:ARG:HD2 | 18:CA:199:ARG:HA | 1.86 | 0.40 |
| 18:CB:130:TRP:HD1 | 18:CB:169:HIS:CD2 | 2.40 | 0.40 |
| 19:CC:217:ILE:H | 19:CC:217:ILE:HG12 | 1.67 | 0.40 |
| 20:CD:169:VAL:HG11 | 20:CD:299:ALA:HB1 | 2.04 | 0.40 |
| 20:CD:302:ILE:HA | 20:CD:302:ILE:HD13 | 1.84 | 0.40 |
| 22:CG:349:ALA:HA | 22:CG:398:MET:H | 1.86 | 0.40 |
| 23:CH:219:ARG:HA | 23:CH:219:ARG:HD3 | 1.85 | 0.40 |
| 24:CI:809:ARG:HB3 | 24:CI:877:LEU:HD12 | 2.03 | 0.40 |
| 24:CI:867:MET:HB2 | 44:C1:1156:C:C5 | 2.57 | 0.40 |
| 24:CI:982:LEU:HA | 24:CI:982:LEU:HD13 | 1.74 | 0.40 |
| 24:CI:1112:LYS:NZ | 44:C1:1080:G:O6 | 2.55 | 0.40 |
| 26:CK:241:HIS:HB3 | 26:CK:258:GLY:HA3 | 2.03 | 0.40 |
| 26:CK:248:ASN:HB3 | 26:CK:251:SER:N | 2.37 | 0.40 |
| 28:CM:61:LEU:HD23 | 28:CM:61:LEU:HA | 1.81 | 0.40 |
| 28:CM:359:GLU:OE1 | 28:CM:359:GLU:N | 2.54 | 0.40 |
| 30:CP:216:GLU:HG2 | 30:CP:218:TRP:HD1 | 1.87 | 0.40 |
| 31:CQ:142:PHE:CE1 | 31:CQ:155:ALA:HB1 | 2.56 | 0.40 |
| 31:CQ:223:GLU:HG3 | 31:CQ:255:MET:HE3 | 2.04 | 0.40 |
| 32:CR:275:LYS:HA | 32:CR:275:LYS:HD2 | 1.85 | 0.40 |
| 32:CR:705:LEU:HD12 | 32:CR:706:PRO:HD2 | 2.04 | 0.40 |
| 32:CS:70:HIS:HB2 | 32:CS:73:LYS:HG2 | 2.03 | 0.40 |
| 35:Ce:161:LYS:HA | 35:Ce:192:THR:O | 2.22 | 0.40 |
| 36:Cg:157:ALA:O | 36:Cg:160:SER:OG | 2.31 | 0.40 |
| 43:CU:213:LEU:HD13 | 43:CU:213:LEU:HA | 1.89 | 0.40 |
| 44:C1:9:G:N1 | 44:C1:27:A:C6 | 2.89 | 0.40 |
| 44:C1:1539:G:H2' | 44:C1:1540:A:C8 | 2.56 | 0.40 |
| 45:C2:156:C:H2' | 45:C2:157:G:C8 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:UV:169:LEU:HG | 46:UV:228:PRO:HG2 | 2.02 | 0.40 |
| 46:UV:854:LEU:HG | 46:UV:858:HIS:CE1 | 2.57 | 0.40 |
| 46:UV:999:THR:HG23 | 46:UV:1085:LYS:NZ | 2.36 | 0.40 |
| 47:CV:58:VAL:HB | 47:CV:186:LYS:HD2 | 2.02 | 0.40 |
| 48:UH:494:TRP:CD1 | 48:UH:498:MET:HE3 | 2.56 | 0.40 |
| 48:UH:596:LYS:O | 48:UH:600:ARG:HB2 | 2.21 | 0.40 |
| 50:US:178:ILE:HG21 | 50:US:181:LEU:HD23 | 2.03 | 0.40 |
| 50:US:352:LEU:O | 50:US:357:ARG:NH2 | 2.44 | 0.40 |
| 52:CX:253:ILE:HD12 | 52:CX:253:ILE:HA | 1.93 | 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 | UA | 835/904 (92%) | 730 (87%) | 103 (12%) | 2 (0%) | 43 78 |
| 2 | UB | 502/907 (55%) | 466 (93%) | 36 (7%) | 0 | 100 100 |
| 3 | UC | 72/648 (11%) | 67 (93%) | 5 (7%) | 0 | 100 100 |
| 4 | UD | 754/884 (85%) | 689 (91%) | 65 (9%) | 0 | 100 100 |
| 5 | UF | 325/414 (78%) | 304 (94%) | 21 (6%) | 0 | 100 100 |
| 6 | UG | 446/558 (80%) | 384 (86%) | 60 (14%) | 2 (0%) | 30 67 |
| 7 | UJ | 796/1802 (44%) | 750 (94%) | 45 (6%) | 1 (0%) | 48 83 |
| 8 | UK | 211/270 (78%) | 201 (95%) | 10 (5%) | 0 | 100 100 |
| 9 | UL | 767/962 (80%) | 685 (89%) | 82 (11%) | 0 | 100 100 |
| 10 | UM | 645/912 (71%) | 605 (94%) | 39 (6%) | 1 (0%) | 43 78 |
| 11 | UN | 150/938 (16%) | 143 (95%) | 6 (4%) | 1 (1%) | 18 55 |
| 12 | UO | 498/557 (89%) | 450 (90%) | 48 (10%) | 0 | 100 100 |
| 13 | UQ | 775/960 (81%) | 691 (89%) | 81 (10%) | 3 (0%) | 30 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 14 | UR | 437/618 (71%) | 399 (91%) | 38 (9%) | 0 | 100 | 100 |
| 15 | UU | 890/1049 (85%) | 786 (88%) | 103 (12%) | 1 (0%) | 48 | 83 |
| 16 | UX | 188/193 (97%) | 174 (93%) | 14 (7%) | 0 | 100 | 100 |
| 17 | UZ | 229/391 (59%) | 211 (92%) | 18 (8%) | 0 | 100 | 100 |
| 18 | CA | 238/313 (76%) | 213 (90%) | 25 (10%) | 0 | 100 | 100 |
| 18 | CB | 235/313 (75%) | 211 (90%) | 24 (10%) | 0 | 100 | 100 |
| 19 | CC | 383/523 (73%) | 353 (92%) | 30 (8%) | 0 | 100 | 100 |
| 20 | CD | 416/582 (72%) | 382 (92%) | 34 (8%) | 0 | 100 | 100 |
| 21 | CE | 119/127 (94%) | 107 (90%) | 12 (10%) | 0 | 100 | 100 |
| 21 | CF | 118/127 (93%) | 110 (93%) | 8 (7%) | 0 | 100 | 100 |
| 22 | CG | 368/630 (58%) | 342 (93%) | 26 (7%) | 0 | 100 | 100 |
| 23 | CH | 383/411 (93%) | 348 (91%) | 35 (9%) | 0 | 100 | 100 |
| 24 | CI | 812/1163 (70%) | 737 (91%) | 73 (9%) | 2 (0%) | 43 | 78 |
| 25 | CJ | 177/183 (97%) | 151 (85%) | 26 (15%) | 0 | 100 | 100 |
| 26 | CK | 295/297 (99%) | 271 (92%) | 24 (8%) | 0 | 100 | 100 |
| 27 | CL | 225/785 (29%) | 200 (89%) | 24 (11%) | 1 (0%) | 30 | 67 |
| 28 | CM | 443/446 (99%) | 398 (90%) | 44 (10%) | 1 (0%) | 43 | 78 |
| 29 | CN | 222/252 (88%) | 207 (93%) | 15 (7%) | 0 | 100 | 100 |
| 29 | CO | 211/252 (84%) | 193 (92%) | 16 (8%) | 2 (1%) | 14 | 49 |
| 30 | CP | 185/322 (58%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 31 | CQ | 171/259 (66%) | 165 (96%) | 6 (4%) | 0 | 100 | 100 |
| 32 | CR | 746/1073 (70%) | 699 (94%) | 47 (6%) | 0 | 100 | 100 |
| 32 | CS | 746/1073 (70%) | 699 (94%) | 47 (6%) | 0 | 100 | 100 |
| 33 | CT | 127/203 (63%) | 111 (87%) | 16 (13%) | 0 | 100 | 100 |
| 34 | Cc | 188/212 (89%) | 170 (90%) | 18 (10%) | 0 | 100 | 100 |
| 35 | Ce | 155/203 (76%) | 140 (90%) | 15 (10%) | 0 | 100 | 100 |
| 36 | Cg | 157/190 (83%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 37 | Ch | 47/151 (31%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 38 | Ci | 113/150 (75%) | 103 (91%) | 10 (9%) | 0 | 100 | 100 |
| 39 | Cj | 124/143 (87%) | 104 (84%) | 20 (16%) | 0 | 100 | 100 |
| 40 | Cm | 122/130 (94%) | 116 (95%) | 6 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 41 | Cn | 92/145 (63%) | 86 (94%) | 6 (6%) | 0 | 100 100 |
| 42 | Cp | 59/68 (87%) | 53 (90%) | 6 (10%) | 0 | 100 100 |
| 43 | CU | 123/311 (40%) | 108 (88%) | 15 (12%) | 0 | 100 100 |
| 46 | UV | 1057/1171 (90%) | 946 (90%) | 108 (10%) | 3 (0%) | 36 72 |
| 47 | CV | 144/322 (45%) | 130 (90%) | 13 (9%) | 1 (1%) | 18 55 |
| 48 | UH | 349/930 (38%) | 327 (94%) | 22 (6%) | 0 | 100 100 |
| 49 | UE | 121/410 (30%) | 109 (90%) | 12 (10%) | 0 | 100 100 |
| 49 | UI | 121/410 (30%) | 109 (90%) | 12 (10%) | 0 | 100 100 |
| 50 | US | 443/549 (81%) | 414 (94%) | 28 (6%) | 1 (0%) | 43 78 |
| 51 | Cl | 78/156 (50%) | 72 (92%) | 6 (8%) | 0 | 100 100 |
| 52 | CX | 265/480 (55%) | 252 (95%) | 13 (5%) | 0 | 100 100 |
| 53 | UP | 52/364 (14%) | 42 (81%) | 9 (17%) | 1 (2%) | 6 32 |
| 54 | Cz | 273/1796 (15%) | 257 (94%) | 15 (6%) | 1 (0%) | 30 67 |
| All | All | 19223/30592 (63%) | 17548 (91%) | 1651 (9%) | 24 (0%) | 49 83 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | UG | 176 | LEU |
| 29 | CO | 85 | SER |
| 46 | UV | 1059 | ASP |
| 13 | UQ | 708 | SER |
| 11 | UN | 902 | ARG |
| 47 | CV | 92 | SER |
| 50 | US | 241 | GLU |
| 54 | Cz | 1673 | ARG |
| 1 | UA | 372 | GLY |
| 6 | UG | 56 | PRO |
| 27 | CL | 640 | PRO |
| 29 | CO | 84 | ILE |
| 13 | UQ | 365 | GLY |
| 13 | UQ | 564 | GLU |
| 24 | CI | 308 | THR |
| 24 | CI | 396 | PHE |
| 28 | CM | 336 | MET |
| 46 | UV | 567 | ARG |
| 46 | UV | 735 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | UA | 423 | PRO |
| 7 | UJ | 336 | PRO |
| 10 | UM | 329 | PRO |
| 15 | UU | 190 | ILE |
| 53 | UP | 329 | 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 | UA | 651/775 (84%) | 630 (97%) | 21 (3%) | 34 | 56 |
| 2 | UB | 425/788 (54%) | 421 (99%) | 4 (1%) | 70 | 77 |
| 3 | UC | 61/536 (11%) | 60 (98%) | 1 (2%) | 55 | 69 |
| 4 | UD | 653/738 (88%) | 645 (99%) | 8 (1%) | 63 | 74 |
| 5 | UF | 248/341 (73%) | 248 (100%) | 0 | 100 | 100 |
| 6 | UG | 344/474 (73%) | 330 (96%) | 14 (4%) | 27 | 49 |
| 7 | UJ | 658/1526 (43%) | 651 (99%) | 7 (1%) | 65 | 74 |
| 8 | UK | 159/227 (70%) | 157 (99%) | 2 (1%) | 61 | 72 |
| 9 | UL | 667/821 (81%) | 661 (99%) | 6 (1%) | 70 | 77 |
| 10 | UM | 569/770 (74%) | 565 (99%) | 4 (1%) | 76 | 79 |
| 11 | UN | 123/765 (16%) | 122 (99%) | 1 (1%) | 73 | 78 |
| 12 | UO | 404/456 (89%) | 396 (98%) | 8 (2%) | 48 | 66 |
| 13 | UQ | 650/817 (80%) | 638 (98%) | 12 (2%) | 51 | 67 |
| 14 | UR | 360/524 (69%) | 350 (97%) | 10 (3%) | 38 | 59 |
| 15 | UU | 672/863 (78%) | 651 (97%) | 21 (3%) | 35 | 56 |
| 16 | UX | 150/167 (90%) | 146 (97%) | 4 (3%) | 39 | 60 |
| 17 | UZ | 186/329 (56%) | 184 (99%) | 2 (1%) | 65 | 74 |
| 18 | CA | 175/228 (77%) | 168 (96%) | 7 (4%) | 28 | 49 |
| 18 | CB | 195/228 (86%) | 194 (100%) | 1 (0%) | 81 | 82 |
| 19 | CC | 287/435 (66%) | 287 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 20 | CD | 319/489 (65%) | 314 (98%) | 5 (2%) | 55 69 |
| 21 | CE | 91/108 (84%) | 85 (93%) | 6 (7%) | 15 37 |
| 21 | CF | 88/108 (82%) | 88 (100%) | 0 | 100 100 |
| 22 | CG | 299/525 (57%) | 298 (100%) | 1 (0%) | 86 84 |
| 23 | CH | 303/320 (95%) | 296 (98%) | 7 (2%) | 44 64 |
| 24 | CI | 661/1009 (66%) | 647 (98%) | 14 (2%) | 47 65 |
| 25 | CJ | 147/169 (87%) | 138 (94%) | 9 (6%) | 17 39 |
| 26 | CK | 245/266 (92%) | 232 (95%) | 13 (5%) | 20 42 |
| 27 | CL | 181/642 (28%) | 175 (97%) | 6 (3%) | 33 55 |
| 28 | CM | 364/383 (95%) | 358 (98%) | 6 (2%) | 55 69 |
| 29 | CN | 202/223 (91%) | 201 (100%) | 1 (0%) | 81 82 |
| 29 | CO | 193/223 (86%) | 191 (99%) | 2 (1%) | 68 76 |
| 30 | CP | 164/287 (57%) | 164 (100%) | 0 | 100 100 |
| 31 | CQ | 145/215 (67%) | 145 (100%) | 0 | 100 100 |
| 32 | CR | 654/916 (71%) | 471 (72%) | 183 (28%) | 0 3 |
| 32 | CS | 654/916 (71%) | 471 (72%) | 183 (28%) | 0 3 |
| 33 | CT | 108/167 (65%) | 107 (99%) | 1 (1%) | 70 77 |
| 34 | Cc | 149/178 (84%) | 148 (99%) | 1 (1%) | 76 79 |
| 35 | Ce | 137/177 (77%) | 135 (98%) | 2 (2%) | 57 71 |
| 36 | Cg | 122/162 (75%) | 121 (99%) | 1 (1%) | 73 78 |
| 37 | Ch | 43/130 (33%) | 43 (100%) | 0 | 100 100 |
| 38 | Ci | 74/117 (63%) | 73 (99%) | 1 (1%) | 59 72 |
| 39 | Cj | 92/115 (80%) | 90 (98%) | 2 (2%) | 45 64 |
| 40 | Cm | 103/113 (91%) | 102 (99%) | 1 (1%) | 68 76 |
| 41 | Cn | 70/116 (60%) | 70 (100%) | 0 | 100 100 |
| 42 | Cp | 46/61 (75%) | 45 (98%) | 1 (2%) | 45 64 |
| 43 | CU | 103/260 (40%) | 98 (95%) | 5 (5%) | 22 44 |
| 46 | UV | 908/989 (92%) | 900 (99%) | 8 (1%) | 70 77 |
| 47 | CV | 129/276 (47%) | 129 (100%) | 0 | 100 100 |
| 48 | UH | 301/788 (38%) | 300 (100%) | 1 (0%) | 86 84 |
| 49 | UE | 105/346 (30%) | 74 (70%) | 31 (30%) | 0 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 49 | UI | 105/346 (30%) | 74 (70%) | 31 (30%) | 0 3 |
| 50 | US | 404/493 (82%) | 402 (100%) | 2 (0%) | 81 82 |
| 51 | Cl | 71/135 (53%) | 71 (100%) | 0 | 100 100 |
| 52 | CX | 227/411 (55%) | 227 (100%) | 0 | 100 100 |
| 53 | UP | 44/314 (14%) | 44 (100%) | 0 | 100 100 |
| 54 | Cz | 235/1533 (15%) | 235 (100%) | 0 | 100 100 |
| All | All | 15923/25834 (62%) | 15266 (96%) | 657 (4%) | 28 49 |

All (657) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | UA | 8 | SER |
| 1 | UA | 43 | VAL |
| 1 | UA | 45 | ASN |
| 1 | UA | 68 | ASN |
| 1 | UA | 121 | VAL |
| 1 | UA | 127 | THR |
| 1 | UA | 167 | LEU |
| 1 | UA | 219 | VAL |
| 1 | UA | 269 | LEU |
| 1 | UA | 296 | SER |
| 1 | UA | 347 | VAL |
| 1 | UA | 356 | VAL |
| 1 | UA | 415 | ARG |
| 1 | UA | 439 | VAL |
| 1 | UA | 450 | ILE |
| 1 | UA | 560 | ILE |
| 1 | UA | 577 | THR |
| 1 | UA | 580 | TYR |
| 1 | UA | 602 | THR |
| 1 | UA | 611 | THR |
| 1 | UA | 777 | VAL |
| 2 | UB | 48 | LEU |
| 2 | UB | 90 | LEU |
| 2 | UB | 111 | ASN |
| 2 | UB | 828 | ASN |
| 3 | UC | 643 | VAL |
| 4 | UD | 112 | THR |
| 4 | UD | 137 | VAL |
| 4 | UD | 162 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | UD | 224 | THR |
| 4 | UD | 248 | ASP |
| 4 | UD | 267 | THR |
| 4 | UD | 484 | VAL |
| 4 | UD | 549 | VAL |
| 6 | UG | 153 | LEU |
| 6 | UG | 172 | CYS |
| 6 | UG | 179 | THR |
| 6 | UG | 233 | THR |
| 6 | UG | 260 | THR |
| 6 | UG | 265 | THR |
| 6 | UG | 275 | ILE |
| 6 | UG | 290 | THR |
| 6 | UG | 303 | VAL |
| 6 | UG | 356 | THR |
| 6 | UG | 358 | VAL |
| 6 | UG | 365 | THR |
| 6 | UG | 419 | ILE |
| 6 | UG | 466 | ILE |
| 7 | UJ | 44 | THR |
| 7 | UJ | 45 | PHE |
| 7 | UJ | 84 | THR |
| 7 | UJ | 163 | GLU |
| 7 | UJ | 288 | ILE |
| 7 | UJ | 643 | THR |
| 7 | UJ | 720 | LEU |
| 8 | UK | 265 | VAL |
| 8 | UK | 269 | LYS |
| 9 | UL | 82 | VAL |
| 9 | UL | 209 | ILE |
| 9 | UL | 284 | VAL |
| 9 | UL | 298 | VAL |
| 9 | UL | 481 | ILE |
| 9 | UL | 610 | VAL |
| 10 | UM | 210 | PHE |
| 10 | UM | 436 | VAL |
| 10 | UM | 675 | VAL |
| 10 | UM | 745 | LEU |
| 11 | UN | 923 | VAL |
| 12 | UO | 5 | VAL |
| 12 | UO | 125 | VAL |
| 12 | UO | 149 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | UO | 190 | VAL |
| 12 | UO | 270 | THR |
| 12 | UO | 277 | THR |
| 12 | UO | 323 | ILE |
| 12 | UO | 519 | LEU |
| 13 | UQ | 244 | LEU |
| 13 | UQ | 316 | VAL |
| 13 | UQ | 358 | VAL |
| 13 | UQ | 378 | VAL |
| 13 | UQ | 389 | VAL |
| 13 | UQ | 449 | ASP |
| 13 | UQ | 452 | VAL |
| 13 | UQ | 497 | THR |
| 13 | UQ | 537 | THR |
| 13 | UQ | 622 | THR |
| 13 | UQ | 837 | VAL |
| 13 | UQ | 920 | VAL |
| 14 | UR | 152 | THR |
| 14 | UR | 157 | LEU |
| 14 | UR | 271 | ASP |
| 14 | UR | 272 | THR |
| 14 | UR | 277 | ILE |
| 14 | UR | 279 | SER |
| 14 | UR | 314 | LEU |
| 14 | UR | 471 | ARG |
| 14 | UR | 500 | LEU |
| 14 | UR | 535 | VAL |
| 15 | UU | 40 | THR |
| 15 | UU | 41 | ILE |
| 15 | UU | 54 | ILE |
| 15 | UU | 81 | ASN |
| 15 | UU | 192 | MET |
| 15 | UU | 222 | LEU |
| 15 | UU | 276 | VAL |
| 15 | UU | 354 | THR |
| 15 | UU | 377 | ILE |
| 15 | UU | 409 | LEU |
| 15 | UU | 547 | VAL |
| 15 | UU | 554 | THR |
| 15 | UU | 618 | THR |
| 15 | UU | 692 | VAL |
| 15 | UU | 714 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | UU | 738 | THR |
| 15 | UU | 842 | THR |
| 15 | UU | 858 | ASP |
| 15 | UU | 892 | ILE |
| 15 | UU | 929 | LEU |
| 15 | UU | 1012 | LEU |
| 16 | UX | 19 | VAL |
| 16 | UX | 37 | VAL |
| 16 | UX | 76 | LEU |
| 16 | UX | 92 | THR |
| 17 | UZ | 161 | ASN |
| 17 | UZ | 213 | ASN |
| 18 | CA | 83 | VAL |
| 18 | CA | 91 | LEU |
| 18 | CA | 177 | THR |
| 18 | CA | 260 | SER |
| 18 | CA | 291 | THR |
| 18 | CA | 292 | LEU |
| 18 | CA | 307 | LEU |
| 18 | CB | 167 | VAL |
| 20 | CD | 338 | THR |
| 20 | CD | 350 | VAL |
| 20 | CD | 371 | LEU |
| 20 | CD | 372 | SER |
| 20 | CD | 442 | ILE |
| 21 | CE | 25 | VAL |
| 21 | CE | 53 | VAL |
| 21 | CE | 59 | THR |
| 21 | CE | 64 | ILE |
| 21 | CE | 71 | ILE |
| 21 | CE | 94 | VAL |
| 22 | CG | 312 | VAL |
| 23 | CH | 73 | THR |
| 23 | CH | 83 | THR |
| 23 | CH | 128 | LEU |
| 23 | CH | 196 | PHE |
| 23 | CH | 208 | LEU |
| 23 | CH | 337 | THR |
| 23 | CH | 410 | VAL |
| 24 | CI | 197 | LEU |
| 24 | CI | 256 | THR |
| 24 | CI | 367 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | CI | 393 | VAL |
| 24 | CI | 827 | LEU |
| 24 | CI | 863 | THR |
| 24 | CI | 872 | THR |
| 24 | CI | 915 | VAL |
| 24 | CI | 939 | ASN |
| 24 | CI | 985 | ASP |
| 24 | CI | 986 | ILE |
| 24 | CI | 1019 | ILE |
| 24 | CI | 1034 | THR |
| 24 | CI | 1058 | LEU |
| 25 | CJ | 5 | LEU |
| 25 | CJ | 32 | VAL |
| 25 | CJ | 38 | ILE |
| 25 | CJ | 88 | LEU |
| 25 | CJ | 116 | THR |
| 25 | CJ | 123 | THR |
| 25 | CJ | 140 | VAL |
| 25 | CJ | 158 | VAL |
| 25 | CJ | 159 | THR |
| 26 | CK | 18 | LEU |
| 26 | CK | 81 | SER |
| 26 | CK | 87 | ARG |
| 26 | CK | 88 | VAL |
| 26 | CK | 90 | VAL |
| 26 | CK | 92 | THR |
| 26 | CK | 107 | ILE |
| 26 | CK | 123 | ILE |
| 26 | CK | 125 | PRO |
| 26 | CK | 229 | THR |
| 26 | CK | 237 | ILE |
| 26 | CK | 239 | VAL |
| 26 | CK | 269 | THR |
| 27 | CL | 534 | THR |
| 27 | CL | 619 | ILE |
| 27 | CL | 626 | ILE |
| 27 | CL | 630 | LEU |
| 27 | CL | 648 | THR |
| 27 | CL | 669 | VAL |
| 28 | CM | 7 | THR |
| 28 | CM | 47 | VAL |
| 28 | CM | 79 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | CM | 106 | VAL |
| 28 | CM | 223 | ILE |
| 28 | CM | 307 | ILE |
| 29 | CN | 30 | ASN |
| 29 | CO | 169 | ASP |
| 29 | CO | 236 | VAL |
| 32 | CR | 2 | THR |
| 32 | CR | 4 | GLN |
| 32 | CR | 7 | VAL |
| 32 | CR | 9 | SER |
| 32 | CR | 15 | ILE |
| 32 | CR | 23 | LYS |
| 32 | CR | 25 | SER |
| 32 | CR | 29 | VAL |
| 32 | CR | 30 | VAL |
| 32 | CR | 36 | GLU |
| 32 | CR | 38 | ILE |
| 32 | CR | 39 | VAL |
| 32 | CR | 41 | LEU |
| 32 | CR | 46 | SER |
| 32 | CR | 49 | ASP |
| 32 | CR | 51 | ARG |
| 32 | CR | 52 | GLN |
| 32 | CR | 54 | LYS |
| 32 | CR | 55 | SER |
| 32 | CR | 56 | VAL |
| 32 | CR | 62 | LYS |
| 32 | CR | 65 | LEU |
| 32 | CR | 73 | LYS |
| 32 | CR | 80 | LYS |
| 32 | CR | 84 | ARG |
| 32 | CR | 86 | ILE |
| 32 | CR | 87 | ARG |
| 32 | CR | 88 | GLU |
| 32 | CR | 96 | GLU |
| 32 | CR | 97 | LEU |
| 32 | CR | 99 | ILE |
| 32 | CR | 101 | LEU |
| 32 | CR | 102 | ASN |
| 32 | CR | 105 | ARG |
| 32 | CR | 107 | CYS |
| 32 | CR | 110 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CR | 112 | THR |
| 32 | CR | 113 | ASP |
| 32 | CR | 115 | ILE |
| 32 | CR | 119 | THR |
| 32 | CR | 123 | CYS |
| 32 | CR | 124 | ILE |
| 32 | CR | 125 | LEU |
| 32 | CR | 131 | ILE |
| 32 | CR | 136 | LEU |
| 32 | CR | 142 | THR |
| 32 | CR | 149 | VAL |
| 32 | CR | 150 | VAL |
| 32 | CR | 151 | LEU |
| 32 | CR | 153 | LEU |
| 32 | CR | 159 | LEU |
| 32 | CR | 160 | LYS |
| 32 | CR | 162 | LEU |
| 32 | CR | 165 | MET |
| 32 | CR | 181 | VAL |
| 32 | CR | 188 | ARG |
| 32 | CR | 192 | SER |
| 32 | CR | 195 | SER |
| 32 | CR | 198 | SER |
| 32 | CR | 201 | VAL |
| 32 | CR | 202 | ILE |
| 32 | CR | 206 | LEU |
| 32 | CR | 211 | ILE |
| 32 | CR | 212 | SER |
| 32 | CR | 217 | VAL |
| 32 | CR | 251 | SER |
| 32 | CR | 252 | LEU |
| 32 | CR | 253 | ILE |
| 32 | CR | 266 | LEU |
| 32 | CR | 277 | LEU |
| 32 | CR | 278 | ARG |
| 32 | CR | 284 | THR |
| 32 | CR | 291 | LYS |
| 32 | CR | 297 | VAL |
| 32 | CR | 308 | SER |
| 32 | CR | 316 | SER |
| 32 | CR | 318 | GLU |
| 32 | CR | 319 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CR | 322 | THR |
| 32 | CR | 378 | HIS |
| 32 | CR | 379 | VAL |
| 32 | CR | 382 | GLN |
| 32 | CR | 386 | VAL |
| 32 | CR | 387 | VAL |
| 32 | CR | 388 | ILE |
| 32 | CR | 390 | GLU |
| 32 | CR | 394 | ILE |
| 32 | CR | 403 | MET |
| 32 | CR | 410 | MET |
| 32 | CR | 412 | SER |
| 32 | CR | 414 | ILE |
| 32 | CR | 415 | SER |
| 32 | CR | 418 | GLU |
| 32 | CR | 420 | THR |
| 32 | CR | 425 | SER |
| 32 | CR | 427 | LYS |
| 32 | CR | 430 | LYS |
| 32 | CR | 432 | LEU |
| 32 | CR | 433 | ARG |
| 32 | CR | 476 | GLU |
| 32 | CR | 479 | ARG |
| 32 | CR | 484 | ASP |
| 32 | CR | 487 | GLU |
| 32 | CR | 488 | LYS |
| 32 | CR | 492 | THR |
| 32 | CR | 494 | LEU |
| 32 | CR | 502 | ARG |
| 32 | CR | 512 | ASP |
| 32 | CR | 514 | SER |
| 32 | CR | 517 | GLU |
| 32 | CR | 526 | LEU |
| 32 | CR | 532 | VAL |
| 32 | CR | 533 | SER |
| 32 | CR | 534 | GLU |
| 32 | CR | 535 | LYS |
| 32 | CR | 539 | GLN |
| 32 | CR | 541 | VAL |
| 32 | CR | 545 | VAL |
| 32 | CR | 548 | HIS |
| 32 | CR | 554 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CR | 556 | LEU |
| 32 | CR | 558 | LEU |
| 32 | CR | 559 | MET |
| 32 | CR | 566 | GLU |
| 32 | CR | 569 | VAL |
| 32 | CR | 576 | GLU |
| 32 | CR | 584 | CYS |
| 32 | CR | 594 | ILE |
| 32 | CR | 596 | LYS |
| 32 | CR | 625 | ASP |
| 32 | CR | 626 | GLU |
| 32 | CR | 631 | SER |
| 32 | CR | 651 | SER |
| 32 | CR | 654 | LEU |
| 32 | CR | 655 | GLN |
| 32 | CR | 658 | VAL |
| 32 | CR | 704 | GLU |
| 32 | CR | 711 | LYS |
| 32 | CR | 712 | LEU |
| 32 | CR | 713 | SER |
| 32 | CR | 716 | ARG |
| 32 | CR | 718 | GLU |
| 32 | CR | 723 | VAL |
| 32 | CR | 725 | VAL |
| 32 | CR | 732 | GLN |
| 32 | CR | 745 | VAL |
| 32 | CR | 747 | LEU |
| 32 | CR | 750 | THR |
| 32 | CR | 753 | ASP |
| 32 | CR | 759 | THR |
| 32 | CR | 760 | CYS |
| 32 | CR | 768 | ASP |
| 32 | CR | 773 | SER |
| 32 | CR | 784 | LYS |
| 32 | CR | 788 | SER |
| 32 | CR | 789 | LEU |
| 32 | CR | 793 | LYS |
| 32 | CR | 800 | ILE |
| 32 | CR | 801 | LEU |
| 32 | CR | 806 | GLU |
| 32 | CR | 808 | SER |
| 32 | CR | 824 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CR | 830 | ASP |
| 32 | CR | 832 | LEU |
| 32 | CR | 834 | THR |
| 32 | CR | 848 | LEU |
| 32 | CR | 858 | MET |
| 32 | CR | 860 | THR |
| 32 | CR | 861 | ILE |
| 32 | CR | 863 | GLN |
| 32 | CR | 864 | LEU |
| 32 | CR | 867 | THR |
| 32 | CR | 870 | LEU |
| 32 | CR | 872 | GLU |
| 32 | CR | 887 | LEU |
| 32 | CR | 893 | ASP |
| 32 | CR | 894 | ILE |
| 32 | CR | 902 | ASN |
| 32 | CR | 907 | GLN |
| 32 | CR | 908 | VAL |
| 32 | CR | 909 | LEU |
| 32 | CR | 913 | MET |
| 32 | CR | 914 | LYS |
| 32 | CS | 2 | THR |
| 32 | CS | 4 | GLN |
| 32 | CS | 7 | VAL |
| 32 | CS | 9 | SER |
| 32 | CS | 15 | ILE |
| 32 | CS | 23 | LYS |
| 32 | CS | 25 | SER |
| 32 | CS | 29 | VAL |
| 32 | CS | 30 | VAL |
| 32 | CS | 36 | GLU |
| 32 | CS | 38 | ILE |
| 32 | CS | 39 | VAL |
| 32 | CS | 41 | LEU |
| 32 | CS | 46 | SER |
| 32 | CS | 49 | ASP |
| 32 | CS | 51 | ARG |
| 32 | CS | 52 | GLN |
| 32 | CS | 54 | LYS |
| 32 | CS | 55 | SER |
| 32 | CS | 56 | VAL |
| 32 | CS | 62 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CS | 65 | LEU |
| 32 | CS | 73 | LYS |
| 32 | CS | 80 | LYS |
| 32 | CS | 84 | ARG |
| 32 | CS | 86 | ILE |
| 32 | CS | 87 | ARG |
| 32 | CS | 88 | GLU |
| 32 | CS | 96 | GLU |
| 32 | CS | 97 | LEU |
| 32 | CS | 99 | ILE |
| 32 | CS | 101 | LEU |
| 32 | CS | 102 | ASN |
| 32 | CS | 105 | ARG |
| 32 | CS | 107 | CYS |
| 32 | CS | 110 | LYS |
| 32 | CS | 112 | THR |
| 32 | CS | 113 | ASP |
| 32 | CS | 115 | ILE |
| 32 | CS | 119 | THR |
| 32 | CS | 123 | CYS |
| 32 | CS | 124 | ILE |
| 32 | CS | 125 | LEU |
| 32 | CS | 131 | ILE |
| 32 | CS | 136 | LEU |
| 32 | CS | 142 | THR |
| 32 | CS | 149 | VAL |
| 32 | CS | 150 | VAL |
| 32 | CS | 151 | LEU |
| 32 | CS | 153 | LEU |
| 32 | CS | 159 | LEU |
| 32 | CS | 160 | LYS |
| 32 | CS | 162 | LEU |
| 32 | CS | 165 | MET |
| 32 | CS | 181 | VAL |
| 32 | CS | 188 | ARG |
| 32 | CS | 192 | SER |
| 32 | CS | 195 | SER |
| 32 | CS | 198 | SER |
| 32 | CS | 201 | VAL |
| 32 | CS | 202 | ILE |
| 32 | CS | 206 | LEU |
| 32 | CS | 211 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CS | 212 | SER |
| 32 | CS | 217 | VAL |
| 32 | CS | 251 | SER |
| 32 | CS | 252 | LEU |
| 32 | CS | 253 | ILE |
| 32 | CS | 266 | LEU |
| 32 | CS | 277 | LEU |
| 32 | CS | 278 | ARG |
| 32 | CS | 284 | THR |
| 32 | CS | 291 | LYS |
| 32 | CS | 297 | VAL |
| 32 | CS | 308 | SER |
| 32 | CS | 316 | SER |
| 32 | CS | 318 | GLU |
| 32 | CS | 319 | ASN |
| 32 | CS | 322 | THR |
| 32 | CS | 378 | HIS |
| 32 | CS | 379 | VAL |
| 32 | CS | 382 | GLN |
| 32 | CS | 386 | VAL |
| 32 | CS | 387 | VAL |
| 32 | CS | 388 | ILE |
| 32 | CS | 390 | GLU |
| 32 | CS | 394 | ILE |
| 32 | CS | 403 | MET |
| 32 | CS | 410 | MET |
| 32 | CS | 412 | SER |
| 32 | CS | 414 | ILE |
| 32 | CS | 415 | SER |
| 32 | CS | 418 | GLU |
| 32 | CS | 420 | THR |
| 32 | CS | 425 | SER |
| 32 | CS | 427 | LYS |
| 32 | CS | 430 | LYS |
| 32 | CS | 432 | LEU |
| 32 | CS | 433 | ARG |
| 32 | CS | 476 | GLU |
| 32 | CS | 479 | ARG |
| 32 | CS | 484 | ASP |
| 32 | CS | 487 | GLU |
| 32 | CS | 488 | LYS |
| 32 | CS | 492 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CS | 494 | LEU |
| 32 | CS | 502 | ARG |
| 32 | CS | 512 | ASP |
| 32 | CS | 514 | SER |
| 32 | CS | 517 | GLU |
| 32 | CS | 526 | LEU |
| 32 | CS | 532 | VAL |
| 32 | CS | 533 | SER |
| 32 | CS | 534 | GLU |
| 32 | CS | 535 | LYS |
| 32 | CS | 539 | GLN |
| 32 | CS | 541 | VAL |
| 32 | CS | 545 | VAL |
| 32 | CS | 548 | HIS |
| 32 | CS | 554 | ASN |
| 32 | CS | 556 | LEU |
| 32 | CS | 558 | LEU |
| 32 | CS | 559 | MET |
| 32 | CS | 566 | GLU |
| 32 | CS | 569 | VAL |
| 32 | CS | 576 | GLU |
| 32 | CS | 584 | CYS |
| 32 | CS | 594 | ILE |
| 32 | CS | 596 | LYS |
| 32 | CS | 625 | ASP |
| 32 | CS | 626 | GLU |
| 32 | CS | 631 | SER |
| 32 | CS | 651 | SER |
| 32 | CS | 654 | LEU |
| 32 | CS | 655 | GLN |
| 32 | CS | 658 | VAL |
| 32 | CS | 704 | GLU |
| 32 | CS | 711 | LYS |
| 32 | CS | 712 | LEU |
| 32 | CS | 713 | SER |
| 32 | CS | 716 | ARG |
| 32 | CS | 718 | GLU |
| 32 | CS | 723 | VAL |
| 32 | CS | 725 | VAL |
| 32 | CS | 732 | GLN |
| 32 | CS | 745 | VAL |
| 32 | CS | 747 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CS | 750 | THR |
| 32 | CS | 753 | ASP |
| 32 | CS | 759 | THR |
| 32 | CS | 760 | CYS |
| 32 | CS | 768 | ASP |
| 32 | CS | 773 | SER |
| 32 | CS | 784 | LYS |
| 32 | CS | 788 | SER |
| 32 | CS | 789 | LEU |
| 32 | CS | 793 | LYS |
| 32 | CS | 800 | ILE |
| 32 | CS | 801 | LEU |
| 32 | CS | 806 | GLU |
| 32 | CS | 808 | SER |
| 32 | CS | 824 | LEU |
| 32 | CS | 830 | ASP |
| 32 | CS | 832 | LEU |
| 32 | CS | 834 | THR |
| 32 | CS | 848 | LEU |
| 32 | CS | 858 | MET |
| 32 | CS | 860 | THR |
| 32 | CS | 861 | ILE |
| 32 | CS | 863 | GLN |
| 32 | CS | 864 | LEU |
| 32 | CS | 867 | THR |
| 32 | CS | 870 | LEU |
| 32 | CS | 872 | GLU |
| 32 | CS | 887 | LEU |
| 32 | CS | 893 | ASP |
| 32 | CS | 894 | ILE |
| 32 | CS | 902 | ASN |
| 32 | CS | 907 | GLN |
| 32 | CS | 908 | VAL |
| 32 | CS | 909 | LEU |
| 32 | CS | 913 | MET |
| 32 | CS | 914 | LYS |
| 33 | CT | 86 | THR |
| 34 | Cc | 134 | THR |
| 35 | Ce | 34 | GLU |
| 35 | Ce | 181 | GLU |
| 36 | Cg | 97 | LEU |
| 38 | Ci | 131 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | Cj | 10 | PHE |
| 39 | Cj | 69 | VAL |
| 40 | Cm | 25 | VAL |
| 42 | Cp | 49 | VAL |
| 43 | CU | 116 | LEU |
| 43 | CU | 120 | LEU |
| 43 | CU | 126 | ASP |
| 43 | CU | 251 | ASN |
| 43 | CU | 254 | VAL |
| 46 | UV | 131 | MET |
| 46 | UV | 155 | ASP |
| 46 | UV | 307 | LEU |
| 46 | UV | 443 | LEU |
| 46 | UV | 507 | LYS |
| 46 | UV | 810 | LEU |
| 46 | UV | 941 | THR |
| 46 | UV | 1080 | THR |
| 48 | UH | 574 | SER |
| 49 | UE | 155 | THR |
| 49 | UE | 162 | ARG |
| 49 | UE | 167 | ASP |
| 49 | UE | 169 | LEU |
| 49 | UE | 180 | ILE |
| 49 | UE | 191 | SER |
| 49 | UE | 195 | THR |
| 49 | UE | 197 | LEU |
| 49 | UE | 198 | SER |
| 49 | UE | 199 | LYS |
| 49 | UE | 214 | LEU |
| 49 | UE | 215 | MET |
| 49 | UE | 219 | GLN |
| 49 | UE | 236 | ILE |
| 49 | UE | 238 | ARG |
| 49 | UE | 241 | GLU |
| 49 | UE | 242 | LEU |
| 49 | UE | 243 | SER |
| 49 | UE | 244 | ARG |
| 49 | UE | 246 | LEU |
| 49 | UE | 250 | SER |
| 49 | UE | 251 | ARG |
| 49 | UE | 253 | LEU |
| 49 | UE | 256 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | UE | 257 | LEU |
| 49 | UE | 263 | LEU |
| 49 | UE | 266 | LEU |
| 49 | UE | 269 | GLN |
| 49 | UE | 273 | ARG |
| 49 | UE | 277 | LYS |
| 49 | UE | 278 | MET |
| 50 | US | 168 | GLU |
| 50 | US | 506 | THR |
| 49 | UI | 155 | THR |
| 49 | UI | 162 | ARG |
| 49 | UI | 167 | ASP |
| 49 | UI | 169 | LEU |
| 49 | UI | 180 | ILE |
| 49 | UI | 191 | SER |
| 49 | UI | 195 | THR |
| 49 | UI | 197 | LEU |
| 49 | UI | 198 | SER |
| 49 | UI | 199 | LYS |
| 49 | UI | 214 | LEU |
| 49 | UI | 215 | MET |
| 49 | UI | 219 | GLN |
| 49 | UI | 236 | ILE |
| 49 | UI | 238 | ARG |
| 49 | UI | 241 | GLU |
| 49 | UI | 242 | LEU |
| 49 | UI | 243 | SER |
| 49 | UI | 244 | ARG |
| 49 | UI | 246 | LEU |
| 49 | UI | 250 | SER |
| 49 | UI | 251 | ARG |
| 49 | UI | 253 | LEU |
| 49 | UI | 256 | LEU |
| 49 | UI | 257 | LEU |
| 49 | UI | 263 | LEU |
| 49 | UI | 266 | LEU |
| 49 | UI | 269 | GLN |
| 49 | UI | 273 | ARG |
| 49 | UI | 277 | LYS |
| 49 | UI | 278 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (316) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | UA | 9 | ASN |
| 1 | UA | 78 | GLN |
| 1 | UA | 144 | HIS |
| 1 | UA | 207 | GLN |
| 1 | UA | 253 | GLN |
| 1 | UA | 321 | GLN |
| 1 | UA | 336 | GLN |
| 1 | UA | 467 | HIS |
| 1 | UA | 543 | GLN |
| 2 | UB | 22 | GLN |
| 2 | UB | 27 | GLN |
| 2 | UB | 525 | ASN |
| 2 | UB | 542 | GLN |
| 2 | UB | 551 | GLN |
| 2 | UB | 701 | GLN |
| 2 | UB | 741 | HIS |
| 2 | UB | 751 | GLN |
| 2 | UB | 765 | ASN |
| 2 | UB | 802 | HIS |
| 2 | UB | 824 | HIS |
| 3 | UC | 584 | GLN |
| 4 | UD | 235 | ASN |
| 4 | UD | 309 | GLN |
| 4 | UD | 322 | HIS |
| 4 | UD | 324 | HIS |
| 4 | UD | 370 | GLN |
| 4 | UD | 485 | GLN |
| 4 | UD | 673 | ASN |
| 4 | UD | 697 | GLN |
| 4 | UD | 807 | ASN |
| 5 | UF | 45 | HIS |
| 5 | UF | 89 | GLN |
| 5 | UF | 289 | GLN |
| 6 | UG | 49 | GLN |
| 6 | UG | 96 | GLN |
| 6 | UG | 114 | GLN |
| 6 | UG | 127 | GLN |
| 6 | UG | 206 | ASN |
| 6 | UG | 221 | HIS |
| 6 | UG | 243 | GLN |
| 6 | UG | 277 | GLN |
| 6 | UG | 378 | GLN |
| 6 | UG | 427 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | UG | 452 | ASN |
| 7 | UJ | 43 | GLN |
| 7 | UJ | 85 | GLN |
| 7 | UJ | 103 | HIS |
| 7 | UJ | 131 | ASN |
| 7 | UJ | 184 | GLN |
| 7 | UJ | 295 | GLN |
| 7 | UJ | 379 | ASN |
| 7 | UJ | 404 | HIS |
| 7 | UJ | 515 | ASN |
| 7 | UJ | 670 | HIS |
| 7 | UJ | 766 | GLN |
| 7 | UJ | 845 | GLN |
| 8 | UK | 13 | HIS |
| 9 | UL | 23 | ASN |
| 9 | UL | 107 | ASN |
| 9 | UL | 145 | GLN |
| 9 | UL | 207 | HIS |
| 9 | UL | 296 | HIS |
| 9 | UL | 398 | ASN |
| 9 | UL | 453 | ASN |
| 9 | UL | 457 | GLN |
| 9 | UL | 504 | ASN |
| 9 | UL | 515 | GLN |
| 9 | UL | 930 | GLN |
| 10 | UM | 58 | GLN |
| 10 | UM | 203 | GLN |
| 10 | UM | 236 | GLN |
| 10 | UM | 520 | GLN |
| 10 | UM | 628 | ASN |
| 10 | UM | 644 | ASN |
| 10 | UM | 652 | HIS |
| 10 | UM | 691 | ASN |
| 10 | UM | 733 | GLN |
| 10 | UM | 741 | GLN |
| 10 | UM | 772 | ASN |
| 10 | UM | 776 | ASN |
| 10 | UM | 827 | GLN |
| 10 | UM | 840 | ASN |
| 11 | UN | 348 | HIS |
| 11 | UN | 362 | GLN |
| 11 | UN | 916 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | UO | 143 | HIS |
| 12 | UO | 284 | GLN |
| 12 | UO | 306 | ASN |
| 12 | UO | 329 | HIS |
| 12 | UO | 333 | HIS |
| 13 | UQ | 112 | GLN |
| 13 | UQ | 262 | HIS |
| 13 | UQ | 310 | GLN |
| 13 | UQ | 352 | HIS |
| 13 | UQ | 394 | HIS |
| 13 | UQ | 438 | GLN |
| 13 | UQ | 474 | ASN |
| 13 | UQ | 783 | ASN |
| 13 | UQ | 917 | HIS |
| 13 | UQ | 924 | GLN |
| 14 | UR | 312 | ASN |
| 14 | UR | 364 | GLN |
| 14 | UR | 370 | GLN |
| 14 | UR | 498 | ASN |
| 15 | UU | 81 | ASN |
| 15 | UU | 197 | ASN |
| 15 | UU | 236 | GLN |
| 15 | UU | 257 | ASN |
| 15 | UU | 379 | HIS |
| 15 | UU | 392 | HIS |
| 15 | UU | 427 | GLN |
| 15 | UU | 571 | GLN |
| 15 | UU | 575 | HIS |
| 15 | UU | 577 | GLN |
| 15 | UU | 621 | HIS |
| 15 | UU | 711 | ASN |
| 15 | UU | 774 | GLN |
| 15 | UU | 963 | ASN |
| 15 | UU | 1002 | HIS |
| 16 | UX | 141 | HIS |
| 17 | UZ | 90 | ASN |
| 17 | UZ | 105 | GLN |
| 17 | UZ | 110 | ASN |
| 17 | UZ | 276 | GLN |
| 18 | CA | 78 | HIS |
| 18 | CA | 249 | GLN |
| 18 | CB | 235 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | CB | 299 | HIS |
| 19 | CC | 67 | ASN |
| 19 | CC | 139 | ASN |
| 19 | CC | 173 | ASN |
| 19 | CC | 175 | ASN |
| 19 | CC | 179 | GLN |
| 19 | CC | 192 | ASN |
| 19 | CC | 245 | ASN |
| 19 | CC | 272 | GLN |
| 19 | CC | 321 | HIS |
| 19 | CC | 394 | ASN |
| 20 | CD | 106 | ASN |
| 20 | CD | 124 | GLN |
| 20 | CD | 128 | ASN |
| 20 | CD | 263 | GLN |
| 20 | CD | 280 | ASN |
| 20 | CD | 314 | ASN |
| 20 | CD | 404 | ASN |
| 21 | CE | 46 | ASN |
| 21 | CE | 76 | ASN |
| 21 | CF | 60 | GLN |
| 21 | CF | 67 | HIS |
| 22 | CG | 198 | GLN |
| 22 | CG | 243 | GLN |
| 22 | CG | 245 | HIS |
| 22 | CG | 274 | ASN |
| 22 | CG | 301 | ASN |
| 22 | CG | 302 | GLN |
| 22 | CG | 430 | HIS |
| 22 | CG | 436 | HIS |
| 22 | CG | 462 | GLN |
| 23 | CH | 90 | ASN |
| 23 | CH | 199 | GLN |
| 23 | CH | 232 | ASN |
| 23 | CH | 323 | GLN |
| 24 | CI | 165 | ASN |
| 24 | CI | 202 | HIS |
| 24 | CI | 221 | ASN |
| 24 | CI | 248 | ASN |
| 24 | CI | 287 | HIS |
| 24 | CI | 366 | ASN |
| 24 | CI | 374 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | CI | 380 | GLN |
| 24 | CI | 612 | ASN |
| 24 | CI | 753 | ASN |
| 24 | CI | 767 | GLN |
| 24 | CI | 930 | ASN |
| 24 | CI | 1006 | ASN |
| 24 | CI | 1011 | GLN |
| 25 | CJ | 27 | HIS |
| 25 | CJ | 59 | HIS |
| 26 | CK | 8 | GLN |
| 26 | CK | 48 | ASN |
| 26 | CK | 121 | ASN |
| 26 | CK | 159 | HIS |
| 26 | CK | 190 | HIS |
| 27 | CL | 514 | ASN |
| 27 | CL | 569 | HIS |
| 28 | CM | 41 | GLN |
| 28 | CM | 120 | ASN |
| 28 | CM | 143 | ASN |
| 28 | CM | 206 | ASN |
| 28 | CM | 277 | ASN |
| 28 | CM | 370 | GLN |
| 29 | CN | 111 | GLN |
| 29 | CN | 156 | ASN |
| 29 | CN | 199 | ASN |
| 29 | CO | 93 | HIS |
| 29 | CO | 111 | GLN |
| 29 | CO | 115 | GLN |
| 30 | CP | 147 | ASN |
| 30 | CP | 159 | GLN |
| 30 | CP | 167 | ASN |
| 30 | CP | 190 | ASN |
| 31 | CQ | 137 | GLN |
| 31 | CQ | 224 | ASN |
| 31 | CQ | 247 | ASN |
| 32 | CR | 4 | GLN |
| 32 | CR | 20 | GLN |
| 32 | CR | 53 | ASN |
| 32 | CR | 102 | ASN |
| 32 | CR | 126 | GLN |
| 32 | CR | 170 | HIS |
| 32 | CR | 207 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | CR | 365 | HIS |
| 32 | CR | 485 | ASN |
| 32 | CR | 491 | ASN |
| 32 | CR | 565 | HIS |
| 32 | CR | 587 | GLN |
| 32 | CR | 731 | GLN |
| 32 | CR | 758 | HIS |
| 32 | CR | 838 | HIS |
| 32 | CR | 846 | ASN |
| 32 | CR | 902 | ASN |
| 32 | CR | 907 | GLN |
| 32 | CS | 4 | GLN |
| 32 | CS | 20 | GLN |
| 32 | CS | 53 | ASN |
| 32 | CS | 102 | ASN |
| 32 | CS | 126 | GLN |
| 32 | CS | 170 | HIS |
| 32 | CS | 382 | GLN |
| 32 | CS | 485 | ASN |
| 32 | CS | 491 | ASN |
| 32 | CS | 565 | HIS |
| 32 | CS | 587 | GLN |
| 32 | CS | 731 | GLN |
| 32 | CS | 758 | HIS |
| 32 | CS | 838 | HIS |
| 32 | CS | 846 | ASN |
| 32 | CS | 852 | HIS |
| 32 | CS | 902 | ASN |
| 32 | CS | 907 | GLN |
| 32 | CS | 922 | HIS |
| 33 | CT | 126 | ASN |
| 34 | Cc | 50 | GLN |
| 34 | Cc | 87 | HIS |
| 34 | Cc | 91 | ASN |
| 34 | Cc | 109 | HIS |
| 34 | Cc | 145 | GLN |
| 34 | Cc | 187 | ASN |
| 34 | Cc | 211 | ASN |
| 35 | Ce | 77 | HIS |
| 36 | Cg | 108 | GLN |
| 38 | Ci | 93 | HIS |
| 39 | Cj | 74 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | Cj | 77 | GLN |
| 39 | Cj | 83 | GLN |
| 39 | Cj | 107 | GLN |
| 40 | Cm | 64 | GLN |
| 40 | Cm | 80 | ASN |
| 46 | UV | 77 | HIS |
| 46 | UV | 119 | GLN |
| 46 | UV | 192 | ASN |
| 46 | UV | 205 | ASN |
| 46 | UV | 260 | GLN |
| 46 | UV | 270 | ASN |
| 46 | UV | 281 | GLN |
| 46 | UV | 399 | GLN |
| 46 | UV | 415 | HIS |
| 46 | UV | 416 | GLN |
| 46 | UV | 417 | HIS |
| 46 | UV | 494 | ASN |
| 46 | UV | 542 | ASN |
| 46 | UV | 615 | GLN |
| 46 | UV | 677 | HIS |
| 46 | UV | 782 | GLN |
| 46 | UV | 813 | HIS |
| 46 | UV | 858 | HIS |
| 46 | UV | 938 | GLN |
| 46 | UV | 974 | GLN |
| 47 | CV | 55 | ASN |
| 47 | CV | 89 | GLN |
| 47 | CV | 91 | HIS |
| 47 | CV | 199 | ASN |
| 48 | UH | 477 | ASN |
| 48 | UH | 590 | ASN |
| 48 | UH | 862 | HIS |
| 49 | UE | 183 | ASN |
| 49 | UE | 219 | GLN |
| 49 | UE | 269 | GLN |
| 50 | US | 151 | GLN |
| 50 | US | 152 | HIS |
| 50 | US | 188 | ASN |
| 50 | US | 206 | HIS |
| 50 | US | 225 | ASN |
| 50 | US | 260 | GLN |
| 50 | US | 261 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | US | 264 | GLN |
| 50 | US | 372 | HIS |
| 50 | US | 419 | HIS |
| 50 | US | 464 | GLN |
| 51 | Cl | 21 | ASN |
| 52 | CX | 290 | ASN |
| 52 | CX | 322 | GLN |
| 52 | CX | 352 | GLN |
| 52 | CX | 364 | ASN |
| 52 | CX | 411 | HIS |
| 52 | CX | 423 | ASN |
| 52 | CX | 440 | HIS |
| 49 | UI | 183 | ASN |
| 49 | UI | 269 | GLN |
| 54 | Cz | 1519 | GLN |
| 54 | Cz | 1530 | GLN |
| 54 | Cz | 1549 | ASN |
| 54 | Cz | 1556 | ASN |
| 54 | Cz | 1568 | GLN |
| 54 | Cz | 1631 | ASN |
| 54 | Cz | 1675 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 44 | C1 | 1088/2323 (46%) | 374 (34%) | 31 (2%) |
| 45 | C2 | 226/230 (98%) | 84 (37%) | 8 (3%) |
| All | All | 1314/2553 (51%) | 458 (34%) | 39 (2%) |

All (458) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 2 | G |
| 44 | C1 | 3 | G |
| 44 | C1 | 4 | G |
| 44 | C1 | 5 | G |
| 44 | C1 | 7 | A |
| 44 | C1 | 13 | G |
| 44 | C1 | 14 | G |
| 44 | C1 | 15 | G |
| 44 | C1 | 16 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 17 | C |
| 44 | C1 | 18 | G |
| 44 | C1 | 19 | C |
| 44 | C1 | 20 | C |
| 44 | C1 | 23 | G |
| 44 | C1 | 26 | C |
| 44 | C1 | 38 | G |
| 44 | C1 | 40 | A |
| 44 | C1 | 41 | G |
| 44 | C1 | 42 | C |
| 44 | C1 | 43 | C |
| 44 | C1 | 47 | G |
| 44 | C1 | 49 | G |
| 44 | C1 | 56 | C |
| 44 | C1 | 57 | C |
| 44 | C1 | 59 | U |
| 44 | C1 | 60 | A |
| 44 | C1 | 61 | G |
| 44 | C1 | 63 | C |
| 44 | C1 | 66 | G |
| 44 | C1 | 68 | U |
| 44 | C1 | 71 | A |
| 44 | C1 | 72 | U |
| 44 | C1 | 73 | A |
| 44 | C1 | 74 | C |
| 44 | C1 | 77 | C |
| 44 | C1 | 89 | G |
| 44 | C1 | 90 | A |
| 44 | C1 | 93 | G |
| 44 | C1 | 96 | C |
| 44 | C1 | 104 | U |
| 44 | C1 | 105 | A |
| 44 | C1 | 107 | C |
| 44 | C1 | 121 | G |
| 44 | C1 | 126 | C |
| 44 | C1 | 127 | C |
| 44 | C1 | 128 | G |
| 44 | C1 | 132 | A |
| 44 | C1 | 134 | C |
| 44 | C1 | 135 | A |
| 44 | C1 | 136 | C |
| 44 | C1 | 143 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 152 | G |
| 44 | C1 | 154 | C |
| 44 | C1 | 155 | G |
| 44 | C1 | 158 | C |
| 44 | C1 | 159 | C |
| 44 | C1 | 160 | C |
| 44 | C1 | 161 | A |
| 44 | C1 | 162 | G |
| 44 | C1 | 163 | C |
| 44 | C1 | 166 | A |
| 44 | C1 | 169 | G |
| 44 | C1 | 170 | C |
| 44 | C1 | 182 | C |
| 44 | C1 | 183 | C |
| 44 | C1 | 185 | G |
| 44 | C1 | 192 | A |
| 44 | C1 | 201 | G |
| 44 | C1 | 203 | C |
| 44 | C1 | 205 | C |
| 44 | C1 | 206 | C |
| 44 | C1 | 207 | U |
| 44 | C1 | 208 | A |
| 44 | C1 | 210 | G |
| 44 | C1 | 216 | A |
| 44 | C1 | 220 | A |
| 44 | C1 | 222 | U |
| 44 | C1 | 223 | A |
| 44 | C1 | 228 | G |
| 44 | C1 | 234 | G |
| 44 | C1 | 236 | C |
| 44 | C1 | 237 | G |
| 44 | C1 | 242 | U |
| 44 | C1 | 243 | U |
| 44 | C1 | 244 | G |
| 44 | C1 | 251 | G |
| 44 | C1 | 257 | G |
| 44 | C1 | 258 | C |
| 44 | C1 | 259 | U |
| 44 | C1 | 260 | U |
| 44 | C1 | 262 | G |
| 44 | C1 | 265 | G |
| 44 | C1 | 266 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 267 | U |
| 44 | C1 | 268 | G |
| 44 | C1 | 269 | G |
| 44 | C1 | 272 | A |
| 44 | C1 | 273 | G |
| 44 | C1 | 276 | C |
| 44 | C1 | 277 | U |
| 44 | C1 | 278 | A |
| 44 | C1 | 281 | U |
| 44 | C1 | 282 | C |
| 44 | C1 | 283 | A |
| 44 | C1 | 285 | A |
| 44 | C1 | 291 | C |
| 44 | C1 | 292 | G |
| 44 | C1 | 339 | C |
| 44 | C1 | 340 | G |
| 44 | C1 | 346 | C |
| 44 | C1 | 347 | C |
| 44 | C1 | 349 | C |
| 44 | C1 | 351 | U |
| 44 | C1 | 352 | G |
| 44 | C1 | 353 | G |
| 44 | C1 | 357 | G |
| 44 | C1 | 360 | U |
| 44 | C1 | 371 | U |
| 44 | C1 | 372 | U |
| 44 | C1 | 379 | G |
| 44 | C1 | 382 | U |
| 44 | C1 | 383 | G |
| 44 | C1 | 384 | C |
| 44 | C1 | 386 | G |
| 44 | C1 | 398 | C |
| 44 | C1 | 401 | C |
| 44 | C1 | 402 | U |
| 44 | C1 | 403 | G |
| 44 | C1 | 407 | A |
| 44 | C1 | 416 | U |
| 44 | C1 | 423 | U |
| 44 | C1 | 425 | C |
| 44 | C1 | 427 | G |
| 44 | C1 | 432 | G |
| 44 | C1 | 435 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 436 | A |
| 44 | C1 | 439 | A |
| 44 | C1 | 440 | G |
| 44 | C1 | 441 | A |
| 44 | C1 | 442 | U |
| 44 | C1 | 443 | G |
| 44 | C1 | 454 | C |
| 44 | C1 | 458 | A |
| 44 | C1 | 459 | C |
| 44 | C1 | 467 | C |
| 44 | C1 | 468 | C |
| 44 | C1 | 469 | G |
| 44 | C1 | 471 | C |
| 44 | C1 | 473 | G |
| 44 | C1 | 474 | A |
| 44 | C1 | 475 | C |
| 44 | C1 | 477 | A |
| 44 | C1 | 483 | U |
| 44 | C1 | 484 | G |
| 44 | C1 | 491 | G |
| 44 | C1 | 492 | C |
| 44 | C1 | 499 | G |
| 44 | C1 | 500 | C |
| 44 | C1 | 501 | U |
| 44 | C1 | 502 | A |
| 44 | C1 | 504 | C |
| 44 | C1 | 581 | C |
| 44 | C1 | 582 | G |
| 44 | C1 | 583 | A |
| 44 | C1 | 584 | U |
| 44 | C1 | 585 | A |
| 44 | C1 | 586 | G |
| 44 | C1 | 587 | U |
| 44 | C1 | 594 | G |
| 44 | C1 | 596 | U |
| 44 | C1 | 603 | G |
| 44 | C1 | 604 | C |
| 44 | C1 | 609 | A |
| 44 | C1 | 610 | G |
| 44 | C1 | 613 | A |
| 44 | C1 | 614 | U |
| 44 | C1 | 621 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 627 | A |
| 44 | C1 | 1054 | A |
| 44 | C1 | 1059 | A |
| 44 | C1 | 1061 | A |
| 44 | C1 | 1062 | C |
| 44 | C1 | 1064 | G |
| 44 | C1 | 1069 | A |
| 44 | C1 | 1070 | G |
| 44 | C1 | 1076 | U |
| 44 | C1 | 1077 | U |
| 44 | C1 | 1078 | U |
| 44 | C1 | 1079 | C |
| 44 | C1 | 1080 | G |
| 44 | C1 | 1081 | G |
| 44 | C1 | 1083 | U |
| 44 | C1 | 1085 | U |
| 44 | C1 | 1086 | U |
| 44 | C1 | 1088 | U |
| 44 | C1 | 1089 | A |
| 44 | C1 | 1094 | G |
| 44 | C1 | 1095 | A |
| 44 | C1 | 1097 | U |
| 44 | C1 | 1098 | G |
| 44 | C1 | 1103 | C |
| 44 | C1 | 1104 | A |
| 44 | C1 | 1120 | C |
| 44 | C1 | 1123 | G |
| 44 | C1 | 1124 | G |
| 44 | C1 | 1125 | A |
| 44 | C1 | 1126 | A |
| 44 | C1 | 1127 | C |
| 44 | C1 | 1128 | A |
| 44 | C1 | 1129 | A |
| 44 | C1 | 1140 | A |
| 44 | C1 | 1141 | G |
| 44 | C1 | 1147 | U |
| 44 | C1 | 1148 | G |
| 44 | C1 | 1149 | C |
| 44 | C1 | 1150 | C |
| 44 | C1 | 1154 | A |
| 44 | C1 | 1158 | G |
| 44 | C1 | 1159 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 1163 | A |
| 44 | C1 | 1164 | A |
| 44 | C1 | 1166 | U |
| 44 | C1 | 1167 | C |
| 44 | C1 | 1168 | C |
| 44 | C1 | 1169 | A |
| 44 | C1 | 1170 | G |
| 44 | C1 | 1178 | A |
| 44 | C1 | 1179 | G |
| 44 | C1 | 1186 | U |
| 44 | C1 | 1218 | G |
| 44 | C1 | 1219 | A |
| 44 | C1 | 1222 | C |
| 44 | C1 | 1223 | U |
| 44 | C1 | 1444 | A |
| 44 | C1 | 1447 | A |
| 44 | C1 | 1448 | A |
| 44 | C1 | 1449 | U |
| 44 | C1 | 1450 | A |
| 44 | C1 | 1451 | G |
| 44 | C1 | 1452 | G |
| 44 | C1 | 1461 | G |
| 44 | C1 | 1469 | A |
| 44 | C1 | 1471 | U |
| 44 | C1 | 1479 | U |
| 44 | C1 | 1480 | G |
| 44 | C1 | 1481 | U |
| 44 | C1 | 1483 | A |
| 44 | C1 | 1484 | G |
| 44 | C1 | 1486 | G |
| 44 | C1 | 1489 | G |
| 44 | C1 | 1491 | A |
| 44 | C1 | 1497 | U |
| 44 | C1 | 1498 | G |
| 44 | C1 | 1499 | G |
| 44 | C1 | 1507 | G |
| 44 | C1 | 1516 | C |
| 44 | C1 | 1517 | A |
| 44 | C1 | 1518 | A |
| 44 | C1 | 1519 | C |
| 44 | C1 | 1520 | U |
| 44 | C1 | 1525 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 1527 | G |
| 44 | C1 | 1529 | A |
| 44 | C1 | 1536 | A |
| 44 | C1 | 1545 | U |
| 44 | C1 | 1546 | U |
| 44 | C1 | 1547 | C |
| 44 | C1 | 1549 | U |
| 44 | C1 | 1551 | A |
| 44 | C1 | 1554 | C |
| 44 | C1 | 1555 | A |
| 44 | C1 | 1624 | A |
| 44 | C1 | 1625 | G |
| 44 | C1 | 1628 | A |
| 44 | C1 | 1635 | G |
| 44 | C1 | 1636 | G |
| 44 | C1 | 1637 | C |
| 44 | C1 | 1638 | G |
| 44 | C1 | 1639 | U |
| 44 | C1 | 1642 | A |
| 44 | C1 | 1643 | U |
| 44 | C1 | 1644 | U |
| 44 | C1 | 1645 | U |
| 44 | C1 | 1656 | C |
| 44 | C1 | 1657 | G |
| 44 | C1 | 1665 | A |
| 44 | C1 | 1667 | G |
| 44 | C1 | 1668 | A |
| 44 | C1 | 1670 | A |
| 44 | C1 | 1673 | U |
| 44 | C1 | 1675 | A |
| 44 | C1 | 1676 | A |
| 44 | C1 | 1677 | A |
| 44 | C1 | 1678 | A |
| 44 | C1 | 1699 | U |
| 44 | C1 | 1700 | A |
| 44 | C1 | 1701 | U |
| 44 | C1 | 1703 | G |
| 44 | C1 | 1710 | G |
| 44 | C1 | 1711 | G |
| 44 | C1 | 1712 | C |
| 44 | C1 | 1713 | U |
| 44 | C1 | 1729 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 1730 | G |
| 44 | C1 | 1735 | A |
| 44 | C1 | 1740 | C |
| 44 | C1 | 1742 | C |
| 44 | C1 | 1743 | C |
| 44 | C1 | 1744 | A |
| 44 | C1 | 1748 | G |
| 44 | C1 | 1751 | G |
| 44 | C1 | 2047 | G |
| 44 | C1 | 2048 | C |
| 44 | C1 | 2054 | A |
| 44 | C1 | 2055 | C |
| 44 | C1 | 2056 | U |
| 44 | C1 | 2057 | G |
| 44 | C1 | 2061 | G |
| 44 | C1 | 2070 | A |
| 44 | C1 | 2071 | G |
| 44 | C1 | 2073 | A |
| 44 | C1 | 2074 | C |
| 44 | C1 | 2075 | U |
| 44 | C1 | 2076 | C |
| 44 | C1 | 2077 | C |
| 44 | C1 | 2078 | C |
| 44 | C1 | 2085 | G |
| 44 | C1 | 2086 | A |
| 44 | C1 | 2087 | G |
| 44 | C1 | 2088 | A |
| 44 | C1 | 2107 | A |
| 44 | C1 | 2109 | A |
| 44 | C1 | 2115 | U |
| 44 | C1 | 2118 | U |
| 44 | C1 | 2120 | C |
| 44 | C1 | 2121 | U |
| 44 | C1 | 2156 | A |
| 44 | C1 | 2157 | G |
| 44 | C1 | 2158 | G |
| 44 | C1 | 2162 | C |
| 44 | C1 | 2167 | G |
| 44 | C1 | 2173 | G |
| 44 | C1 | 2177 | G |
| 44 | C1 | 2178 | U |
| 44 | C1 | 2179 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 2183 | A |
| 44 | C1 | 2184 | G |
| 44 | C1 | 2185 | C |
| 44 | C1 | 2197 | A |
| 44 | C1 | 2201 | C |
| 44 | C1 | 2202 | C |
| 44 | C1 | 2205 | G |
| 44 | C1 | 2210 | U |
| 44 | C1 | 2211 | U |
| 44 | C1 | 2212 | G |
| 44 | C1 | 2213 | U |
| 44 | C1 | 2214 | A |
| 44 | C1 | 2215 | C |
| 44 | C1 | 2217 | C |
| 44 | C1 | 2220 | C |
| 44 | C1 | 2222 | C |
| 44 | C1 | 2223 | C |
| 44 | C1 | 2227 | C |
| 44 | C1 | 2328 | G |
| 44 | C1 | 2329 | A |
| 44 | C1 | 2330 | G |
| 44 | C1 | 2351 | G |
| 44 | C1 | 2352 | U |
| 44 | C1 | 2362 | U |
| 44 | C1 | 2363 | G |
| 44 | C1 | 2364 | A |
| 44 | C1 | 2365 | A |
| 44 | C1 | 2366 | C |
| 44 | C1 | 2374 | G |
| 45 | C2 | 2 | G |
| 45 | C2 | 6 | C |
| 45 | C2 | 8 | A |
| 45 | C2 | 9 | U |
| 45 | C2 | 10 | A |
| 45 | C2 | 15 | A |
| 45 | C2 | 23 | A |
| 45 | C2 | 24 | U |
| 45 | C2 | 29 | A |
| 45 | C2 | 30 | U |
| 45 | C2 | 32 | G |
| 45 | C2 | 33 | U |
| 45 | C2 | 36 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | C2 | 37 | U |
| 45 | C2 | 39 | U |
| 45 | C2 | 40 | C |
| 45 | C2 | 43 | C |
| 45 | C2 | 47 | U |
| 45 | C2 | 48 | G |
| 45 | C2 | 57 | A |
| 45 | C2 | 58 | A |
| 45 | C2 | 61 | G |
| 45 | C2 | 62 | A |
| 45 | C2 | 63 | G |
| 45 | C2 | 64 | C |
| 45 | C2 | 70 | A |
| 45 | C2 | 81 | G |
| 45 | C2 | 82 | U |
| 45 | C2 | 84 | G |
| 45 | C2 | 90 | C |
| 45 | C2 | 91 | G |
| 45 | C2 | 92 | A |
| 45 | C2 | 94 | A |
| 45 | C2 | 95 | U |
| 45 | C2 | 100 | G |
| 45 | C2 | 104 | C |
| 45 | C2 | 105 | C |
| 45 | C2 | 111 | G |
| 45 | C2 | 124 | U |
| 45 | C2 | 125 | U |
| 45 | C2 | 126 | U |
| 45 | C2 | 127 | A |
| 45 | C2 | 128 | C |
| 45 | C2 | 136 | C |
| 45 | C2 | 140 | C |
| 45 | C2 | 142 | G |
| 45 | C2 | 145 | A |
| 45 | C2 | 147 | G |
| 45 | C2 | 148 | G |
| 45 | C2 | 153 | G |
| 45 | C2 | 156 | C |
| 45 | C2 | 160 | U |
| 45 | C2 | 162 | C |
| 45 | C2 | 163 | C |
| 45 | C2 | 164 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | C2 | 165 | C |
| 45 | C2 | 166 | G |
| 45 | C2 | 167 | U |
| 45 | C2 | 168 | C |
| 45 | C2 | 170 | C |
| 45 | C2 | 174 | G |
| 45 | C2 | 178 | U |
| 45 | C2 | 179 | A |
| 45 | C2 | 181 | A |
| 45 | C2 | 182 | G |
| 45 | C2 | 187 | U |
| 45 | C2 | 189 | G |
| 45 | C2 | 190 | C |
| 45 | C2 | 193 | U |
| 45 | C2 | 198 | U |
| 45 | C2 | 199 | G |
| 45 | C2 | 200 | U |
| 45 | C2 | 201 | A |
| 45 | C2 | 244 | G |
| 45 | C2 | 247 | G |
| 45 | C2 | 250 | G |
| 45 | C2 | 255 | U |
| 45 | C2 | 256 | G |
| 45 | C2 | 257 | G |
| 45 | C2 | 259 | A |
| 45 | C2 | 260 | G |
| 45 | C2 | 261 | U |
| 45 | C2 | 262 | C |
| 45 | C2 | 267 | C |

All (39) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 67 | G |
| 44 | C1 | 89 | G |
| 44 | C1 | 135 | A |
| 44 | C1 | 150 | C |
| 44 | C1 | 205 | C |
| 44 | C1 | 207 | U |
| 44 | C1 | 209 | A |
| 44 | C1 | 259 | U |
| 44 | C1 | 260 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | C1 | 277 | U |
| 44 | C1 | 281 | U |
| 44 | C1 | 401 | C |
| 44 | C1 | 424 | U |
| 44 | C1 | 582 | G |
| 44 | C1 | 593 | G |
| 44 | C1 | 1068 | C |
| 44 | C1 | 1077 | U |
| 44 | C1 | 1085 | U |
| 44 | C1 | 1087 | G |
| 44 | C1 | 1163 | A |
| 44 | C1 | 1485 | A |
| 44 | C1 | 1638 | G |
| 44 | C1 | 1712 | C |
| 44 | C1 | 1734 | G |
| 44 | C1 | 2054 | A |
| 44 | C1 | 2070 | A |
| 44 | C1 | 2077 | C |
| 44 | C1 | 2156 | A |
| 44 | C1 | 2177 | G |
| 44 | C1 | 2214 | A |
| 44 | C1 | 2219 | C |
| 45 | C2 | 23 | A |
| 45 | C2 | 35 | G |
| 45 | C2 | 38 | G |
| 45 | C2 | 61 | G |
| 45 | C2 | 91 | G |
| 45 | C2 | 94 | A |
| 45 | C2 | 255 | U |
| 45 | C2 | 259 | A |

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 45 | C2 | 3 |
| 2 | UB | 1 |
| 48 | UH | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C2 | 206:G | O3' | 240:C | P | 18.53 |
| 1 | C2 | 105:C | O3' | 110:A | P | 15.27 |
| 1 | C2 | 119:C | O3' | 123:A | P | 11.89 |
| 1 | UB | 679:ASN | C | 680:PHE | N | 1.20 |
| 1 | UH | 730:PHE | C | 731:LYS | N | 1.18 |

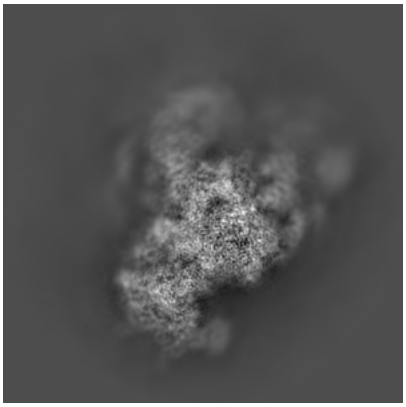
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10055. These allow visual inspection of the internal detail of the map and identification of artifacts.

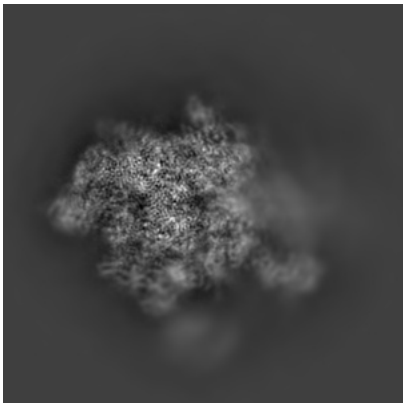
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

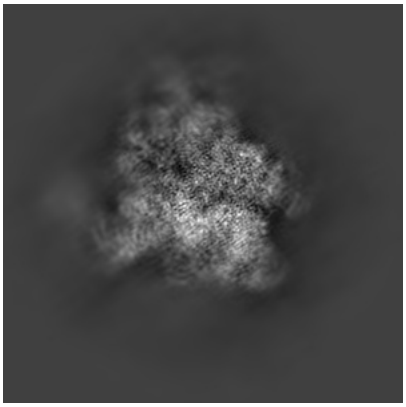
### 6.1.1 Primary map



X



Y

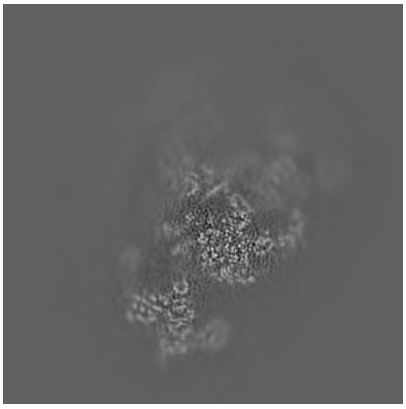


Z

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

## 6.2 Central slices

### 6.2.1 Primary map



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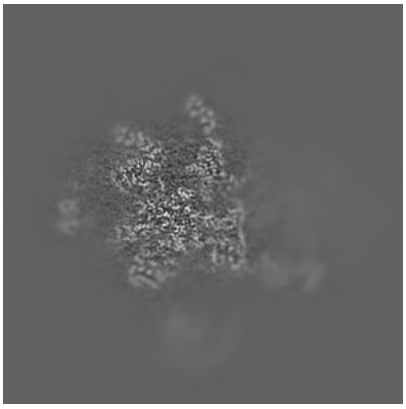
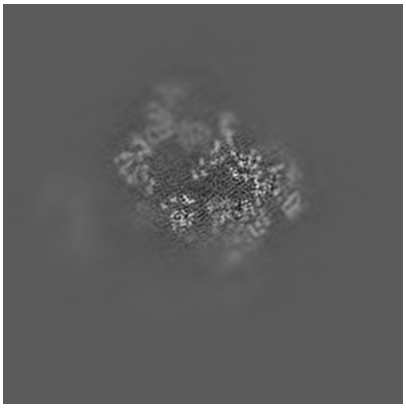


Y Index: 240

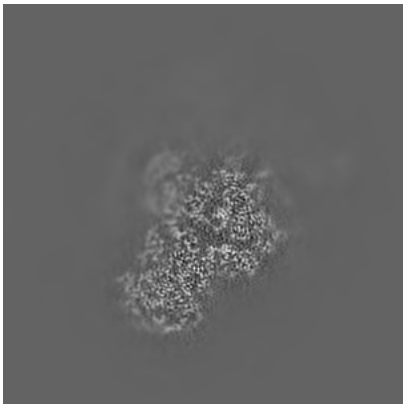


Z Index: 240

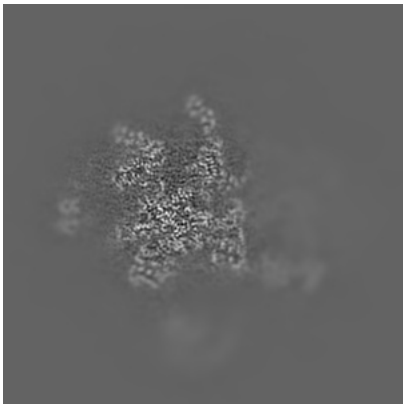
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

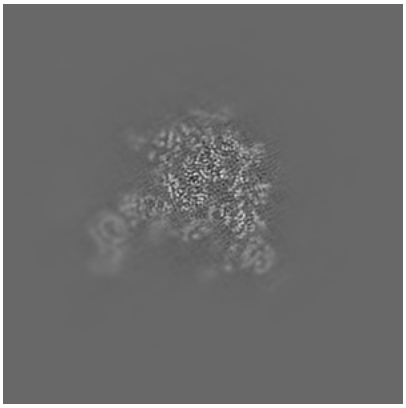
### 6.3.1 Primary map



X Index: 279



Y Index: 241

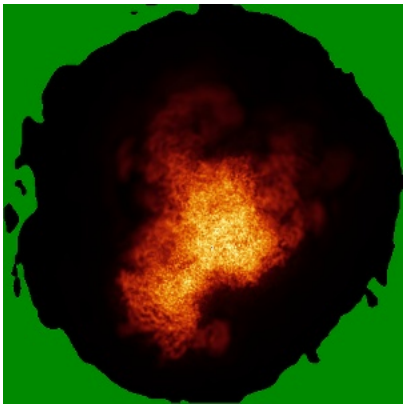


Z Index: 187

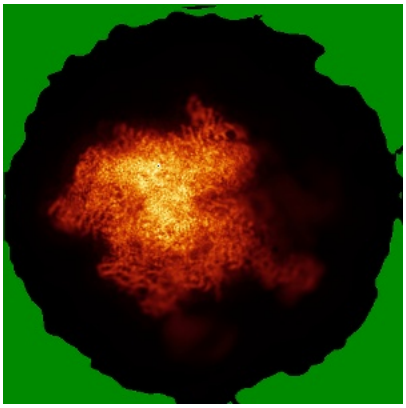
The images above show the largest variance slices of the map in three orthogonal directions.

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

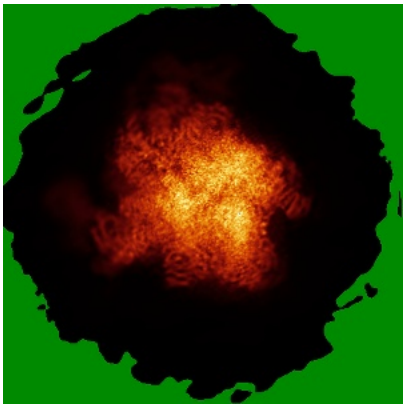
### 6.4.1 Primary map



X



Y



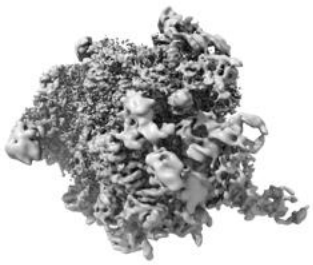
Z

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.

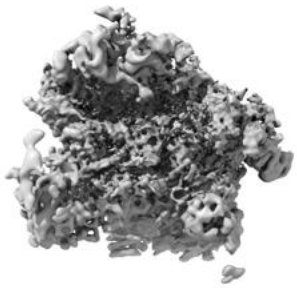
## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

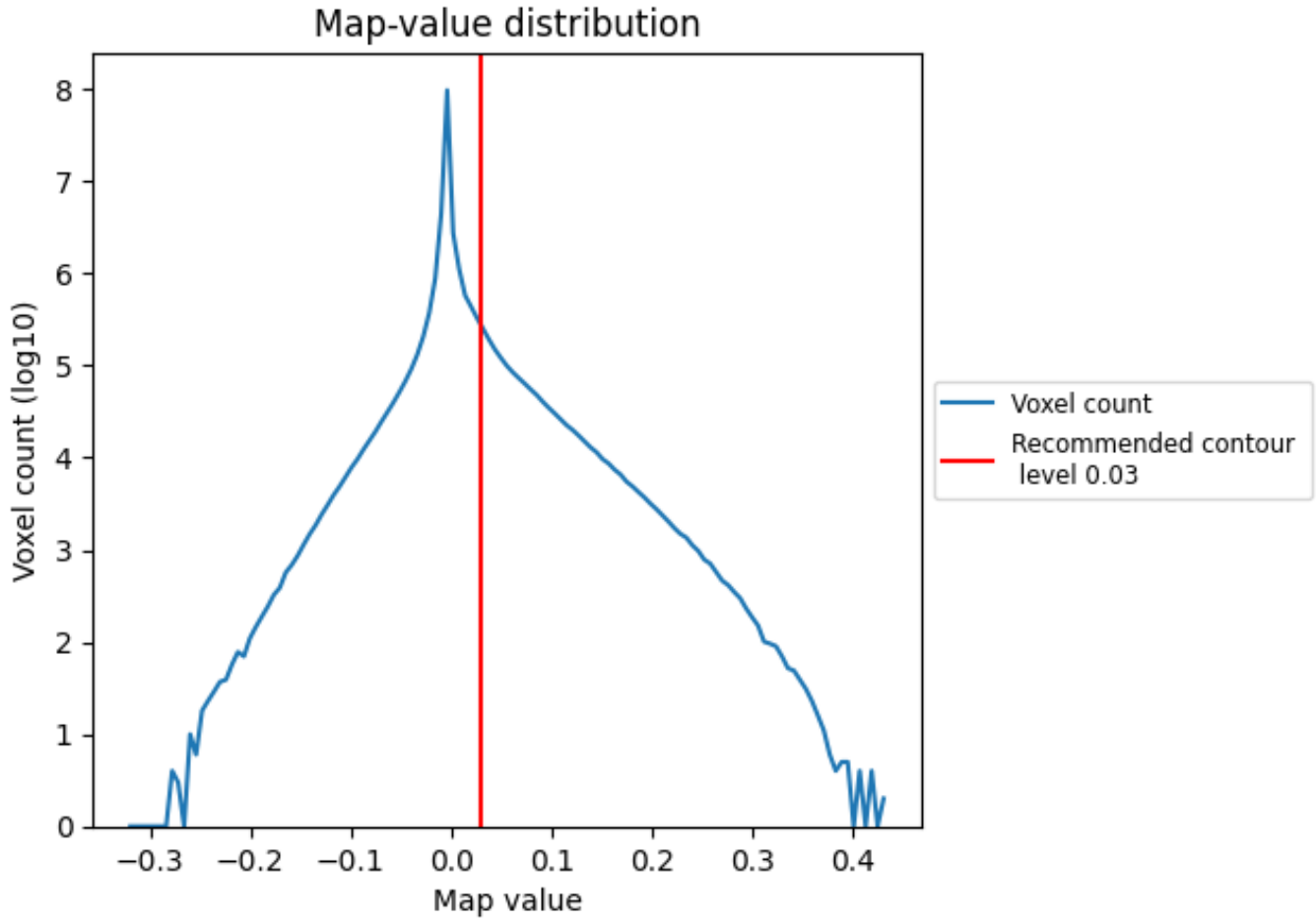
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

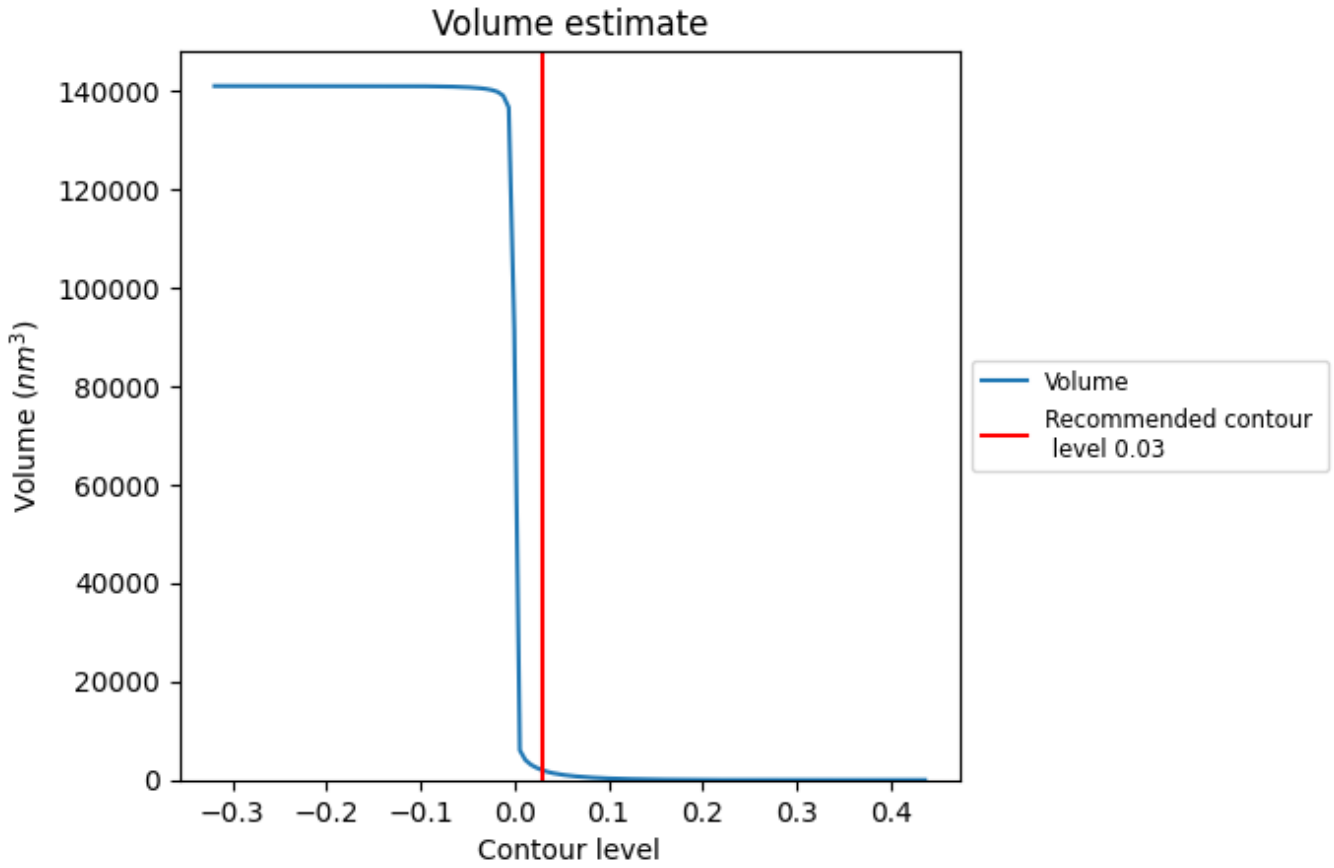
This section contains the results of statistical analysis of the map.

## 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.

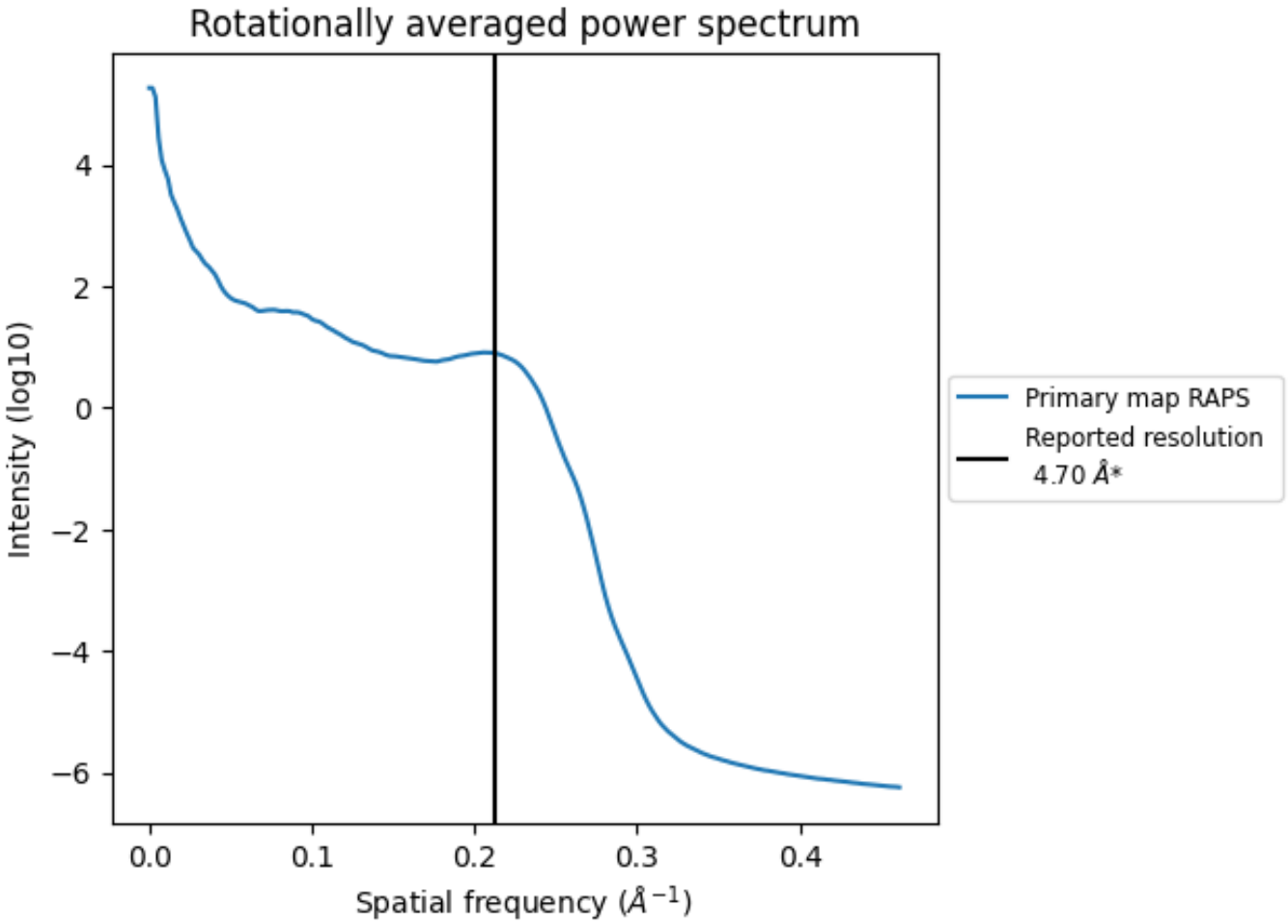
## 7.2 Volume estimate




The volume at the recommended contour level is 1965 $nm^3$; this corresponds to an approximate mass of 1775 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)

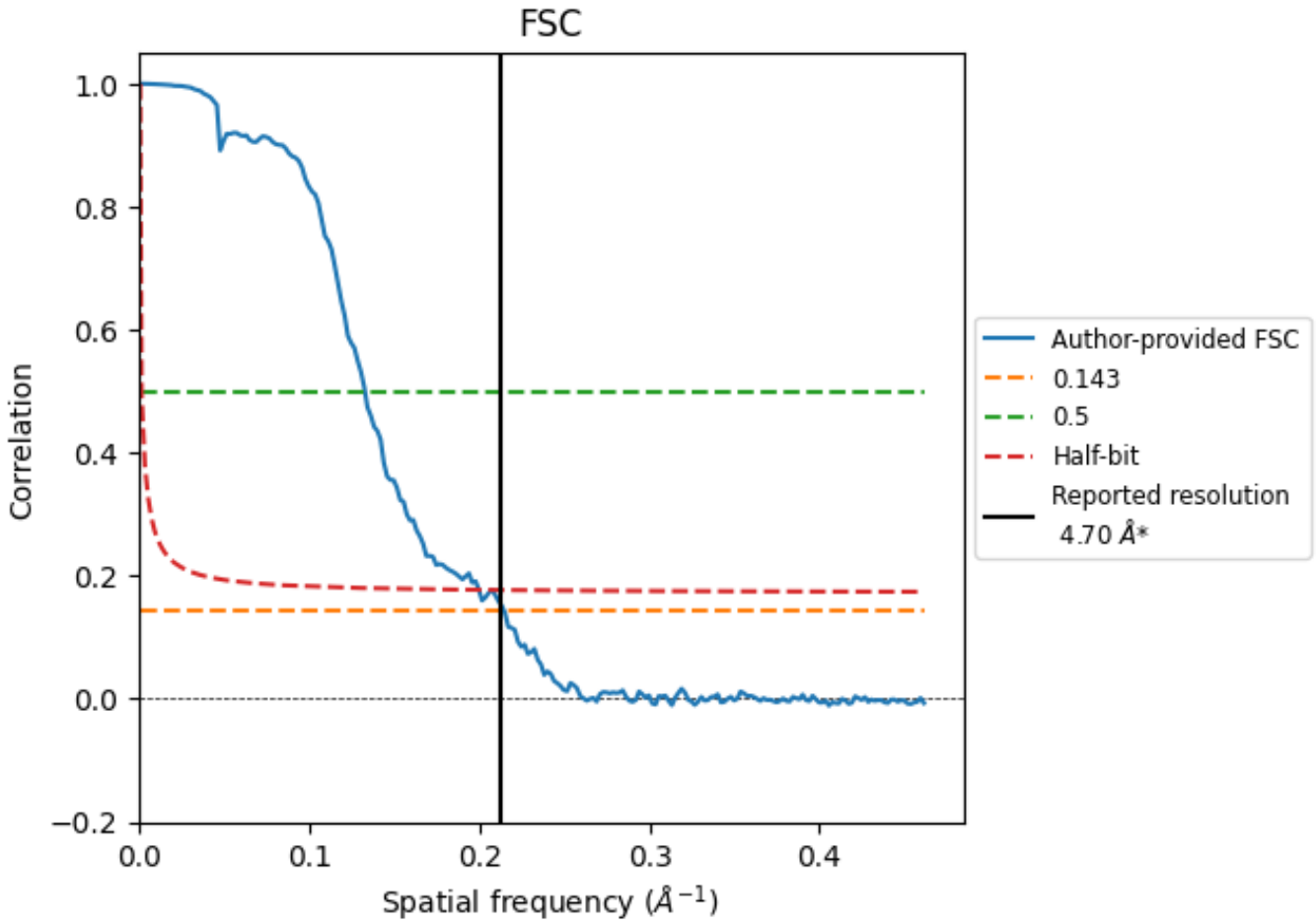



*Reported resolution corresponds to spatial frequency of 0.213 Å$^{-1}$

# 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 0.213 $Å^{-1}$

## 8.2 Resolution estimates (i)

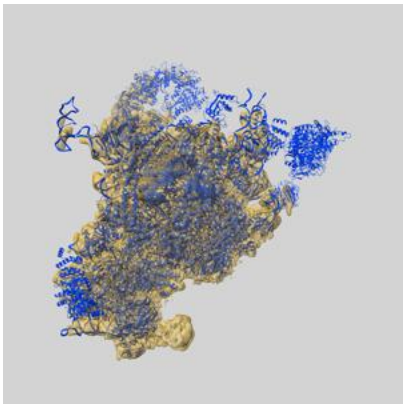
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.70 | - | - |
| Author-provided FSC curve | 4.66 | 7.52 | 5.00 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

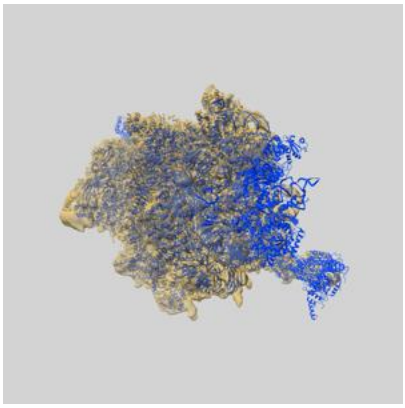
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10055 and PDB model 6RXY. Per-residue inclusion information can be found in section 3 on page 14.

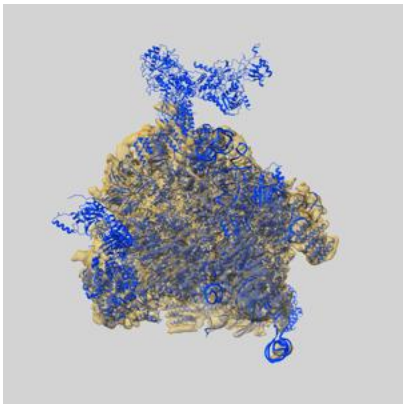
## 9.1 Map-model overlay



X



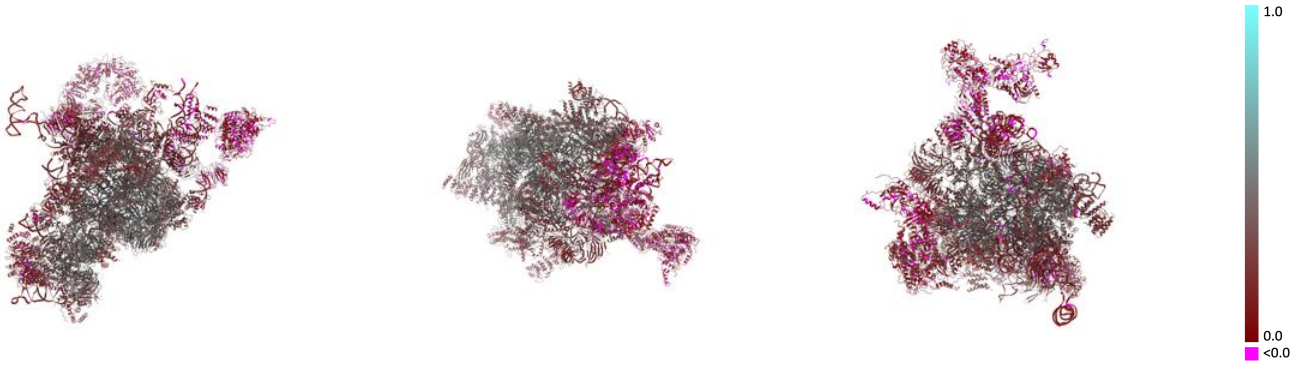
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

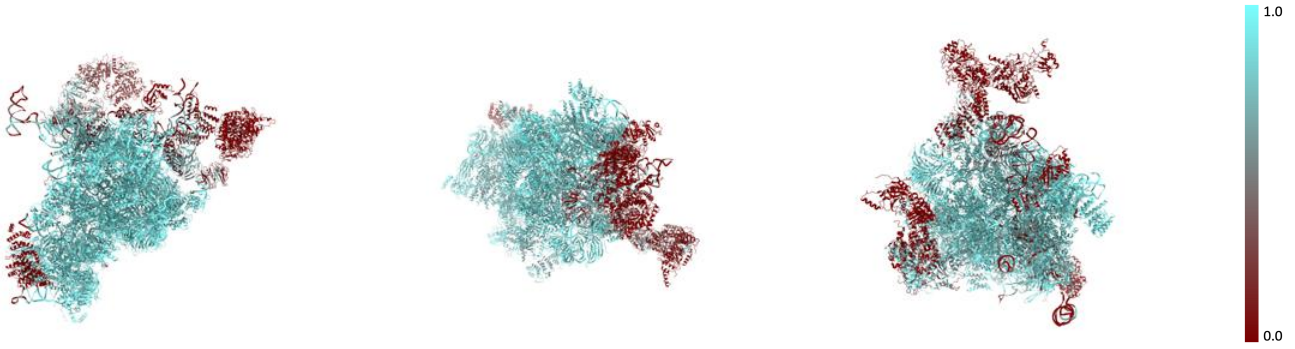
## 9.2 Q-score mapped to coordinate model (i)




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.

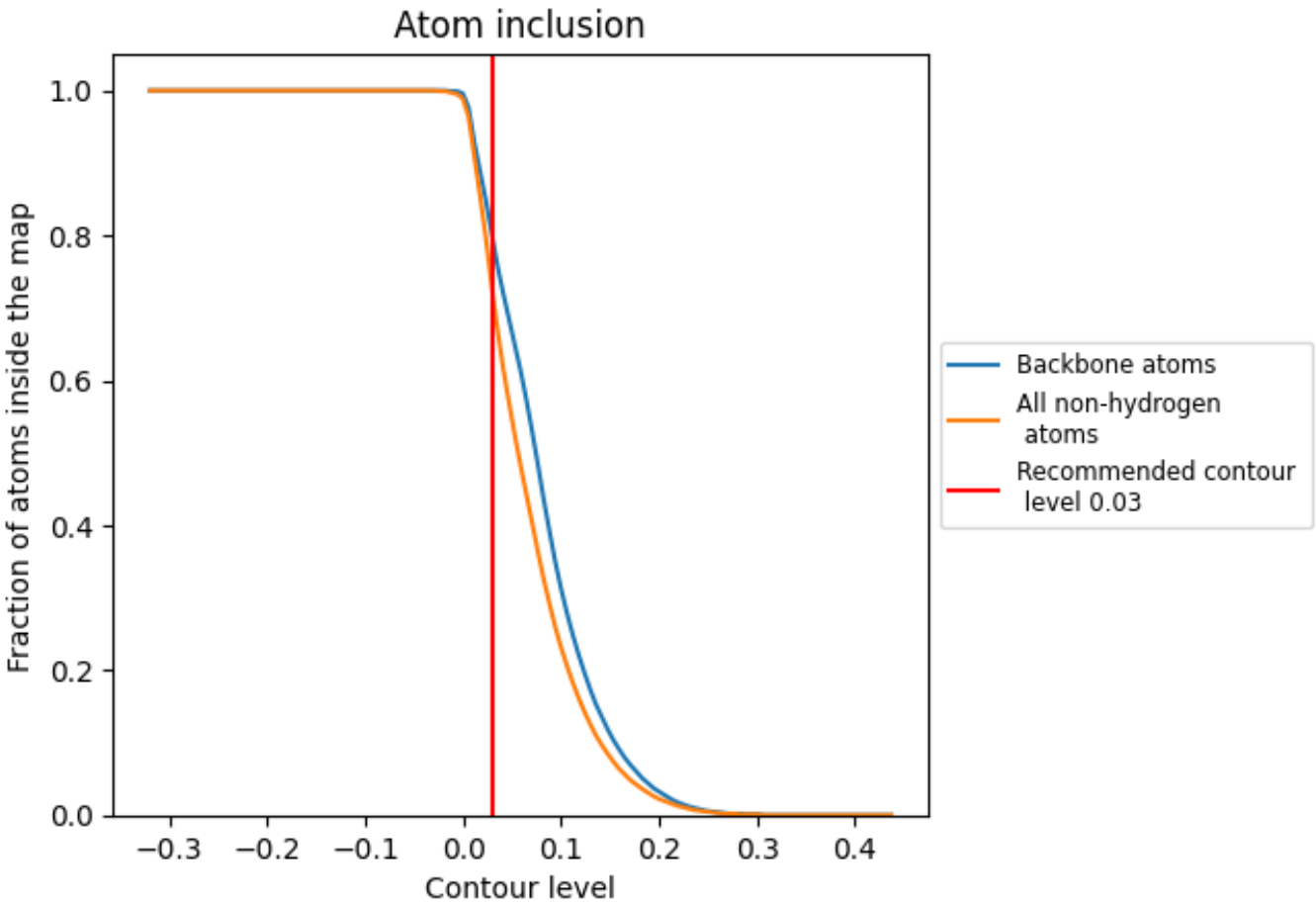
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.03).

## 9.4 Atom inclusion (i)




At the recommended contour level, 80% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

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

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7220 | 0.2860 |
| C1 | 0.8230 | 0.2910 |
| C2 | 0.7840 | 0.2890 |
| CA | 0.8910 | 0.4010 |
| CB | 0.7880 | 0.2650 |
| CC | 0.8330 | 0.2940 |
| CD | 0.8600 | 0.3010 |
| CE | 0.9210 | 0.4520 |
| CF | 0.6880 | 0.2260 |
| CG | 0.6170 | 0.1410 |
| CH | 0.8490 | 0.3060 |
| CI | 0.8290 | 0.3190 |
| CJ | 0.9340 | 0.4690 |
| CK | 0.9170 | 0.4410 |
| CL | 0.9010 | 0.3840 |
| CM | 0.9090 | 0.3920 |
| CN | 0.8400 | 0.3450 |
| CO | 0.7810 | 0.2220 |
| CP | 0.4010 | 0.1470 |
| CQ | 0.8350 | 0.2360 |
| CR | 0.4630 | 0.1440 |
| CS | 0.0680 | 0.0790 |
| CT | 0.8930 | 0.4100 |
| CU | 0.6210 | 0.2920 |
| CV | 0.0000 | 0.0470 |
| CX | 0.6830 | 0.1390 |
| Cc | 0.9180 | 0.4140 |
| Ce | 0.0050 | 0.1440 |
| Cg | 0.4200 | 0.1990 |
| Ch | 0.1500 | 0.0740 |
| Ci | 0.4970 | 0.1250 |
| Cj | 0.9350 | 0.4730 |
| Cl | 0.6350 | 0.2730 |
| Cm | 0.2660 | 0.2370 |
| Cn | 0.8600 | 0.3770 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| Cp | 0.9150 | 0.4210 |
| Cz | 0.1530 | 0.1050 |
| UA | 0.9300 | 0.4450 |
| UB | 0.8650 | 0.2900 |
| UC | 0.7850 | 0.3260 |
| UD | 0.8940 | 0.3560 |
| UE | 0.8470 | 0.3050 |
| UF | 0.8890 | 0.2880 |
| UG | 0.9090 | 0.4320 |
| UH | 0.8530 | 0.2590 |
| UI | 0.7400 | 0.1610 |
| UJ | 0.4900 | 0.2670 |
| UK | 0.9130 | 0.4090 |
| UL | 0.8620 | 0.2650 |
| UM | 0.5660 | 0.1270 |
| UN | 0.8970 | 0.3630 |
| UO | 0.9160 | 0.4160 |
| UP | 0.8970 | 0.3780 |
| UQ | 0.9150 | 0.3900 |
| UR | 0.9330 | 0.4440 |
| US | 0.8450 | 0.2750 |
| UU | 0.9310 | 0.4210 |
| UV | 0.0000 | 0.0550 |
| UX | 0.8750 | 0.3830 |
| UZ | 0.8520 | 0.3060 |