



Full wwPDB EM Validation Report ⓘ

Nov 26, 2022 – 11:56 AM EST

PDB ID : 7SUK
EMDB ID : EMD-25441
Title : Structure of Bfr2-Lcp5 Complex Observed in the Small Subunit Processome
Isolated from R2TP-depleted Yeast Cells
Authors : Rai, J.; Zhao, Y.; Li, H.
Deposited on : 2021-11-17
Resolution : 3.99 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

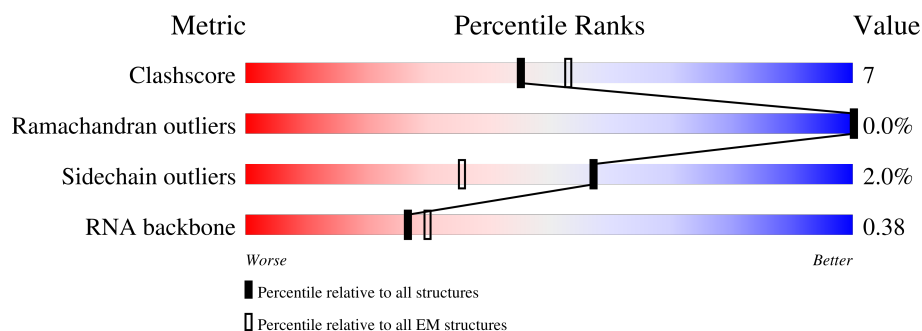
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.99 Å.

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









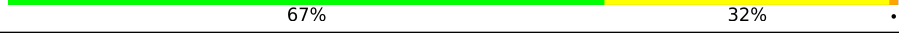
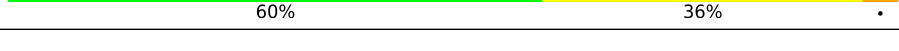
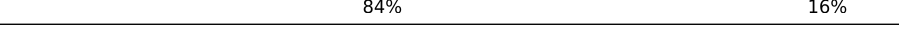
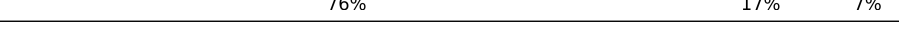
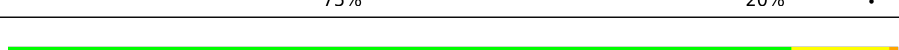

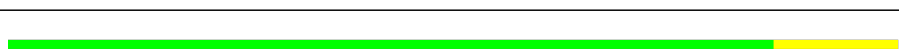

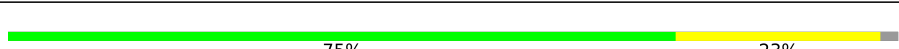





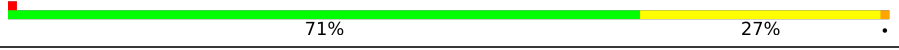
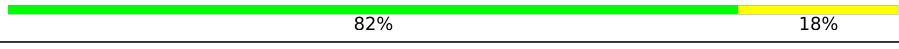

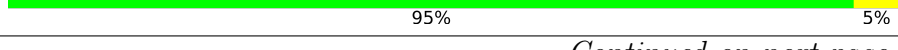

| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | NA | 245 | |
| 2 | SA | 413 | |
| 3 | NB | 180 | |
| 4 | L0 | 700 | |
| 5 | L2 | 333 | |
| 6 | L3 | 127 | |
| 7 | L4 | 228 | |

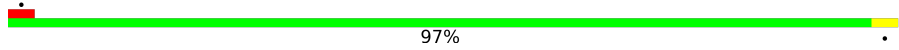

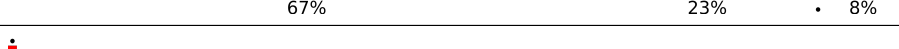
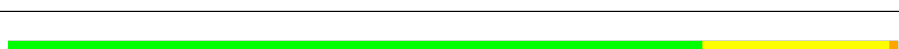



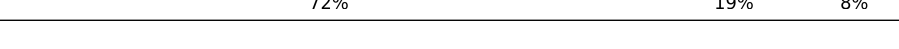



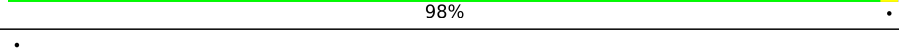

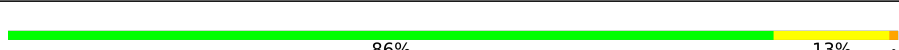


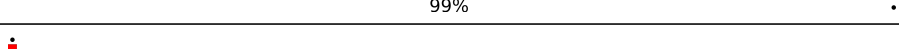







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | L5 | 213 |  |
| 9 | L7 | 190 |  |
| 10 | L8 | 200 |  |
| 11 | L9 | 175 |  |
| 12 | LC | 125 |  |
| 13 | LD | 156 |  |
| 14 | LE | 127 |  |
| 15 | LF | 90 |  |
| 16 | LG | 63 |  |
| 17 | LH | 896 |  |
| 18 | LJ | 513 |  |
| 19 | LK | 123 |  |
| 20 | LL | 555 |  |
| 21 | LM | 431 |  |
| 22 | LN | 748 |  |
| 23 | LO | 855 |  |
| 24 | LP | 420 |  |
| 25 | LQ | 939 |  |
| 26 | LS | 594 |  |
| 27 | LT | 921 |  |
| 28 | LU | 465 |  |
| 29 | LV | 362 |  |
| 30 | LW | 438 |  |
| 31 | LZ | 182 |  |
| 32 | NG | 111 |  |


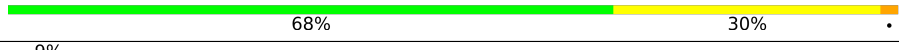
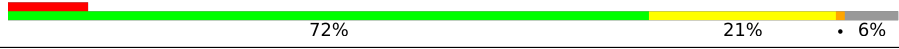


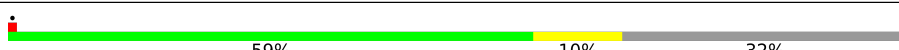
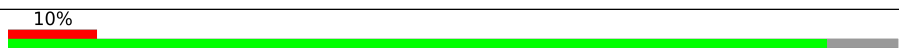
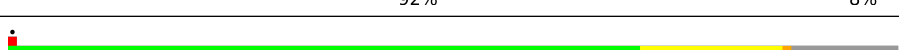
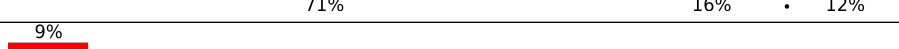
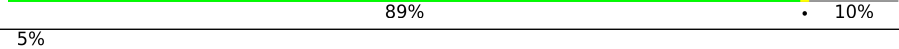

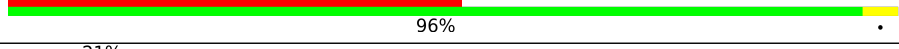
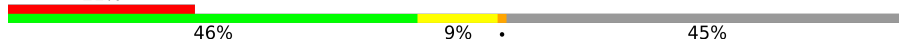
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 33 | NK | 175 |  |
| 34 | SC | 247 |  |
| 34 | SD | 247 |  |
| 35 | SE | 121 |  |
| 35 | SF | 121 |  |
| 36 | SG | 464 |  |
| 37 | SH | 360 |  |
| 38 | SI | 1123 |  |
| 39 | SJ | 236 |  |
| 39 | SK | 236 |  |
| 40 | SL | 183 |  |
| 41 | SM | 290 |  |
| 42 | SN | 247 |  |
| 43 | SO | 179 |  |
| 44 | SQ | 167 |  |
| 45 | SR | 104 |  |
| 46 | SS | 197 |  |
| 47 | ST | 806 |  |
| 48 | SY | 248 |  |
| 49 | SZ | 261 |  |
| 50 | NJ | 265 |  |
| 51 | NH | 1141 |  |
| 52 | NI | 187 |  |
| 53 | 8 | 1807 |  |
| 54 | SU | 513 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 55 | LI | 687 |  |
| 56 | ND | 60 |  |
| 57 | LR | 811 |  |
| 58 | NE | 240 |  |
| 59 | SB | 436 |  |
| 60 | SV | 92 |  |
| 61 | SP | 2418 |  |
| 62 | LX | 923 |  |
| 62 | LY | 923 |  |
| 63 | L6 | 219 |  |
| 64 | NF | 124 |  |
| 65 | 5 | 534 |  |
| 66 | 6 | 357 |  |

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 213241 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 U3 small nucleolar RNA-associated protein MPP10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | NA | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1034 | 297 | 332 | 4 | | |

- Molecule 2 is a protein called Nucleolar protein 56.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | SA | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2854 | 1815 | 490 | 541 | 8 | | |

- Molecule 3 is a protein called Something about silencing protein 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 3 | NB | 142 | Total | C | N | O | | 0 | 0 |
| | | | 1098 | 677 | 218 | 203 | | | |

- Molecule 4 is a RNA chain called 5' ETS.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 4 | L0 | 488 | Total | C | N | O | P | 0 | 0 |
| | | | 10405 | 4650 | 1838 | 3429 | 488 | | |

- Molecule 5 is a RNA chain called U3 snoRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5 | L2 | 169 | Total | C | N | O | P | 0 | 0 |
| | | | 3585 | 1605 | 629 | 1182 | 169 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|--------------|
| L2 | 200 | C | G | conflict | GB 751247007 |

- Molecule 6 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | L3 | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 901 | 569 | 168 | 162 | 2 | | |

- Molecule 7 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | L4 | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1810 | 1158 | 330 | 319 | 3 | | |

- Molecule 8 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | L5 | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1669 | 1045 | 307 | 314 | 3 | | |

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | L7 | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1321 | 854 | 227 | 240 | | | |

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | L8 | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1349 | 839 | 267 | 241 | 2 | | |

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | L9 | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1415 | 895 | 273 | 246 | 1 | | |

- Molecule 12 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | LC | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 973 | 625 | 174 | 174 | | | |

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | LD | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1027 | 660 | 194 | 170 | 3 | | |

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | LE | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1003 | 640 | 183 | 177 | 3 | | |

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | LF | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 715 | 458 | 131 | 126 | | | |

- Molecule 16 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16 | LG | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | |

- Molecule 17 is a protein called NET1-associated nuclear protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 17 | LH | 834 | Total | C | N | O | S | 0 | 0 |
| | | | 6633 | 4215 | 1121 | 1278 | 19 | | |

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18 | LJ | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3911 | 2462 | 702 | 735 | 12 | | |

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | LK | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 898 | 567 | 166 | 163 | 2 | | |

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | LL | 475 | Total | C | N | O | S | 0 | 0 |
| | | | 3772 | 2400 | 649 | 710 | 13 | | |

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21 | LM | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3443 | 2224 | 566 | 641 | 12 | | |

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 22 | LN | 678 | Total | C | N | O | S | 0 | 0 |
| | | | 5344 | 3384 | 930 | 1009 | 21 | | |

- Molecule 23 is a protein called Periodic tryptophan protein 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 23 | LO | 834 | Total | C | N | O | S | 0 | 0 |
| | | | 6635 | 4223 | 1140 | 1253 | 19 | | |

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24 | LP | 359 | Total | C | N | O | S | 0 | 0 |
| | | | 2709 | 1723 | 486 | 488 | 12 | | |

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 25 | LQ | 848 | Total | C | N | O | S | 0 | 0 |
| | | | 6640 | 4244 | 1116 | 1253 | 27 | | |

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26 | LS | 481 | Total | C | N | O | S | 0 | 0 |
| | | | 3791 | 2399 | 668 | 714 | 10 | | |

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 27 | LT | 850 | Total | C | N | O | S | 0 | 0 |
| | | | 6697 | 4253 | 1154 | 1269 | 21 | | |

- Molecule 28 is a protein called Protein SOF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28 | LU | 457 | Total | C | N | O | S | 0 | 0 |
| | | | 3725 | 2328 | 679 | 702 | 16 | | |

- Molecule 29 is a protein called Ribosome biogenesis protein ENP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29 | LV | 362 | Total | C | N | O | S | 0 | 0 |
| | | | 2840 | 1789 | 487 | 555 | 9 | | |

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30 | LW | 438 | Total | C | N | O | S | 0 | 0 |
| | | | 3428 | 2163 | 601 | 652 | 12 | | |

- Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | LZ | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1530 | 967 | 287 | 269 | 7 | | |

- Molecule 32 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 32 | NG | 111 | Total | C | N | O | | 0 | 0 |
| | | | 543 | 321 | 111 | 111 | | | |

- Molecule 33 is a protein called KRR1 small subunit processome component.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 33 | NK | 175 | Total | C | N | O | | 0 | 0 |
| | | | 868 | 518 | 175 | 175 | | | |

- Molecule 34 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34 | SC | 242 | Total | C | N | O | S | 0 | 0 |
| | | | 1881 | 1193 | 338 | 340 | 10 | | |
| 34 | SD | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1782 | 1131 | 320 | 321 | 10 | | |

- Molecule 35 is a protein called Ribonucloprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | SE | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 916 | 583 | 158 | 171 | 4 | | |
| 35 | SF | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 916 | 583 | 158 | 171 | 4 | | |

- Molecule 36 is a protein called RRP9 isoform 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36 | SG | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3428 | 2185 | 596 | 637 | 10 | | |

- Molecule 37 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37 | SH | 360 | Total | C | N | O | S | 0 | 0 |
| | | | 2781 | 1781 | 473 | 516 | 11 | | |

- Molecule 38 is a protein called Ribosome biogenesis protein BMS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 38 | SI | 802 | Total | C | N | O | S | 0 | 0 |
| | | | 6412 | 4108 | 1142 | 1133 | 29 | | |

- Molecule 39 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39 | SJ | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1701 | 1079 | 296 | 315 | 11 | | |
| 39 | SK | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1799 | 1142 | 313 | 333 | 11 | | |

- Molecule 40 is a protein called rRNA-processing protein FCF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 40 | SL | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1395 | 890 | 255 | 240 | 10 | | |

- Molecule 41 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41 | SM | 282 | Total | C | N | O | S | 0 | 0 |
| | | | 2296 | 1441 | 430 | 418 | 7 | | |

- Molecule 42 is a protein called Ribosome biogenesis protein UTP30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42 | SN | 247 | Total | C | N | O | S | 0 | 0 |
| | | | 2006 | 1284 | 356 | 358 | 8 | | |

- Molecule 43 is a protein called Pre-rRNA-processing protein PNO1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | SO | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 998 | 606 | 199 | 192 | 1 | | |

- Molecule 44 is a protein called rRNA-processing protein FCF2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | SQ | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1137 | 721 | 211 | 201 | 4 | | |

- Molecule 45 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | SR | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 792 | 506 | 145 | 139 | 2 | | |

- Molecule 46 is a protein called U3 small nucleolar RNA-associated protein 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | SS | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1466 | 905 | 282 | 277 | 2 | | |

- Molecule 47 is a protein called Nucleolar complex protein 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47 | ST | 599 | Total | C | N | O | S | 0 | 0 |
| | | | 4473 | 2830 | 809 | 823 | 11 | | |

- Molecule 48 is a protein called U3 small nucleolar RNA-associated protein 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48 | SY | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 2016 | 1251 | 388 | 370 | 7 | | |

- Molecule 49 is a protein called Essential nuclear protein 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 49 | SZ | 261 | Total | C | N | O | 0 | 0 |
| | | | 1295 | 773 | 261 | 261 | | |

- Molecule 50 is a protein called rRNA biogenesis protein RRP5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 50 | NJ | 265 | Total | C | N | O | 0 | 0 |
| | | | 1314 | 784 | 265 | 265 | | |

- Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 22.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 51 | NH | 1082 | Total | C | N | O | 0 | 0 |
| | | | 5362 | 3198 | 1082 | 1082 | | |

- Molecule 52 is a protein called Ribosomal RNA-processing protein 7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 52 | NI | 169 | Total | C | N | O | 0 | 0 |
| | | | 841 | 503 | 169 | 169 | | |

- Molecule 53 is a RNA chain called 18S pre-rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 53 | 8 | 1192 | Total | C | N | O | P | 0 | 0 |
| | | | 25439 | 11367 | 4542 | 8338 | 1192 | | |

- Molecule 54 is a protein called Nucleolar complex protein 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 54 | SU | 481 | Total | C | N | O | S | 0 | 0 |
| | | | 3650 | 2355 | 611 | 672 | 12 | | |

- Molecule 55 is a protein called U3 small nucleolar RNA-associated protein 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55 | LI | 441 | Total | C | N | O | S | 0 | 0 |
| | | | 2690 | 1672 | 492 | 523 | 3 | | |

- Molecule 56 is a protein called Bud site selection protein 21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|-------|
| 56 | ND | 60 | Total | C | N | O | | 0 | 0 |
| | | | 495 | 310 | 101 | 84 | | | |

- Molecule 57 is a protein called U3 small nucleolar RNA-associated protein 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 57 | LR | 762 | Total | C | N | O | S | 0 | 0 |
| | | | 5957 | 3779 | 1006 | 1144 | 28 | | |

- Molecule 58 is a protein called Protein FAF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58 | NE | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1235 | 759 | 252 | 221 | 3 | | |

- Molecule 59 is a protein called Nucleolar protein 58.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59 | SB | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 2985 | 1852 | 543 | 582 | 8 | | |

- Molecule 60 is a protein called Regulator of rDNA transcription protein 14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 60 | SV | 63 | Total | C | N | O | | 0 | 0 |
| | | | 381 | 234 | 69 | 78 | | | |

- Molecule 61 is a protein called U3 small nucleolar RNA-associated protein 20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 61 | SP | 2234 | Total | C | N | O | 0 | 0 |
| | | | 11108 | 6640 | 2234 | 2234 | | |

- Molecule 62 is a protein called RNA cytidine acetyltransferase.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|-----|-------|----------|-------|------|------|------|---------|-------|---|
| 62 | LY | 835 | Total | C | N | O | 0 | 0 | |
| | | | 4132 | 2462 | 835 | 835 | | | |
| 62 | LX | 812 | Total | C | N | O | S | 0 | 0 |
| | | | 5892 | 3727 | 1041 | 1099 | 25 | | |

- Molecule 63 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63 | L6 | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1327 | 834 | 256 | 235 | 2 | | |

- Molecule 64 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 64 | NF | 124 | Total | C | N | O | 0 | 0 |
| | | | 614 | 367 | 123 | 124 | | |

- Molecule 65 is a protein called Protein BFR2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65 | 5 | 296 | Total | C | N | O | S | 0 | 0 |
| | | | 2389 | 1496 | 422 | 467 | 4 | | |

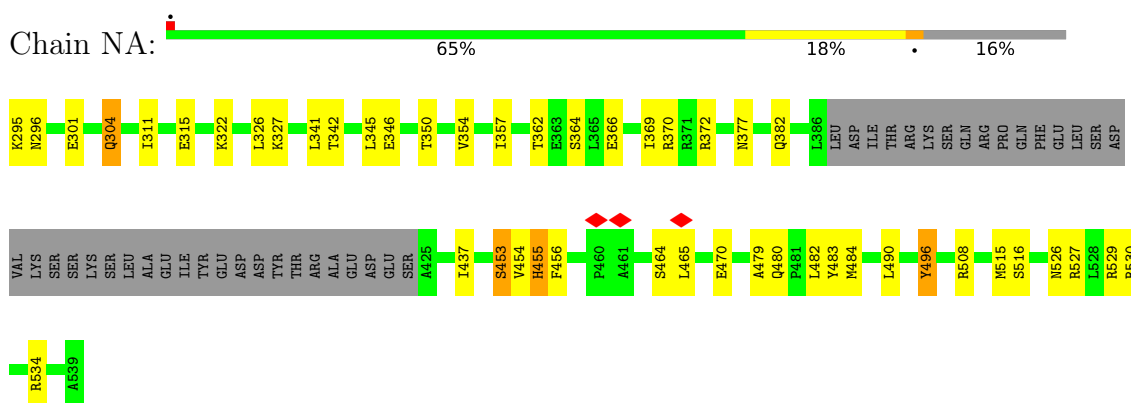
- Molecule 66 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 66 | 6 | 277 | Total | C | N | O | S | 0 | 0 |
| | | | 2244 | 1371 | 426 | 438 | 9 | | |

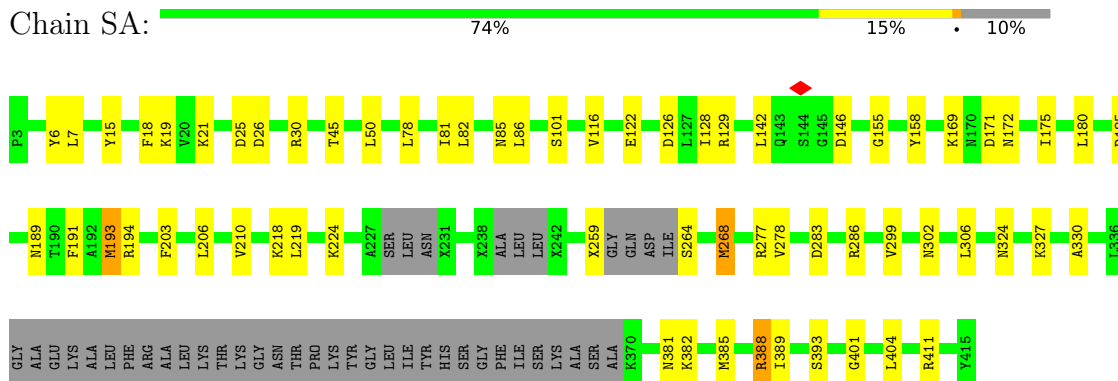
3 Residue-property plots

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

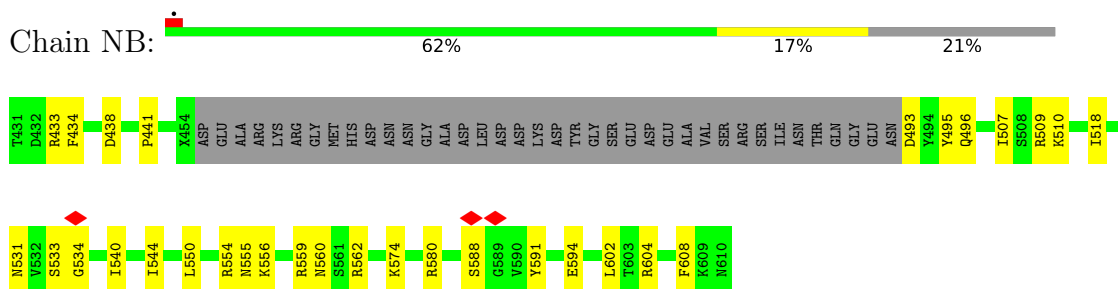
- Molecule 1: U3 small nucleolar RNA-associated protein MPP10



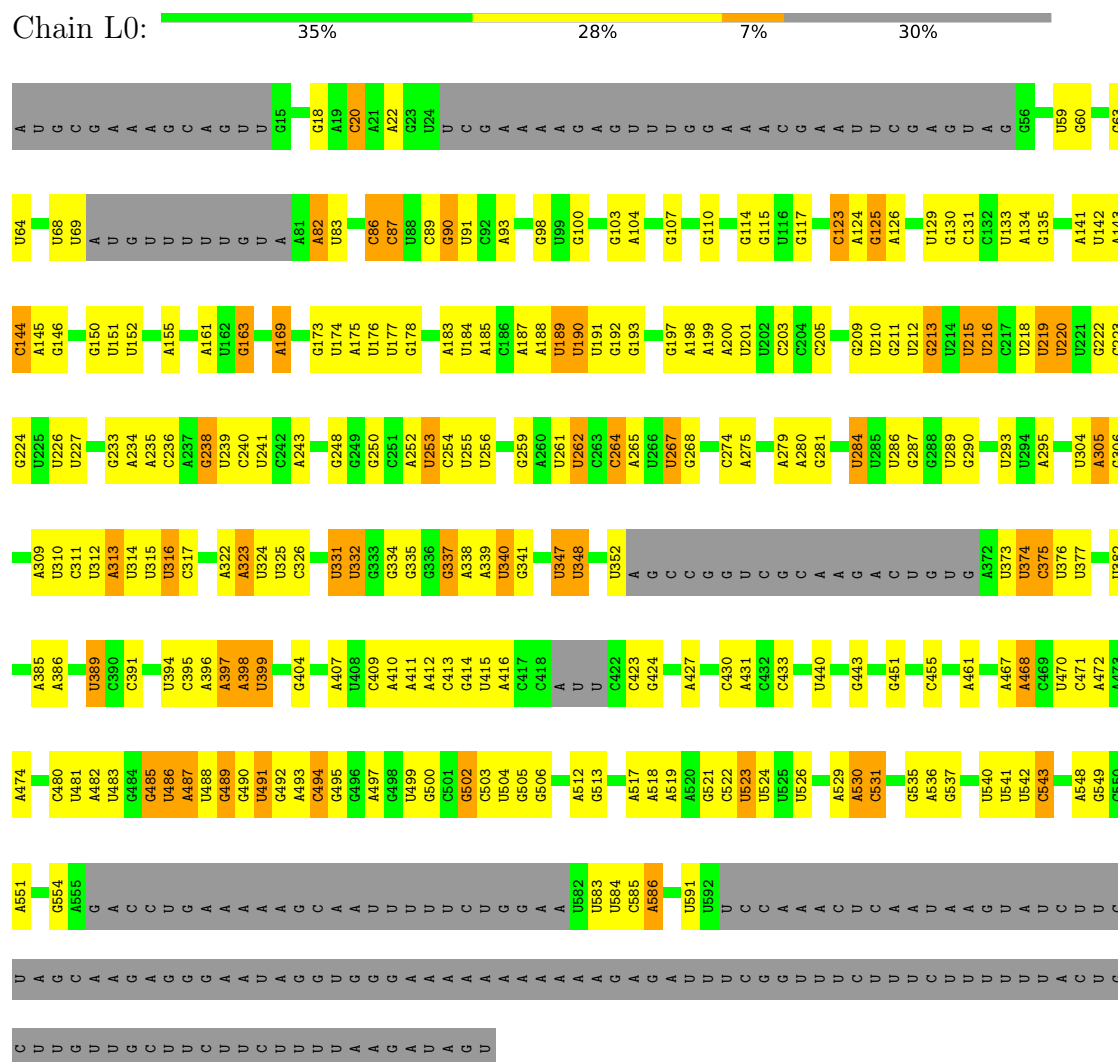
- Molecule 2: Nucleolar protein 56



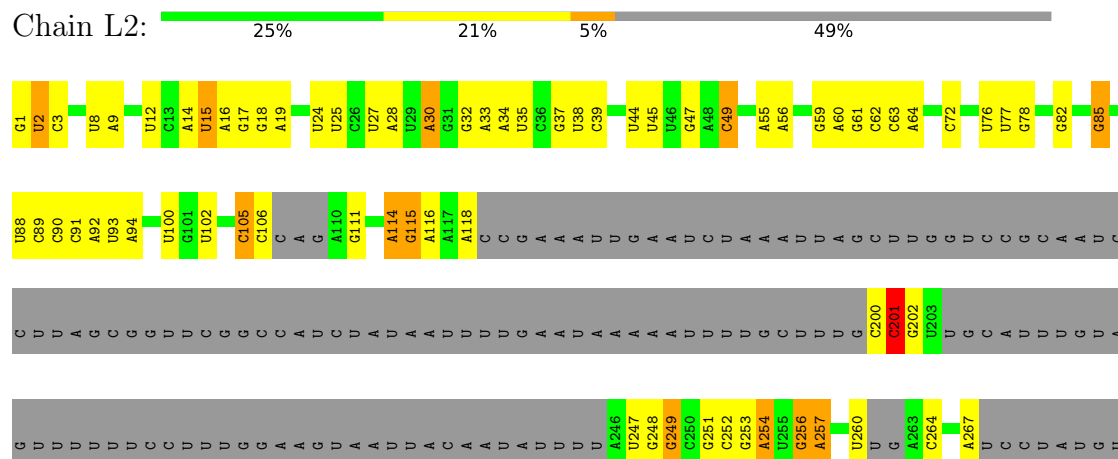
- Molecule 3: Something about silencing protein 10



• Molecule 4: 5' ETS

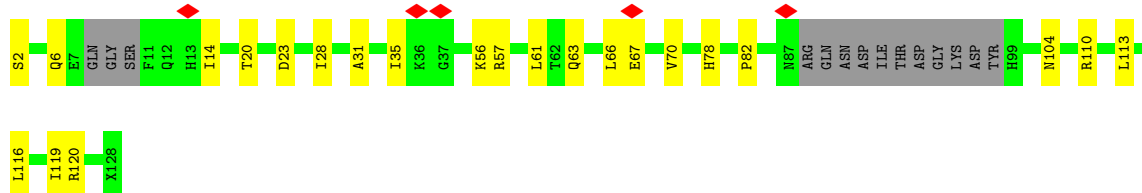


• Molecule 5: U3 snoRNA

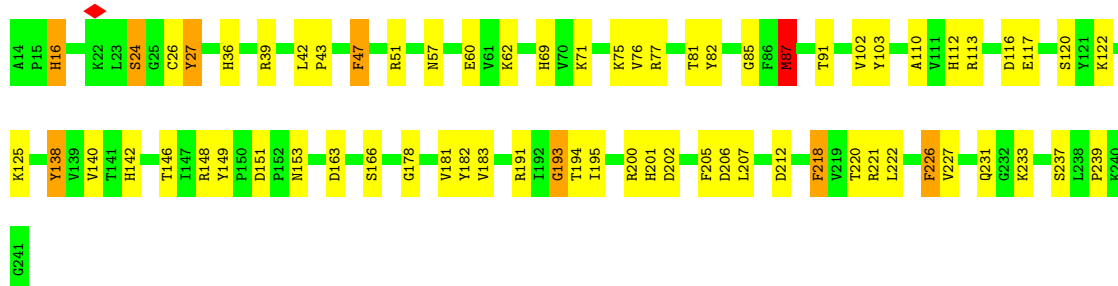




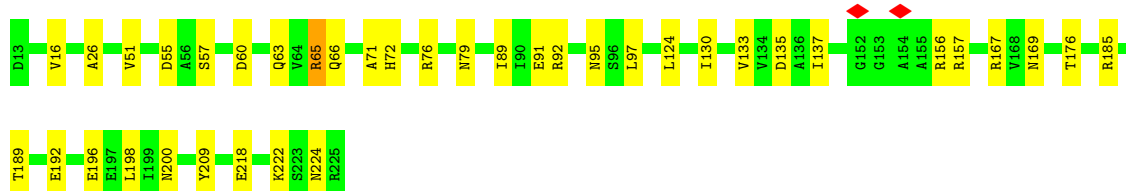
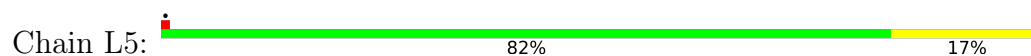
• Molecule 6: 40S ribosomal protein S18-A



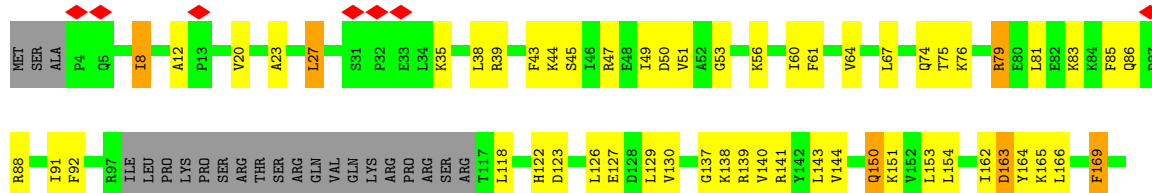
• Molecule 7: 40S ribosomal protein S4-A



• Molecule 8: 40S ribosomal protein S5

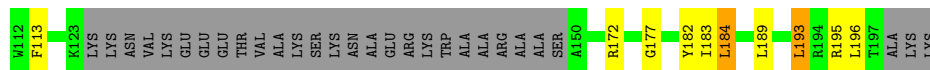
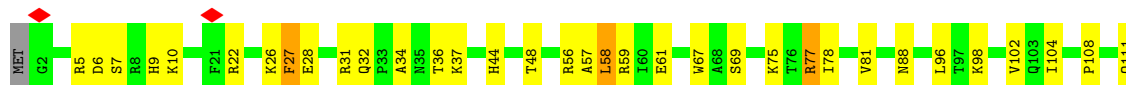


• Molecule 9: 40S ribosomal protein S7-A





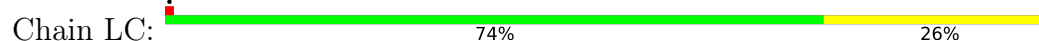
- Molecule 10: 40S ribosomal protein S8-A



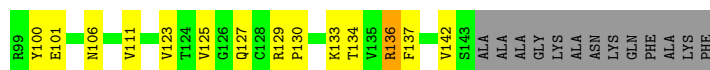
- Molecule 11: 40S ribosomal protein S9-A



- Molecule 12: 40S ribosomal protein S16-A

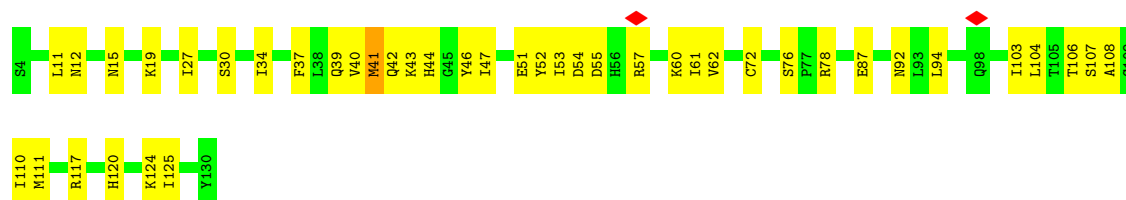


- Molecule 13: 40S ribosomal protein S11-A

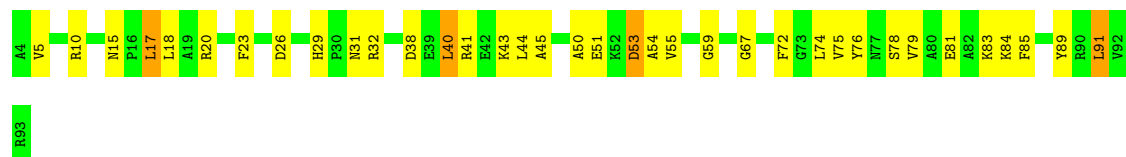


- Molecule 14: 40S ribosomal protein S22-A

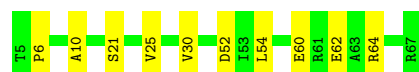




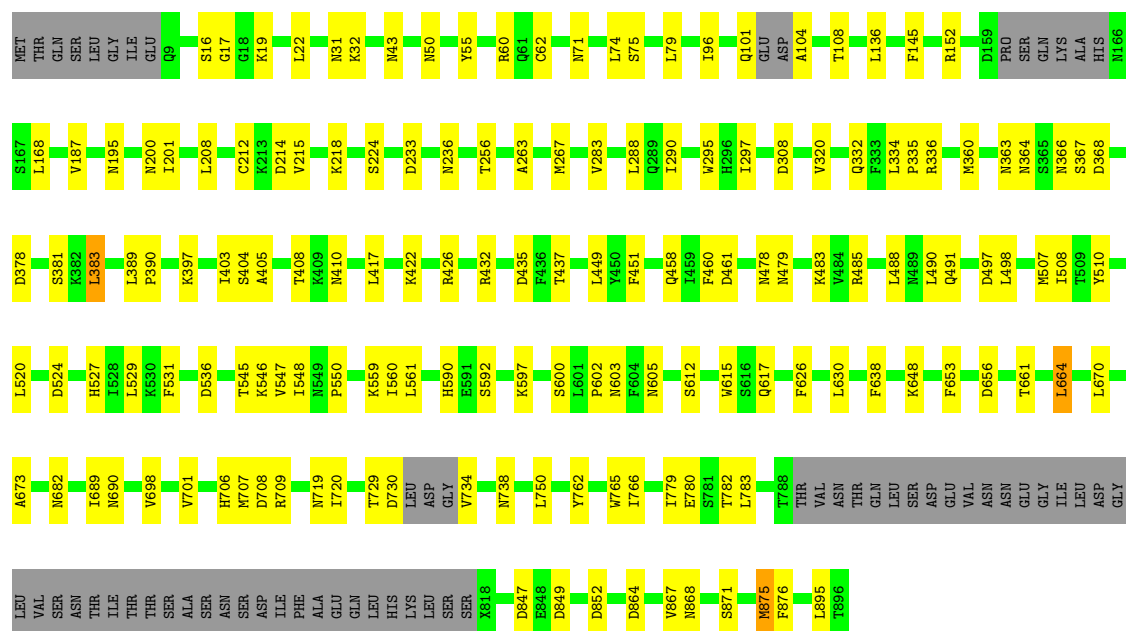
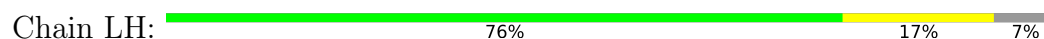
- Molecule 15: 40S ribosomal protein S24-A



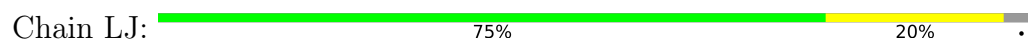
- Molecule 16: 40S ribosomal protein S28-A

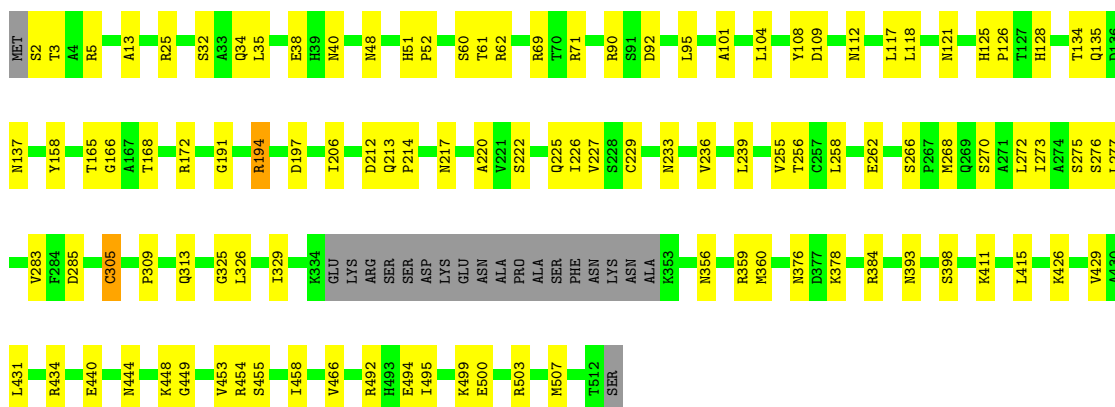


- Molecule 17: NET1-associated nuclear protein 1



- Molecule 18: U3 small nucleolar RNA-associated protein 15





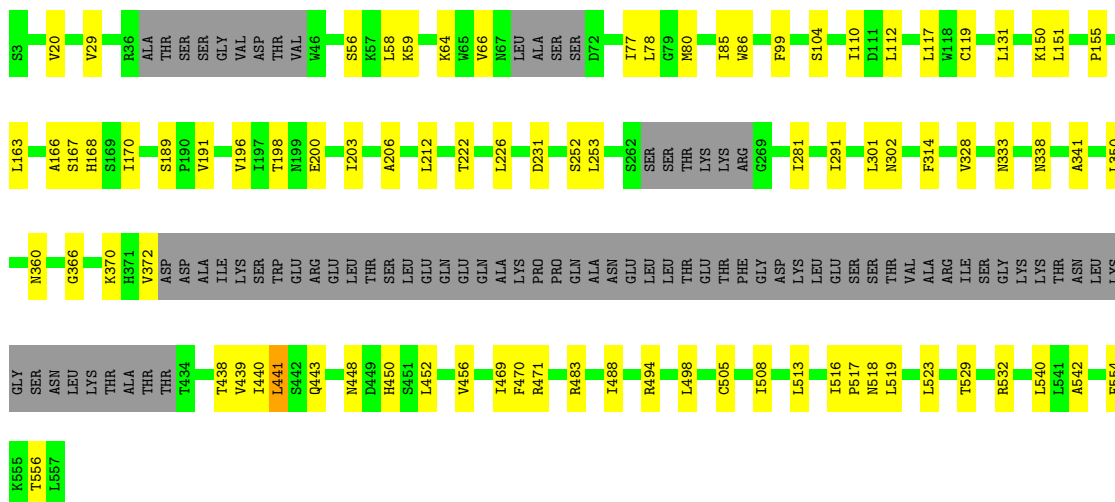
- Molecule 19: U3 small nucleolar RNA-associated protein 9

Chain LK: 88% 11% .



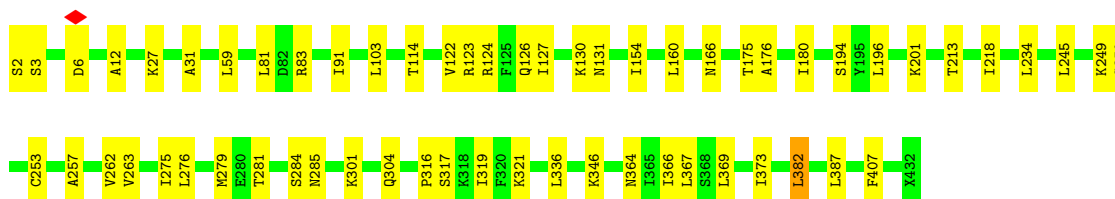
- Molecule 20: U3 small nucleolar RNA-associated protein 5

Chain LL: 70% 15% 14%

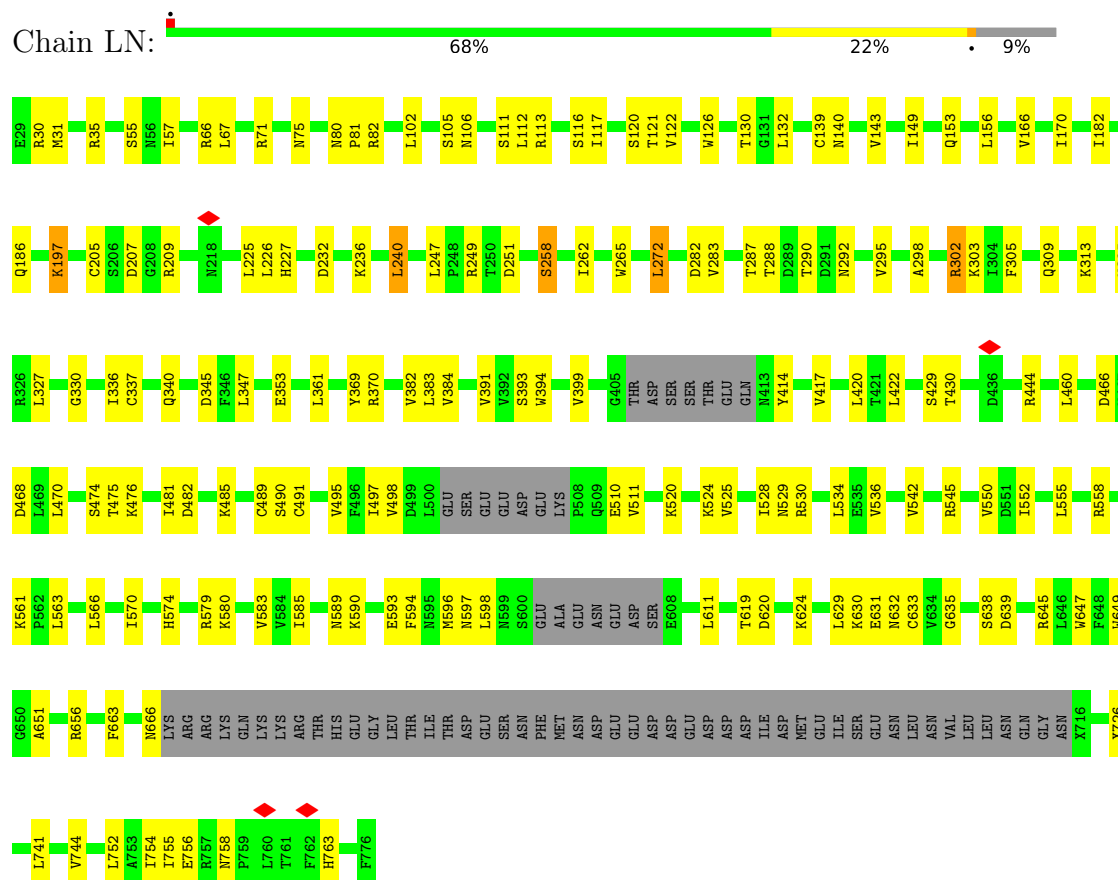


- Molecule 21: U3 small nucleolar RNA-associated protein 10

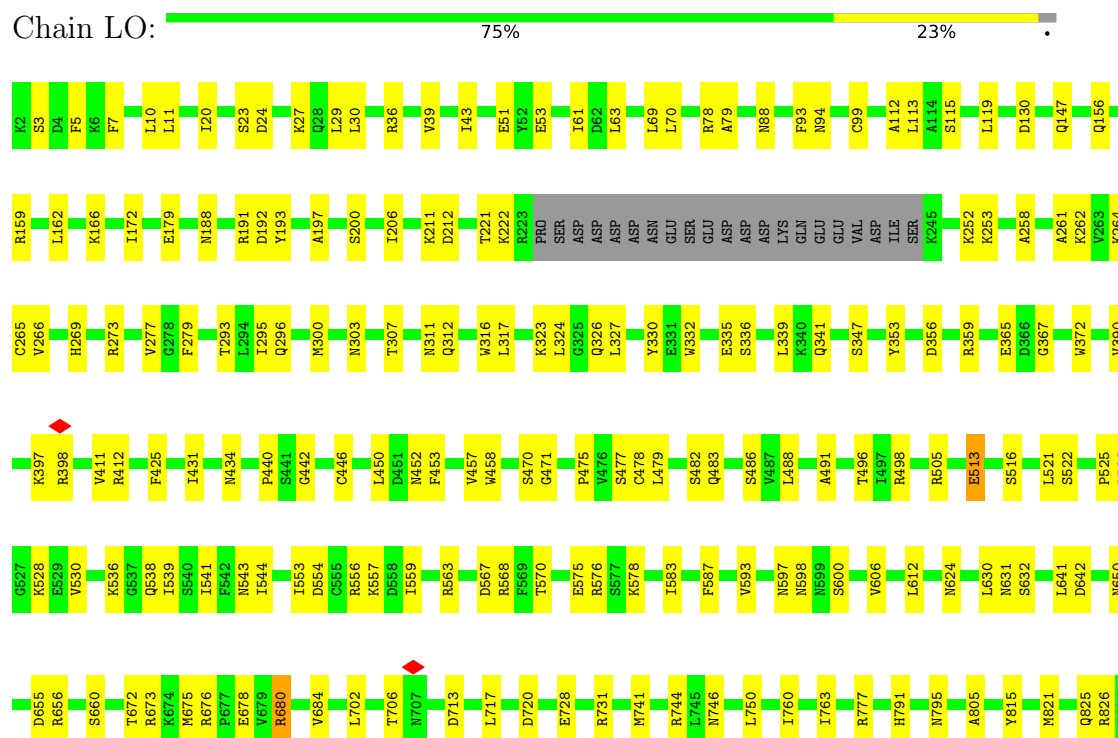
Chain LM: 86% 14%



- Molecule 22: U3 small nucleolar RNA-associated protein 4



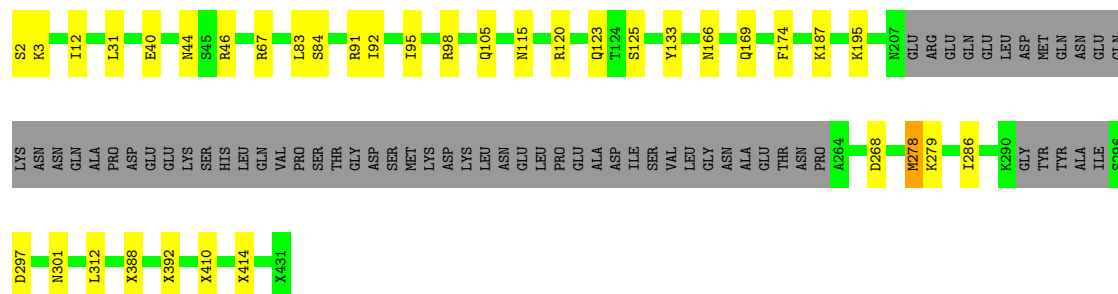
• Molecule 23: Periodic tryptophan protein 2





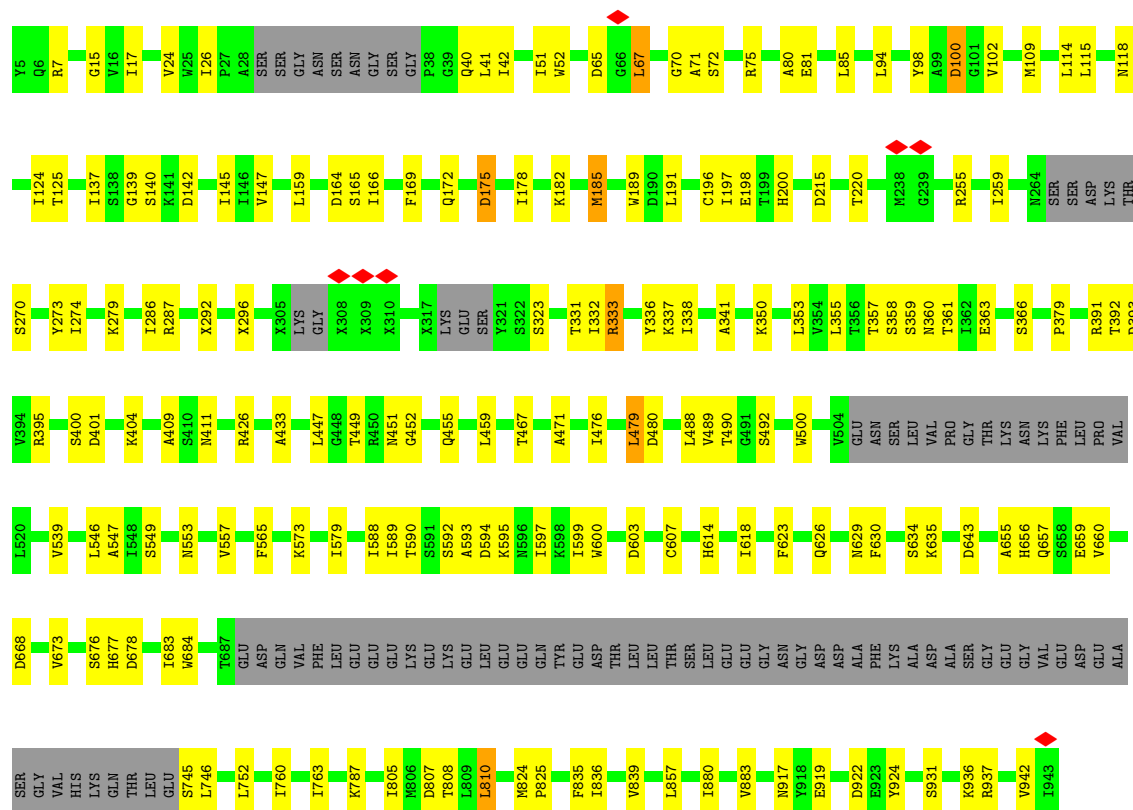
• Molecule 24: U3 small nucleolar RNA-associated protein 6

Chain LP: 77% 8% 15%



• Molecule 25: U3 small nucleolar RNA-associated protein 12

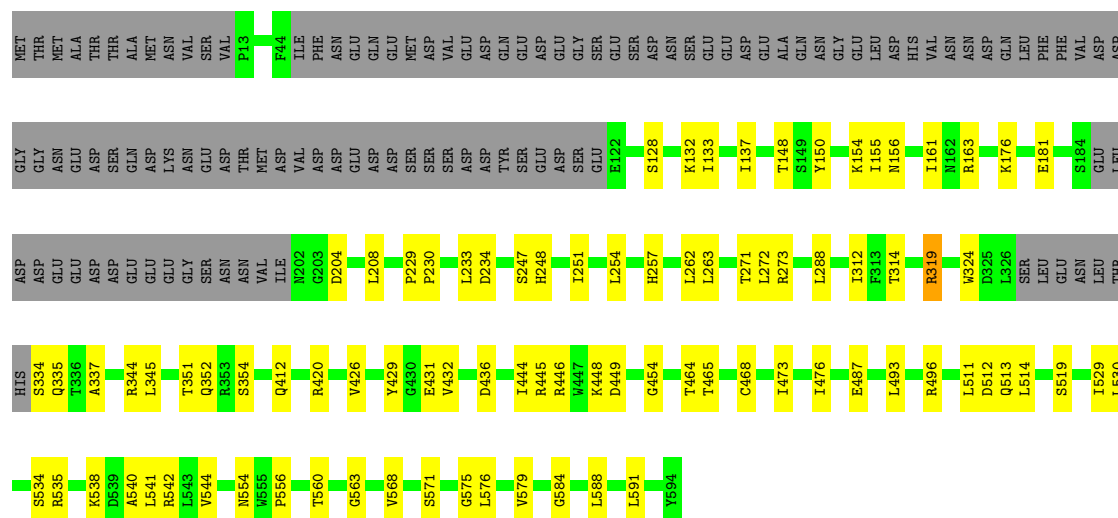
Chain LQ: 71% 18% 10%



• Molecule 26: U3 small nucleolar RNA-associated protein 18

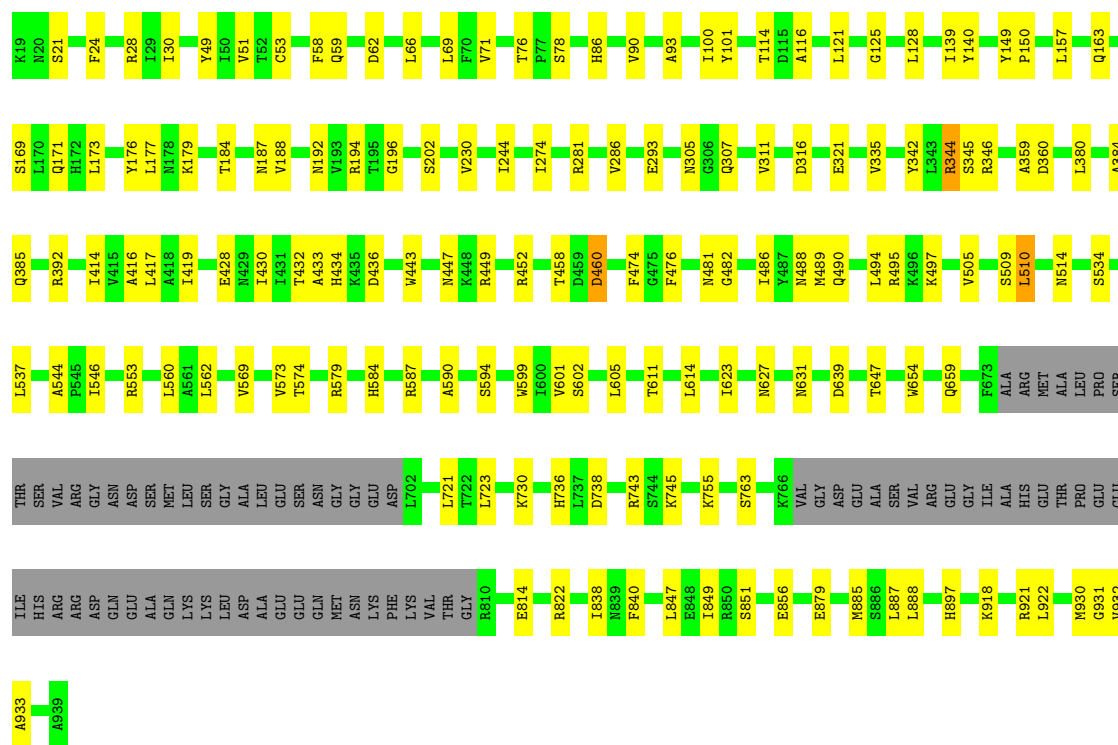
Chain LS: 66% 15% 19%





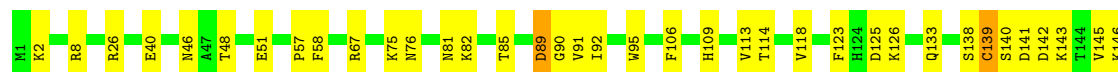
• Molecule 27: U3 small nucleolar RNA-associated protein 21

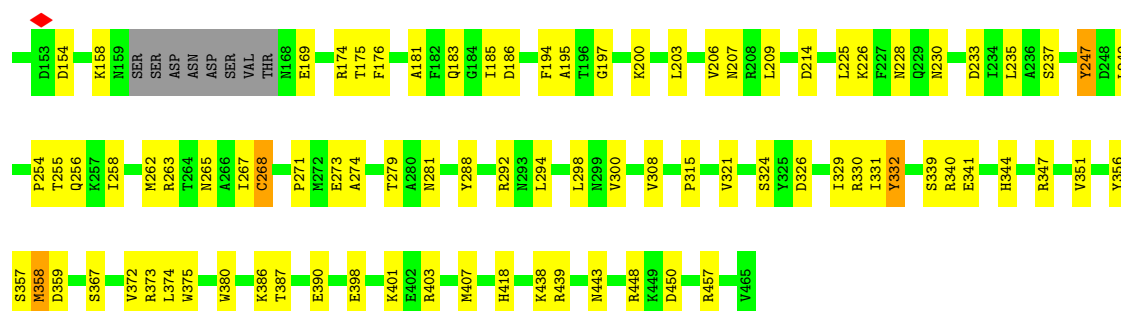
Chain LT: 76% 16% 8%



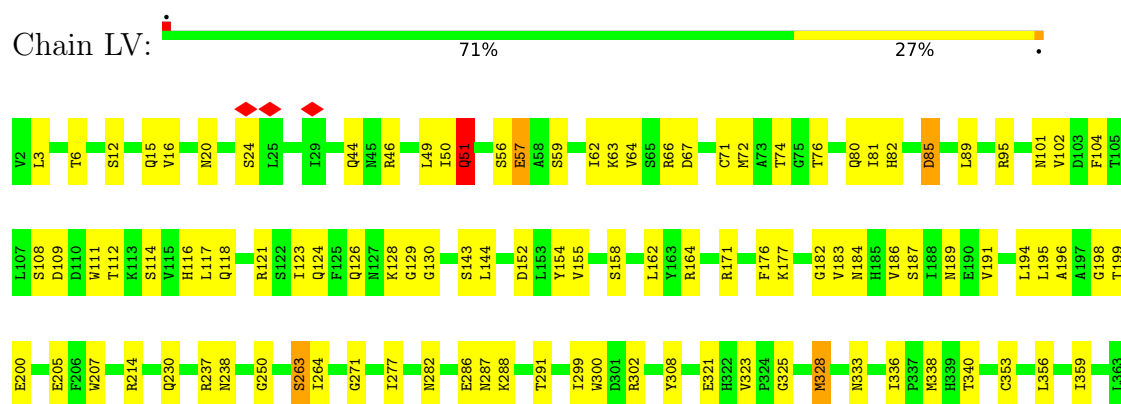
• Molecule 28: Protein SOF1

Chain LU: 72% 25% 3%

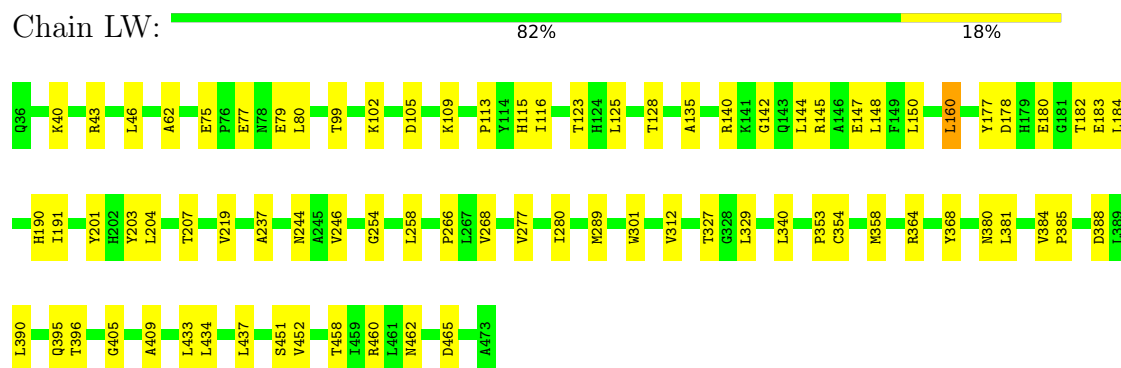




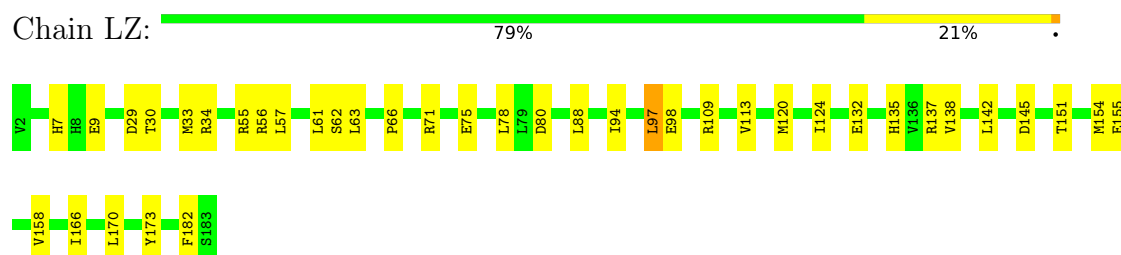
- Molecule 29: Ribosome biogenesis protein ENP2



- Molecule 30: U3 small nucleolar RNA-associated protein 7



- Molecule 31: U3 small nucleolar ribonucleoprotein protein IMP3

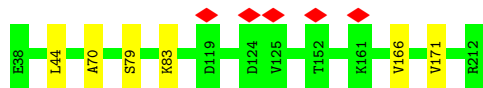


- Molecule 32: 40S ribosomal protein S14-B

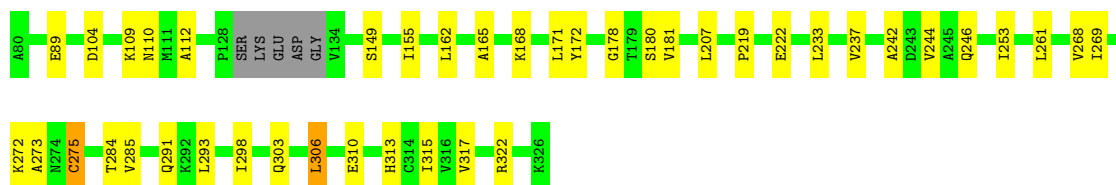
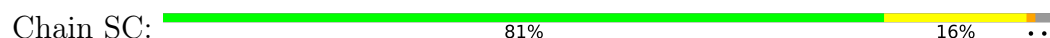




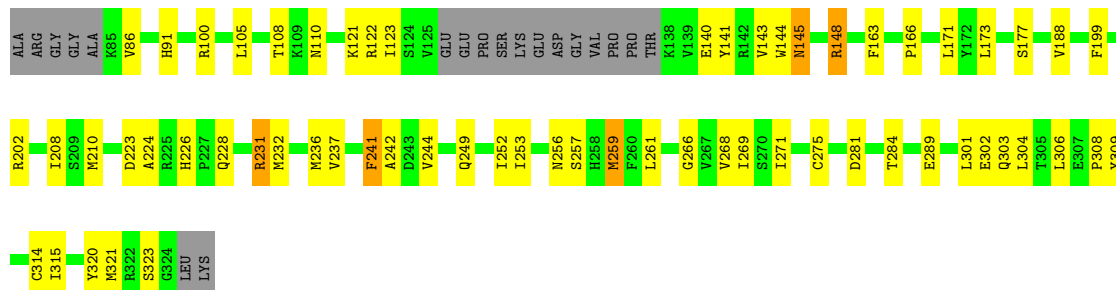
- Molecule 33: KRR1 small subunit processome component



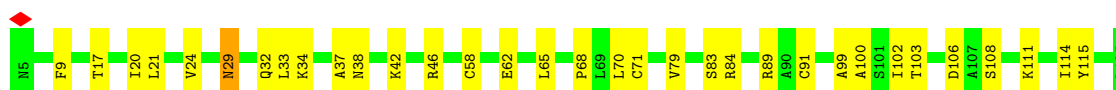
- Molecule 34: rRNA 2'-O-methyltransferase fibrillarin



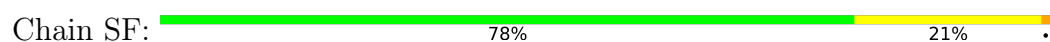
- Molecule 34: rRNA 2'-O-methyltransferase fibrillarin



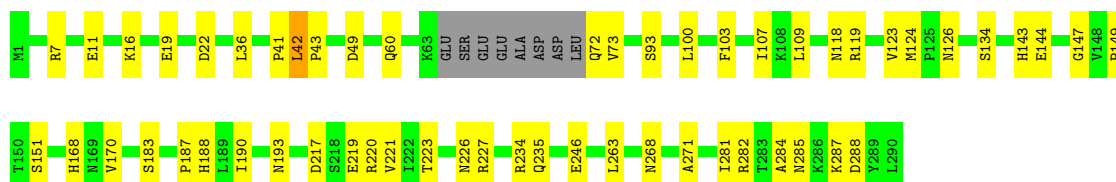
- Molecule 35: Ribonucloprotein



- Molecule 35: Ribonucloprotein

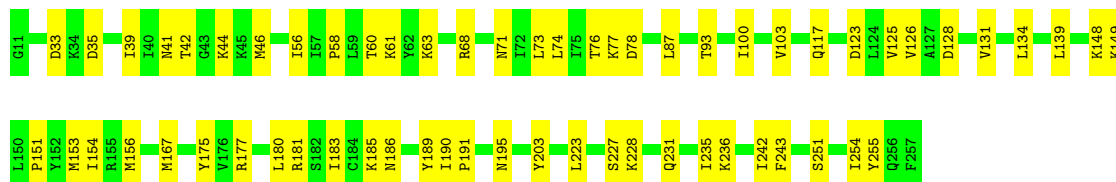


- Molecule 36: RRP9 isoform 1



- Molecule 42: Ribosome biogenesis protein UTP30

Chain SN: 75% 25%



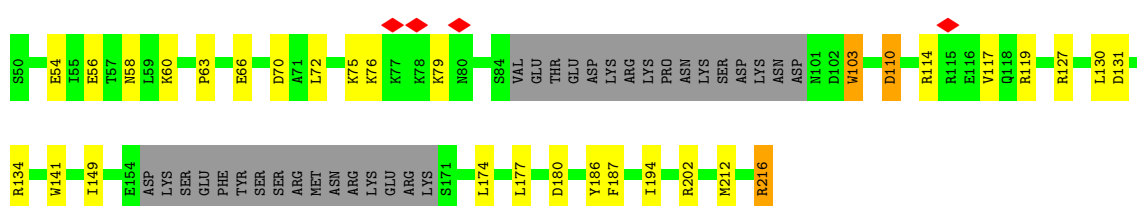
- Molecule 43: Pre-rRNA-processing protein PNO1

Chain SO: 98%



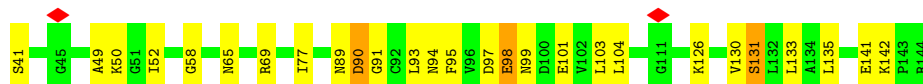
- Molecule 44: rRNA-processing protein FCF2

Chain SQ: 62% 17% 19%



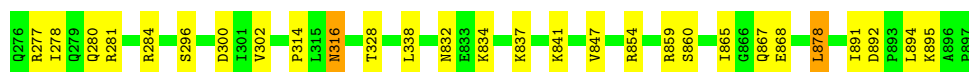
- Molecule 45: 40S ribosomal protein S23-A

Chain SR: 74% 23%

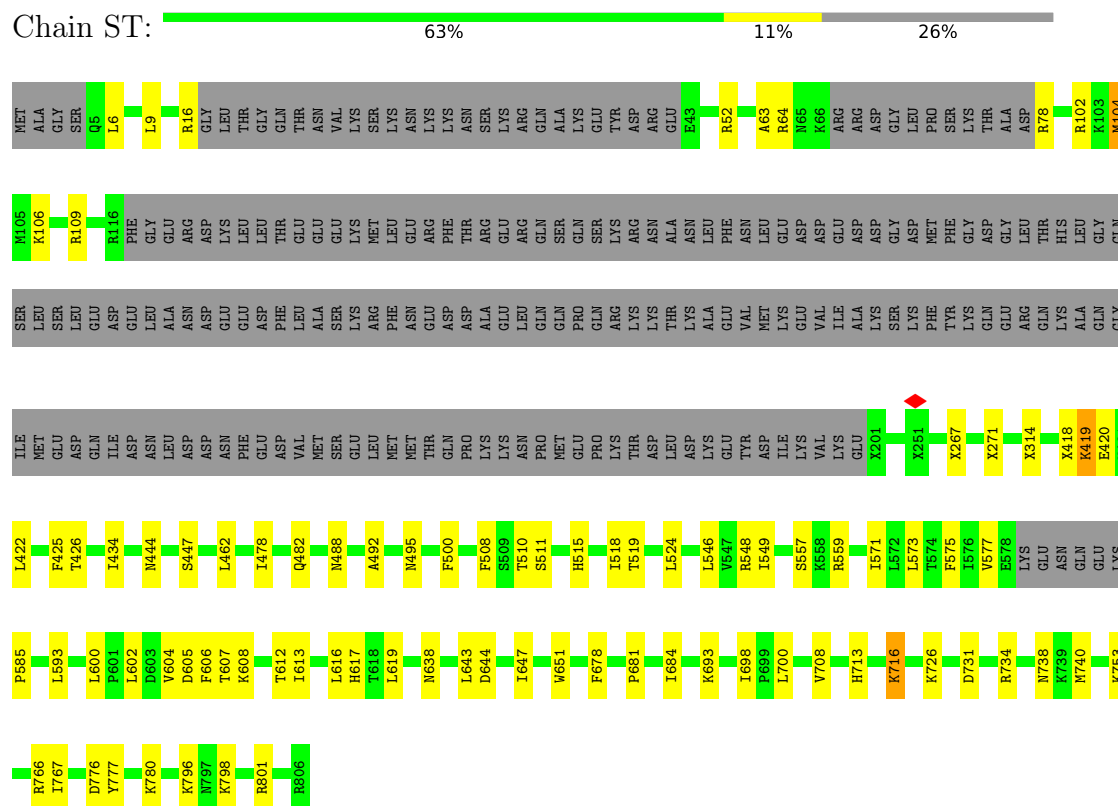


- Molecule 46: U3 small nucleolar RNA-associated protein 14

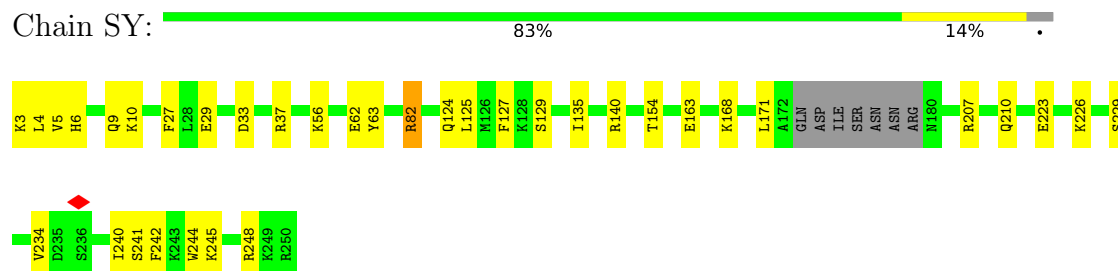
Chain SS: 86% 13%



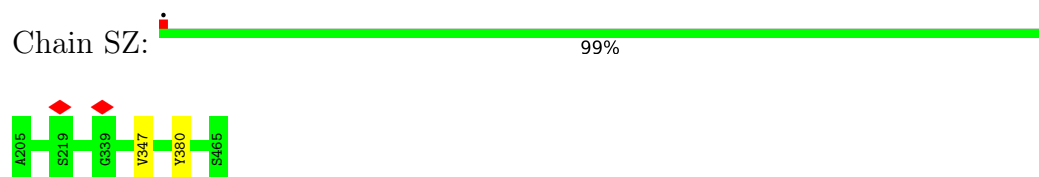
- Molecule 47: Nucleolar complex protein 14



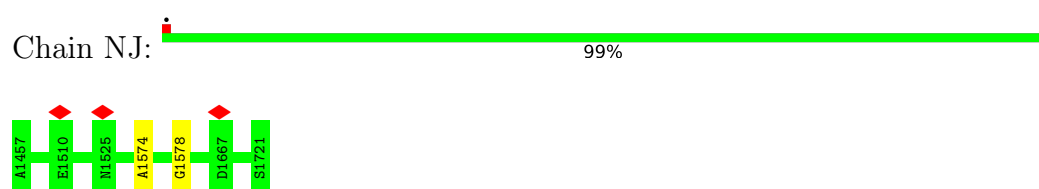
- Molecule 48: U3 small nucleolar RNA-associated protein 11



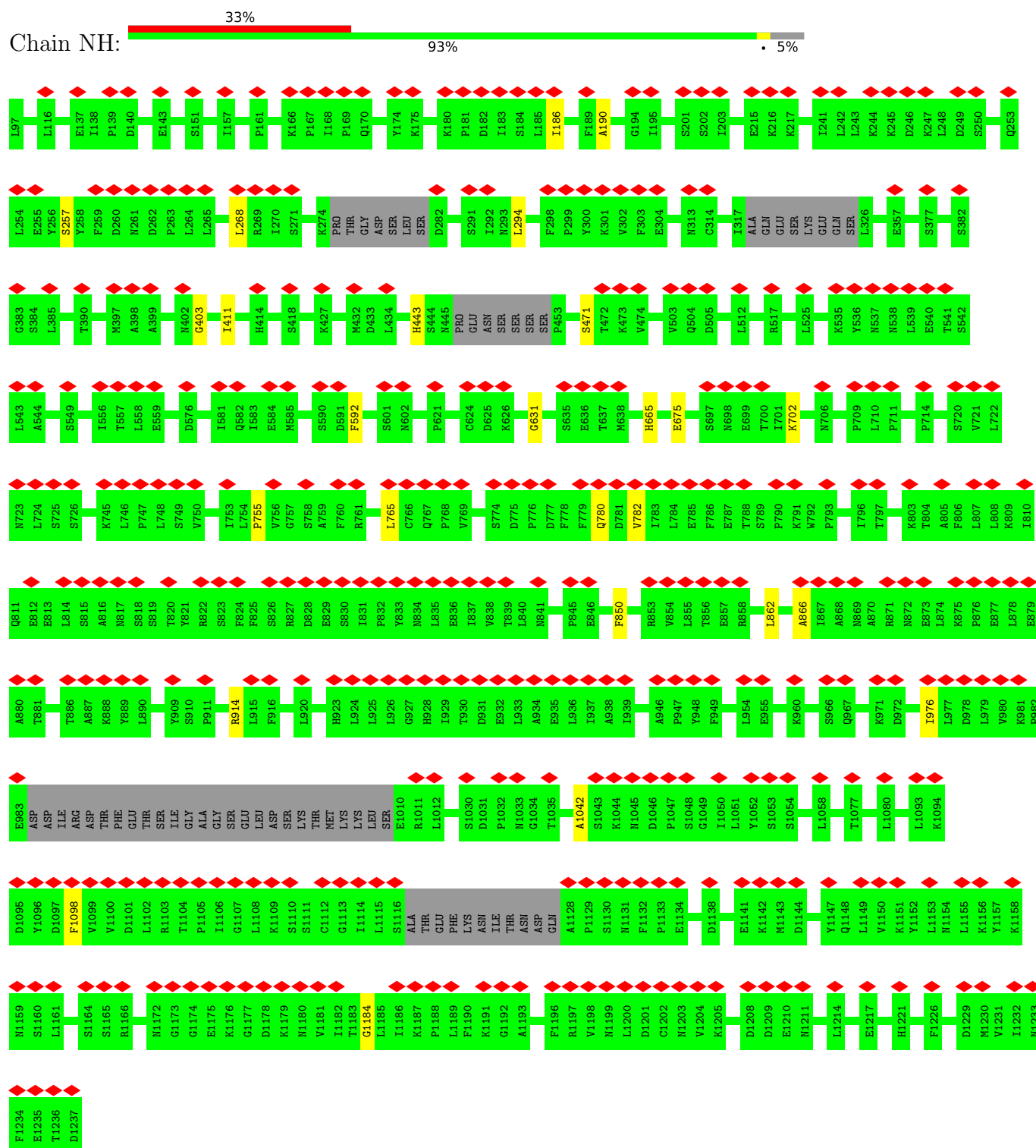
- Molecule 49: Essential nuclear protein 1



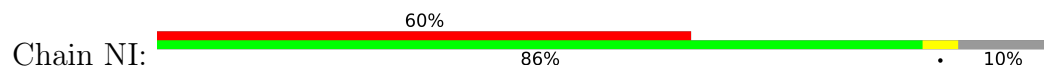
- Molecule 50: rRNA biogenesis protein RRP5



• Molecule 51: U3 small nucleolar RNA-associated protein 22

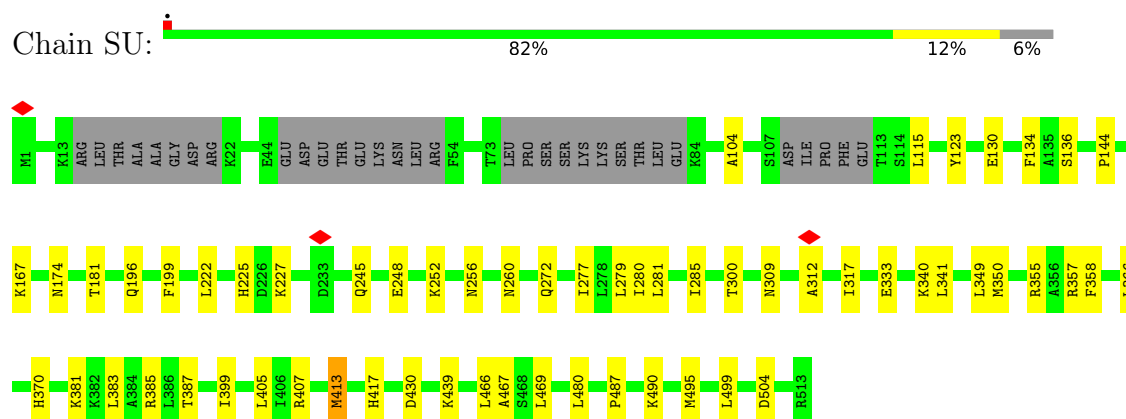


• Molecule 52: Ribosomal RNA-processing protein 7

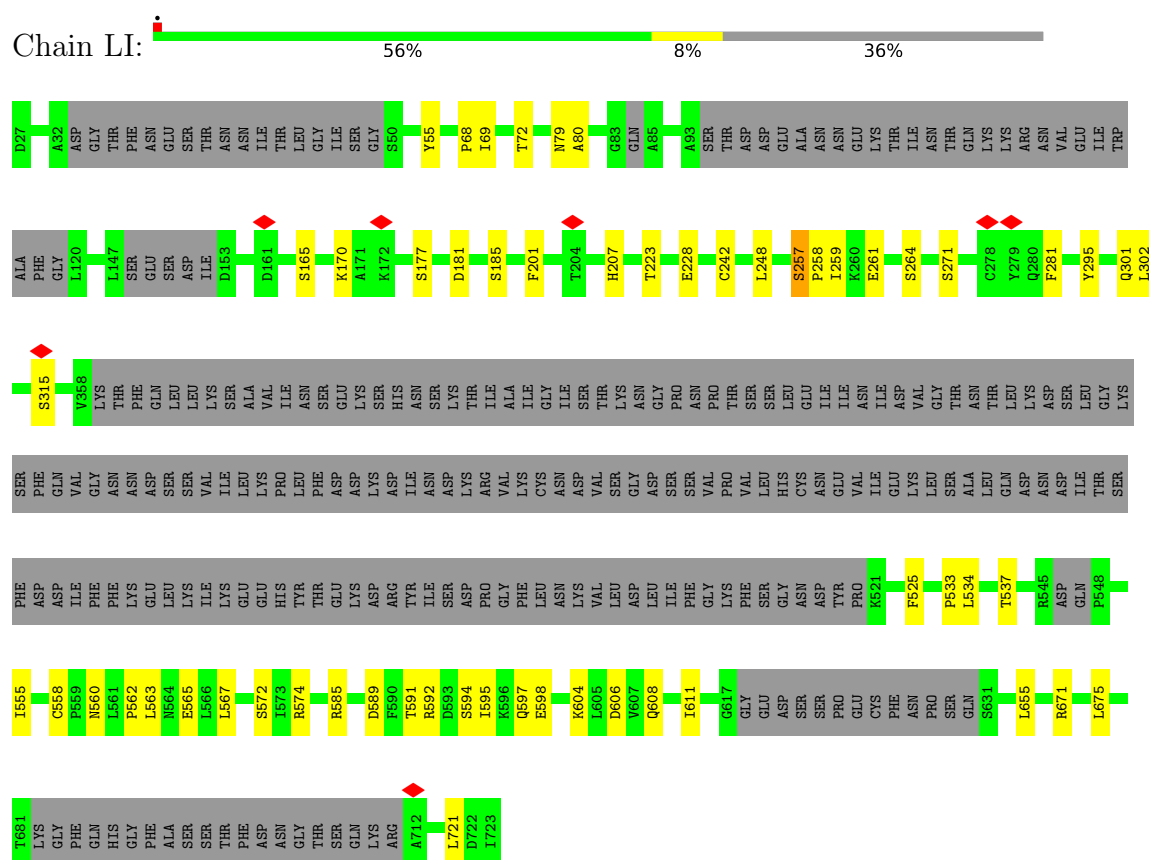




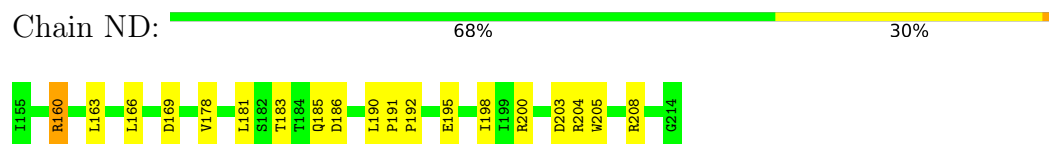
- Molecule 54: Nucleolar complex protein 4



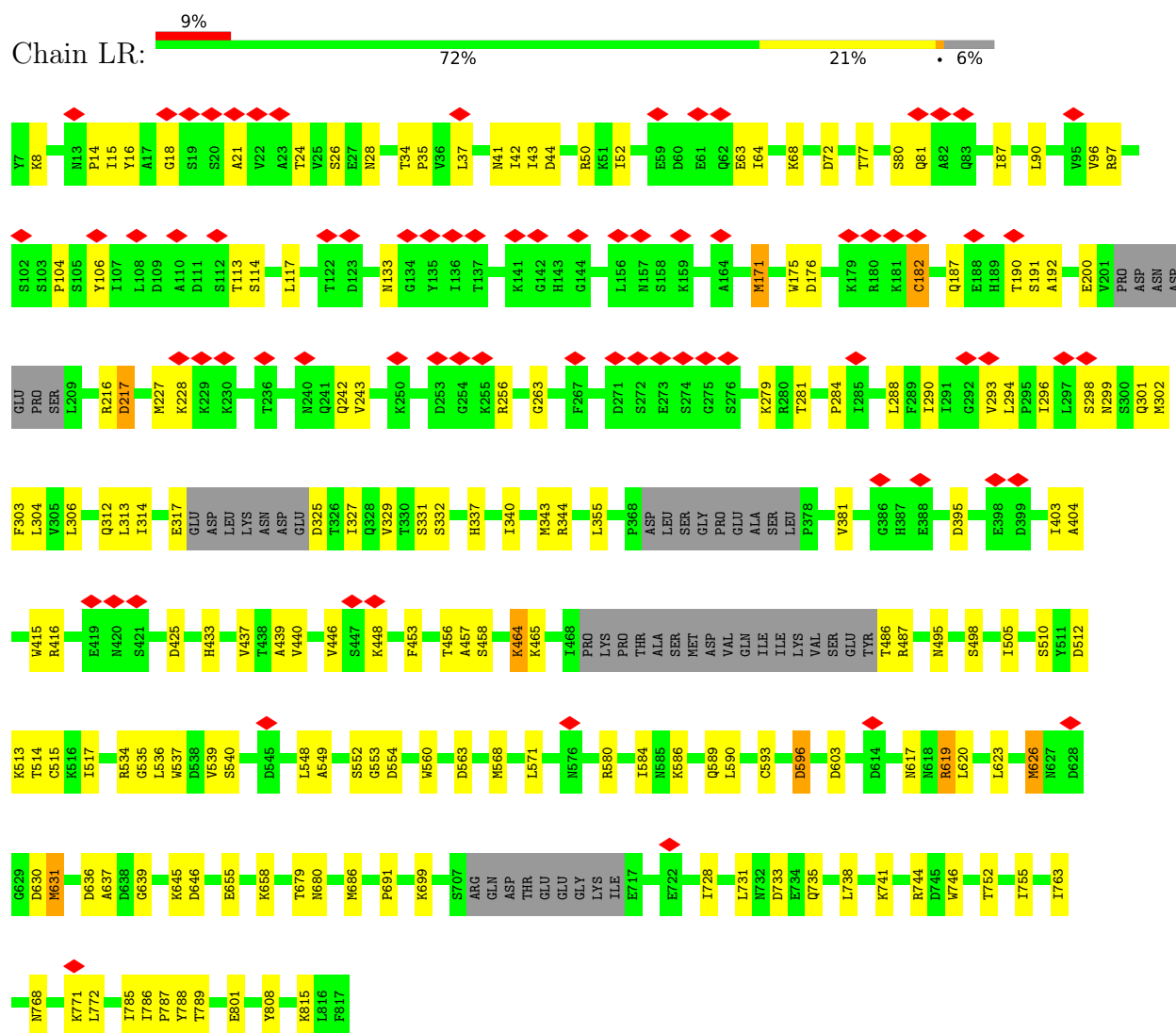
- Molecule 55: U3 small nucleolar RNA-associated protein 8



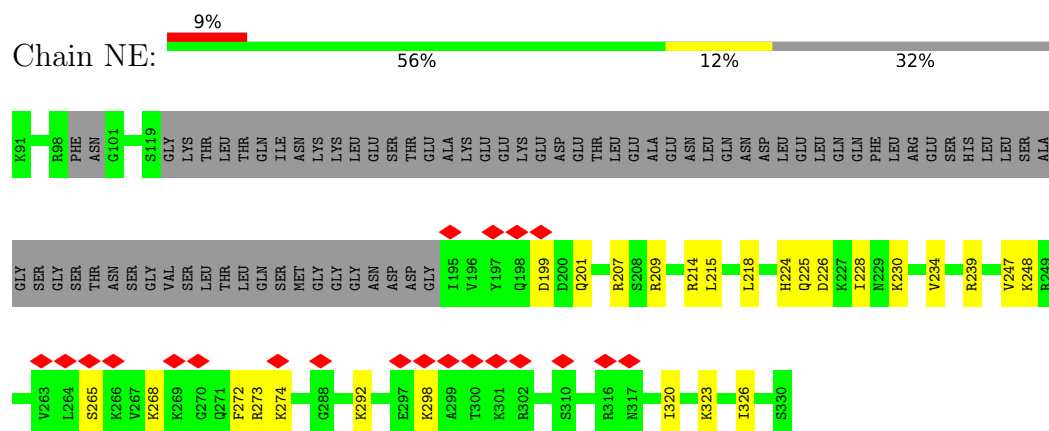
- Molecule 56: Bud site selection protein 21



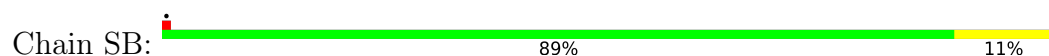
- Molecule 57: U3 small nucleolar RNA-associated protein 13

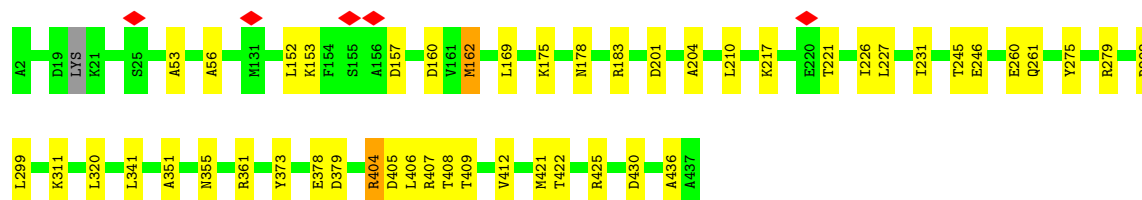


• Molecule 58: Protein FAF1

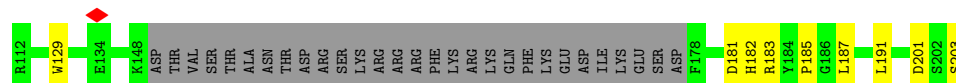


• Molecule 59: Nucleolar protein 58

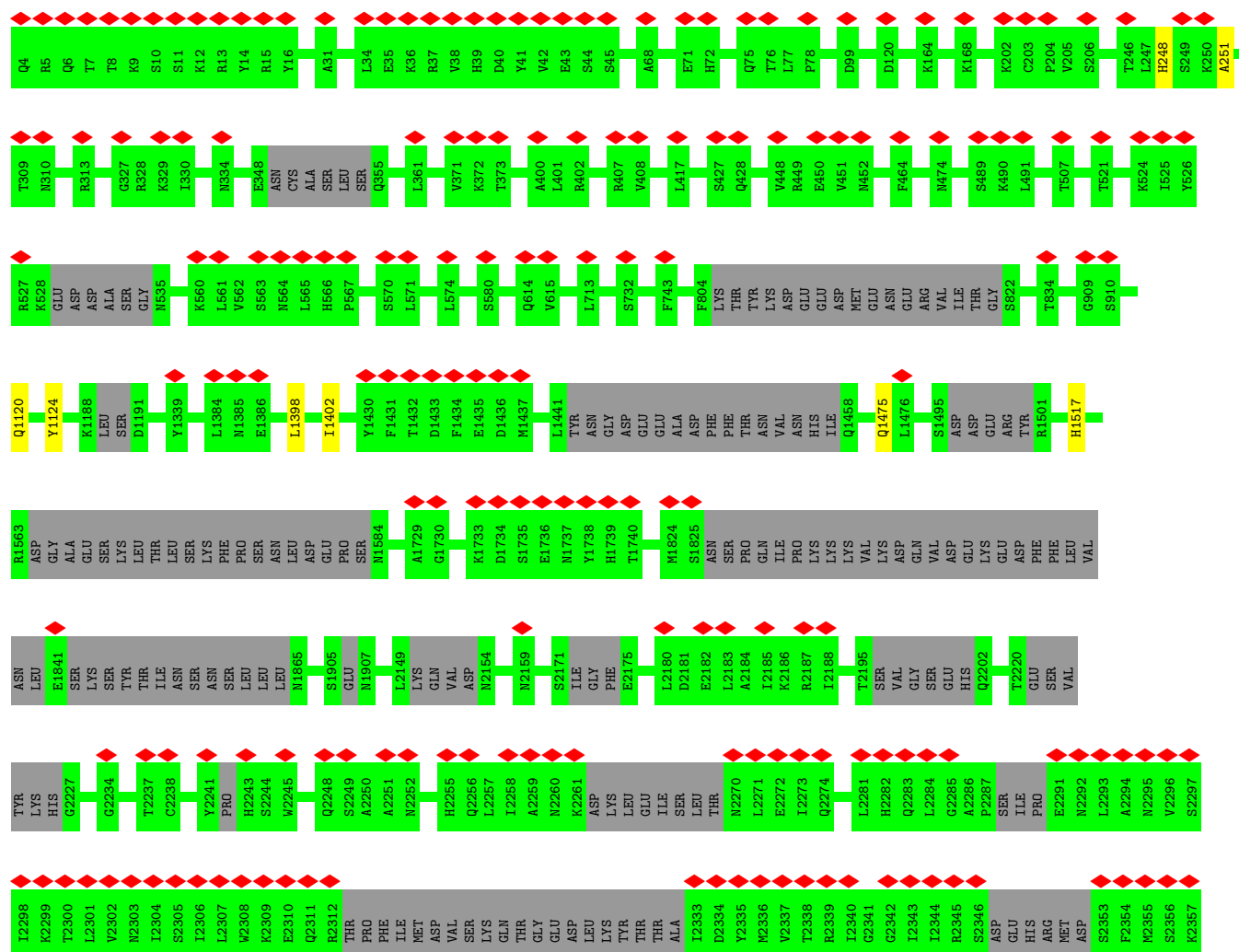




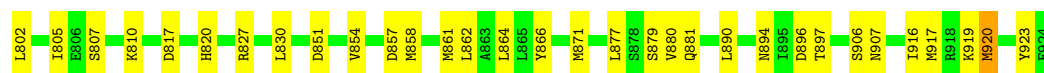
- Molecule 60: Regulator of rDNA transcription protein 14



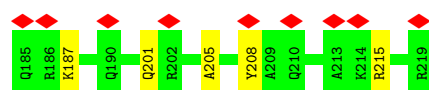
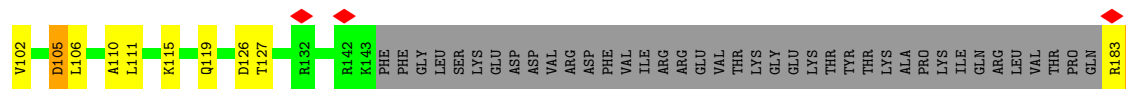
- Molecule 61: U3 small nucleolar RNA-associated protein 20



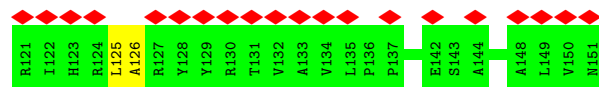
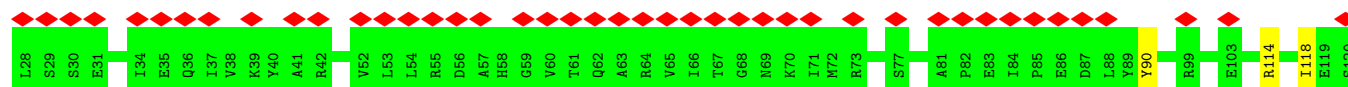




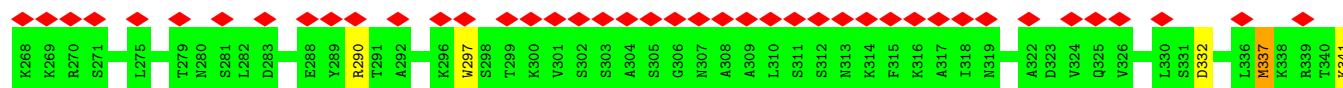
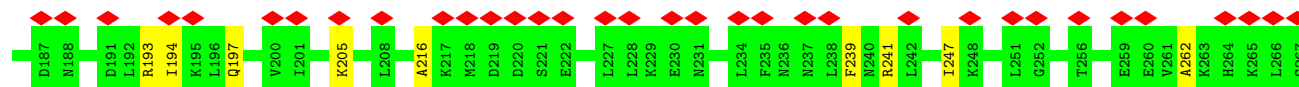
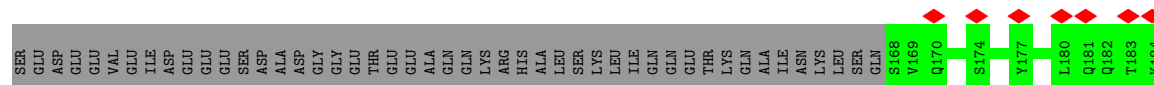
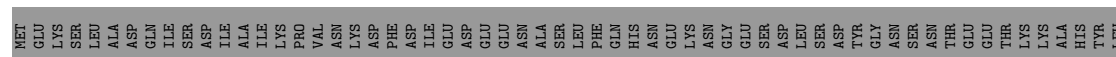
• Molecule 63: 40S ribosomal protein S6-A

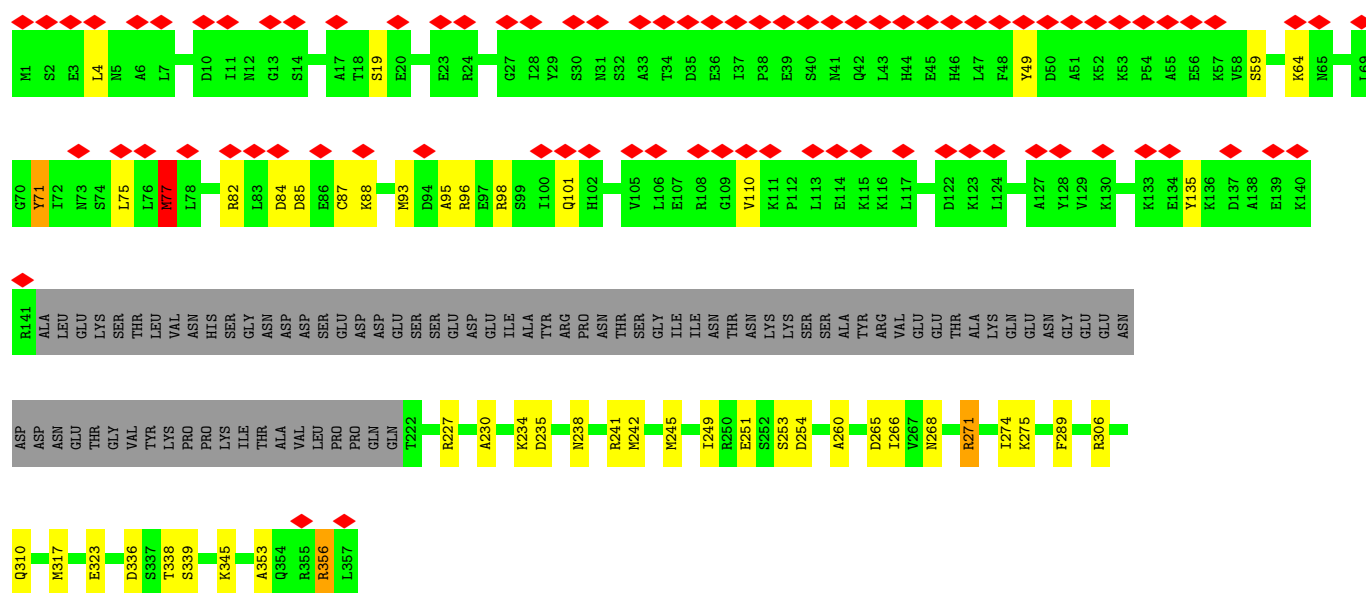


• Molecule 64: 40S ribosomal protein S13



• Molecule 65: Protein BFR2





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 199534 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.074 | Depositor |
| Minimum defocus (nm) | 1300 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.065 | Depositor |
| Minimum map value | -0.009 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.007 | Depositor |
| Map size (Å) | 463.968, 463.968, 463.968 | wwPDB |
| Map dimensions | 432, 432, 432 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.074, 1.074, 1.074 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | NA | 0.28 | 0/1685 | 0.62 | 2/2261 (0.1%) |
| 2 | SA | 0.27 | 0/2769 | 0.51 | 2/3728 (0.1%) |
| 3 | NB | 0.31 | 0/1042 | 0.68 | 1/1377 (0.1%) |
| 4 | L0 | 0.39 | 0/11634 | 1.11 | 71/18120 (0.4%) |
| 5 | L2 | 0.39 | 0/4001 | 1.11 | 22/6215 (0.4%) |
| 6 | L3 | 0.27 | 0/871 | 0.61 | 0/1171 |
| 7 | L4 | 0.32 | 0/1849 | 0.68 | 1/2497 (0.0%) |
| 8 | L5 | 0.29 | 0/1690 | 0.65 | 1/2285 (0.0%) |
| 9 | L7 | 0.32 | 0/1342 | 0.78 | 2/1807 (0.1%) |
| 10 | L8 | 0.33 | 0/1372 | 0.81 | 4/1834 (0.2%) |
| 11 | L9 | 0.37 | 0/1437 | 0.91 | 7/1924 (0.4%) |
| 12 | LC | 0.39 | 0/990 | 0.81 | 2/1335 (0.1%) |
| 13 | LD | 0.31 | 0/1050 | 0.76 | 3/1415 (0.2%) |
| 14 | LE | 0.33 | 0/1020 | 0.77 | 1/1371 (0.1%) |
| 15 | LF | 0.37 | 0/727 | 1.01 | 8/977 (0.8%) |
| 16 | LG | 0.43 | 0/499 | 0.97 | 2/670 (0.3%) |
| 17 | LH | 0.28 | 0/6694 | 0.57 | 6/9070 (0.1%) |
| 18 | LJ | 0.29 | 0/3993 | 0.59 | 2/5413 (0.0%) |
| 19 | LK | 0.25 | 0/735 | 0.55 | 0/987 |
| 20 | LL | 0.27 | 0/3840 | 0.56 | 0/5208 |
| 21 | LM | 0.28 | 0/3470 | 0.53 | 2/4694 (0.0%) |
| 22 | LN | 0.28 | 0/5369 | 0.60 | 4/7272 (0.1%) |
| 23 | LO | 0.33 | 0/6780 | 0.60 | 3/9175 (0.0%) |
| 24 | LP | 0.29 | 0/2281 | 0.52 | 0/3059 |
| 25 | LQ | 0.27 | 0/6574 | 0.58 | 7/8881 (0.1%) |
| 26 | LS | 0.30 | 0/3875 | 0.54 | 0/5254 |
| 27 | LT | 0.30 | 0/6834 | 0.59 | 5/9238 (0.1%) |
| 28 | LU | 0.30 | 0/3802 | 0.63 | 2/5118 (0.0%) |
| 29 | LV | 0.31 | 0/2902 | 0.68 | 2/3941 (0.1%) |
| 30 | LW | 0.30 | 0/3505 | 0.57 | 2/4748 (0.0%) |
| 31 | LZ | 0.38 | 0/1559 | 0.76 | 4/2097 (0.2%) |
| 32 | NG | 0.26 | 0/542 | 0.48 | 0/750 |
| 33 | NK | 0.24 | 0/867 | 0.41 | 0/1208 |
| 34 | SC | 0.33 | 0/1917 | 0.64 | 1/2588 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 34 | SD | 0.31 | 0/1815 | 0.69 | 3/2448 (0.1%) |
| 35 | SE | 0.38 | 0/928 | 0.73 | 1/1262 (0.1%) |
| 35 | SF | 0.38 | 0/928 | 0.75 | 2/1262 (0.2%) |
| 36 | SG | 0.27 | 0/3498 | 0.60 | 3/4712 (0.1%) |
| 37 | SH | 0.29 | 0/2832 | 0.58 | 1/3825 (0.0%) |
| 38 | SI | 0.30 | 0/6403 | 0.66 | 9/8616 (0.1%) |
| 39 | SJ | 0.27 | 0/1727 | 0.58 | 0/2329 |
| 39 | SK | 0.30 | 0/1828 | 0.59 | 0/2470 |
| 40 | SL | 0.32 | 0/1418 | 0.70 | 3/1906 (0.2%) |
| 41 | SM | 0.32 | 0/2337 | 0.69 | 4/3148 (0.1%) |
| 42 | SN | 0.33 | 0/2041 | 0.67 | 2/2745 (0.1%) |
| 43 | SO | 0.26 | 0/1003 | 0.55 | 0/1381 |
| 44 | SQ | 0.31 | 0/1156 | 0.71 | 4/1536 (0.3%) |
| 45 | SR | 0.36 | 0/804 | 0.79 | 4/1074 (0.4%) |
| 46 | SS | 0.28 | 0/1230 | 0.69 | 3/1660 (0.2%) |
| 47 | ST | 0.26 | 0/3826 | 0.57 | 3/5125 (0.1%) |
| 48 | SY | 0.29 | 0/2042 | 0.59 | 0/2704 |
| 49 | SZ | 0.23 | 0/1294 | 0.38 | 0/1804 |
| 50 | NJ | 0.23 | 0/1313 | 0.33 | 0/1830 |
| 51 | NH | 0.24 | 0/5357 | 0.41 | 0/7463 |
| 52 | NI | 0.23 | 0/838 | 0.43 | 0/1166 |
| 53 | 8 | 2.20 | 5/28439 (0.0%) | 1.13 | 168/44273 (0.4%) |
| 54 | SU | 0.27 | 0/3736 | 0.53 | 2/5086 (0.0%) |
| 55 | LI | 0.26 | 0/2703 | 0.58 | 3/3703 (0.1%) |
| 56 | ND | 0.32 | 0/499 | 0.76 | 1/659 (0.2%) |
| 57 | LR | 0.28 | 1/6058 (0.0%) | 0.58 | 3/8201 (0.0%) |
| 58 | NE | 0.27 | 0/1240 | 0.65 | 1/1645 (0.1%) |
| 59 | SB | 0.27 | 0/3012 | 0.55 | 2/4091 (0.0%) |
| 60 | SV | 0.36 | 0/385 | 0.66 | 2/529 (0.4%) |
| 61 | SP | 0.23 | 0/11085 | 0.34 | 0/15445 |
| 62 | LX | 0.28 | 0/5994 | 0.58 | 6/8139 (0.1%) |
| 62 | LY | 0.24 | 0/4128 | 0.41 | 0/5747 |
| 63 | L6 | 1.96 | 1/1341 (0.1%) | 0.91 | 5/1789 (0.3%) |
| 64 | NF | 0.24 | 0/613 | 0.47 | 0/853 |
| 65 | 5 | 0.27 | 0/2422 | 0.57 | 2/3257 (0.1%) |
| 66 | 6 | 0.29 | 0/2271 | 0.66 | 2/3029 (0.1%) |
| All | All | 0.86 | 7/218061 (0.0%) | 0.75 | 408/304600 (0.1%) |

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 | NA | 0 | 1 |
| 7 | L4 | 0 | 2 |
| 9 | L7 | 0 | 1 |
| 11 | L9 | 0 | 1 |
| 15 | LF | 0 | 2 |
| 22 | LN | 0 | 1 |
| 29 | LV | 0 | 2 |
| 34 | SD | 0 | 1 |
| 35 | SE | 0 | 2 |
| 35 | SF | 0 | 1 |
| 38 | SI | 0 | 1 |
| 55 | LI | 0 | 1 |
| 57 | LR | 0 | 1 |
| 63 | L6 | 0 | 1 |
| 65 | 5 | 0 | 1 |
| 66 | 6 | 0 | 1 |
| All | All | 0 | 20 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 53 | 8 | 140 | A | N7-C5 | 187.02 | 2.51 | 1.39 |
| 53 | 8 | 140 | A | N9-C4 | 185.66 | 2.49 | 1.37 |
| 53 | 8 | 140 | A | C8-N7 | 156.00 | 2.40 | 1.31 |
| 53 | 8 | 140 | A | N9-C8 | 150.09 | 2.57 | 1.37 |
| 53 | 8 | 140 | A | C5-C4 | 135.64 | 2.33 | 1.38 |
| 63 | L6 | 184 | LEU | CA-CB | 70.71 | 3.16 | 1.53 |
| 57 | LR | 104 | PRO | CG-CD | -5.93 | 1.31 | 1.50 |

All (408) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 53 | 8 | 140 | A | N7-C8-N9 | -24.47 | 101.57 | 113.80 |
| 53 | 8 | 140 | A | N1-C2-N3 | 22.84 | 140.72 | 129.30 |
| 53 | 8 | 140 | A | C6-N1-C2 | 20.60 | 130.96 | 118.60 |
| 53 | 8 | 140 | A | C4-C5-C6 | -18.93 | 107.53 | 117.00 |
| 53 | 8 | 140 | A | C5-N7-C8 | 17.31 | 112.56 | 103.90 |
| 53 | 8 | 140 | A | C6-C5-N7 | 17.27 | 144.39 | 132.30 |
| 63 | L6 | 184 | LEU | CA-CB-CG | 17.07 | 154.55 | 115.30 |
| 53 | 8 | 140 | A | N3-C4-C5 | -15.55 | 115.91 | 126.80 |
| 57 | LR | 104 | PRO | CA-N-CD | -11.81 | 94.96 | 111.50 |
| 53 | 8 | 140 | A | N3-C4-N9 | 11.53 | 136.62 | 127.40 |
| 53 | 8 | 140 | A | C8-N9-C4 | 11.37 | 110.35 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 27 | LT | 460 | ASP | CB-CG-OD1 | 11.30 | 128.47 | 118.30 |
| 38 | SI | 348 | ASP | CB-CG-OD1 | 10.64 | 127.88 | 118.30 |
| 16 | LG | 6 | PRO | CA-N-CD | -10.39 | 96.95 | 111.50 |
| 15 | LF | 53 | ASP | CB-CG-OD2 | 10.01 | 127.31 | 118.30 |
| 53 | 8 | 1215 | C | N1-C2-O2 | 10.00 | 124.90 | 118.90 |
| 53 | 8 | 1619 | C | N1-C2-O2 | 9.84 | 124.81 | 118.90 |
| 5 | L2 | 200 | C | N1-C2-O2 | 9.76 | 124.76 | 118.90 |
| 53 | 8 | 1215 | C | C2-N1-C1' | 9.63 | 129.39 | 118.80 |
| 11 | L9 | 18 | PRO | CA-N-CD | -9.54 | 98.14 | 111.50 |
| 53 | 8 | 519 | C | C2-N1-C1' | 9.23 | 128.96 | 118.80 |
| 57 | LR | 104 | PRO | N-CD-CG | -9.21 | 89.38 | 103.20 |
| 11 | L9 | 25 | ASP | CB-CG-OD1 | 9.16 | 126.55 | 118.30 |
| 53 | 8 | 1220 | C | N1-C2-O2 | 9.07 | 124.34 | 118.90 |
| 11 | L9 | 89 | ASP | CB-CG-OD2 | 9.07 | 126.46 | 118.30 |
| 3 | NB | 550 | LEU | CA-CB-CG | 9.01 | 136.03 | 115.30 |
| 53 | 8 | 241 | U | C2-N1-C1' | 8.97 | 128.47 | 117.70 |
| 53 | 8 | 1619 | C | C2-N1-C1' | 8.97 | 128.67 | 118.80 |
| 12 | LC | 64 | ASP | CB-CG-OD2 | 8.87 | 126.28 | 118.30 |
| 53 | 8 | 1123 | C | N3-C2-O2 | -8.87 | 115.69 | 121.90 |
| 15 | LF | 18 | LEU | CA-CB-CG | 8.82 | 135.58 | 115.30 |
| 53 | 8 | 1215 | C | N3-C2-O2 | -8.77 | 115.76 | 121.90 |
| 10 | L8 | 193 | LEU | CA-CB-CG | 8.75 | 135.43 | 115.30 |
| 23 | LO | 720 | ASP | CB-CG-OD2 | 8.69 | 126.12 | 118.30 |
| 40 | SL | 68 | ASP | CB-CG-OD2 | 8.67 | 126.10 | 118.30 |
| 53 | 8 | 241 | U | N1-C2-O2 | 8.64 | 128.85 | 122.80 |
| 13 | LD | 71 | LEU | CA-CB-CG | 8.61 | 135.10 | 115.30 |
| 11 | L9 | 63 | ASP | CB-CG-OD2 | 8.57 | 126.01 | 118.30 |
| 53 | 8 | 258 | C | N1-C2-O2 | 8.54 | 124.02 | 118.90 |
| 41 | SM | 41 | PRO | CA-N-CD | -8.53 | 99.56 | 111.50 |
| 4 | L0 | 216 | U | N1-C2-O2 | 8.50 | 128.75 | 122.80 |
| 5 | L2 | 201 | C | N1-C2-O2 | 8.43 | 123.96 | 118.90 |
| 53 | 8 | 99 | C | C5-C6-N1 | 8.40 | 125.20 | 121.00 |
| 63 | L6 | 184 | LEU | CB-CA-C | 8.39 | 126.14 | 110.20 |
| 53 | 8 | 954 | G | C4-N9-C1' | 8.35 | 137.36 | 126.50 |
| 4 | L0 | 203 | C | N1-C2-O2 | 8.33 | 123.90 | 118.90 |
| 4 | L0 | 216 | U | N3-C2-O2 | -8.30 | 116.39 | 122.20 |
| 53 | 8 | 519 | C | N1-C2-O2 | 8.29 | 123.88 | 118.90 |
| 4 | L0 | 284 | U | N1-C2-O2 | 8.25 | 128.57 | 122.80 |
| 4 | L0 | 347 | U | N1-C2-O2 | 8.24 | 128.57 | 122.80 |
| 55 | LI | 589 | ASP | CB-CG-OD2 | 8.15 | 125.64 | 118.30 |
| 53 | 8 | 1123 | C | N1-C2-O2 | 8.14 | 123.79 | 118.90 |
| 36 | SG | 115 | ASP | CB-CG-OD1 | 8.14 | 125.62 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 53 | 8 | 241 | U | N3-C2-O2 | -8.12 | 116.52 | 122.20 |
| 4 | L0 | 284 | U | N3-C2-O2 | -8.10 | 116.53 | 122.20 |
| 4 | L0 | 347 | U | N3-C2-O2 | -8.09 | 116.54 | 122.20 |
| 53 | 8 | 99 | C | C6-N1-C2 | -7.92 | 117.13 | 120.30 |
| 53 | 8 | 1619 | C | N3-C2-O2 | -7.89 | 116.37 | 121.90 |
| 62 | LX | 762 | MET | CB-CG-SD | 7.82 | 135.86 | 112.40 |
| 4 | L0 | 332 | U | N1-C2-O2 | 7.75 | 128.22 | 122.80 |
| 63 | L6 | 57 | ASP | CB-CG-OD2 | 7.71 | 125.24 | 118.30 |
| 4 | L0 | 91 | U | C5-C6-N1 | 7.70 | 126.55 | 122.70 |
| 27 | LT | 436 | ASP | CB-CG-OD2 | 7.69 | 125.22 | 118.30 |
| 53 | 8 | 1220 | C | N3-C2-O2 | -7.68 | 116.53 | 121.90 |
| 4 | L0 | 543 | C | C2-N1-C1' | 7.65 | 127.22 | 118.80 |
| 5 | L2 | 200 | C | C2-N1-C1' | 7.62 | 127.19 | 118.80 |
| 53 | 8 | 1215 | C | C6-N1-C2 | -7.61 | 117.25 | 120.30 |
| 46 | SS | 878 | LEU | CA-CB-CG | 7.58 | 132.72 | 115.30 |
| 23 | LO | 741 | MET | CA-CB-CG | 7.57 | 126.18 | 113.30 |
| 5 | L2 | 200 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 4 | L0 | 399 | U | C2-N1-C1' | 7.52 | 126.72 | 117.70 |
| 4 | L0 | 332 | U | C2-N1-C1' | 7.50 | 126.69 | 117.70 |
| 5 | L2 | 201 | C | N3-C2-O2 | -7.48 | 116.66 | 121.90 |
| 53 | 8 | 954 | G | N3-C4-N9 | 7.48 | 130.49 | 126.00 |
| 4 | L0 | 241 | U | C2-N1-C1' | 7.45 | 126.64 | 117.70 |
| 22 | LN | 598 | LEU | CA-CB-CG | 7.41 | 132.34 | 115.30 |
| 4 | L0 | 531 | C | C2-N1-C1' | 7.39 | 126.93 | 118.80 |
| 15 | LF | 17 | LEU | CA-CB-CG | 7.38 | 132.27 | 115.30 |
| 53 | 8 | 954 | G | C8-N9-C1' | -7.37 | 117.42 | 127.00 |
| 53 | 8 | 1066 | C | N3-C2-O2 | -7.35 | 116.75 | 121.90 |
| 5 | L2 | 312 | U | N3-C2-O2 | -7.34 | 117.06 | 122.20 |
| 53 | 8 | 1066 | C | N1-C2-O2 | 7.33 | 123.30 | 118.90 |
| 41 | SM | 41 | PRO | C-N-CA | 7.32 | 139.99 | 121.70 |
| 47 | ST | 9 | LEU | CA-CB-CG | 7.32 | 132.13 | 115.30 |
| 23 | LO | 642 | ASP | CB-CG-OD2 | 7.28 | 124.86 | 118.30 |
| 4 | L0 | 215 | U | N1-C2-O2 | 7.28 | 127.90 | 122.80 |
| 4 | L0 | 110 | G | C4-N9-C1' | 7.25 | 135.92 | 126.50 |
| 17 | LH | 383 | LEU | CA-CB-CG | 7.23 | 131.93 | 115.30 |
| 29 | LV | 286 | GLU | CA-CB-CG | 7.23 | 129.31 | 113.40 |
| 4 | L0 | 332 | U | N3-C2-O2 | -7.23 | 117.14 | 122.20 |
| 4 | L0 | 215 | U | N3-C2-O2 | -7.21 | 117.16 | 122.20 |
| 53 | 8 | 975 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 4 | L0 | 215 | U | C2-N1-C1' | 7.16 | 126.29 | 117.70 |
| 53 | 8 | 1773 | C | N1-C2-O2 | 7.15 | 123.19 | 118.90 |
| 34 | SC | 306 | LEU | CA-CB-CG | 7.11 | 131.66 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | 8 | 975 | C | C6-N1-C2 | -7.10 | 117.46 | 120.30 |
| 38 | SI | 263 | LEU | CA-CB-CG | 7.09 | 131.61 | 115.30 |
| 4 | L0 | 216 | U | C2-N1-C1' | 7.05 | 126.16 | 117.70 |
| 8 | L5 | 55 | ASP | CB-CG-OD2 | 7.05 | 124.64 | 118.30 |
| 4 | L0 | 110 | G | N3-C4-N9 | 7.04 | 130.22 | 126.00 |
| 25 | LQ | 67 | LEU | CA-CB-CG | 7.04 | 131.49 | 115.30 |
| 53 | 8 | 190 | C | O4'-C1'-N1 | 7.04 | 113.83 | 108.20 |
| 63 | L6 | 20 | ASP | CB-CG-OD2 | 7.03 | 124.63 | 118.30 |
| 4 | L0 | 455 | C | C2-N1-C1' | 7.01 | 126.51 | 118.80 |
| 53 | 8 | 975 | C | N1-C2-O2 | 6.92 | 123.05 | 118.90 |
| 4 | L0 | 399 | U | N1-C2-O2 | 6.90 | 127.63 | 122.80 |
| 53 | 8 | 482 | U | N3-C2-O2 | -6.89 | 117.37 | 122.20 |
| 44 | SQ | 180 | ASP | CB-CG-OD2 | 6.89 | 124.50 | 118.30 |
| 10 | L8 | 96 | LEU | CA-CB-CG | 6.88 | 131.12 | 115.30 |
| 53 | 8 | 343 | C | N1-C2-O2 | 6.87 | 123.02 | 118.90 |
| 5 | L2 | 200 | C | C6-N1-C2 | -6.84 | 117.56 | 120.30 |
| 53 | 8 | 482 | U | N1-C2-O2 | 6.84 | 127.59 | 122.80 |
| 53 | 8 | 1115 | U | N3-C2-O2 | -6.84 | 117.42 | 122.20 |
| 4 | L0 | 203 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 47 | ST | 740 | MET | CA-CB-CG | 6.83 | 124.91 | 113.30 |
| 53 | 8 | 1115 | U | N1-C2-O2 | 6.82 | 127.58 | 122.80 |
| 53 | 8 | 38 | C | N1-C2-O2 | 6.81 | 122.99 | 118.90 |
| 11 | L9 | 157 | ASP | CB-CG-OD2 | 6.79 | 124.41 | 118.30 |
| 5 | L2 | 100 | U | N3-C2-O2 | -6.78 | 117.45 | 122.20 |
| 5 | L2 | 312 | U | N1-C2-O2 | 6.76 | 127.53 | 122.80 |
| 53 | 8 | 1220 | C | C6-N1-C2 | -6.76 | 117.59 | 120.30 |
| 53 | 8 | 54 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 53 | 8 | 517 | U | C2-N1-C1' | 6.74 | 125.79 | 117.70 |
| 4 | L0 | 64 | U | C2-N1-C1' | 6.73 | 125.78 | 117.70 |
| 53 | 8 | 150 | U | C2-N1-C1' | 6.73 | 125.78 | 117.70 |
| 53 | 8 | 1773 | C | C2-N1-C1' | 6.72 | 126.19 | 118.80 |
| 53 | 8 | 536 | C | C2-N1-C1' | 6.68 | 126.15 | 118.80 |
| 53 | 8 | 1571 | C | N3-C2-O2 | -6.67 | 117.23 | 121.90 |
| 53 | 8 | 1573 | A | P-O3'-C3' | 6.67 | 127.70 | 119.70 |
| 31 | LZ | 88 | LEU | CA-CB-CG | 6.63 | 130.55 | 115.30 |
| 4 | L0 | 110 | G | N3-C4-C5 | -6.62 | 125.29 | 128.60 |
| 44 | SQ | 72 | LEU | CA-CB-CG | 6.61 | 130.49 | 115.30 |
| 53 | 8 | 519 | C | C6-N1-C1' | -6.61 | 112.87 | 120.80 |
| 4 | L0 | 64 | U | N3-C2-O2 | -6.56 | 117.61 | 122.20 |
| 53 | 8 | 482 | U | C2-N1-C1' | 6.55 | 125.56 | 117.70 |
| 53 | 8 | 282 | C | N1-C2-O2 | 6.54 | 122.83 | 118.90 |
| 55 | LI | 721 | LEU | CA-CB-CG | 6.52 | 130.30 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4 | L0 | 284 | U | C2-N1-C1' | 6.51 | 125.51 | 117.70 |
| 53 | 8 | 1262 | U | N3-C2-O2 | -6.47 | 117.67 | 122.20 |
| 53 | 8 | 1773 | C | N3-C2-O2 | -6.46 | 117.38 | 121.90 |
| 53 | 8 | 990 | C | N1-C2-O2 | 6.44 | 122.77 | 118.90 |
| 27 | LT | 489 | MET | CB-CG-SD | 6.44 | 131.72 | 112.40 |
| 53 | 8 | 343 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 53 | 8 | 1057 | U | P-O3'-C3' | 6.43 | 127.42 | 119.70 |
| 25 | LQ | 752 | LEU | CA-CB-CG | 6.43 | 130.09 | 115.30 |
| 53 | 8 | 975 | C | C2-N1-C1' | 6.43 | 125.87 | 118.80 |
| 53 | 8 | 1571 | C | N1-C2-O2 | 6.42 | 122.75 | 118.90 |
| 53 | 8 | 258 | C | N3-C2-O2 | -6.40 | 117.42 | 121.90 |
| 28 | LU | 374 | LEU | CA-CB-CG | 6.40 | 130.01 | 115.30 |
| 35 | SE | 65 | LEU | CA-CB-CG | 6.39 | 130.00 | 115.30 |
| 5 | L2 | 100 | U | N1-C2-O2 | 6.38 | 127.26 | 122.80 |
| 4 | L0 | 543 | C | C6-N1-C2 | -6.36 | 117.75 | 120.30 |
| 53 | 8 | 532 | U | O5'-P-OP1 | 6.36 | 118.33 | 110.70 |
| 53 | 8 | 885 | G | N1-C6-O6 | -6.36 | 116.09 | 119.90 |
| 4 | L0 | 399 | U | C5-C6-N1 | 6.35 | 125.88 | 122.70 |
| 21 | LM | 367 | LEU | CA-CB-CG | 6.35 | 129.91 | 115.30 |
| 4 | L0 | 64 | U | N1-C2-O2 | 6.35 | 127.24 | 122.80 |
| 4 | L0 | 317 | C | N1-C2-O2 | 6.34 | 122.70 | 118.90 |
| 4 | L0 | 399 | U | N3-C2-O2 | -6.33 | 117.77 | 122.20 |
| 53 | 8 | 377 | G | C4-N9-C1' | 6.33 | 134.73 | 126.50 |
| 54 | SU | 499 | LEU | CA-CB-CG | 6.33 | 129.85 | 115.30 |
| 53 | 8 | 880 | C | C6-N1-C2 | -6.31 | 117.77 | 120.30 |
| 53 | 8 | 917 | U | C2-N1-C1' | 6.31 | 125.27 | 117.70 |
| 22 | LN | 225 | LEU | CA-CB-CG | 6.30 | 129.80 | 115.30 |
| 53 | 8 | 1215 | C | C6-N1-C1' | -6.30 | 113.24 | 120.80 |
| 18 | LJ | 313 | GLN | CA-CB-CG | 6.30 | 127.26 | 113.40 |
| 53 | 8 | 517 | U | N1-C2-O2 | 6.28 | 127.19 | 122.80 |
| 53 | 8 | 1123 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 53 | 8 | 54 | C | N1-C2-O2 | 6.24 | 122.64 | 118.90 |
| 15 | LF | 91 | LEU | CA-CB-CG | 6.23 | 129.63 | 115.30 |
| 58 | NE | 215 | LEU | CA-CB-CG | 6.23 | 129.62 | 115.30 |
| 4 | L0 | 110 | G | C8-N9-C1' | -6.22 | 118.92 | 127.00 |
| 5 | L2 | 49 | C | N1-C2-O2 | 6.20 | 122.62 | 118.90 |
| 27 | LT | 537 | LEU | CA-CB-CG | 6.19 | 129.55 | 115.30 |
| 4 | L0 | 241 | U | N3-C2-O2 | -6.18 | 117.87 | 122.20 |
| 7 | L4 | 87 | MET | CA-CB-CG | 6.18 | 123.81 | 113.30 |
| 45 | SR | 98 | GLU | CA-CB-CG | 6.18 | 127.00 | 113.40 |
| 4 | L0 | 144 | C | C2-N1-C1' | 6.17 | 125.59 | 118.80 |
| 53 | 8 | 589 | C | C2-N1-C1' | 6.17 | 125.58 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5 | L2 | 201 | C | C6-N1-C2 | -6.16 | 117.83 | 120.30 |
| 53 | 8 | 954 | G | N3-C4-C5 | -6.15 | 125.52 | 128.60 |
| 53 | 8 | 258 | C | C2-N1-C1' | 6.15 | 125.57 | 118.80 |
| 53 | 8 | 50 | C | C2-N1-C1' | 6.14 | 125.56 | 118.80 |
| 40 | SL | 117 | LEU | CA-CB-CG | 6.13 | 129.41 | 115.30 |
| 38 | SI | 1145 | MET | CA-CB-CG | 6.12 | 123.70 | 113.30 |
| 53 | 8 | 1619 | C | C6-N1-C1' | -6.12 | 113.46 | 120.80 |
| 53 | 8 | 343 | C | C2-N1-C1' | 6.11 | 125.52 | 118.80 |
| 53 | 8 | 1773 | C | C6-N1-C2 | -6.10 | 117.86 | 120.30 |
| 53 | 8 | 1619 | C | C6-N1-C2 | -6.09 | 117.86 | 120.30 |
| 53 | 8 | 519 | C | N3-C2-O2 | -6.08 | 117.64 | 121.90 |
| 56 | ND | 203 | ASP | CB-CG-OD2 | 6.07 | 123.76 | 118.30 |
| 4 | L0 | 340 | U | C2-N1-C1' | 6.07 | 124.98 | 117.70 |
| 53 | 8 | 354 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 63 | L6 | 63 | MET | CB-CG-SD | 6.03 | 130.49 | 112.40 |
| 53 | 8 | 199 | G | P-O3'-C3' | 6.02 | 126.93 | 119.70 |
| 5 | L2 | 200 | C | C5-C6-N1 | 6.02 | 124.01 | 121.00 |
| 28 | LU | 358 | MET | CA-CB-CG | 6.02 | 123.53 | 113.30 |
| 53 | 8 | 99 | C | C2-N1-C1' | 6.02 | 125.42 | 118.80 |
| 66 | 6 | 77 | MET | CB-CG-SD | 6.01 | 130.44 | 112.40 |
| 62 | LX | 209 | PRO | CA-N-CD | -6.01 | 103.08 | 111.50 |
| 53 | 8 | 1220 | C | C2-N1-C1' | 5.99 | 125.39 | 118.80 |
| 11 | L9 | 147 | MET | CB-CG-SD | 5.99 | 130.36 | 112.40 |
| 4 | L0 | 190 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 53 | 8 | 880 | C | C5-C6-N1 | 5.97 | 123.99 | 121.00 |
| 4 | L0 | 543 | C | C5-C6-N1 | 5.97 | 123.98 | 121.00 |
| 53 | 8 | 517 | U | N3-C2-O2 | -5.96 | 118.02 | 122.20 |
| 38 | SI | 555 | MET | CB-CG-SD | 5.96 | 130.28 | 112.40 |
| 42 | SN | 156 | MET | CB-CG-SD | 5.95 | 130.24 | 112.40 |
| 53 | 8 | 937 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 30 | LW | 160 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 53 | 8 | 0 | U | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 21 | LM | 234 | LEU | CA-CB-CG | 5.92 | 128.92 | 115.30 |
| 53 | 8 | 106 | U | N1-C2-O2 | 5.92 | 126.94 | 122.80 |
| 53 | 8 | -3 | U | P-O3'-C3' | 5.91 | 126.79 | 119.70 |
| 4 | L0 | 394 | U | C2-N1-C1' | 5.90 | 124.78 | 117.70 |
| 4 | L0 | 340 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 14 | LE | 94 | LEU | CA-CB-CG | 5.88 | 128.83 | 115.30 |
| 53 | 8 | 282 | C | C5-C6-N1 | 5.87 | 123.93 | 121.00 |
| 53 | 8 | 354 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 4 | L0 | 190 | U | N1-C2-O2 | 5.84 | 126.89 | 122.80 |
| 15 | LF | 40 | LEU | CA-CB-CG | 5.83 | 128.71 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 53 | 8 | 1638 | G | P-O3'-C3' | 5.83 | 126.70 | 119.70 |
| 53 | 8 | 294 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 53 | 8 | 448 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 15 | LF | 85 | PHE | CB-CG-CD1 | 5.81 | 124.87 | 120.80 |
| 53 | 8 | 1262 | U | N1-C2-O2 | 5.81 | 126.86 | 122.80 |
| 53 | 8 | 208 | U | C2-N1-C1' | 5.80 | 124.66 | 117.70 |
| 53 | 8 | 354 | C | C5-C6-N1 | 5.79 | 123.90 | 121.00 |
| 45 | SR | 93 | LEU | CA-CB-CG | 5.79 | 128.61 | 115.30 |
| 53 | 8 | 211 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 53 | 8 | 1115 | U | C2-N1-C1' | 5.79 | 124.64 | 117.70 |
| 4 | L0 | 241 | U | N1-C2-O2 | 5.78 | 126.85 | 122.80 |
| 53 | 8 | 54 | C | N3-C2-O2 | -5.78 | 117.85 | 121.90 |
| 5 | L2 | 312 | U | C2-N1-C1' | 5.78 | 124.63 | 117.70 |
| 1 | NA | 515 | MET | CA-CB-CG | 5.77 | 123.11 | 113.30 |
| 53 | 8 | 1215 | C | C5-C6-N1 | 5.77 | 123.88 | 121.00 |
| 31 | LZ | 170 | LEU | CA-CB-CG | 5.76 | 128.54 | 115.30 |
| 53 | 8 | 448 | C | C2-N1-C1' | 5.76 | 125.13 | 118.80 |
| 53 | 8 | 294 | C | C2-N1-C1' | 5.75 | 125.13 | 118.80 |
| 38 | SI | 608 | LEU | CA-CB-CG | 5.75 | 128.53 | 115.30 |
| 4 | L0 | 203 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 41 | SM | 124 | MET | CB-CG-SD | 5.75 | 129.64 | 112.40 |
| 30 | LW | 125 | LEU | CA-CB-CG | 5.74 | 128.49 | 115.30 |
| 34 | SD | 232 | MET | CA-CB-CG | 5.71 | 123.02 | 113.30 |
| 53 | 8 | 241 | U | C6-N1-C1' | -5.71 | 113.20 | 121.20 |
| 60 | SV | 185 | PRO | CA-N-CD | -5.70 | 103.51 | 111.50 |
| 53 | 8 | 917 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 4 | L0 | 20 | C | N1-C2-O2 | 5.69 | 122.31 | 118.90 |
| 53 | 8 | 106 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 35 | SF | 31 | ARG | CA-CB-CG | 5.69 | 125.91 | 113.40 |
| 4 | L0 | 203 | C | C2-N1-C1' | 5.69 | 125.05 | 118.80 |
| 53 | 8 | 885 | G | C5-C6-O6 | 5.67 | 132.00 | 128.60 |
| 17 | LH | 288 | LEU | CA-CB-CG | 5.67 | 128.34 | 115.30 |
| 25 | LQ | 810 | LEU | CA-CB-CG | 5.67 | 128.34 | 115.30 |
| 53 | 8 | 207 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 57 | LR | 631 | MET | CA-CB-CG | 5.67 | 122.93 | 113.30 |
| 4 | L0 | 91 | U | C2-N1-C1' | 5.66 | 124.49 | 117.70 |
| 2 | SA | 7 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 |
| 17 | LH | 664 | LEU | CA-CB-CG | 5.64 | 128.28 | 115.30 |
| 55 | LI | 534 | LEU | CA-CB-CG | 5.64 | 128.28 | 115.30 |
| 53 | 8 | 519 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 31 | LZ | 97 | LEU | CA-CB-CG | 5.62 | 128.22 | 115.30 |
| 38 | SI | 812 | MET | CA-CB-CG | 5.61 | 122.83 | 113.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | 8 | 38 | C | N3-C2-O2 | -5.60 | 117.98 | 121.90 |
| 15 | LF | 44 | LEU | CA-CB-CG | 5.60 | 128.17 | 115.30 |
| 37 | SH | 350 | MET | CB-CG-SD | 5.59 | 129.18 | 112.40 |
| 53 | 8 | 1686 | C | C2-N1-C1' | 5.58 | 124.94 | 118.80 |
| 53 | 8 | 347 | G | C4-N9-C1' | 5.58 | 133.75 | 126.50 |
| 62 | LX | 164 | MET | CG-SD-CE | 5.57 | 109.11 | 100.20 |
| 53 | 8 | 990 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 53 | 8 | 211 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 65 | 5 | 337 | MET | CA-CB-CG | 5.56 | 122.75 | 113.30 |
| 46 | SS | 892 | ASP | CB-CG-OD2 | 5.55 | 123.30 | 118.30 |
| 35 | SF | 50 | GLU | CA-CB-CG | 5.55 | 125.61 | 113.40 |
| 53 | 8 | 347 | G | C8-N9-C1' | -5.55 | 119.79 | 127.00 |
| 66 | 6 | 71 | TYR | CB-CG-CD1 | -5.54 | 117.68 | 121.00 |
| 60 | SV | 185 | PRO | N-CD-CG | -5.54 | 94.89 | 103.20 |
| 22 | LN | 272 | LEU | CA-CB-CG | 5.54 | 128.03 | 115.30 |
| 44 | SQ | 110 | ASP | CB-CG-OD1 | 5.54 | 123.28 | 118.30 |
| 47 | ST | 104 | MET | CB-CG-SD | 5.52 | 128.96 | 112.40 |
| 34 | SD | 210 | MET | CA-CB-CG | 5.51 | 122.68 | 113.30 |
| 45 | SR | 133 | LEU | CA-CB-CG | 5.49 | 127.93 | 115.30 |
| 4 | L0 | 531 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 4 | L0 | 543 | C | N1-C2-O2 | 5.47 | 122.19 | 118.90 |
| 53 | 8 | 519 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 5 | L2 | 72 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 62 | LX | 15 | ARG | CA-CB-CG | 5.46 | 125.42 | 113.40 |
| 4 | L0 | 264 | C | C2-N1-C1' | 5.46 | 124.80 | 118.80 |
| 38 | SI | 956 | MET | CB-CG-SD | 5.45 | 128.76 | 112.40 |
| 27 | LT | 494 | LEU | CA-CB-CG | 5.45 | 127.83 | 115.30 |
| 53 | 8 | 1620 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 4 | L0 | 347 | U | C2-N1-C1' | 5.43 | 124.22 | 117.70 |
| 17 | LH | 208 | LEU | CA-CB-CG | 5.43 | 127.78 | 115.30 |
| 5 | L2 | 72 | C | N3-C2-O2 | -5.41 | 118.11 | 121.90 |
| 53 | 8 | 1148 | C | C2-N1-C1' | 5.41 | 124.75 | 118.80 |
| 53 | 8 | 465 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 25 | LQ | 479 | LEU | CA-CB-CG | 5.41 | 127.74 | 115.30 |
| 29 | LV | 328 | MET | CA-CB-CG | 5.40 | 122.49 | 113.30 |
| 53 | 8 | 294 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 17 | LH | 507 | MET | CB-CG-SD | 5.39 | 128.56 | 112.40 |
| 4 | L0 | 455 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 65 | 5 | 472 | ILE | CG1-CB-CG2 | -5.37 | 99.58 | 111.40 |
| 53 | 8 | 943 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 53 | 8 | 1220 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 53 | 8 | 207 | U | N1-C2-O2 | 5.36 | 126.56 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | 8 | 372 | G | P-O3'-C3' | 5.36 | 126.13 | 119.70 |
| 53 | 8 | 377 | G | C8-N9-C1' | -5.33 | 120.06 | 127.00 |
| 53 | 8 | 880 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 53 | 8 | 1533 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 34 | SD | 259 | MET | CA-CB-CG | 5.33 | 122.35 | 113.30 |
| 53 | 8 | 1066 | C | C6-N1-C2 | -5.30 | 118.18 | 120.30 |
| 53 | 8 | 937 | C | N3-C2-O2 | -5.29 | 118.19 | 121.90 |
| 53 | 8 | 1448 | G | N3-C4-C5 | -5.29 | 125.95 | 128.60 |
| 4 | L0 | 394 | U | N3-C2-O2 | -5.28 | 118.50 | 122.20 |
| 25 | LQ | 185 | MET | CB-CG-SD | 5.27 | 128.22 | 112.40 |
| 44 | SQ | 216 | ARG | CA-CB-CG | 5.27 | 124.99 | 113.40 |
| 53 | 8 | 226 | A | C2-N3-C4 | 5.27 | 113.23 | 110.60 |
| 53 | 8 | 954 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 53 | 8 | 305 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 1 | NA | 382 | GLN | CA-CB-CG | 5.26 | 124.98 | 113.40 |
| 25 | LQ | 752 | LEU | CB-CG-CD2 | 5.26 | 119.95 | 111.00 |
| 10 | L8 | 184 | LEU | CB-CG-CD2 | 5.26 | 119.95 | 111.00 |
| 53 | 8 | 140 | A | C4-C5-N7 | -5.26 | 108.07 | 110.70 |
| 53 | 8 | 1175 | U | N1-C2-O2 | 5.26 | 126.48 | 122.80 |
| 16 | LG | 6 | PRO | N-CD-CG | -5.25 | 95.32 | 103.20 |
| 53 | 8 | 347 | G | N3-C4-N9 | 5.25 | 129.15 | 126.00 |
| 4 | L0 | 443 | G | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 |
| 53 | 8 | 917 | U | N3-C2-O2 | -5.25 | 118.53 | 122.20 |
| 4 | L0 | 374 | U | C2-N1-C1' | 5.24 | 123.99 | 117.70 |
| 53 | 8 | 941 | A | C4-N9-C1' | 5.24 | 135.74 | 126.30 |
| 53 | 8 | 208 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 59 | SB | 162 | MET | CA-CB-CG | 5.24 | 122.20 | 113.30 |
| 53 | 8 | 1200 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 9 | L7 | 8 | ILE | CG1-CB-CG2 | -5.23 | 99.90 | 111.40 |
| 53 | 8 | 962 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 53 | 8 | 484 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 5 | L2 | 39 | C | C5-C6-N1 | 5.21 | 123.61 | 121.00 |
| 13 | LD | 80 | MET | CB-CG-SD | 5.21 | 128.03 | 112.40 |
| 53 | 8 | 1448 | G | C4-N9-C1' | 5.20 | 133.25 | 126.50 |
| 38 | SI | 347 | LEU | CA-CB-CG | 5.19 | 127.25 | 115.30 |
| 53 | 8 | 1199 | G | C4-N9-C1' | 5.19 | 133.24 | 126.50 |
| 53 | 8 | 1645 | G | C4-N9-C1' | 5.19 | 133.24 | 126.50 |
| 2 | SA | 193 | MET | CA-CB-CG | 5.18 | 122.11 | 113.30 |
| 4 | L0 | 394 | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 4 | L0 | 531 | C | C6-N1-C1' | -5.18 | 114.58 | 120.80 |
| 4 | L0 | 340 | U | C5-C6-N1 | 5.17 | 125.28 | 122.70 |
| 53 | 8 | 377 | G | N3-C4-N9 | 5.17 | 129.10 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 53 | 8 | 448 | C | C5-C6-N1 | 5.17 | 123.58 | 121.00 |
| 38 | SI | 230 | MET | CB-CG-SD | 5.16 | 127.88 | 112.40 |
| 59 | SB | 421 | MET | CB-CG-SD | 5.15 | 127.86 | 112.40 |
| 62 | LX | 164 | MET | CA-CB-CG | 5.15 | 122.06 | 113.30 |
| 4 | L0 | 537 | G | N3-C4-N9 | 5.15 | 129.09 | 126.00 |
| 22 | LN | 240 | LEU | CA-CB-CG | 5.15 | 127.14 | 115.30 |
| 53 | 8 | 241 | U | C5-C6-N1 | 5.14 | 125.27 | 122.70 |
| 53 | 8 | 343 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 5 | L2 | 201 | C | C2-N1-C1' | 5.14 | 124.45 | 118.80 |
| 4 | L0 | 541 | U | N1-C2-O2 | 5.14 | 126.40 | 122.80 |
| 4 | L0 | 144 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 41 | SM | 42 | LEU | CA-CB-CG | 5.13 | 127.11 | 115.30 |
| 4 | L0 | 212 | U | C5-C6-N1 | 5.13 | 125.27 | 122.70 |
| 31 | LZ | 63 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 53 | 8 | 1653 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 53 | 8 | 1057 | U | OP1-P-O3' | 5.13 | 116.48 | 105.20 |
| 53 | 8 | 1191 | U | C2-N1-C1' | 5.12 | 123.84 | 117.70 |
| 46 | SS | 894 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 53 | 8 | 97 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 4 | L0 | 91 | U | C5-C4-O4 | -5.11 | 122.83 | 125.90 |
| 53 | 8 | 50 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 53 | 8 | 990 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 5 | L2 | 39 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 9 | L7 | 27 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 5 | L2 | 49 | C | N3-C2-O2 | -5.10 | 118.33 | 121.90 |
| 53 | 8 | 415 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 62 | LX | 44 | MET | CA-CB-CG | 5.09 | 121.96 | 113.30 |
| 4 | L0 | 317 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 4 | L0 | 347 | U | C5-C6-N1 | 5.09 | 125.25 | 122.70 |
| 11 | L9 | 25 | ASP | CB-CG-OD2 | -5.09 | 113.72 | 118.30 |
| 4 | L0 | 389 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 4 | L0 | 455 | C | C5-C6-N1 | 5.09 | 123.55 | 121.00 |
| 25 | LQ | 175 | ASP | CB-CG-OD1 | 5.09 | 122.88 | 118.30 |
| 4 | L0 | 455 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 12 | LC | 107 | LYS | CB-CG-CD | 5.08 | 124.81 | 111.60 |
| 53 | 8 | 937 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 13 | LD | 80 | MET | CB-CA-C | 5.08 | 120.56 | 110.40 |
| 15 | LF | 74 | LEU | CA-CB-CG | 5.08 | 126.98 | 115.30 |
| 54 | SU | 413 | MET | CB-CG-SD | 5.08 | 127.63 | 112.40 |
| 18 | LJ | 360 | MET | CA-CB-CG | 5.07 | 121.92 | 113.30 |
| 53 | 8 | 98 | U | C5-C6-N1 | 5.07 | 125.23 | 122.70 |
| 5 | L2 | 27 | U | N1-C2-O2 | 5.07 | 126.35 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5 | L2 | 102 | U | N1-C2-O2 | 5.06 | 126.34 | 122.80 |
| 53 | 8 | 1448 | G | N3-C4-N9 | 5.06 | 129.03 | 126.00 |
| 42 | SN | 156 | MET | CG-SD-CE | 5.06 | 108.29 | 100.20 |
| 40 | SL | 97 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 53 | 8 | 448 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 53 | 8 | 589 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 53 | 8 | 1646 | C | N1-C2-O2 | 5.04 | 121.92 | 118.90 |
| 17 | LH | 498 | LEU | CA-CB-CG | 5.03 | 126.88 | 115.30 |
| 36 | SG | 333 | MET | CA-CB-CG | 5.03 | 121.85 | 113.30 |
| 4 | L0 | 502 | G | C4-N9-C1' | 5.03 | 133.03 | 126.50 |
| 45 | SR | 101 | GLU | CA-CB-CG | 5.02 | 124.44 | 113.40 |
| 10 | L8 | 61 | GLU | CA-CB-CG | 5.02 | 124.44 | 113.40 |
| 53 | 8 | 305 | C | C2-N1-C1' | 5.02 | 124.32 | 118.80 |
| 53 | 8 | 377 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 53 | 8 | 1200 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 4 | L0 | 542 | U | C2-N1-C1' | 5.01 | 123.71 | 117.70 |
| 53 | 8 | 37 | U | N1-C2-O2 | 5.00 | 126.30 | 122.80 |
| 4 | L0 | 241 | U | C6-N1-C1' | -5.00 | 114.20 | 121.20 |
| 36 | SG | 114 | LYS | CA-CB-CG | 5.00 | 124.40 | 113.40 |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 65 | 5 | 450 | LEU | Peptide |
| 66 | 6 | 338 | THR | Peptide |
| 7 | L4 | 193 | GLY | Peptide |
| 7 | L4 | 195 | ILE | Peptide |
| 63 | L6 | 68 | LEU | Peptide |
| 9 | L7 | 12 | ALA | Peptide |
| 11 | L9 | 57 | ARG | Sidechain |
| 15 | LF | 31 | ASN | Peptide |
| 15 | LF | 51 | GLU | Peptide |
| 55 | LI | 257 | SER | Peptide |
| 22 | LN | 30 | ARG | Sidechain |
| 57 | LR | 626 | MET | Peptide |
| 29 | LV | 51 | GLN | Peptide |
| 29 | LV | 57 | GLU | Peptide |
| 1 | NA | 453 | SER | Peptide |
| 34 | SD | 321 | MET | Peptide |
| 35 | SE | 89 | ARG | Sidechain |
| 35 | SE | 9 | PHE | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 35 | SF | 9 | PHE | Peptide |
| 38 | SI | 198 | VAL | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | NA | 1667 | 0 | 1701 | 37 | 0 |
| 2 | SA | 2854 | 0 | 2792 | 42 | 0 |
| 3 | NB | 1098 | 0 | 1102 | 24 | 0 |
| 4 | L0 | 10405 | 0 | 5231 | 90 | 0 |
| 5 | L2 | 3585 | 0 | 1819 | 34 | 0 |
| 6 | L3 | 901 | 0 | 907 | 15 | 0 |
| 7 | L4 | 1810 | 0 | 1865 | 42 | 0 |
| 8 | L5 | 1669 | 0 | 1724 | 24 | 0 |
| 9 | L7 | 1321 | 0 | 1390 | 42 | 0 |
| 10 | L8 | 1349 | 0 | 1372 | 26 | 0 |
| 11 | L9 | 1415 | 0 | 1497 | 31 | 0 |
| 12 | LC | 973 | 0 | 1029 | 25 | 0 |
| 13 | LD | 1027 | 0 | 1084 | 24 | 0 |
| 14 | LE | 1003 | 0 | 1040 | 27 | 0 |
| 15 | LF | 715 | 0 | 744 | 14 | 0 |
| 16 | LG | 497 | 0 | 535 | 6 | 0 |
| 17 | LH | 6633 | 0 | 6510 | 99 | 0 |
| 18 | LJ | 3911 | 0 | 3906 | 68 | 0 |
| 19 | LK | 898 | 0 | 811 | 10 | 0 |
| 20 | LL | 3772 | 0 | 3806 | 55 | 0 |
| 21 | LM | 3443 | 0 | 3559 | 41 | 0 |
| 22 | LN | 5344 | 0 | 5301 | 100 | 0 |
| 23 | LO | 6635 | 0 | 6525 | 118 | 0 |
| 24 | LP | 2709 | 0 | 2371 | 26 | 0 |
| 25 | LQ | 6640 | 0 | 6503 | 108 | 0 |
| 26 | LS | 3791 | 0 | 3772 | 55 | 0 |
| 27 | LT | 6697 | 0 | 6676 | 99 | 0 |
| 28 | LU | 3725 | 0 | 3679 | 93 | 0 |
| 29 | LV | 2840 | 0 | 2685 | 68 | 0 |
| 30 | LW | 3428 | 0 | 3407 | 53 | 0 |
| 31 | LZ | 1530 | 0 | 1572 | 24 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 32 | NG | 543 | 0 | 277 | 3 | 0 |
| 33 | NK | 868 | 0 | 379 | 3 | 0 |
| 34 | SC | 1881 | 0 | 1928 | 28 | 0 |
| 34 | SD | 1782 | 0 | 1826 | 35 | 0 |
| 35 | SE | 916 | 0 | 964 | 19 | 0 |
| 35 | SF | 916 | 0 | 964 | 20 | 0 |
| 36 | SG | 3428 | 0 | 3446 | 76 | 0 |
| 37 | SH | 2781 | 0 | 2878 | 60 | 0 |
| 38 | SI | 6412 | 0 | 6498 | 127 | 0 |
| 39 | SJ | 1701 | 0 | 1767 | 29 | 0 |
| 39 | SK | 1799 | 0 | 1872 | 33 | 0 |
| 40 | SL | 1395 | 0 | 1476 | 29 | 0 |
| 41 | SM | 2296 | 0 | 2325 | 42 | 0 |
| 42 | SN | 2006 | 0 | 2118 | 39 | 0 |
| 43 | SO | 998 | 0 | 631 | 3 | 0 |
| 44 | SQ | 1137 | 0 | 1188 | 20 | 0 |
| 45 | SR | 792 | 0 | 847 | 23 | 0 |
| 46 | SS | 1466 | 0 | 1257 | 22 | 0 |
| 47 | ST | 4473 | 0 | 4057 | 53 | 0 |
| 48 | SY | 2016 | 0 | 2093 | 28 | 0 |
| 49 | SZ | 1295 | 0 | 571 | 2 | 0 |
| 50 | NJ | 1314 | 0 | 610 | 1 | 0 |
| 51 | NH | 5362 | 0 | 2295 | 13 | 0 |
| 52 | NI | 841 | 0 | 365 | 4 | 0 |
| 53 | 8 | 25439 | 0 | 12823 | 271 | 0 |
| 54 | SU | 3650 | 0 | 3365 | 37 | 0 |
| 55 | LI | 2690 | 0 | 1931 | 33 | 0 |
| 56 | ND | 495 | 0 | 561 | 13 | 0 |
| 57 | LR | 5957 | 0 | 5992 | 109 | 0 |
| 58 | NE | 1235 | 0 | 1243 | 20 | 0 |
| 59 | SB | 2985 | 0 | 2703 | 32 | 0 |
| 60 | SV | 381 | 0 | 255 | 6 | 0 |
| 61 | SP | 11108 | 0 | 4748 | 4 | 0 |
| 62 | LX | 5892 | 0 | 5420 | 87 | 0 |
| 62 | LY | 4132 | 0 | 1819 | 5 | 0 |
| 63 | L6 | 1327 | 0 | 1403 | 38 | 0 |
| 64 | NF | 614 | 0 | 279 | 7 | 0 |
| 65 | 5 | 2389 | 0 | 2411 | 36 | 0 |
| 66 | 6 | 2244 | 0 | 2245 | 38 | 0 |
| All | All | 213241 | 0 | 176745 | 2553 | 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 7.

All (2553) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:8:140:A:C4 | 53:8:140:A:C5 | 2.33 | 1.17 |
| 53:8:140:A:C4 | 63:L6:184:LEU:HA | 1.94 | 1.02 |
| 45:SR:41:SER:N | 53:8:600:U:HO2' | 1.68 | 0.91 |
| 53:8:140:A:C8 | 53:8:140:A:N7 | 2.40 | 0.88 |
| 53:8:140:A:C8 | 63:L6:184:LEU:CB | 2.59 | 0.86 |
| 53:8:140:A:C5 | 63:L6:184:LEU:HB2 | 2.10 | 0.85 |
| 53:8:140:A:N9 | 63:L6:184:LEU:HB3 | 1.92 | 0.83 |
| 53:8:140:A:C5 | 63:L6:184:LEU:CB | 2.64 | 0.81 |
| 53:8:140:A:C4 | 53:8:140:A:N9 | 2.49 | 0.80 |
| 53:8:140:A:C4 | 63:L6:184:LEU:CB | 2.65 | 0.80 |
| 27:LT:432:THR:HG1 | 27:LT:443:TRP:HE1 | 1.29 | 0.79 |
| 53:8:140:A:C5 | 53:8:140:A:N7 | 2.51 | 0.79 |
| 53:8:140:A:N9 | 63:L6:184:LEU:CB | 2.48 | 0.76 |
| 53:8:140:A:C8 | 63:L6:184:LEU:CA | 2.70 | 0.74 |
| 53:8:1695:G:N2 | 53:8:1706:C:C2 | 2.56 | 0.74 |
| 53:8:140:A:N7 | 63:L6:184:LEU:CB | 2.51 | 0.73 |
| 53:8:140:A:C4 | 63:L6:184:LEU:CA | 2.72 | 0.73 |
| 53:8:140:A:C8 | 53:8:140:A:N9 | 2.57 | 0.73 |
| 53:8:984:G:H1 | 53:8:1017:U:H3 | 1.36 | 0.72 |
| 53:8:1588:G:H1 | 53:8:1608:U:H3 | 1.39 | 0.70 |
| 53:8:140:A:C5 | 63:L6:184:LEU:CA | 2.74 | 0.70 |
| 28:LU:85:THR:HG1 | 28:LU:95:TRP:HE1 | 1.37 | 0.70 |
| 27:LT:584:HIS:HE2 | 27:LT:602:SER:HG | 1.39 | 0.70 |
| 5:L2:85:G:N7 | 59:SB:361:ARG:NH1 | 2.41 | 0.68 |
| 46:SS:316:ASN:HD21 | 46:SS:895:LYS:H | 1.42 | 0.68 |
| 29:LV:64:VAL:HG11 | 29:LV:323:VAL:HG22 | 1.76 | 0.67 |
| 31:LZ:109:ARG:HH22 | 31:LZ:155:GLU:HB2 | 1.59 | 0.67 |
| 62:LX:60:LYS:HG3 | 62:LX:61:LYS:HG2 | 1.76 | 0.67 |
| 25:LQ:137:ILE:HG23 | 25:LQ:147:VAL:HG22 | 1.75 | 0.66 |
| 53:8:140:A:N9 | 63:L6:184:LEU:CA | 2.59 | 0.66 |
| 18:LJ:108:TYR:HB3 | 18:LJ:117:LEU:H | 1.60 | 0.66 |
| 17:LH:630:LEU:HB2 | 17:LH:653:PHE:HB2 | 1.77 | 0.66 |
| 37:SH:315:LYS:HD2 | 37:SH:348:GLU:HB2 | 1.77 | 0.66 |
| 2:SA:191:PHE:HB3 | 2:SA:278:VAL:HG22 | 1.78 | 0.66 |
| 17:LH:17:GLY:HA2 | 17:LH:50:ASN:HD21 | 1.59 | 0.66 |
| 53:8:314:C:H42 | 53:8:354:C:H42 | 1.44 | 0.66 |
| 7:L4:71:LYS:HG2 | 7:L4:91:THR:HB | 1.77 | 0.66 |
| 22:LN:265:TRP:HA | 22:LN:272:LEU:HA | 1.78 | 0.66 |
| 62:LX:27:VAL:HG23 | 62:LX:150:ILE:HB | 1.78 | 0.66 |
| 27:LT:723:LEU:HD22 | 27:LT:879:GLU:HB2 | 1.76 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:8:140:A:C4 | 63:L6:184:LEU:HB2 | 2.30 | 0.65 |
| 39:SJ:44:VAL:HG12 | 39:SJ:113:TYR:HB2 | 1.78 | 0.65 |
| 57:LR:495:ASN:H | 57:LR:510:SER:HA | 1.61 | 0.65 |
| 9:L7:43:PHE:HB2 | 9:L7:60:ILE:HD11 | 1.77 | 0.65 |
| 25:LQ:588:ILE:HB | 25:LQ:600:TRP:HB2 | 1.77 | 0.65 |
| 25:LQ:594:ASP:HB2 | 53:8:1137:A:H1' | 1.78 | 0.65 |
| 37:SH:141:MET:HA | 37:SH:144:PHE:HB2 | 1.78 | 0.65 |
| 37:SH:181:HIS:HB3 | 37:SH:310:ARG:HH21 | 1.61 | 0.65 |
| 39:SK:51:GLU:HG2 | 39:SK:68:LEU:HD23 | 1.79 | 0.65 |
| 1:NA:516:SER:HB2 | 57:LR:691:PRO:HD2 | 1.79 | 0.65 |
| 10:L8:22:ARG:HH12 | 53:8:384:G:H5'' | 1.62 | 0.65 |
| 42:SN:63:LYS:HG2 | 42:SN:185:LYS:HB2 | 1.79 | 0.65 |
| 41:SM:100:LEU:HA | 41:SM:103:PHE:HB3 | 1.79 | 0.65 |
| 7:L4:151:ASP:HA | 63:L6:215:ARG:HH12 | 1.62 | 0.64 |
| 53:8:151:G:H22 | 53:8:163:G:H1 | 1.44 | 0.64 |
| 14:LE:51:GLU:HB2 | 14:LE:62:VAL:HB | 1.79 | 0.64 |
| 25:LQ:392:THR:HG21 | 25:LQ:411:ASN:H | 1.61 | 0.64 |
| 22:LN:482:ASP:HB2 | 22:LN:485:LYS:HB2 | 1.78 | 0.64 |
| 47:ST:647:ILE:HA | 47:ST:651:TRP:HB2 | 1.80 | 0.64 |
| 35:SE:58:CYS:HA | 35:SE:84:ARG:HD3 | 1.80 | 0.64 |
| 34:SD:171:LEU:HB2 | 34:SD:237:VAL:HG11 | 1.78 | 0.64 |
| 10:L8:44:HIS:HB3 | 10:L8:56:ARG:HB2 | 1.81 | 0.63 |
| 38:SI:828:ARG:NH1 | 45:SR:94:ASN:O | 2.28 | 0.63 |
| 1:NA:484:MET:SD | 23:LO:359:ARG:NH1 | 2.71 | 0.63 |
| 53:8:273:G:H1 | 53:8:284:G:H1' | 1.64 | 0.63 |
| 53:8:1711:C:N4 | 53:8:1713:G:N7 | 2.46 | 0.63 |
| 5:L2:12:U:H3 | 53:8:1112:G:H1 | 1.46 | 0.63 |
| 39:SK:44:VAL:HG22 | 39:SK:113:TYR:HB2 | 1.78 | 0.63 |
| 20:LL:281:ILE:HG12 | 20:LL:328:VAL:HB | 1.80 | 0.63 |
| 23:LO:717:LEU:HD23 | 23:LO:744:ARG:HG2 | 1.80 | 0.63 |
| 38:SI:924:VAL:O | 47:ST:109:ARG:NH1 | 2.30 | 0.63 |
| 30:LW:434:LEU:HD11 | 31:LZ:9:GLU:HB2 | 1.80 | 0.63 |
| 34:SC:149:SER:HB2 | 34:SC:180:SER:HB2 | 1.80 | 0.63 |
| 62:LX:641:ASN:HB3 | 62:LX:644:TYR:HB2 | 1.81 | 0.63 |
| 7:L4:206:ASP:HB2 | 7:L4:222:LEU:HB3 | 1.78 | 0.63 |
| 23:LO:20:ILE:H | 23:LO:307:THR:HG21 | 1.62 | 0.63 |
| 65:5:337:MET:SD | 65:5:341:LYS:NZ | 2.72 | 0.63 |
| 55:LI:604:LYS:HG3 | 55:LI:608:GLN:HE22 | 1.64 | 0.63 |
| 28:LU:315:PRO:HB2 | 46:SS:891:ILE:HD11 | 1.80 | 0.63 |
| 9:L7:140:VAL:HG12 | 9:L7:150:GLN:HB3 | 1.81 | 0.62 |
| 11:L9:60:LEU:HD21 | 11:L9:93:LEU:HB3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:SI:52:ARG:HH22 | 53:8:28:A:H4' | 1.64 | 0.62 |
| 9:L7:150:GLN:HE22 | 9:L7:181:ILE:HD13 | 1.64 | 0.62 |
| 57:LR:395:ASP:HB3 | 57:LR:404:ALA:HB3 | 1.81 | 0.62 |
| 29:LV:50:ILE:HG22 | 29:LV:51:GLN:HG3 | 1.81 | 0.62 |
| 36:SG:333:MET:HG3 | 36:SG:335:ARG:HG2 | 1.80 | 0.62 |
| 45:SR:98:GLU:OE2 | 45:SR:99:ASN:ND2 | 2.33 | 0.62 |
| 53:8:140:A:N7 | 63:L6:184:LEU:CA | 2.63 | 0.62 |
| 4:L0:551:A:N1 | 4:L0:586:A:N6 | 2.47 | 0.61 |
| 22:LN:139:CYS:SG | 22:LN:140:ASN:N | 2.72 | 0.61 |
| 27:LT:885:MET:HA | 27:LT:888:LEU:HB2 | 1.83 | 0.61 |
| 48:SY:10:LYS:NZ | 53:8:552:G:N7 | 2.48 | 0.61 |
| 57:LR:548:LEU:HB3 | 57:LR:560:TRP:HB2 | 1.81 | 0.61 |
| 57:LR:728:ILE:HA | 57:LR:731:LEU:HD12 | 1.82 | 0.61 |
| 63:L6:72:ARG:HA | 63:L6:98:ARG:HA | 1.80 | 0.61 |
| 1:NA:346:GLU:HB2 | 47:ST:766:ARG:HH12 | 1.65 | 0.61 |
| 6:L3:14:ILE:HG22 | 6:L3:23:ASP:HA | 1.80 | 0.61 |
| 23:LO:162:LEU:HB3 | 23:LO:172:ILE:HG12 | 1.83 | 0.61 |
| 27:LT:587:ARG:HH21 | 27:LT:605:LEU:HD11 | 1.65 | 0.61 |
| 30:LW:190:HIS:HD1 | 30:LW:207:THR:HG1 | 1.44 | 0.61 |
| 38:SI:944:ASN:ND2 | 38:SI:991:PHE:O | 2.33 | 0.61 |
| 42:SN:42:THR:H | 42:SN:195:ASN:HB2 | 1.64 | 0.61 |
| 14:LE:41:MET:HG2 | 14:LE:47:ILE:HG12 | 1.83 | 0.61 |
| 62:LX:786:LEU:HA | 62:LX:890:LEU:HD21 | 1.82 | 0.61 |
| 18:LJ:213:GLN:NE2 | 18:LJ:233:ASN:OD1 | 2.34 | 0.61 |
| 40:SL:27:LYS:NZ | 40:SL:28:ASN:OD1 | 2.33 | 0.61 |
| 62:LY:899:ALA:HB1 | 62:LY:905:PRO:HA | 1.83 | 0.61 |
| 2:SA:155:GLY:HA2 | 34:SC:233:LEU:HD23 | 1.83 | 0.61 |
| 4:L0:123:C:N4 | 54:SU:134:PHE:O | 2.34 | 0.61 |
| 22:LN:247:LEU:HD23 | 22:LN:292:ASN:HB3 | 1.83 | 0.61 |
| 27:LT:28:ARG:HH11 | 27:LT:30:ILE:HD13 | 1.66 | 0.61 |
| 27:LT:509:SER:OG | 27:LT:510:LEU:N | 2.34 | 0.61 |
| 22:LN:186:GLN:NE2 | 22:LN:205:CYS:SG | 2.74 | 0.61 |
| 25:LQ:26:ILE:HB | 25:LQ:40:GLN:HB2 | 1.83 | 0.61 |
| 39:SK:24:VAL:HG12 | 54:SU:487:PRO:HB2 | 1.81 | 0.61 |
| 4:L0:135:G:O2' | 20:LL:494:ARG:NH1 | 2.33 | 0.60 |
| 9:L7:162:ILE:HA | 9:L7:165:LYS:HG2 | 1.83 | 0.60 |
| 35:SE:17:THR:HA | 35:SE:20:ILE:HG22 | 1.83 | 0.60 |
| 18:LJ:197:ASP:HB2 | 18:LJ:206:ILE:HD11 | 1.84 | 0.60 |
| 21:LM:194:SER:HB2 | 27:LT:335:VAL:HG11 | 1.81 | 0.60 |
| 27:LT:311:VAL:HG22 | 27:LT:321:GLU:HG2 | 1.83 | 0.60 |
| 29:LV:288:LYS:HB3 | 29:LV:299:ILE:HD11 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:L7:166:LEU:HD13 | 9:L7:183:PHE:HB2 | 1.82 | 0.60 |
| 23:LO:673:ARG:HG3 | 23:LO:675:MET:H | 1.67 | 0.60 |
| 53:8:185:U:H3' | 53:8:186:C:H4' | 1.83 | 0.60 |
| 57:LR:64:ILE:HA | 57:LR:80:SER:HA | 1.82 | 0.60 |
| 29:LV:263:SER:OG | 29:LV:264:ILE:N | 2.35 | 0.60 |
| 66:6:238:ASN:OD1 | 66:6:241:ARG:NH2 | 2.35 | 0.60 |
| 4:L0:219:U:H5' | 56:ND:204:ARG:HH12 | 1.66 | 0.60 |
| 12:LC:98:ASP:OD2 | 27:LT:488:ASN:ND2 | 2.35 | 0.60 |
| 23:LO:440:PRO:HG3 | 23:LO:483:GLN:HA | 1.84 | 0.60 |
| 42:SN:103:VAL:HG11 | 42:SN:131:VAL:HG21 | 1.82 | 0.60 |
| 21:LM:366:ILE:HA | 21:LM:369:LEU:HB2 | 1.84 | 0.60 |
| 62:LX:621:GLN:HB3 | 62:LX:784:ARG:HH12 | 1.66 | 0.60 |
| 47:ST:700:LEU:HD21 | 54:SU:467:ALA:HB2 | 1.84 | 0.60 |
| 57:LR:171:MET:HB3 | 57:LR:187:GLN:HA | 1.84 | 0.60 |
| 17:LH:497:ASP:HB2 | 17:LH:510:TYR:HB3 | 1.83 | 0.59 |
| 23:LO:10:LEU:HD13 | 23:LO:702:LEU:HD23 | 1.84 | 0.59 |
| 57:LR:540:SER:HB2 | 57:LR:549:ALA:HB3 | 1.84 | 0.59 |
| 2:SA:385:MET:HG2 | 35:SF:63:ILE:HB | 1.83 | 0.59 |
| 57:LR:290:ILE:HA | 57:LR:306:LEU:HA | 1.84 | 0.59 |
| 4:L0:174:U:O2' | 4:L0:222:G:N2 | 2.35 | 0.59 |
| 36:SG:368:LEU:HD23 | 36:SG:371:ARG:HD3 | 1.83 | 0.59 |
| 36:SG:481:ILE:HD13 | 36:SG:486:VAL:HG13 | 1.84 | 0.59 |
| 36:SG:541:ALA:HB3 | 36:SG:564:TYR:HB3 | 1.84 | 0.59 |
| 38:SI:925:ASN:OD1 | 47:ST:109:ARG:NH1 | 2.35 | 0.59 |
| 15:LF:83:LYS:HE3 | 15:LF:91:LEU:HD12 | 1.85 | 0.59 |
| 44:SQ:131:ASP:HB3 | 44:SQ:134:ARG:HG2 | 1.85 | 0.59 |
| 5:L2:82:G:N7 | 35:SE:38:ASN:ND2 | 2.47 | 0.59 |
| 12:LC:121:SER:OG | 12:LC:123:ARG:NH1 | 2.36 | 0.59 |
| 28:LU:226:LYS:HG2 | 28:LU:268:CYS:HA | 1.85 | 0.59 |
| 28:LU:332:TYR:HB3 | 28:LU:339:SER:HA | 1.83 | 0.59 |
| 38:SI:1122:ALA:HB2 | 44:SQ:194:ILE:HD12 | 1.83 | 0.59 |
| 13:LD:87:ARG:HH21 | 13:LD:106:ASN:HD21 | 1.50 | 0.59 |
| 28:LU:133:GLN:HE22 | 28:LU:169:GLU:HG2 | 1.67 | 0.59 |
| 4:L0:87:C:O2 | 17:LH:332:GLN:NE2 | 2.36 | 0.59 |
| 13:LD:33:ARG:NH2 | 13:LD:53:TYR:O | 2.36 | 0.59 |
| 18:LJ:275:SER:HB3 | 18:LJ:305:CYS:HB3 | 1.84 | 0.59 |
| 22:LN:470:LEU:HD11 | 22:LN:498:VAL:HG11 | 1.85 | 0.59 |
| 23:LO:347:SER:HB2 | 23:LO:365:GLU:H | 1.68 | 0.59 |
| 15:LF:54:ALA:HB2 | 15:LF:79:VAL:HG12 | 1.84 | 0.58 |
| 23:LO:79:ALA:HB3 | 23:LO:93:PHE:HB3 | 1.85 | 0.58 |
| 29:LV:121:ARG:HH12 | 53:8:340:U:H5'' | 1.66 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:NA:370:ARG:HH22 | 47:ST:52:ARG:HD3 | 1.69 | 0.58 |
| 2:SA:185:ASP:O | 2:SA:189:ASN:ND2 | 2.36 | 0.58 |
| 4:L0:335:G:H1 | 4:L0:389:U:H3 | 1.51 | 0.58 |
| 5:L2:256:G:N7 | 35:SF:38:ASN:ND2 | 2.51 | 0.58 |
| 22:LN:489:CYS:HB2 | 22:LN:534:LEU:HD11 | 1.85 | 0.58 |
| 27:LT:128:LEU:HB3 | 27:LT:140:TYR:HB2 | 1.85 | 0.58 |
| 36:SG:198:LYS:HE2 | 36:SG:212:LYS:HB2 | 1.84 | 0.58 |
| 2:SA:277:ARG:NH2 | 59:SB:261:GLN:OE1 | 2.36 | 0.58 |
| 17:LH:320:VAL:HG22 | 17:LH:335:PRO:HA | 1.84 | 0.58 |
| 22:LN:166:VAL:HG22 | 22:LN:182:ILE:HG12 | 1.85 | 0.58 |
| 57:LR:439:ALA:HB3 | 57:LR:457:ALA:HB3 | 1.85 | 0.58 |
| 63:L6:67:VAL:H | 63:L6:100:ALA:HB2 | 1.68 | 0.58 |
| 11:L9:57:ARG:NH2 | 40:SL:87:MET:O | 2.36 | 0.58 |
| 35:SF:22:ASP:O | 35:SF:26:GLN:NE2 | 2.36 | 0.58 |
| 62:LX:585:VAL:HB | 62:LX:639:ALA:HB3 | 1.85 | 0.58 |
| 9:L7:163:ASP:OD1 | 9:L7:163:ASP:N | 2.34 | 0.58 |
| 28:LU:114:THR:HG1 | 28:LU:139:CYS:HG | 1.51 | 0.58 |
| 36:SG:333:MET:SD | 36:SG:350:LYS:NZ | 2.76 | 0.58 |
| 36:SG:442:ILE:HA | 36:SG:472:PRO:HA | 1.84 | 0.58 |
| 41:SM:123:VAL:HG23 | 41:SM:126:ASN:HB2 | 1.86 | 0.58 |
| 63:L6:105:ASP:OD2 | 63:L6:105:ASP:N | 2.35 | 0.58 |
| 10:L8:98:LYS:HD2 | 10:L8:172:ARG:HG2 | 1.84 | 0.58 |
| 29:LV:162:LEU:HB3 | 29:LV:176:PHE:HB2 | 1.85 | 0.58 |
| 1:NA:366:GLU:HA | 1:NA:369:ILE:HD12 | 1.86 | 0.58 |
| 38:SI:1059:ARG:NH1 | 48:SY:33:ASP:OD2 | 2.35 | 0.58 |
| 62:LX:12:SER:O | 62:LX:16:ASN:ND2 | 2.37 | 0.58 |
| 66:6:64:LYS:HB2 | 66:6:110:VAL:HG11 | 1.85 | 0.58 |
| 4:L0:471:C:OP1 | 21:LM:27:LYS:NZ | 2.37 | 0.58 |
| 22:LN:384:VAL:HG23 | 22:LN:391:VAL:HG12 | 1.86 | 0.58 |
| 30:LW:354:CYS:SG | 30:LW:364:ARG:NH2 | 2.77 | 0.58 |
| 37:SH:289:VAL:O | 37:SH:317:GLN:NE2 | 2.36 | 0.58 |
| 1:NA:470:GLU:HG3 | 1:NA:490:LEU:HB2 | 1.86 | 0.58 |
| 25:LQ:447:LEU:HB3 | 25:LQ:455:GLN:HB2 | 1.86 | 0.58 |
| 54:SU:350:MET:O | 54:SU:355:ARG:NH1 | 2.37 | 0.58 |
| 65:5:337:MET:O | 66:6:96:ARG:NH2 | 2.37 | 0.58 |
| 8:L5:76:ARG:NH1 | 12:LC:120:ASP:OD2 | 2.37 | 0.58 |
| 26:LS:254:LEU:HD22 | 26:LS:263:LEU:HD11 | 1.86 | 0.58 |
| 42:SN:93:THR:HG22 | 42:SN:177:ARG:HB2 | 1.86 | 0.58 |
| 57:LR:440:VAL:HG12 | 57:LR:456:THR:HG22 | 1.85 | 0.58 |
| 34:SD:105:LEU:HD21 | 48:SY:124:GLN:HA | 1.86 | 0.57 |
| 53:8:538:A:H5' | 53:8:543:C:H41 | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:L7:74:GLN:HG2 | 9:L7:92:PHE:HD2 | 1.68 | 0.57 |
| 26:LS:568:VAL:HG23 | 26:LS:579:VAL:HG22 | 1.87 | 0.57 |
| 45:SR:41:SER:N | 53:8:600:U:O2' | 2.36 | 0.57 |
| 53:8:376:C:O2' | 53:8:378:A:N7 | 2.36 | 0.57 |
| 53:8:965:U:H5'' | 64:NF:126:ALA:HB2 | 1.86 | 0.57 |
| 65:5:193:ARG:HH11 | 66:6:75:LEU:HD13 | 1.69 | 0.57 |
| 1:NA:483:TYR:OH | 27:LT:736:HIS:ND1 | 2.37 | 0.57 |
| 25:LQ:196:CYS:SG | 25:LQ:197:ILE:N | 2.76 | 0.57 |
| 36:SG:402:ILE:HA | 36:SG:417:SER:HA | 1.86 | 0.57 |
| 38:SI:761:GLN:O | 38:SI:765:ASN:ND2 | 2.38 | 0.57 |
| 44:SQ:110:ASP:O | 44:SQ:114:ARG:NH2 | 2.38 | 0.57 |
| 48:SY:140:ARG:NH1 | 56:ND:166:LEU:O | 2.37 | 0.57 |
| 48:SY:154:THR:HA | 48:SY:168:LYS:HG3 | 1.86 | 0.57 |
| 53:8:1161:C:H1' | 53:8:1619:C:H41 | 1.69 | 0.57 |
| 9:L7:151:LYS:HE2 | 9:L7:184:GLU:HB3 | 1.86 | 0.57 |
| 22:LN:583:VAL:HG22 | 22:LN:593:GLU:HG3 | 1.86 | 0.57 |
| 27:LT:28:ARG:HH21 | 27:LT:71:VAL:HG11 | 1.69 | 0.57 |
| 37:SH:123:ALA:HB1 | 37:SH:261:ILE:HG21 | 1.85 | 0.57 |
| 44:SQ:202:ARG:O | 53:8:1489:U:N3 | 2.37 | 0.57 |
| 47:ST:478:ILE:HG12 | 47:ST:524:LEU:HD13 | 1.86 | 0.57 |
| 61:SP:1475:GLN:HA | 61:SP:1517:HIS:HA | 1.85 | 0.57 |
| 10:L8:98:LYS:HB3 | 53:8:329:G:H5'' | 1.87 | 0.57 |
| 17:LH:602:PRO:HB3 | 55:LI:591:THR:HB | 1.87 | 0.57 |
| 26:LS:312:ILE:HB | 26:LS:324:TRP:HB3 | 1.87 | 0.57 |
| 29:LV:56:SER:HA | 29:LV:336:ILE:HA | 1.86 | 0.57 |
| 35:SF:22:ASP:OD2 | 36:SG:342:ARG:NH2 | 2.37 | 0.57 |
| 40:SL:171:PRO:HA | 40:SL:184:LYS:HB2 | 1.86 | 0.57 |
| 57:LR:786:ILE:HG13 | 57:LR:787:PRO:HD3 | 1.86 | 0.57 |
| 65:5:444:ALA:O | 65:5:448:ASN:ND2 | 2.38 | 0.57 |
| 1:NA:326:LEU:O | 38:SI:930:LYS:NZ | 2.32 | 0.57 |
| 18:LJ:48:ASN:ND2 | 18:LJ:51:HIS:O | 2.38 | 0.57 |
| 21:LM:123:ARG:O | 21:LM:126:GLN:NE2 | 2.37 | 0.57 |
| 25:LQ:760:ILE:HA | 25:LQ:763:ILE:HB | 1.85 | 0.57 |
| 53:8:966:A:OP2 | 64:NF:126:ALA:N | 2.26 | 0.57 |
| 3:NB:507:ILE:HG22 | 3:NB:510:LYS:HE3 | 1.87 | 0.57 |
| 4:L0:337:G:OP1 | 58:NE:209:ARG:NH2 | 2.38 | 0.57 |
| 8:L5:60:ASP:HA | 8:L5:65:ARG:HH22 | 1.70 | 0.57 |
| 26:LS:538:LYS:HE2 | 26:LS:563:GLY:HA2 | 1.87 | 0.57 |
| 41:SM:282:ARG:NH2 | 53:8:560:U:OP2 | 2.37 | 0.57 |
| 57:LR:313:LEU:HB3 | 57:LR:331:SER:HB3 | 1.86 | 0.57 |
| 28:LU:298:LEU:O | 28:LU:457:ARG:NH1 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:8:579:A:H4' | 53:8:580:A:H5' | 1.87 | 0.57 |
| 55:LI:165:SER:HA | 55:LI:181:ASP:HA | 1.85 | 0.57 |
| 7:L4:200:ARG:NH1 | 7:L4:206:ASP:OD1 | 2.37 | 0.57 |
| 17:LH:867:VAL:HG22 | 17:LH:895:LEU:HD21 | 1.87 | 0.57 |
| 25:LQ:114:LEU:HG | 25:LQ:115:LEU:HG | 1.85 | 0.57 |
| 62:LX:104:ARG:NH1 | 62:LX:105:TYR:O | 2.38 | 0.57 |
| 20:LL:516:ILE:HD12 | 20:LL:517:PRO:HD2 | 1.87 | 0.56 |
| 38:SI:1062:ARG:NH2 | 53:8:1490:C:OP1 | 2.38 | 0.56 |
| 14:LE:15:ASN:ND2 | 14:LE:72:CYS:O | 2.38 | 0.56 |
| 25:LQ:433:ALA:HA | 25:LQ:449:THR:HA | 1.87 | 0.56 |
| 29:LV:66:ARG:HH12 | 29:LV:108:SER:HB2 | 1.68 | 0.56 |
| 35:SE:24:VAL:HG12 | 35:SE:102:ILE:HD11 | 1.85 | 0.56 |
| 39:SK:190:GLN:NE2 | 39:SK:244:GLY:O | 2.38 | 0.56 |
| 4:L0:293:U:H3 | 23:LO:632:SER:HB3 | 1.70 | 0.56 |
| 22:LN:481:ILE:HA | 22:LN:536:VAL:HG21 | 1.87 | 0.56 |
| 26:LS:448:LYS:NZ | 26:LS:449:ASP:O | 2.34 | 0.56 |
| 28:LU:344:HIS:NE2 | 28:LU:418:HIS:O | 2.39 | 0.56 |
| 37:SH:281:GLU:OE1 | 38:SI:625:TRP:NE1 | 2.38 | 0.56 |
| 41:SM:93:SER:O | 41:SM:119:ARG:NH1 | 2.39 | 0.56 |
| 53:8:111:U:HO2' | 53:8:112:A:H8 | 1.53 | 0.56 |
| 53:8:140:A:C5 | 63:L6:184:LEU:HA | 2.41 | 0.56 |
| 53:8:312:A:H2 | 53:8:315:A:H5' | 1.71 | 0.56 |
| 63:L6:10:ASN:ND2 | 63:L6:127:THR:O | 2.37 | 0.56 |
| 1:NA:480:GLN:O | 27:LT:743:ARG:NH2 | 2.39 | 0.56 |
| 4:L0:274:C:H2' | 4:L0:275:A:H8 | 1.70 | 0.56 |
| 11:L9:77:ILE:HG21 | 11:L9:91:LYS:HA | 1.87 | 0.56 |
| 15:LF:15:ASN:HB3 | 15:LF:20:ARG:HB2 | 1.87 | 0.56 |
| 17:LH:536:ASP:N | 17:LH:536:ASP:OD1 | 2.38 | 0.56 |
| 28:LU:258:ILE:HD12 | 28:LU:294:LEU:HB3 | 1.86 | 0.56 |
| 53:8:877:G:O2' | 53:8:942:G:N2 | 2.39 | 0.56 |
| 9:L7:20:VAL:HA | 9:L7:23:ALA:HB3 | 1.86 | 0.56 |
| 17:LH:559:LYS:HG2 | 17:LH:612:SER:HA | 1.86 | 0.56 |
| 31:LZ:151:THR:HB | 31:LZ:154:MET:HB2 | 1.87 | 0.56 |
| 42:SN:74:LEU:HD23 | 42:SN:100:ILE:HD12 | 1.88 | 0.56 |
| 45:SR:65:ASN:HB3 | 45:SR:90:ASP:HB2 | 1.88 | 0.56 |
| 28:LU:262:MET:O | 28:LU:281:ASN:ND2 | 2.39 | 0.56 |
| 30:LW:178:ASP:HB2 | 30:LW:184:LEU:HD21 | 1.87 | 0.56 |
| 36:SG:523:LYS:NZ | 36:SG:524:ILE:O | 2.38 | 0.56 |
| 55:LI:555:ILE:O | 55:LI:585:ARG:NH1 | 2.39 | 0.56 |
| 4:L0:375:C:OP2 | 46:SS:834:LYS:NZ | 2.39 | 0.56 |
| 7:L4:24:SER:HB2 | 66:6:289:PHE:HZ | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:L9:79:ARG:HD2 | 66:6:323:GLU:HB3 | 1.87 | 0.56 |
| 17:LH:682:ASN:HB2 | 17:LH:689:ILE:HD11 | 1.88 | 0.56 |
| 39:SK:83:ASP:N | 39:SK:83:ASP:OD1 | 2.39 | 0.56 |
| 40:SL:163:ARG:HD2 | 53:8:15:U:H4' | 1.88 | 0.56 |
| 9:L7:150:GLN:NE2 | 9:L7:180:GLN:O | 2.38 | 0.56 |
| 10:L8:67:TRP:HA | 10:L8:183:ILE:HG22 | 1.88 | 0.56 |
| 26:LS:272:LEU:HD12 | 26:LS:288:LEU:HD23 | 1.87 | 0.56 |
| 27:LT:510:LEU:O | 27:LT:553:ARG:NH1 | 2.39 | 0.56 |
| 37:SH:256:TYR:HD1 | 37:SH:283:ILE:HG12 | 1.69 | 0.56 |
| 42:SN:56:ILE:HD13 | 42:SN:183:ILE:HG13 | 1.88 | 0.56 |
| 53:8:1468:U:H2' | 53:8:1469:A:H8 | 1.71 | 0.56 |
| 5:L2:34:A:N7 | 31:LZ:7:HIS:ND1 | 2.51 | 0.56 |
| 9:L7:164:TYR:HD2 | 46:SS:278:ILE:HD13 | 1.69 | 0.56 |
| 29:LV:126:GLN:NE2 | 29:LV:129:GLY:O | 2.39 | 0.56 |
| 37:SH:111:LYS:NZ | 38:SI:921:GLU:OE2 | 2.37 | 0.56 |
| 57:LR:416:ARG:H | 57:LR:425:ASP:HB2 | 1.71 | 0.56 |
| 17:LH:690:ASN:HD22 | 17:LH:750:LEU:HB2 | 1.70 | 0.56 |
| 36:SG:356:ARG:NH1 | 66:6:260:ALA:O | 2.38 | 0.56 |
| 37:SH:330:LYS:NZ | 38:SI:554:TYR:O | 2.39 | 0.56 |
| 41:SM:42:LEU:HD12 | 58:NE:218:LEU:HB3 | 1.88 | 0.56 |
| 15:LF:5:VAL:O | 15:LF:43:LYS:NZ | 2.38 | 0.55 |
| 20:LL:167:SER:O | 20:LL:168:HIS:ND1 | 2.39 | 0.55 |
| 47:ST:616:LEU:HB3 | 47:ST:619:LEU:HB2 | 1.86 | 0.55 |
| 4:L0:169:A:N7 | 22:LN:236:LYS:NZ | 2.53 | 0.55 |
| 11:L9:17:ARG:NH2 | 53:8:22:A:OP1 | 2.40 | 0.55 |
| 14:LE:41:MET:SD | 14:LE:41:MET:N | 2.70 | 0.55 |
| 28:LU:90:GLY:HA2 | 28:LU:113:VAL:HG23 | 1.89 | 0.55 |
| 28:LU:457:ARG:NH2 | 53:8:1:U:O4 | 2.39 | 0.55 |
| 34:SD:320:TYR:OH | 34:SD:323:SER:OG | 2.24 | 0.55 |
| 57:LR:513:LYS:HG2 | 57:LR:535:GLY:HA2 | 1.88 | 0.55 |
| 57:LR:596:ASP:OD1 | 57:LR:596:ASP:N | 2.39 | 0.55 |
| 23:LO:88:ASN:ND2 | 27:LT:659:GLN:O | 2.40 | 0.55 |
| 47:ST:482:GLN:HB2 | 47:ST:524:LEU:HD11 | 1.87 | 0.55 |
| 53:8:235:G:N2 | 53:8:236:A:N7 | 2.53 | 0.55 |
| 57:LR:296:ILE:HG22 | 57:LR:298:SER:H | 1.71 | 0.55 |
| 57:LR:679:THR:OG1 | 57:LR:680:ASN:N | 2.39 | 0.55 |
| 39:SK:70:CYS:SG | 53:8:1192:C:N4 | 2.79 | 0.55 |
| 57:LR:227:MET:N | 57:LR:227:MET:SD | 2.78 | 0.55 |
| 4:L0:89:C:OP1 | 26:LS:319:ARG:NH1 | 2.39 | 0.55 |
| 23:LO:411:VAL:HG23 | 23:LO:425:PHE:HB2 | 1.89 | 0.55 |
| 23:LO:624:ASN:ND2 | 23:LO:676:ARG:O | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:SD:314:CYS:SG | 34:SD:315:ILE:N | 2.79 | 0.55 |
| 53:8:911:U:OP1 | 57:LR:534:ARG:NE | 2.38 | 0.55 |
| 1:NA:534:ARG:NH2 | 53:8:1641:C:OP2 | 2.39 | 0.55 |
| 3:NB:544:ILE:O | 38:SI:193:ARG:NH2 | 2.40 | 0.55 |
| 17:LH:71:ASN:HD22 | 17:LH:74:LEU:HG | 1.70 | 0.55 |
| 17:LH:368:ASP:HB3 | 17:LH:389:LEU:HD13 | 1.88 | 0.55 |
| 20:LL:110:ILE:HD12 | 20:LL:119:CYS:HB3 | 1.88 | 0.55 |
| 34:SC:171:LEU:HB2 | 34:SC:237:VAL:HG11 | 1.88 | 0.55 |
| 47:ST:422:LEU:HA | 47:ST:425:PHE:HB3 | 1.87 | 0.55 |
| 19:LK:496:LEU:HA | 19:LK:499:ILE:HD12 | 1.89 | 0.55 |
| 22:LN:542:VAL:HG23 | 22:LN:552:ILE:HG13 | 1.88 | 0.55 |
| 30:LW:40:LYS:HA | 30:LW:43:ARG:HG2 | 1.89 | 0.55 |
| 36:SG:164:GLN:NE2 | 36:SG:528:GLU:O | 2.40 | 0.55 |
| 39:SJ:100:LEU:O | 39:SJ:105:ASN:ND2 | 2.38 | 0.55 |
| 39:SK:144:LEU:HB2 | 39:SK:150:ILE:HD11 | 1.88 | 0.55 |
| 47:ST:548:ARG:NH2 | 47:ST:638:ASN:OD1 | 2.39 | 0.55 |
| 58:NE:265:SER:O | 58:NE:273:ARG:NH1 | 2.40 | 0.55 |
| 10:L8:81:VAL:HA | 10:L8:102:VAL:HA | 1.87 | 0.55 |
| 12:LC:31:VAL:HG22 | 12:LC:67:VAL:HB | 1.88 | 0.55 |
| 29:LV:152:ASP:OD1 | 29:LV:152:ASP:N | 2.40 | 0.55 |
| 38:SI:855:GLN:HE21 | 38:SI:1016:ASN:HD22 | 1.55 | 0.55 |
| 47:ST:734:ARG:O | 47:ST:738:ASN:ND2 | 2.39 | 0.55 |
| 5:L2:15:U:OP2 | 58:NE:224:HIS:NE2 | 2.38 | 0.55 |
| 9:L7:162:ILE:O | 9:L7:166:LEU:N | 2.39 | 0.55 |
| 14:LE:11:LEU:HD21 | 14:LE:37:PHE:HE1 | 1.72 | 0.55 |
| 21:LM:196:LEU:HD11 | 21:LM:213:THR:HG21 | 1.89 | 0.55 |
| 23:LO:556:ARG:NH2 | 23:LO:575:GLU:OE1 | 2.40 | 0.55 |
| 28:LU:228:ASN:ND2 | 28:LU:230:ASN:O | 2.39 | 0.55 |
| 39:SJ:168:THR:HA | 39:SJ:171:LEU:HB2 | 1.89 | 0.55 |
| 4:L0:391:C:O2 | 31:LZ:55:ARG:NH1 | 2.40 | 0.55 |
| 8:L5:92:ARG:NH2 | 8:L5:169:ASN:OD1 | 2.40 | 0.55 |
| 20:LL:203:ILE:HD11 | 20:LL:212:LEU:HB3 | 1.89 | 0.55 |
| 21:LM:166:ASN:ND2 | 59:SB:408:THR:O | 2.40 | 0.55 |
| 25:LQ:338:ILE:HG22 | 25:LQ:355:LEU:HD21 | 1.87 | 0.55 |
| 34:SD:242:ALA:HB2 | 34:SD:253:ILE:HD11 | 1.89 | 0.55 |
| 36:SG:460:ARG:HA | 36:SG:463:GLN:HB2 | 1.89 | 0.55 |
| 48:SY:140:ARG:NH2 | 56:ND:169:ASP:OD1 | 2.40 | 0.55 |
| 4:L0:489:G:O6 | 24:LP:120:ARG:NH1 | 2.40 | 0.54 |
| 9:L7:64:VAL:HG13 | 9:L7:67:LEU:HB2 | 1.89 | 0.54 |
| 14:LE:27:ILE:HB | 14:LE:61:ILE:HB | 1.89 | 0.54 |
| 14:LE:78:ARG:HH21 | 14:LE:124:LYS:HG3 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LJ:90:ARG:HH21 | 18:LJ:137:ASN:HB3 | 1.72 | 0.54 |
| 19:LK:456:LEU:HD23 | 55:LI:675:LEU:HD22 | 1.89 | 0.54 |
| 20:LL:469:ILE:HG21 | 20:LL:505:CYS:HA | 1.89 | 0.54 |
| 21:LM:245:LEU:HB3 | 21:LM:257:ALA:HB2 | 1.89 | 0.54 |
| 28:LU:265:ASN:ND2 | 28:LU:308:VAL:O | 2.39 | 0.54 |
| 28:LU:438:LYS:NZ | 53:8:0:U:OP1 | 2.40 | 0.54 |
| 48:SY:234:VAL:HG22 | 48:SY:240:ILE:HG22 | 1.89 | 0.54 |
| 18:LJ:90:ARG:NH2 | 18:LJ:137:ASN:O | 2.40 | 0.54 |
| 28:LU:450:ASP:OD1 | 28:LU:450:ASP:N | 2.40 | 0.54 |
| 30:LW:115:HIS:HB3 | 30:LW:128:THR:HB | 1.89 | 0.54 |
| 31:LZ:62:SER:O | 58:NE:207:ARG:NH1 | 2.40 | 0.54 |
| 53:8:523:G:H21 | 53:8:529:A:H62 | 1.54 | 0.54 |
| 53:8:966:A:OP2 | 64:NF:125:LEU:N | 2.40 | 0.54 |
| 7:L4:43:PRO:HB3 | 7:L4:81:THR:HA | 1.90 | 0.54 |
| 38:SI:60:ASP:O | 38:SI:239:ASN:ND2 | 2.40 | 0.54 |
| 54:SU:181:THR:HB | 54:SU:225:HIS:HE1 | 1.71 | 0.54 |
| 55:LI:301:GLN:HA | 55:LI:315:SER:HA | 1.89 | 0.54 |
| 57:LR:15:ILE:HG12 | 57:LR:43:ILE:HD13 | 1.89 | 0.54 |
| 17:LH:19:LYS:HE2 | 17:LH:366:ASN:HD21 | 1.71 | 0.54 |
| 34:SD:91:HIS:NE2 | 48:SY:163:GLU:O | 2.37 | 0.54 |
| 35:SF:13:ASP:O | 35:SF:17:THR:OG1 | 2.24 | 0.54 |
| 53:8:1670:G:O2' | 53:8:1731:A:N6 | 2.39 | 0.54 |
| 55:LI:207:HIS:HA | 55:LI:223:THR:HA | 1.89 | 0.54 |
| 4:L0:238:G:N2 | 4:L0:274:C:O2 | 2.37 | 0.54 |
| 26:LS:556:PRO:HB2 | 26:LS:560:THR:HG21 | 1.90 | 0.54 |
| 36:SG:137:GLY:HA3 | 36:SG:500:LYS:HD2 | 1.89 | 0.54 |
| 36:SG:498:VAL:HG23 | 36:SG:511:LEU:HB2 | 1.90 | 0.54 |
| 47:ST:488:ASN:HB2 | 47:ST:492:ALA:HB2 | 1.90 | 0.54 |
| 53:8:126:A:H61 | 53:8:290:G:H1 | 1.55 | 0.54 |
| 57:LR:593:CYS:HB2 | 57:LR:620:LEU:HG | 1.89 | 0.54 |
| 10:L8:88:ASN:OD1 | 10:L8:88:ASN:N | 2.41 | 0.54 |
| 17:LH:529:LEU:HB3 | 17:LH:547:VAL:HB | 1.89 | 0.54 |
| 20:LL:189:SER:HB2 | 20:LL:206:ALA:HB1 | 1.89 | 0.54 |
| 26:LS:128:SER:O | 26:LS:132:LYS:NZ | 2.40 | 0.54 |
| 34:SD:173:LEU:HB3 | 34:SD:242:ALA:HA | 1.90 | 0.54 |
| 37:SH:156:ARG:HH21 | 37:SH:230:TRP:HE1 | 1.54 | 0.54 |
| 57:LR:763:ILE:HG23 | 57:LR:772:LEU:HD13 | 1.90 | 0.54 |
| 17:LH:437:THR:OG1 | 17:LH:706:HIS:ND1 | 2.41 | 0.54 |
| 21:LM:59:LEU:HD21 | 21:LM:114:THR:HG22 | 1.90 | 0.54 |
| 28:LU:123:PHE:HA | 28:LU:207:ASN:HD21 | 1.73 | 0.54 |
| 29:LV:67:ASP:OD1 | 29:LV:67:ASP:N | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:LV:112:THR:HA | 29:LV:128:LYS:HD3 | 1.89 | 0.54 |
| 29:LV:353:CYS:HB3 | 29:LV:356:LEU:HB2 | 1.89 | 0.54 |
| 30:LW:289:MET:HG2 | 30:LW:301:TRP:HB2 | 1.90 | 0.54 |
| 38:SI:344:ARG:NH1 | 53:8:426:G:O6 | 2.41 | 0.54 |
| 39:SJ:116:THR:HG22 | 39:SJ:118:ARG:H | 1.72 | 0.54 |
| 39:SK:88:ARG:NH1 | 53:8:1191:U:O2 | 2.40 | 0.54 |
| 39:SK:199:ASP:N | 39:SK:199:ASP:OD1 | 2.39 | 0.54 |
| 4:L0:146:G:N2 | 20:LL:360:ASN:OD1 | 2.38 | 0.54 |
| 11:L9:53:ARG:NH2 | 11:L9:99:LEU:O | 2.40 | 0.54 |
| 23:LO:99:CYS:HB3 | 23:LO:113:LEU:HD11 | 1.90 | 0.54 |
| 23:LO:112:ALA:HB1 | 23:LO:119:LEU:HD11 | 1.88 | 0.54 |
| 28:LU:82:LYS:NZ | 28:LU:154:ASP:OD2 | 2.40 | 0.54 |
| 39:SJ:63:ASP:N | 39:SJ:63:ASP:OD1 | 2.40 | 0.54 |
| 4:L0:83:U:H2' | 22:LN:327:LEU:HD22 | 1.90 | 0.54 |
| 10:L8:31:ARG:HH21 | 10:L8:48:THR:HG22 | 1.73 | 0.54 |
| 17:LH:664:LEU:HB3 | 17:LH:670:LEU:HD12 | 1.88 | 0.54 |
| 22:LN:122:VAL:HB | 56:ND:192:PRO:HG3 | 1.90 | 0.54 |
| 22:LN:590:LYS:NZ | 22:LN:619:THR:O | 2.41 | 0.54 |
| 25:LQ:109:MET:N | 25:LQ:109:MET:SD | 2.80 | 0.54 |
| 30:LW:451:SER:OG | 30:LW:452:VAL:N | 2.41 | 0.54 |
| 39:SJ:35:ASP:N | 39:SJ:35:ASP:OD1 | 2.41 | 0.54 |
| 66:6:336:ASP:OD1 | 66:6:336:ASP:N | 2.40 | 0.54 |
| 7:L4:221:ARG:NH1 | 53:8:111:U:OP1 | 2.41 | 0.54 |
| 8:L5:51:VAL:HG11 | 8:L5:130:ILE:HG12 | 1.90 | 0.54 |
| 9:L7:138:LYS:NZ | 9:L7:139:ARG:O | 2.41 | 0.54 |
| 17:LH:404:SER:OG | 17:LH:405:ALA:N | 2.40 | 0.54 |
| 21:LM:124:ARG:NH1 | 21:LM:124:ARG:O | 2.41 | 0.54 |
| 28:LU:340:ARG:NH1 | 28:LU:341:GLU:OE1 | 2.41 | 0.54 |
| 34:SD:122:ARG:NH1 | 34:SD:140:GLU:OE2 | 2.41 | 0.54 |
| 39:SJ:183:ASP:N | 39:SJ:183:ASP:OD1 | 2.41 | 0.54 |
| 7:L4:57:ASN:ND2 | 53:8:446:A:OP1 | 2.41 | 0.53 |
| 26:LS:148:THR:OG1 | 26:LS:163:ARG:NH2 | 2.41 | 0.53 |
| 27:LT:342:TYR:HH | 27:LT:345:SER:HG | 1.56 | 0.53 |
| 36:SG:305:ARG:HG2 | 36:SG:317:ILE:HG23 | 1.90 | 0.53 |
| 37:SH:155:LYS:NZ | 37:SH:163:GLY:O | 2.40 | 0.53 |
| 42:SN:181:ARG:NH1 | 60:SV:203:SER:O | 2.41 | 0.53 |
| 62:LX:131:THR:HG22 | 62:LX:134:LEU:H | 1.73 | 0.53 |
| 1:NA:530:ARG:HH12 | 53:8:1642:G:H5'' | 1.73 | 0.53 |
| 7:L4:182:TYR:N | 7:L4:226:PHE:O | 2.40 | 0.53 |
| 17:LH:708:ASP:OD1 | 17:LH:708:ASP:N | 2.41 | 0.53 |
| 22:LN:345:ASP:HB2 | 22:LN:361:LEU:HB2 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:LS:204:ASP:OD1 | 26:LS:204:ASP:N | 2.41 | 0.53 |
| 27:LT:392:ARG:HE | 27:LT:449:ARG:HH22 | 1.55 | 0.53 |
| 53:8:627:C:N4 | 53:8:970:A:OP2 | 2.41 | 0.53 |
| 54:SU:407:ARG:NH2 | 54:SU:490:LYS:O | 2.41 | 0.53 |
| 15:LF:10:ARG:HH22 | 15:LF:26:ASP:HB2 | 1.73 | 0.53 |
| 20:LL:112:LEU:HD11 | 20:LL:131:LEU:HD11 | 1.89 | 0.53 |
| 23:LO:828:ILE:HG21 | 27:LT:930:MET:HB2 | 1.89 | 0.53 |
| 26:LS:436:ASP:OD1 | 26:LS:436:ASP:N | 2.40 | 0.53 |
| 30:LW:258:LEU:HB2 | 30:LW:268:VAL:HG22 | 1.90 | 0.53 |
| 35:SF:58:CYS:HA | 35:SF:84:ARG:HD3 | 1.91 | 0.53 |
| 38:SI:828:ARG:NH1 | 45:SR:94:ASN:OD1 | 2.41 | 0.53 |
| 41:SM:220:ARG:NH1 | 41:SM:235:GLN:OE1 | 2.42 | 0.53 |
| 54:SU:466:LEU:HA | 54:SU:469:LEU:HD12 | 1.90 | 0.53 |
| 55:LI:567:LEU:HD21 | 55:LI:595:ILE:HD11 | 1.90 | 0.53 |
| 62:LX:736:PHE:O | 62:LX:740:ASN:ND2 | 2.42 | 0.53 |
| 4:L0:334:G:OP1 | 31:LZ:56:ARG:NH2 | 2.41 | 0.53 |
| 8:L5:57:SER:OG | 8:L5:167:ARG:NH1 | 2.39 | 0.53 |
| 14:LE:87:GLU:OE1 | 14:LE:117:ARG:NH2 | 2.37 | 0.53 |
| 18:LJ:134:THR:OG1 | 18:LJ:135:GLN:OE1 | 2.25 | 0.53 |
| 23:LO:36:ARG:NH2 | 23:LO:53:GLU:OE1 | 2.39 | 0.53 |
| 23:LO:597:ASN:HA | 23:LO:680:ARG:HB2 | 1.90 | 0.53 |
| 26:LS:465:THR:HG23 | 26:LS:468:CYS:H | 1.72 | 0.53 |
| 37:SH:340:LYS:HG3 | 37:SH:351:ILE:HB | 1.90 | 0.53 |
| 45:SR:97:ASP:N | 45:SR:97:ASP:OD1 | 2.40 | 0.53 |
| 6:L3:110:ARG:HH22 | 6:L3:113:LEU:HD12 | 1.73 | 0.53 |
| 7:L4:87:MET:O | 7:L4:122:LYS:NZ | 2.42 | 0.53 |
| 23:LO:567:ASP:OD1 | 23:LO:576:ARG:NH2 | 2.40 | 0.53 |
| 23:LO:598:ASN:ND2 | 23:LO:600:SER:OG | 2.41 | 0.53 |
| 27:LT:346:ARG:NH1 | 27:LT:384:ALA:O | 2.42 | 0.53 |
| 38:SI:67:PRO:O | 38:SI:114:ARG:NH2 | 2.41 | 0.53 |
| 62:LX:635:ILE:HB | 62:LX:725:VAL:HG12 | 1.90 | 0.53 |
| 63:L6:98:ARG:NH2 | 63:L6:105:ASP:OD2 | 2.34 | 0.53 |
| 1:NA:311:ILE:HB | 38:SI:1032:LEU:HD13 | 1.90 | 0.53 |
| 4:L0:313:A:N6 | 30:LW:79:GLU:OE1 | 2.40 | 0.53 |
| 12:LC:42:GLU:OE2 | 12:LC:45:ARG:NH1 | 2.41 | 0.53 |
| 17:LH:461:ASP:OD1 | 17:LH:461:ASP:N | 2.41 | 0.53 |
| 23:LO:834:GLU:HA | 23:LO:837:ASN:HB2 | 1.89 | 0.53 |
| 29:LV:109:ASP:OD1 | 29:LV:109:ASP:N | 2.41 | 0.53 |
| 29:LV:189:ASN:HB3 | 29:LV:194:LEU:H | 1.73 | 0.53 |
| 29:LV:205:GLU:OE1 | 29:LV:207:TRP:NE1 | 2.41 | 0.53 |
| 34:SD:166:PRO:HA | 34:SD:188:VAL:HA | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:SF:6:PRO:HB3 | 36:SG:465:GLN:HE21 | 1.72 | 0.53 |
| 38:SI:870:ARG:NH2 | 53:8:573:C:O2' | 2.41 | 0.53 |
| 42:SN:58:PRO:HA | 42:SN:186:ASN:HD22 | 1.74 | 0.53 |
| 47:ST:314:UNK:O | 47:ST:559:ARG:NH2 | 2.42 | 0.53 |
| 54:SU:245:GLN:HB3 | 54:SU:248:GLU:HG2 | 1.90 | 0.53 |
| 4:L0:490:G:HO2' | 4:L0:494:C:HO2' | 1.55 | 0.53 |
| 28:LU:183:GLN:N | 28:LU:197:GLY:O | 2.38 | 0.53 |
| 36:SG:484:SER:OG | 36:SG:485:ASN:N | 2.42 | 0.53 |
| 38:SI:124:ASP:OD1 | 38:SI:124:ASP:N | 2.35 | 0.53 |
| 41:SM:281:ILE:HD11 | 53:8:564:G:H4' | 1.90 | 0.53 |
| 53:8:378:A:O2' | 66:6:306:ARG:NH2 | 2.42 | 0.53 |
| 53:8:1052:U:H3 | 53:8:1066:C:H42 | 1.55 | 0.53 |
| 57:LR:325:ASP:OD1 | 57:LR:325:ASP:N | 2.41 | 0.53 |
| 17:LH:297:ILE:O | 17:LH:485:ARG:NH2 | 2.42 | 0.53 |
| 23:LO:828:ILE:HA | 23:LO:832:ALA:HB3 | 1.91 | 0.53 |
| 27:LT:230:VAL:HB | 27:LT:244:ILE:HB | 1.91 | 0.53 |
| 28:LU:357:SER:OG | 28:LU:358:MET:N | 2.42 | 0.53 |
| 31:LZ:137:ARG:HA | 31:LZ:142:LEU:HA | 1.91 | 0.53 |
| 42:SN:33:ASP:OD1 | 42:SN:33:ASP:N | 2.42 | 0.53 |
| 53:8:110:U:H4' | 66:6:227:ARG:HH21 | 1.74 | 0.53 |
| 53:8:364:G:H1 | 53:8:380:U:H3 | 1.57 | 0.53 |
| 53:8:964:U:O2' | 64:NF:125:LEU:O | 2.27 | 0.53 |
| 20:LL:448:ASN:OD1 | 20:LL:483:ARG:NH1 | 2.42 | 0.53 |
| 22:LN:589:ASN:OD1 | 22:LN:632:ASN:ND2 | 2.42 | 0.53 |
| 24:LP:12:ILE:HG21 | 30:LW:62:ALA:HB1 | 1.90 | 0.53 |
| 53:8:956:C:H2' | 53:8:957:G:C8 | 2.44 | 0.53 |
| 55:LI:261:GLU:HA | 55:LI:271:SER:HA | 1.90 | 0.53 |
| 62:LX:879:SER:OG | 62:LX:880:VAL:N | 2.42 | 0.53 |
| 3:NB:433:ARG:O | 39:SJ:211:ARG:NH1 | 2.42 | 0.53 |
| 14:LE:92:ASN:O | 40:SL:79:LYS:NZ | 2.42 | 0.53 |
| 23:LO:156:GLN:NE2 | 23:LO:200:SER:O | 2.42 | 0.53 |
| 30:LW:266:PRO:O | 46:SS:832:ASN:ND2 | 2.41 | 0.53 |
| 31:LZ:145:ASP:OD1 | 31:LZ:145:ASP:N | 2.38 | 0.53 |
| 39:SK:165:ASN:ND2 | 53:8:1576:A:OP1 | 2.42 | 0.53 |
| 47:ST:434:ILE:HD11 | 47:ST:500:PHE:HB2 | 1.91 | 0.53 |
| 54:SU:281:LEU:HA | 54:SU:285:ILE:HB | 1.91 | 0.53 |
| 55:LI:558:CYS:O | 55:LI:585:ARG:NH2 | 2.41 | 0.53 |
| 57:LR:631:MET:HB2 | 57:LR:645:LYS:HG3 | 1.91 | 0.53 |
| 11:L9:59:LEU:HD21 | 11:L9:73:GLY:HA2 | 1.90 | 0.52 |
| 17:LH:16:SER:HB3 | 17:LH:783:LEU:HB2 | 1.91 | 0.52 |
| 17:LH:55:TYR:HB3 | 17:LH:383:LEU:HD11 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:LL:56:SER:O | 20:LL:59:LYS:NZ | 2.41 | 0.52 |
| 22:LN:66:ARG:NH1 | 22:LN:80:ASN:OD1 | 2.42 | 0.52 |
| 25:LQ:480:ASP:HB3 | 25:LQ:539:VAL:HG23 | 1.91 | 0.52 |
| 28:LU:330:ARG:NH1 | 28:LU:339:SER:OG | 2.39 | 0.52 |
| 29:LV:46:ARG:NH1 | 29:LV:46:ARG:O | 2.42 | 0.52 |
| 30:LW:144:LEU:HD21 | 30:LW:147:GLU:HB2 | 1.91 | 0.52 |
| 40:SL:157:ASP:OD2 | 40:SL:157:ASP:N | 2.40 | 0.52 |
| 53:8:1083:G:N2 | 53:8:1095:U:OP2 | 2.41 | 0.52 |
| 53:8:1484:G:N2 | 53:8:1606:C:O2 | 2.42 | 0.52 |
| 62:LX:166:MET:N | 62:LX:166:MET:SD | 2.82 | 0.52 |
| 66:6:77:MET:HG2 | 66:6:95:ALA:HB2 | 1.90 | 0.52 |
| 6:L3:104:ASN:OD1 | 6:L3:104:ASN:N | 2.40 | 0.52 |
| 11:L9:57:ARG:HH12 | 40:SL:88:ASP:HA | 1.75 | 0.52 |
| 23:LO:491:ALA:HB2 | 23:LO:521:LEU:HB2 | 1.92 | 0.52 |
| 25:LQ:100:ASP:OD2 | 25:LQ:100:ASP:N | 2.37 | 0.52 |
| 25:LQ:165:SER:OG | 25:LQ:166:ILE:N | 2.42 | 0.52 |
| 28:LU:26:ARG:HH21 | 46:SS:868:GLU:HA | 1.74 | 0.52 |
| 35:SE:29:ASN:ND2 | 48:SY:244:TRP:O | 2.42 | 0.52 |
| 37:SH:37:ARG:NH2 | 37:SH:49:GLU:OE2 | 2.37 | 0.52 |
| 53:8:364:G:N2 | 53:8:380:U:O2 | 2.40 | 0.52 |
| 53:8:1044:U:H3 | 53:8:1074:G:H1 | 1.57 | 0.52 |
| 6:L3:20:THR:HG21 | 6:L3:35:ILE:HG23 | 1.91 | 0.52 |
| 8:L5:63:GLN:HE22 | 8:L5:66:GLN:HE21 | 1.58 | 0.52 |
| 18:LJ:415:LEU:HD11 | 18:LJ:458:ILE:HD13 | 1.91 | 0.52 |
| 22:LN:585:ILE:HG12 | 22:LN:633:CYS:HB3 | 1.92 | 0.52 |
| 25:LQ:595:LYS:HA | 25:LQ:618:ILE:HG13 | 1.90 | 0.52 |
| 28:LU:146:LYS:HG2 | 28:LU:175:THR:HG22 | 1.91 | 0.52 |
| 30:LW:116:ILE:O | 30:LW:380:ASN:ND2 | 2.42 | 0.52 |
| 38:SI:287:ARG:HH21 | 38:SI:297:SER:HB2 | 1.73 | 0.52 |
| 42:SN:177:ARG:NH2 | 60:SV:201:ASP:O | 2.39 | 0.52 |
| 53:8:23:G:H1 | 53:8:602:U:H2' | 1.74 | 0.52 |
| 7:L4:183:VAL:HG21 | 7:L4:220:THR:HG21 | 1.92 | 0.52 |
| 13:LD:91:LEU:HB3 | 13:LD:100:TYR:HB3 | 1.91 | 0.52 |
| 24:LP:120:ARG:HH21 | 24:LP:123:GLN:HB3 | 1.75 | 0.52 |
| 25:LQ:172:GLN:HE22 | 25:LQ:178:ILE:HG13 | 1.74 | 0.52 |
| 25:LQ:807:ASP:HA | 25:LQ:810:LEU:HD13 | 1.91 | 0.52 |
| 36:SG:335:ARG:HD3 | 36:SG:348:LEU:HD21 | 1.91 | 0.52 |
| 53:8:183:U:O2 | 53:8:203:U:N3 | 2.41 | 0.52 |
| 53:8:884:A:H61 | 53:8:927:C:H42 | 1.58 | 0.52 |
| 53:8:929:A:OP2 | 53:8:931:C:N4 | 2.42 | 0.52 |
| 54:SU:317:ILE:HD11 | 54:SU:349:LEU:HD22 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:NA:496:TYR:O | 57:LR:788:TYR:OH | 2.28 | 0.52 |
| 18:LJ:229:CYS:HB2 | 18:LJ:258:LEU:HD13 | 1.92 | 0.52 |
| 23:LO:29:LEU:HD21 | 23:LO:327:LEU:HD21 | 1.92 | 0.52 |
| 23:LO:453:PHE:HB3 | 23:LO:475:PRO:HA | 1.92 | 0.52 |
| 34:SD:281:ASP:HB2 | 34:SD:284:THR:HG23 | 1.92 | 0.52 |
| 36:SG:286:LEU:HD23 | 36:SG:295:LEU:HD11 | 1.91 | 0.52 |
| 45:SR:95:PHE:O | 45:SR:142:LYS:NZ | 2.39 | 0.52 |
| 45:SR:103:LEU:HB2 | 45:SR:126:LYS:HB2 | 1.92 | 0.52 |
| 53:8:593:U:H5'' | 53:8:594:A:H5' | 1.90 | 0.52 |
| 53:8:1274:C:H2' | 53:8:1275:A:H8 | 1.75 | 0.52 |
| 57:LR:568:MET:N | 57:LR:568:MET:SD | 2.82 | 0.52 |
| 65:5:345:ARG:NH2 | 65:5:411:GLU:OE1 | 2.41 | 0.52 |
| 3:NB:580:ARG:NH1 | 40:SL:51:LEU:O | 2.42 | 0.52 |
| 3:NB:588:SER:O | 35:SF:46:ARG:NH1 | 2.42 | 0.52 |
| 9:L7:118:LEU:O | 9:L7:122:HIS:ND1 | 2.42 | 0.52 |
| 11:L9:19:TYR:OH | 53:8:20:G:N1 | 2.42 | 0.52 |
| 12:LC:16:ALA:HB2 | 12:LC:72:GLY:HA3 | 1.91 | 0.52 |
| 18:LJ:356:ASN:OD1 | 18:LJ:359:ARG:NH2 | 2.43 | 0.52 |
| 20:LL:155:PRO:HD3 | 20:LL:196:VAL:HG11 | 1.92 | 0.52 |
| 22:LN:345:ASP:OD1 | 22:LN:345:ASP:N | 2.42 | 0.52 |
| 25:LQ:359:SER:HG | 25:LQ:361:THR:HG1 | 1.55 | 0.52 |
| 26:LS:137:ILE:HD12 | 26:LS:155:ILE:HD12 | 1.92 | 0.52 |
| 35:SF:25:GLN:NE2 | 36:SG:323:ASP:OD1 | 2.40 | 0.52 |
| 37:SH:207:ARG:HE | 37:SH:268:PRO:HG2 | 1.73 | 0.52 |
| 41:SM:49:ASP:OD1 | 41:SM:49:ASP:N | 2.42 | 0.52 |
| 45:SR:49:ALA:HB3 | 45:SR:104:LEU:HB2 | 1.90 | 0.52 |
| 4:L0:491:U:H4' | 24:LP:83:LEU:HD13 | 1.92 | 0.52 |
| 8:L5:156:ARG:NH1 | 8:L5:157:ARG:O | 2.43 | 0.52 |
| 11:L9:100:LYS:NZ | 40:SL:59:ILE:O | 2.43 | 0.52 |
| 27:LT:274:ILE:HG12 | 27:LT:286:VAL:HG12 | 1.92 | 0.52 |
| 28:LU:145:VAL:HB | 28:LU:176:PHE:HB2 | 1.92 | 0.52 |
| 28:LU:254:PRO:HG2 | 46:SS:284:ARG:HE | 1.74 | 0.52 |
| 38:SI:160:GLN:NE2 | 38:SI:197:GLU:O | 2.42 | 0.52 |
| 39:SJ:102:SER:HA | 39:SK:236:VAL:HG21 | 1.91 | 0.52 |
| 39:SJ:188:ARG:HG2 | 39:SJ:191:ASP:H | 1.75 | 0.52 |
| 62:LX:91:MET:SD | 62:LX:91:MET:N | 2.83 | 0.52 |
| 1:NA:496:TYR:OH | 1:NA:508:ARG:NH2 | 2.41 | 0.52 |
| 4:L0:68:U:OP2 | 17:LH:426:ARG:NH1 | 2.42 | 0.52 |
| 13:LD:6:THR:OG1 | 13:LD:7:VAL:N | 2.42 | 0.52 |
| 22:LN:520:LYS:O | 22:LN:524:LYS:NZ | 2.43 | 0.52 |
| 23:LO:303:ASN:HD21 | 23:LO:324:LEU:HD12 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:471:GLY:O | 23:LO:498:ARG:NH2 | 2.39 | 0.52 |
| 25:LQ:479:LEU:HD22 | 25:LQ:490:THR:HG22 | 1.92 | 0.52 |
| 29:LV:116:HIS:HB2 | 29:LV:124:GLN:HB2 | 1.92 | 0.52 |
| 36:SG:242:VAL:HG23 | 36:SG:253:THR:HG22 | 1.92 | 0.52 |
| 47:ST:573:LEU:HB3 | 47:ST:593:LEU:HD11 | 1.91 | 0.52 |
| 47:ST:612:THR:OG1 | 47:ST:613:ILE:N | 2.40 | 0.52 |
| 53:8:505:A:H61 | 53:8:585:A:H2' | 1.75 | 0.52 |
| 53:8:992:A:OP2 | 53:8:993:A:N6 | 2.37 | 0.52 |
| 53:8:1170:G:N2 | 53:8:1571:C:O3' | 2.42 | 0.52 |
| 62:LX:193:GLY:HA2 | 62:LX:212:GLY:H | 1.75 | 0.52 |
| 2:SA:21:LYS:NZ | 2:SA:45:THR:O | 2.42 | 0.52 |
| 2:SA:210:VAL:HG11 | 2:SA:219:LEU:HD12 | 1.92 | 0.52 |
| 26:LS:464:THR:HG21 | 26:LS:476:ILE:HA | 1.92 | 0.52 |
| 27:LT:93:ALA:HB2 | 27:LT:121:LEU:HD22 | 1.91 | 0.52 |
| 27:LT:430:ILE:HB | 27:LT:443:TRP:HB2 | 1.91 | 0.52 |
| 30:LW:135:ALA:HB1 | 30:LW:144:LEU:HD11 | 1.91 | 0.52 |
| 30:LW:244:ASN:HB3 | 30:LW:246:VAL:HG22 | 1.91 | 0.52 |
| 36:SG:241:THR:HG21 | 36:SG:285:SER:HA | 1.91 | 0.52 |
| 39:SK:96:LEU:HD11 | 39:SK:114:ILE:HD11 | 1.91 | 0.52 |
| 65:5:412:ASP:N | 65:5:412:ASP:OD1 | 2.42 | 0.52 |
| 66:6:268:ASN:HD21 | 66:6:271:ARG:HB2 | 1.75 | 0.52 |
| 3:NB:562:ARG:NH1 | 53:8:476:U:OP2 | 2.42 | 0.52 |
| 4:L0:323:A:OP1 | 23:LO:191:ARG:NH1 | 2.43 | 0.52 |
| 22:LN:589:ASN:ND2 | 22:LN:629:LEU:O | 2.42 | 0.52 |
| 26:LS:161:ILE:HD13 | 27:LT:177:LEU:HB2 | 1.92 | 0.52 |
| 27:LT:460:ASP:O | 27:LT:481:ASN:ND2 | 2.43 | 0.52 |
| 38:SI:923:ASP:N | 38:SI:923:ASP:OD1 | 2.43 | 0.52 |
| 47:ST:510:THR:HA | 47:ST:518:ILE:HD13 | 1.91 | 0.52 |
| 47:ST:515:HIS:O | 47:ST:519:THR:OG1 | 2.28 | 0.52 |
| 47:ST:678:PHE:HB3 | 47:ST:681:PRO:HD2 | 1.91 | 0.52 |
| 57:LR:699:LYS:HD3 | 57:LR:755:ILE:HD11 | 1.92 | 0.52 |
| 62:LX:326:PHE:HA | 62:LX:360:LYS:HA | 1.92 | 0.52 |
| 5:L2:314:C:H2' | 5:L2:315:A:H8 | 1.75 | 0.51 |
| 21:LM:262:VAL:HG13 | 21:LM:301:LYS:HG2 | 1.93 | 0.51 |
| 36:SG:203:ASP:O | 36:SG:538:ARG:NH2 | 2.43 | 0.51 |
| 36:SG:308:SER:HB3 | 36:SG:315:LEU:HD21 | 1.92 | 0.51 |
| 38:SI:366:MET:SD | 38:SI:366:MET:N | 2.83 | 0.51 |
| 40:SL:138:ASP:HB3 | 40:SL:160:LEU:HD13 | 1.92 | 0.51 |
| 42:SN:76:THR:OG1 | 42:SN:77:LYS:N | 2.43 | 0.51 |
| 53:8:538:A:N3 | 53:8:540:G:N2 | 2.59 | 0.51 |
| 1:NA:370:ARG:NH2 | 41:SM:246:GLU:OE1 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:L9:36:LEU:HD11 | 11:L9:105:LEU:HD21 | 1.92 | 0.51 |
| 15:LF:29:HIS:HB2 | 15:LF:67:GLY:HA2 | 1.91 | 0.51 |
| 25:LQ:15:GLY:O | 25:LQ:360:ASN:ND2 | 2.43 | 0.51 |
| 25:LQ:393:ASP:N | 25:LQ:393:ASP:OD1 | 2.44 | 0.51 |
| 28:LU:85:THR:OG1 | 28:LU:95:TRP:NE1 | 2.35 | 0.51 |
| 41:SM:36:LEU:O | 58:NE:214:ARG:NH2 | 2.43 | 0.51 |
| 53:8:598:U:H2' | 53:8:599:A:H8 | 1.74 | 0.51 |
| 62:LX:9:ARG:HH22 | 62:LX:214:LYS:HA | 1.75 | 0.51 |
| 6:L3:57:ARG:NH1 | 18:LJ:61:THR:OG1 | 2.41 | 0.51 |
| 7:L4:181:VAL:HA | 7:L4:227:VAL:HA | 1.93 | 0.51 |
| 23:LO:27:LYS:HD3 | 23:LO:43:ILE:HG13 | 1.91 | 0.51 |
| 23:LO:269:HIS:NE2 | 23:LO:312:GLN:O | 2.43 | 0.51 |
| 23:LO:434:ASN:HD21 | 23:LO:450:LEU:HD23 | 1.74 | 0.51 |
| 28:LU:292:ARG:NH1 | 46:SS:296:SER:OG | 2.44 | 0.51 |
| 31:LZ:66:PRO:HA | 31:LZ:71:ARG:HH11 | 1.76 | 0.51 |
| 34:SC:310:GLU:OE1 | 34:SC:313:HIS:ND1 | 2.44 | 0.51 |
| 35:SE:33:LEU:HD11 | 35:SE:100:ALA:HB1 | 1.91 | 0.51 |
| 38:SI:1156:LYS:HD2 | 53:8:18:C:H5' | 1.92 | 0.51 |
| 39:SK:90:ASP:N | 39:SK:90:ASP:OD1 | 2.43 | 0.51 |
| 41:SM:19:GLU:HA | 41:SM:22:ASP:HB2 | 1.91 | 0.51 |
| 47:ST:616:LEU:HD13 | 47:ST:619:LEU:HD12 | 1.93 | 0.51 |
| 51:NH:862:LEU:HA | 51:NH:866:ALA:HB3 | 1.93 | 0.51 |
| 53:8:887:A:C2 | 53:8:925:G:N1 | 2.79 | 0.51 |
| 59:SB:404:ARG:NH1 | 59:SB:405:ASP:O | 2.43 | 0.51 |
| 62:LX:802:LEU:HD23 | 62:LX:805:ILE:HD11 | 1.92 | 0.51 |
| 65:5:450:LEU:O | 65:5:453:ASN:N | 2.41 | 0.51 |
| 18:LJ:212:ASP:OD1 | 18:LJ:212:ASP:N | 2.43 | 0.51 |
| 20:LL:440:ILE:HG12 | 20:LL:452:LEU:HD21 | 1.93 | 0.51 |
| 25:LQ:635:LYS:HA | 25:LQ:659:GLU:HG2 | 1.92 | 0.51 |
| 27:LT:730:LYS:NZ | 27:LT:838:ILE:O | 2.41 | 0.51 |
| 28:LU:140:SER:OG | 28:LU:141:ASP:N | 2.43 | 0.51 |
| 42:SN:242:ILE:HG13 | 42:SN:254:ILE:HG13 | 1.93 | 0.51 |
| 53:8:1208:A:N6 | 53:8:1454:G:N1 | 2.58 | 0.51 |
| 53:8:1220:C:H42 | 53:8:1263:G:H1 | 1.58 | 0.51 |
| 55:LI:606:ASP:N | 55:LI:606:ASP:OD1 | 2.42 | 0.51 |
| 57:LR:34:THR:HG23 | 57:LR:41:ASN:HB2 | 1.91 | 0.51 |
| 57:LR:42:ILE:HG21 | 57:LR:90:LEU:HD11 | 1.91 | 0.51 |
| 62:LX:62:LYS:O | 62:LX:125:GLN:NE2 | 2.43 | 0.51 |
| 5:L2:326:U:OP1 | 35:SE:46:ARG:NH2 | 2.37 | 0.51 |
| 9:L7:51:VAL:HG23 | 9:L7:53:GLY:H | 1.76 | 0.51 |
| 17:LH:709:ARG:HB2 | 17:LH:765:TRP:HD1 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:LJ:266:SER:OG | 18:LJ:268:MET:O | 2.28 | 0.51 |
| 22:LN:232:ASP:OD1 | 22:LN:232:ASP:N | 2.44 | 0.51 |
| 22:LN:597:ASN:N | 22:LN:597:ASN:OD1 | 2.43 | 0.51 |
| 23:LO:300:MET:SD | 23:LO:326:GLN:NE2 | 2.83 | 0.51 |
| 25:LQ:337:LYS:HB3 | 25:LQ:358:SER:HB3 | 1.91 | 0.51 |
| 26:LS:133:ILE:HD12 | 27:LT:194:ARG:HH12 | 1.75 | 0.51 |
| 26:LS:511:LEU:HD13 | 26:LS:544:VAL:HG11 | 1.92 | 0.51 |
| 27:LT:125:GLY:HA2 | 59:SB:430:ASP:HA | 1.92 | 0.51 |
| 34:SC:284:THR:HG22 | 40:SL:64:GLN:HE22 | 1.75 | 0.51 |
| 40:SL:18:ASN:HB3 | 40:SL:21:LYS:HB3 | 1.92 | 0.51 |
| 57:LR:498:SER:OG | 57:LR:539:VAL:O | 2.29 | 0.51 |
| 3:NB:438:ASP:OD1 | 3:NB:438:ASP:N | 2.42 | 0.51 |
| 4:L0:163:G:H4' | 26:LS:354:SER:HB2 | 1.92 | 0.51 |
| 6:L3:56:LYS:HE2 | 6:L3:61:LEU:HG | 1.93 | 0.51 |
| 20:LL:443:GLN:NE2 | 54:SU:333:GLU:O | 2.43 | 0.51 |
| 23:LO:849:LEU:HD22 | 27:LT:897:HIS:HB2 | 1.93 | 0.51 |
| 25:LQ:922:ASP:OD1 | 25:LQ:922:ASP:N | 2.40 | 0.51 |
| 26:LS:412:GLN:OE1 | 26:LS:420:ARG:NH2 | 2.44 | 0.51 |
| 26:LS:473:ILE:HA | 26:LS:476:ILE:HD12 | 1.92 | 0.51 |
| 27:LT:627:ASN:ND2 | 27:LT:647:THR:OG1 | 2.37 | 0.51 |
| 28:LU:67:ARG:HH21 | 40:SL:122:ASP:HA | 1.75 | 0.51 |
| 38:SI:1089:GLN:HB3 | 48:SY:82:ARG:HH21 | 1.75 | 0.51 |
| 38:SI:1150:SER:OG | 38:SI:1154:LYS:NZ | 2.44 | 0.51 |
| 47:ST:605:ASP:OD1 | 47:ST:605:ASP:N | 2.44 | 0.51 |
| 50:NJ:1574:ALA:HA | 50:NJ:1578:GLY:HA3 | 1.93 | 0.51 |
| 57:LR:563:ASP:OD1 | 57:LR:563:ASP:N | 2.42 | 0.51 |
| 62:LX:753:ASP:OD1 | 62:LX:753:ASP:N | 2.43 | 0.51 |
| 66:6:353:ALA:O | 66:6:356:ARG:NH1 | 2.43 | 0.51 |
| 4:L0:183:A:N6 | 4:L0:213:G:O6 | 2.44 | 0.51 |
| 35:SE:42:LYS:HD2 | 35:SE:46:ARG:HH12 | 1.74 | 0.51 |
| 36:SG:185:LEU:HD21 | 36:SG:527:VAL:HG11 | 1.92 | 0.51 |
| 38:SI:288:VAL:HG23 | 38:SI:814:GLY:HA2 | 1.91 | 0.51 |
| 38:SI:767:ILE:O | 38:SI:770:GLN:NE2 | 2.42 | 0.51 |
| 38:SI:968:THR:HG22 | 38:SI:1001:VAL:HG12 | 1.92 | 0.51 |
| 38:SI:974:GLY:HA3 | 38:SI:991:PHE:HD1 | 1.75 | 0.51 |
| 52:NI:15:VAL:HA | 52:NI:38:PHE:HA | 1.92 | 0.51 |
| 57:LR:505:ILE:HB | 57:LR:517:ILE:HD11 | 1.92 | 0.51 |
| 1:NA:341:LEU:O | 6:L3:120:ARG:NH2 | 2.44 | 0.51 |
| 2:SA:172:ASN:HA | 2:SA:175:ILE:HD12 | 1.92 | 0.51 |
| 4:L0:467:A:H61 | 5:L2:49:C:H42 | 1.59 | 0.51 |
| 26:LS:493:LEU:HD21 | 26:LS:530:LEU:HD22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:LV:57:GLU:O | 29:LV:76:THR:OG1 | 2.29 | 0.51 |
| 31:LZ:120:MET:HA | 48:SY:62:GLU:HA | 1.92 | 0.51 |
| 34:SC:89:GLU:OE1 | 44:SQ:141:TRP:NE1 | 2.41 | 0.51 |
| 34:SD:110:ASN:ND2 | 34:SD:141:TYR:O | 2.44 | 0.51 |
| 37:SH:119:LYS:HB3 | 37:SH:165:GLU:HB3 | 1.92 | 0.51 |
| 37:SH:201:SER:HB3 | 37:SH:204:LEU:HD13 | 1.93 | 0.51 |
| 37:SH:361:ASN:HD22 | 37:SH:364:LYS:HD2 | 1.76 | 0.51 |
| 2:SA:86:LEU:HD13 | 2:SA:116:VAL:HG21 | 1.93 | 0.51 |
| 4:L0:248:G:OP2 | 48:SY:82:ARG:NH2 | 2.44 | 0.51 |
| 23:LO:450:LEU:HA | 23:LO:475:PRO:HB3 | 1.92 | 0.51 |
| 23:LO:525:PRO:HG2 | 23:LO:587:PHE:HA | 1.92 | 0.51 |
| 25:LQ:488:LEU:HB3 | 25:LQ:500:TRP:HB2 | 1.91 | 0.51 |
| 28:LU:367:SER:HB3 | 28:LU:373:ARG:HH12 | 1.75 | 0.51 |
| 34:SD:301:LEU:HD23 | 34:SD:302:GLU:HB2 | 1.93 | 0.51 |
| 36:SG:525:GLN:HB2 | 36:SG:540:LEU:HB2 | 1.93 | 0.51 |
| 36:SG:546:GLU:OE2 | 36:SG:551:ARG:NH1 | 2.44 | 0.51 |
| 38:SI:846:VAL:HG22 | 38:SI:855:GLN:HB3 | 1.93 | 0.51 |
| 54:SU:167:LYS:O | 54:SU:272:GLN:NE2 | 2.43 | 0.51 |
| 9:L7:50:ASP:HA | 9:L7:56:LYS:HG3 | 1.92 | 0.51 |
| 10:L8:9:HIS:NE2 | 53:8:321:C:N3 | 2.50 | 0.51 |
| 11:L9:87:SER:HB3 | 11:L9:90:LYS:HG3 | 1.92 | 0.51 |
| 13:LD:64:VAL:HG12 | 13:LD:129:ARG:HH11 | 1.76 | 0.51 |
| 22:LN:370:ARG:NH2 | 22:LN:630:LYS:O | 2.44 | 0.51 |
| 27:LT:307:GLN:NE2 | 59:SB:422:THR:O | 2.39 | 0.51 |
| 27:LT:590:ALA:HB3 | 27:LT:631:ASN:HA | 1.92 | 0.51 |
| 28:LU:403:ARG:NH2 | 46:SS:860:SER:O | 2.44 | 0.51 |
| 29:LV:300:TRP:HA | 29:LV:308:TYR:H | 1.76 | 0.51 |
| 30:LW:113:PRO:HA | 30:LW:395:GLN:HA | 1.93 | 0.51 |
| 34:SD:257:SER:HA | 34:SD:261:LEU:HD23 | 1.92 | 0.51 |
| 39:SJ:167:ILE:HG13 | 39:SJ:171:LEU:HG | 1.92 | 0.51 |
| 39:SK:151:ARG:HB2 | 47:ST:716:LYS:HE3 | 1.93 | 0.51 |
| 53:8:883:C:O2 | 53:8:946:U:N3 | 2.44 | 0.51 |
| 57:LR:580:ARG:HG2 | 57:LR:623:LEU:HB3 | 1.93 | 0.51 |
| 5:L2:59:G:H5' | 23:LO:570:THR:HG23 | 1.93 | 0.50 |
| 7:L4:140:VAL:HG12 | 7:L4:146:THR:HG22 | 1.92 | 0.50 |
| 11:L9:110:GLN:OE1 | 11:L9:126:ARG:NH1 | 2.41 | 0.50 |
| 11:L9:155:HIS:NE2 | 36:SG:321:HIS:O | 2.45 | 0.50 |
| 11:L9:157:ASP:OD2 | 11:L9:158:PHE:N | 2.44 | 0.50 |
| 13:LD:11:ARG:NH2 | 53:8:342:C:O2' | 2.43 | 0.50 |
| 17:LH:490:LEU:HD11 | 18:LJ:426:LYS:HD2 | 1.93 | 0.50 |
| 23:LO:660:SER:HA | 23:LO:672:THR:HA | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:LP:297:ASP:OD1 | 24:LP:297:ASP:N | 2.43 | 0.50 |
| 36:SG:262:VAL:HG13 | 36:SG:271:VAL:HG23 | 1.91 | 0.50 |
| 38:SI:125:LEU:HD21 | 38:SI:899:VAL:HG21 | 1.93 | 0.50 |
| 38:SI:826:LYS:NZ | 38:SI:923:ASP:OD2 | 2.44 | 0.50 |
| 39:SJ:239:SER:HG | 39:SK:239:SER:HG | 1.58 | 0.50 |
| 41:SM:187:PRO:HB3 | 41:SM:220:ARG:HE | 1.75 | 0.50 |
| 2:SA:158:TYR:OH | 34:SC:222:GLU:OE1 | 2.28 | 0.50 |
| 17:LH:531:PHE:HD2 | 17:LH:545:THR:HB | 1.76 | 0.50 |
| 20:LL:64:LYS:HB3 | 20:LL:77:ILE:HD12 | 1.92 | 0.50 |
| 23:LO:78:ARG:NH1 | 23:LO:94:ASN:OD1 | 2.43 | 0.50 |
| 25:LQ:137:ILE:HG12 | 25:LQ:147:VAL:HG13 | 1.92 | 0.50 |
| 25:LQ:336:TYR:HB2 | 25:LQ:357:THR:HB | 1.93 | 0.50 |
| 25:LQ:350:LYS:HD2 | 25:LQ:366:SER:HB3 | 1.91 | 0.50 |
| 38:SI:248:ARG:HG2 | 38:SI:272:TYR:HB2 | 1.93 | 0.50 |
| 57:LR:26:SER:OG | 57:LR:28:ASN:OD1 | 2.30 | 0.50 |
| 9:L7:143:LEU:O | 14:LE:42:GLN:NE2 | 2.45 | 0.50 |
| 14:LE:54:ASP:OD1 | 14:LE:54:ASP:N | 2.45 | 0.50 |
| 18:LJ:40:ASN:HB2 | 18:LJ:60:SER:HB3 | 1.94 | 0.50 |
| 20:LL:231:ASP:N | 20:LL:231:ASP:OD1 | 2.43 | 0.50 |
| 23:LO:30:LEU:HD11 | 23:LO:63:LEU:HD22 | 1.93 | 0.50 |
| 26:LS:257:HIS:HB2 | 26:LS:262:LEU:HB2 | 1.94 | 0.50 |
| 57:LR:18:GLY:HA2 | 57:LR:37:LEU:HG | 1.92 | 0.50 |
| 62:LX:877:LEU:HD21 | 62:LX:919:LYS:HD3 | 1.93 | 0.50 |
| 10:L8:108:PRO:HA | 10:L8:111:GLN:HB2 | 1.93 | 0.50 |
| 17:LH:136:LEU:HD13 | 17:LH:187:VAL:HB | 1.93 | 0.50 |
| 17:LH:215:VAL:HG21 | 17:LH:224:SER:HB3 | 1.92 | 0.50 |
| 18:LJ:217:ASN:HB3 | 18:LJ:229:CYS:HB3 | 1.93 | 0.50 |
| 22:LN:417:VAL:HG11 | 22:LN:460:LEU:HD13 | 1.94 | 0.50 |
| 25:LQ:426:ARG:NH2 | 25:LQ:459:LEU:O | 2.44 | 0.50 |
| 27:LT:738:ASP:OD1 | 27:LT:738:ASP:N | 2.44 | 0.50 |
| 27:LT:851:SER:OG | 43:SO:241:ARG:NH2 | 2.43 | 0.50 |
| 29:LV:184:ASN:ND2 | 29:LV:198:GLY:O | 2.43 | 0.50 |
| 53:8:1491:U:H4' | 53:8:1492:A:H5' | 1.93 | 0.50 |
| 57:LR:96:VAL:HG12 | 57:LR:97:ARG:HD2 | 1.92 | 0.50 |
| 62:LX:215:ASN:N | 62:LX:215:ASN:OD1 | 2.42 | 0.50 |
| 2:SA:330:ALA:HB1 | 2:SA:381:ASN:HA | 1.94 | 0.50 |
| 19:LK:453:PRO:HB3 | 55:LI:675:LEU:HD11 | 1.94 | 0.50 |
| 28:LU:8:ARG:HH22 | 30:LW:409:ALA:HA | 1.76 | 0.50 |
| 37:SH:283:ILE:O | 38:SI:634:ARG:NH1 | 2.45 | 0.50 |
| 38:SI:285:GLY:H | 38:SI:298:VAL:HG23 | 1.75 | 0.50 |
| 40:SL:165:ARG:NH1 | 53:8:19:A:N1 | 2.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:8:992:A:H3' | 53:8:993:A:C8 | 2.47 | 0.50 |
| 57:LR:44:ASP:N | 57:LR:44:ASP:OD1 | 2.39 | 0.50 |
| 59:SB:299:LEU:HD22 | 59:SB:320:LEU:HD23 | 1.94 | 0.50 |
| 4:L0:316:U:OP1 | 30:LW:364:ARG:NH2 | 2.44 | 0.50 |
| 5:L2:306:G:H2' | 5:L2:307:G:C8 | 2.47 | 0.50 |
| 9:L7:139:ARG:NH2 | 14:LE:52:TYR:O | 2.44 | 0.50 |
| 10:L8:77:ARG:NH1 | 10:L8:78:ILE:O | 2.44 | 0.50 |
| 22:LN:466:ASP:OD1 | 22:LN:466:ASP:N | 2.42 | 0.50 |
| 25:LQ:65:ASP:HB2 | 25:LQ:67:LEU:HD22 | 1.94 | 0.50 |
| 34:SD:199:PHE:HE2 | 34:SD:223:ASP:HB2 | 1.75 | 0.50 |
| 56:ND:185:GLN:NE2 | 56:ND:186:ASP:OD2 | 2.45 | 0.50 |
| 57:LR:446:VAL:HG13 | 57:LR:448:LYS:H | 1.76 | 0.50 |
| 1:NA:453:SER:O | 1:NA:455:HIS:N | 2.45 | 0.50 |
| 10:L8:193:LEU:HA | 10:L8:196:LEU:HB2 | 1.93 | 0.50 |
| 25:LQ:7:ARG:NH2 | 25:LQ:70:GLY:O | 2.45 | 0.50 |
| 25:LQ:655:ALA:HB2 | 25:LQ:684:TRP:HZ2 | 1.75 | 0.50 |
| 25:LQ:760:ILE:HD11 | 25:LQ:835:PHE:HB2 | 1.94 | 0.50 |
| 29:LV:89:LEU:HD12 | 63:L6:73:ILE:HG12 | 1.93 | 0.50 |
| 38:SI:287:ARG:HD2 | 38:SI:820:ILE:HD13 | 1.92 | 0.50 |
| 42:SN:39:ILE:HG12 | 42:SN:243:PHE:HB2 | 1.93 | 0.50 |
| 66:6:71:TYR:HD1 | 66:6:75:LEU:HD11 | 1.76 | 0.50 |
| 7:L4:16:HIS:HE2 | 66:6:230:ALA:HA | 1.77 | 0.50 |
| 20:LL:438:THR:HG21 | 20:LL:471:ARG:HB3 | 1.93 | 0.50 |
| 22:LN:226:LEU:O | 22:LN:227:HIS:ND1 | 2.45 | 0.50 |
| 23:LO:853:ASP:N | 23:LO:853:ASP:OD1 | 2.44 | 0.50 |
| 24:LP:166:ASN:HD22 | 46:SS:328:THR:HA | 1.77 | 0.50 |
| 25:LQ:102:VAL:HG12 | 25:LQ:118:ASN:HB3 | 1.94 | 0.50 |
| 25:LQ:547:ALA:HA | 25:LQ:557:VAL:HA | 1.93 | 0.50 |
| 27:LT:573:VAL:HG13 | 27:LT:574:THR:HG23 | 1.93 | 0.50 |
| 37:SH:184:ASP:N | 37:SH:184:ASP:OD1 | 2.45 | 0.50 |
| 39:SJ:129:ARG:O | 53:8:1194:A:N6 | 2.41 | 0.50 |
| 62:LX:920:MET:HA | 62:LX:923:TYR:HB3 | 1.93 | 0.50 |
| 1:NA:479:ALA:O | 23:LO:341:GLN:NE2 | 2.44 | 0.50 |
| 5:L2:253:G:OP2 | 35:SF:95:ARG:NH1 | 2.45 | 0.50 |
| 8:L5:189:THR:OG1 | 8:L5:192:GLU:OE1 | 2.30 | 0.50 |
| 13:LD:14:GLN:OE1 | 13:LD:14:GLN:N | 2.45 | 0.50 |
| 20:LL:439:VAL:HG11 | 54:SU:300:THR:HG21 | 1.92 | 0.50 |
| 25:LQ:880:ILE:HA | 25:LQ:883:VAL:HG12 | 1.93 | 0.50 |
| 25:LQ:917:ASN:ND2 | 25:LQ:919:GLU:OE2 | 2.44 | 0.50 |
| 28:LU:200:LYS:HE3 | 28:LU:214:ASP:HB3 | 1.94 | 0.50 |
| 36:SG:539:ILE:HB | 36:SG:566:ALA:HB3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:SH:327:ARG:NH2 | 38:SI:555:MET:O | 2.36 | 0.50 |
| 38:SI:120:CYS:HB2 | 38:SI:131:ILE:HD13 | 1.92 | 0.50 |
| 47:ST:798:LYS:O | 47:ST:801:ARG:NH2 | 2.45 | 0.50 |
| 57:LR:571:LEU:HD11 | 57:LR:590:LEU:HD23 | 1.94 | 0.50 |
| 57:LR:584:ILE:HG13 | 57:LR:586:LYS:H | 1.77 | 0.50 |
| 62:LX:743:VAL:HG11 | 62:LX:774:LEU:HG | 1.94 | 0.50 |
| 66:6:85:ASP:OD1 | 66:6:85:ASP:N | 2.45 | 0.50 |
| 2:SA:129:ARG:NH1 | 34:SC:261:LEU:O | 2.44 | 0.49 |
| 3:NB:554:ARG:NH2 | 53:8:547:U:OP2 | 2.44 | 0.49 |
| 4:L0:485:G:H1 | 28:LU:386:LYS:H | 1.61 | 0.49 |
| 14:LE:76:SER:HB2 | 58:NE:320:ILE:HG12 | 1.94 | 0.49 |
| 17:LH:22:LEU:HD21 | 17:LH:32:LYS:HD3 | 1.93 | 0.49 |
| 18:LJ:285:ASP:OD1 | 18:LJ:285:ASP:N | 2.42 | 0.49 |
| 22:LN:35:ARG:HA | 22:LN:754:ILE:HB | 1.94 | 0.49 |
| 22:LN:529:ASN:O | 22:LN:545:ARG:NH1 | 2.39 | 0.49 |
| 28:LU:40:GLU:OE2 | 46:SS:865:ILE:N | 2.43 | 0.49 |
| 28:LU:273:GLU:HA | 46:SS:302:VAL:HG21 | 1.94 | 0.49 |
| 41:SM:281:ILE:HB | 41:SM:284:ALA:HB2 | 1.94 | 0.49 |
| 51:NH:443:HIS:HA | 51:NH:471:SER:H | 1.76 | 0.49 |
| 57:LR:344:ARG:NH2 | 57:LR:395:ASP:OD1 | 2.42 | 0.49 |
| 4:L0:499:U:H2' | 4:L0:500:G:H8 | 1.77 | 0.49 |
| 17:LH:214:ASP:N | 17:LH:214:ASP:OD1 | 2.43 | 0.49 |
| 18:LJ:453:VAL:HG11 | 20:LL:532:ARG:HE | 1.76 | 0.49 |
| 21:LM:12:ALA:HB2 | 30:LW:142:GLY:HA3 | 1.94 | 0.49 |
| 23:LO:528:LYS:O | 23:LO:543:ASN:ND2 | 2.44 | 0.49 |
| 23:LO:650:ASN:ND2 | 23:LO:655:ASP:OD2 | 2.42 | 0.49 |
| 25:LQ:634:SER:OG | 25:LQ:635:LYS:N | 2.44 | 0.49 |
| 29:LV:187:SER:HB3 | 29:LV:196:ALA:HB3 | 1.93 | 0.49 |
| 29:LV:200:GLU:HA | 29:LV:230:GLN:HB3 | 1.92 | 0.49 |
| 30:LW:177:TYR:HE1 | 30:LW:183:GLU:HG2 | 1.77 | 0.49 |
| 34:SD:249:GLN:HB3 | 34:SD:269:ILE:HD11 | 1.94 | 0.49 |
| 36:SG:348:LEU:HB3 | 36:SG:357:LEU:HB2 | 1.93 | 0.49 |
| 42:SN:126:VAL:HG22 | 42:SN:154:ILE:HG12 | 1.95 | 0.49 |
| 42:SN:148:LYS:HG2 | 42:SN:149:LYS:HD2 | 1.94 | 0.49 |
| 53:8:223:U:H3 | 53:8:243:G:H22 | 1.59 | 0.49 |
| 55:LI:295:TYR:HA | 55:LI:302:LEU:HA | 1.94 | 0.49 |
| 1:NA:527:ARG:NH1 | 53:8:1641:C:OP1 | 2.39 | 0.49 |
| 4:L0:331:U:H2' | 30:LW:191:ILE:HD12 | 1.93 | 0.49 |
| 4:L0:348:U:OP2 | 4:L0:377:U:N3 | 2.45 | 0.49 |
| 14:LE:53:ILE:N | 14:LE:60:LYS:O | 2.43 | 0.49 |
| 17:LH:520:LEU:HD11 | 20:LL:542:ALA:HB1 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:303:ASN:HA | 23:LO:323:LYS:HE3 | 1.93 | 0.49 |
| 24:LP:2:SER:OG | 24:LP:3:LYS:N | 2.45 | 0.49 |
| 34:SD:100:ARG:NH2 | 60:SV:129:TRP:O | 2.45 | 0.49 |
| 38:SI:279:PRO:HB3 | 38:SI:784:LYS:HA | 1.94 | 0.49 |
| 41:SM:118:ASN:OD1 | 41:SM:118:ASN:N | 2.45 | 0.49 |
| 53:8:140:A:C8 | 63:L6:184:LEU:N | 2.80 | 0.49 |
| 53:8:863:A:H8 | 53:8:865:A:H4' | 1.77 | 0.49 |
| 5:L2:64:A:OP2 | 27:LT:392:ARG:NH1 | 2.46 | 0.49 |
| 7:L4:116:ASP:OD1 | 7:L4:116:ASP:N | 2.46 | 0.49 |
| 9:L7:44:LYS:HZ3 | 9:L7:61:PHE:HB3 | 1.77 | 0.49 |
| 21:LM:281:THR:HG21 | 26:LS:208:LEU:HB2 | 1.93 | 0.49 |
| 22:LN:102:LEU:HD23 | 22:LN:116:SER:HB2 | 1.94 | 0.49 |
| 22:LN:383:LEU:HD22 | 22:LN:394:TRP:HZ3 | 1.78 | 0.49 |
| 25:LQ:215:ASP:OD1 | 25:LQ:215:ASP:N | 2.38 | 0.49 |
| 26:LS:345:LEU:HD11 | 26:LS:352:GLN:HE21 | 1.77 | 0.49 |
| 29:LV:85:ASP:OD1 | 29:LV:85:ASP:N | 2.41 | 0.49 |
| 36:SG:256:ARG:NH1 | 36:SG:282:GLU:OE1 | 2.45 | 0.49 |
| 41:SM:193:ASN:HB3 | 41:SM:226:ASN:HB3 | 1.95 | 0.49 |
| 42:SN:71:ASN:HB2 | 42:SN:123:ASP:H | 1.77 | 0.49 |
| 53:8:965:U:H3' | 64:NF:125:LEU:H | 1.77 | 0.49 |
| 58:NE:224:HIS:ND1 | 58:NE:226:ASP:OD1 | 2.46 | 0.49 |
| 65:5:194:ILE:O | 65:5:197:GLN:NE2 | 2.45 | 0.49 |
| 24:LP:187:LYS:HE2 | 44:SQ:63:PRO:HB2 | 1.95 | 0.49 |
| 25:LQ:807:ASP:N | 25:LQ:807:ASP:OD1 | 2.41 | 0.49 |
| 27:LT:53:CYS:HA | 27:LT:58:PHE:HA | 1.94 | 0.49 |
| 29:LV:291:THR:HG23 | 29:LV:300:TRP:HE1 | 1.77 | 0.49 |
| 34:SC:109:LYS:NZ | 44:SQ:103:TRP:O | 2.40 | 0.49 |
| 36:SG:252:VAL:HA | 36:SG:262:VAL:HA | 1.94 | 0.49 |
| 37:SH:329:ILE:HG23 | 37:SH:333:PHE:HD2 | 1.78 | 0.49 |
| 38:SI:867:THR:OG1 | 38:SI:868:ARG:NH1 | 2.45 | 0.49 |
| 42:SN:243:PHE:HB3 | 42:SN:251:SER:HB2 | 1.93 | 0.49 |
| 53:8:487:G:H2' | 53:8:488:G:H8 | 1.76 | 0.49 |
| 57:LR:537:TRP:HD1 | 57:LR:553:GLY:HA2 | 1.76 | 0.49 |
| 61:SP:1120:GLN:O | 61:SP:1124:TYR:N | 2.45 | 0.49 |
| 5:L2:76:U:OP2 | 26:LS:513:GLN:NE2 | 2.45 | 0.49 |
| 18:LJ:431:LEU:HD21 | 18:LJ:466:VAL:HG22 | 1.93 | 0.49 |
| 22:LN:302:ARG:NH1 | 22:LN:330:GLY:O | 2.45 | 0.49 |
| 42:SN:60:THR:HG23 | 42:SN:61:LYS:HG2 | 1.94 | 0.49 |
| 53:8:479:C:O2 | 53:8:510:G:N2 | 2.45 | 0.49 |
| 53:8:1057:U:O2' | 53:8:1058:U:O2 | 2.31 | 0.49 |
| 55:LI:271:SER:O | 55:LI:281:PHE:N | 2.44 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:L4:163:ASP:OD2 | 7:L4:166:SER:OG | 2.31 | 0.49 |
| 25:LQ:836:ILE:HA | 25:LQ:839:VAL:HG12 | 1.94 | 0.49 |
| 26:LS:576:LEU:HD13 | 26:LS:588:LEU:HD21 | 1.94 | 0.49 |
| 36:SG:443:LEU:HD12 | 36:SG:471:GLN:HB2 | 1.93 | 0.49 |
| 36:SG:491:SER:OG | 36:SG:492:TRP:N | 2.46 | 0.49 |
| 37:SH:29:LYS:NZ | 37:SH:332:ILE:O | 2.42 | 0.49 |
| 37:SH:312:ARG:NH2 | 37:SH:349:ASP:OD2 | 2.46 | 0.49 |
| 38:SI:45:ARG:NE | 53:8:28:A:OP1 | 2.44 | 0.49 |
| 45:SR:89:ASN:HD22 | 48:SY:4:LEU:HB3 | 1.76 | 0.49 |
| 53:8:1506:G:H2' | 53:8:1507:G:H8 | 1.78 | 0.49 |
| 7:L4:117:GLU:O | 7:L4:120:SER:OG | 2.31 | 0.49 |
| 13:LD:92:HIS:N | 13:LD:101:GLU:O | 2.43 | 0.49 |
| 17:LH:524:ASP:OD1 | 17:LH:524:ASP:N | 2.42 | 0.49 |
| 21:LM:130:LYS:HA | 21:LM:130:LYS:HD2 | 1.66 | 0.49 |
| 22:LN:490:SER:OG | 22:LN:491:CYS:N | 2.46 | 0.49 |
| 23:LO:258:ALA:HB1 | 23:LO:261:ALA:HB3 | 1.94 | 0.49 |
| 29:LV:3:LEU:HD22 | 29:LV:15:GLN:H | 1.78 | 0.49 |
| 36:SG:285:SER:N | 36:SG:298:SER:OG | 2.44 | 0.49 |
| 41:SM:183:SER:HB3 | 41:SM:220:ARG:HD3 | 1.95 | 0.49 |
| 62:LX:827:ARG:HA | 62:LX:830:LEU:HD12 | 1.94 | 0.49 |
| 3:NB:493:ASP:OD1 | 3:NB:496:GLN:NE2 | 2.45 | 0.49 |
| 14:LE:103:ILE:HB | 14:LE:110:ILE:HD11 | 1.93 | 0.49 |
| 18:LJ:411:LYS:NZ | 18:LJ:448:LYS:O | 2.42 | 0.49 |
| 20:LL:78:LEU:HB2 | 20:LL:86:TRP:HB2 | 1.95 | 0.49 |
| 22:LN:574:HIS:HE2 | 22:LN:638:SER:HG | 1.61 | 0.49 |
| 38:SI:1049:ASN:OD1 | 38:SI:1049:ASN:N | 2.42 | 0.49 |
| 38:SI:1113:ILE:HG13 | 44:SQ:119:ARG:HD2 | 1.95 | 0.49 |
| 53:8:901:G:H3' | 53:8:902:G:H8 | 1.77 | 0.49 |
| 54:SU:350:MET:HA | 54:SU:355:ARG:HB3 | 1.95 | 0.49 |
| 1:NA:372:ARG:NH2 | 1:NA:377:ASN:O | 2.41 | 0.49 |
| 1:NA:484:MET:HB3 | 23:LO:359:ARG:HH12 | 1.78 | 0.49 |
| 8:L5:97:LEU:HD23 | 8:L5:176:THR:HG23 | 1.95 | 0.49 |
| 27:LT:24:PHE:HB3 | 27:LT:654:TRP:HB3 | 1.94 | 0.49 |
| 27:LT:569:VAL:HB | 27:LT:579:ARG:HB2 | 1.94 | 0.49 |
| 28:LU:140:SER:OG | 28:LU:142:ASP:OD1 | 2.30 | 0.49 |
| 29:LV:287:ASN:HB3 | 29:LV:302:ARG:HG2 | 1.95 | 0.49 |
| 31:LZ:78:LEU:HD22 | 31:LZ:97:LEU:HD11 | 1.95 | 0.49 |
| 34:SC:155:ILE:HD11 | 34:SC:162:LEU:HD13 | 1.92 | 0.49 |
| 36:SG:256:ARG:NH2 | 36:SG:549:LEU:O | 2.46 | 0.49 |
| 53:8:199:G:O2' | 53:8:201:G:N2 | 2.45 | 0.49 |
| 53:8:1049:U:O4 | 53:8:1067:C:N4 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:LR:515:CYS:HB2 | 57:LR:536:LEU:HD22 | 1.95 | 0.49 |
| 6:L3:6:GLN:OE1 | 6:L3:6:GLN:N | 2.46 | 0.48 |
| 10:L8:5:ARG:NH2 | 10:L8:27:PHE:O | 2.46 | 0.48 |
| 17:LH:101:GLN:OE1 | 17:LH:104:ALA:N | 2.46 | 0.48 |
| 18:LJ:453:VAL:HG21 | 20:LL:532:ARG:HG2 | 1.95 | 0.48 |
| 27:LT:188:VAL:H | 27:LT:202:SER:HB3 | 1.78 | 0.48 |
| 27:LT:476:PHE:HD1 | 27:LT:486:ILE:HG12 | 1.78 | 0.48 |
| 30:LW:201:TYR:HB3 | 30:LW:437:LEU:HD23 | 1.95 | 0.48 |
| 38:SI:255:PRO:HA | 38:SI:258:ILE:HD12 | 1.95 | 0.48 |
| 41:SM:143:HIS:HB2 | 41:SM:151:SER:HB3 | 1.94 | 0.48 |
| 53:8:897:C:H2' | 53:8:914:G:H22 | 1.76 | 0.48 |
| 53:8:1193:A:OP2 | 53:8:1195:C:N4 | 2.45 | 0.48 |
| 57:LR:686:MET:HG2 | 57:LR:735:GLN:HB3 | 1.94 | 0.48 |
| 62:LX:9:ARG:NH1 | 62:LX:214:LYS:O | 2.46 | 0.48 |
| 3:NB:574:LYS:HZ3 | 53:8:502:U:H5'' | 1.78 | 0.48 |
| 27:LT:62:ASP:HB2 | 27:LT:69:LEU:HD21 | 1.95 | 0.48 |
| 28:LU:76:ASN:HA | 28:LU:118:VAL:HG21 | 1.94 | 0.48 |
| 30:LW:160:LEU:HD22 | 30:LW:219:VAL:HG11 | 1.96 | 0.48 |
| 30:LW:358:MET:N | 30:LW:358:MET:SD | 2.86 | 0.48 |
| 34:SD:309:TYR:OH | 48:SY:127:PHE:O | 2.27 | 0.48 |
| 36:SG:467:LYS:HA | 36:SG:470:LEU:HD12 | 1.95 | 0.48 |
| 37:SH:156:ARG:NH2 | 37:SH:228:ASP:OD2 | 2.44 | 0.48 |
| 37:SH:323:ILE:HG23 | 38:SI:553:ILE:HG23 | 1.95 | 0.48 |
| 3:NB:556:LYS:HD3 | 3:NB:559:ARG:HD3 | 1.94 | 0.48 |
| 5:L2:201:C:O2 | 5:L2:249:G:N1 | 2.43 | 0.48 |
| 22:LN:156:LEU:HG | 22:LN:170:ILE:HD11 | 1.96 | 0.48 |
| 23:LO:367:GLY:HA2 | 23:LO:390:VAL:HG23 | 1.95 | 0.48 |
| 24:LP:187:LYS:NZ | 44:SQ:66:GLU:OE2 | 2.46 | 0.48 |
| 25:LQ:476:ILE:HD12 | 25:LQ:479:LEU:HD21 | 1.94 | 0.48 |
| 35:SF:11:LEU:HA | 35:SF:80:PHE:HB2 | 1.94 | 0.48 |
| 38:SI:87:ARG:NE | 38:SI:98:LEU:O | 2.42 | 0.48 |
| 38:SI:176:LEU:HD23 | 38:SI:177:PHE:HB3 | 1.94 | 0.48 |
| 38:SI:827:ALA:O | 38:SI:883:ALA:N | 2.38 | 0.48 |
| 39:SJ:31:LEU:HD12 | 39:SJ:109:LYS:HA | 1.95 | 0.48 |
| 47:ST:508:PHE:HB3 | 47:ST:518:ILE:HD11 | 1.95 | 0.48 |
| 53:8:461:G:H2' | 53:8:462:G:H8 | 1.78 | 0.48 |
| 62:LX:776:GLU:OE2 | 62:LX:820:HIS:NE2 | 2.46 | 0.48 |
| 65:5:417:LEU:O | 65:5:421:LEU:N | 2.45 | 0.48 |
| 1:NA:350:THR:HG21 | 38:SI:975:GLU:HG2 | 1.95 | 0.48 |
| 10:L8:58:LEU:O | 10:L8:59:ARG:NH1 | 2.41 | 0.48 |
| 13:LD:123:VAL:HG12 | 13:LD:142:VAL:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:559:ILE:HG21 | 23:LO:578:LYS:HA | 1.95 | 0.48 |
| 25:LQ:805:ILE:O | 25:LQ:808:THR:OG1 | 2.31 | 0.48 |
| 25:LQ:836:ILE:HD12 | 25:LQ:857:LEU:HD13 | 1.95 | 0.48 |
| 27:LT:721:LEU:HD13 | 27:LT:922:LEU:HD23 | 1.95 | 0.48 |
| 29:LV:191:VAL:HG23 | 65:5:484:LYS:HE2 | 1.96 | 0.48 |
| 34:SC:207:LEU:HG | 34:SC:219:PRO:HB3 | 1.94 | 0.48 |
| 34:SD:208:ILE:HD12 | 59:SB:152:LEU:HD22 | 1.96 | 0.48 |
| 46:SS:300:ASP:OD2 | 46:SS:300:ASP:N | 2.45 | 0.48 |
| 47:ST:63:ALA:HB1 | 53:8:1463:C:H4' | 1.95 | 0.48 |
| 47:ST:64:ARG:HA | 47:ST:78:ARG:HG2 | 1.95 | 0.48 |
| 51:NH:257:SER:HA | 51:NH:592:PHE:H | 1.78 | 0.48 |
| 51:NH:976:ILE:HA | 51:NH:1042:ALA:HB3 | 1.95 | 0.48 |
| 53:8:875:G:N2 | 53:8:953:G:N3 | 2.61 | 0.48 |
| 54:SU:104:ALA:HB1 | 54:SU:115:LEU:HD21 | 1.95 | 0.48 |
| 62:LX:789:LEU:HD23 | 62:LX:890:LEU:HD23 | 1.95 | 0.48 |
| 5:L2:47:G:O2' | 30:LW:180:GLU:OE1 | 2.30 | 0.48 |
| 11:L9:58:ASP:N | 11:L9:58:ASP:OD1 | 2.45 | 0.48 |
| 22:LN:282:ASP:OD1 | 22:LN:282:ASP:N | 2.37 | 0.48 |
| 25:LQ:273:TYR:OH | 25:LQ:341:ALA:O | 2.32 | 0.48 |
| 25:LQ:549:SER:HB3 | 25:LQ:579:ILE:HD11 | 1.96 | 0.48 |
| 27:LT:176:TYR:HB3 | 27:LT:179:LYS:HB2 | 1.93 | 0.48 |
| 28:LU:89:ASP:HB2 | 28:LU:91:VAL:HG12 | 1.96 | 0.48 |
| 30:LW:388:ASP:OD1 | 30:LW:388:ASP:N | 2.40 | 0.48 |
| 41:SM:42:LEU:HD23 | 41:SM:43:PRO:HD2 | 1.94 | 0.48 |
| 62:LX:487:ASN:HD21 | 62:LX:493:ASP:HB2 | 1.78 | 0.48 |
| 63:L6:39:GLU:HG3 | 63:L6:46:LYS:HG3 | 1.94 | 0.48 |
| 28:LU:138:SER:OG | 28:LU:139:CYS:N | 2.47 | 0.48 |
| 29:LV:118:GLN:OE1 | 29:LV:124:GLN:NE2 | 2.47 | 0.48 |
| 38:SI:126:ASN:N | 38:SI:126:ASN:OD1 | 2.47 | 0.48 |
| 42:SN:87:LEU:O | 42:SN:93:THR:OG1 | 2.31 | 0.48 |
| 52:NI:39:ALA:HA | 52:NI:55:LEU:HA | 1.95 | 0.48 |
| 57:LR:619:ARG:O | 57:LR:637:ALA:N | 2.42 | 0.48 |
| 62:LX:537:MET:O | 62:LX:541:TYR:N | 2.46 | 0.48 |
| 2:SA:306:LEU:HD13 | 2:SA:404:LEU:HB3 | 1.96 | 0.48 |
| 9:L7:174:ASN:N | 9:L7:174:ASN:OD1 | 2.46 | 0.48 |
| 11:L9:38:ASN:N | 11:L9:38:ASN:OD1 | 2.47 | 0.48 |
| 18:LJ:168:THR:OG1 | 18:LJ:194:ARG:NH2 | 2.47 | 0.48 |
| 23:LO:470:SER:OG | 41:SM:134:SER:O | 2.29 | 0.48 |
| 25:LQ:565:PHE:O | 37:SH:207:ARG:NH2 | 2.46 | 0.48 |
| 25:LQ:597:ILE:HD13 | 25:LQ:630:PHE:HE2 | 1.79 | 0.48 |
| 38:SI:826:LYS:HE3 | 38:SI:926:ILE:HG22 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:SY:241:SER:OG | 48:SY:242:PHE:N | 2.46 | 0.48 |
| 53:8:1514:U:H2' | 53:8:1515:A:H8 | 1.78 | 0.48 |
| 53:8:1541:G:H21 | 53:8:1569:A:H62 | 1.60 | 0.48 |
| 62:LX:34:ARG:NH1 | 62:LX:64:LEU:O | 2.46 | 0.48 |
| 62:LX:769:ARG:NH1 | 62:LX:770:GLU:O | 2.47 | 0.48 |
| 65:5:290:ARG:HH12 | 66:6:101:GLN:HE21 | 1.61 | 0.48 |
| 65:5:471:PRO:HD2 | 65:5:472:ILE:HD12 | 1.94 | 0.48 |
| 7:L4:191:ARG:HH22 | 7:L4:218:PHE:HB3 | 1.78 | 0.48 |
| 8:L5:124:LEU:HD11 | 18:LJ:117:LEU:HD21 | 1.96 | 0.48 |
| 15:LF:55:VAL:HG23 | 15:LF:75:VAL:HB | 1.96 | 0.48 |
| 18:LJ:35:LEU:HD23 | 18:LJ:326:LEU:HD13 | 1.96 | 0.48 |
| 23:LO:23:SER:OG | 23:LO:24:ASP:N | 2.46 | 0.48 |
| 25:LQ:745:SER:OG | 25:LQ:746:LEU:N | 2.46 | 0.48 |
| 29:LV:338:MET:N | 29:LV:338:MET:SD | 2.86 | 0.48 |
| 36:SG:259:LYS:HB2 | 36:SG:259:LYS:HE3 | 1.71 | 0.48 |
| 56:ND:190:LEU:HD12 | 56:ND:191:PRO:HD2 | 1.95 | 0.48 |
| 59:SB:227:LEU:HD23 | 59:SB:231:ILE:HG22 | 1.95 | 0.48 |
| 65:5:480:THR:OG1 | 65:5:481:SER:N | 2.44 | 0.48 |
| 2:SA:25:ASP:OD1 | 2:SA:25:ASP:N | 2.47 | 0.48 |
| 8:L5:72:HIS:O | 12:LC:79:TYR:OH | 2.32 | 0.48 |
| 17:LH:656:ASP:OD1 | 17:LH:656:ASP:N | 2.43 | 0.48 |
| 18:LJ:220:ALA:HA | 18:LJ:226:ILE:HG22 | 1.94 | 0.48 |
| 22:LN:106:ASN:H | 22:LN:153:GLN:HG2 | 1.79 | 0.48 |
| 23:LO:130:ASP:N | 23:LO:130:ASP:OD1 | 2.42 | 0.48 |
| 23:LO:296:GLN:NE2 | 23:LO:332:TRP:O | 2.47 | 0.48 |
| 28:LU:329:ILE:HD11 | 28:LU:351:VAL:HG21 | 1.95 | 0.48 |
| 37:SH:228:ASP:OD2 | 37:SH:230:TRP:NE1 | 2.47 | 0.48 |
| 40:SL:130:CYS:HB2 | 40:SL:132:HIS:CE1 | 2.49 | 0.48 |
| 48:SY:168:LYS:HA | 48:SY:171:LEU:HG | 1.96 | 0.48 |
| 53:8:1003:A:H1' | 53:8:1005:A:H62 | 1.79 | 0.48 |
| 53:8:1512:G:H2' | 53:8:1513:G:H8 | 1.79 | 0.48 |
| 59:SB:162:MET:SD | 59:SB:275:TYR:OH | 2.66 | 0.48 |
| 59:SB:217:LYS:O | 59:SB:221:THR:OG1 | 2.31 | 0.48 |
| 62:LX:723:LEU:O | 62:LX:764:ASN:N | 2.47 | 0.48 |
| 1:NA:322:LYS:HE3 | 1:NA:327:LYS:HG2 | 1.96 | 0.48 |
| 2:SA:306:LEU:HD21 | 2:SA:382:LYS:HB3 | 1.96 | 0.48 |
| 8:L5:16:VAL:HG21 | 27:LT:534:SER:HB3 | 1.95 | 0.48 |
| 17:LH:849:ASP:H | 17:LH:852:ASP:HB2 | 1.78 | 0.48 |
| 17:LH:864:ASP:OD1 | 17:LH:864:ASP:N | 2.47 | 0.48 |
| 18:LJ:125:HIS:NE2 | 39:SK:19:LEU:O | 2.45 | 0.48 |
| 20:LL:66:VAL:HG22 | 20:LL:112:LEU:HD22 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:LM:275:ILE:HG22 | 21:LM:279:MET:HE1 | 1.96 | 0.48 |
| 23:LO:252:LYS:NZ | 23:LO:253:LYS:O | 2.44 | 0.48 |
| 31:LZ:138:VAL:HG22 | 31:LZ:158:VAL:HG12 | 1.96 | 0.48 |
| 36:SG:417:SER:HB3 | 36:SG:421:ASN:HB2 | 1.95 | 0.48 |
| 40:SL:22:ASP:OD1 | 40:SL:22:ASP:N | 2.40 | 0.48 |
| 41:SM:268:ASN:OD1 | 48:SY:56:LYS:NZ | 2.44 | 0.48 |
| 53:8:261:U:O2' | 53:8:262:U:O4' | 2.31 | 0.48 |
| 53:8:375:U:H5'' | 53:8:376:C:H5' | 1.95 | 0.48 |
| 57:LR:279:LYS:NZ | 57:LR:317:GLU:O | 2.47 | 0.48 |
| 57:LR:619:ARG:NH1 | 57:LR:620:LEU:O | 2.47 | 0.48 |
| 57:LR:630:ASP:HB3 | 57:LR:646:ASP:HB2 | 1.96 | 0.48 |
| 62:LX:771:SER:HB2 | 62:LX:773:TRP:CE2 | 2.49 | 0.48 |
| 7:L4:110:ALA:HB1 | 36:SG:112:LEU:HD23 | 1.96 | 0.47 |
| 17:LH:479:ASN:HD22 | 18:LJ:3:THR:HG21 | 1.79 | 0.47 |
| 25:LQ:72:SER:HA | 25:LQ:75:ARG:HH22 | 1.79 | 0.47 |
| 26:LS:334:SER:OG | 26:LS:335:GLN:N | 2.47 | 0.47 |
| 29:LV:95:ARG:NH2 | 29:LV:129:GLY:O | 2.47 | 0.47 |
| 33:NK:70:ALA:HB3 | 33:NK:83:LYS:H | 1.78 | 0.47 |
| 34:SC:110:ASN:ND2 | 34:SC:112:ALA:O | 2.47 | 0.47 |
| 35:SE:102:ILE:HG21 | 35:SE:114:ILE:HD11 | 1.96 | 0.47 |
| 39:SK:119:GLY:O | 39:SK:165:ASN:ND2 | 2.44 | 0.47 |
| 53:8:513:U:H2' | 53:8:514:G:C8 | 2.49 | 0.47 |
| 62:LX:29:VAL:HA | 62:LX:152:LEU:HB3 | 1.96 | 0.47 |
| 62:LX:157:SER:HA | 62:LX:160:GLN:HB2 | 1.96 | 0.47 |
| 1:NA:301:GLU:OE2 | 1:NA:304:GLN:NE2 | 2.47 | 0.47 |
| 8:L5:26:ALA:N | 12:LC:27:GLY:O | 2.44 | 0.47 |
| 17:LH:435:ASP:OD1 | 17:LH:435:ASP:N | 2.41 | 0.47 |
| 21:LM:81:LEU:O | 21:LM:124:ARG:NH2 | 2.47 | 0.47 |
| 26:LS:272:LEU:HD11 | 26:LS:314:THR:HG21 | 1.96 | 0.47 |
| 27:LT:128:LEU:HB2 | 27:LT:150:PRO:HG2 | 1.96 | 0.47 |
| 29:LV:154:TYR:HB3 | 29:LV:164:ARG:HA | 1.94 | 0.47 |
| 36:SG:346:ALA:HB3 | 36:SG:359:PHE:HB2 | 1.95 | 0.47 |
| 37:SH:208:MET:HB3 | 37:SH:243:ILE:HD12 | 1.96 | 0.47 |
| 47:ST:726:LYS:NZ | 53:8:1461:C:OP2 | 2.44 | 0.47 |
| 57:LR:21:ALA:HB3 | 57:LR:35:PRO:HG3 | 1.96 | 0.47 |
| 2:SA:26:ASP:OD2 | 28:LU:81:ASN:ND2 | 2.43 | 0.47 |
| 2:SA:126:ASP:OD1 | 34:SC:322:ARG:NH2 | 2.47 | 0.47 |
| 2:SA:142:LEU:HA | 24:LP:105:GLN:HE21 | 1.79 | 0.47 |
| 2:SA:169:LYS:HA | 2:SA:299:VAL:HG22 | 1.96 | 0.47 |
| 4:L0:490:G:H21 | 4:L0:495:G:H1' | 1.78 | 0.47 |
| 18:LJ:191:GLY:H | 18:LJ:214:PRO:HA | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LJ:227:VAL:HG23 | 18:LJ:236:VAL:HG12 | 1.95 | 0.47 |
| 20:LL:488:ILE:HG13 | 20:LL:529:THR:HG21 | 1.96 | 0.47 |
| 22:LN:66:ARG:HH21 | 22:LN:528:ILE:HD11 | 1.79 | 0.47 |
| 22:LN:468:ASP:OD1 | 22:LN:468:ASP:N | 2.45 | 0.47 |
| 22:LN:510:GLU:O | 22:LN:558:ARG:NH1 | 2.42 | 0.47 |
| 27:LT:21:SER:HB2 | 27:LT:623:ILE:HG12 | 1.97 | 0.47 |
| 28:LU:125:ASP:OD1 | 28:LU:125:ASP:N | 2.46 | 0.47 |
| 28:LU:380:TRP:NE1 | 28:LU:398:GLU:OE2 | 2.46 | 0.47 |
| 38:SI:125:LEU:HD22 | 38:SI:912:ARG:HD2 | 1.96 | 0.47 |
| 42:SN:41:ASN:ND2 | 53:8:1499:G:O2' | 2.47 | 0.47 |
| 45:SR:126:LYS:HG2 | 45:SR:131:SER:HA | 1.96 | 0.47 |
| 65:5:488:ASP:OD1 | 65:5:488:ASP:N | 2.42 | 0.47 |
| 3:NB:531:ASN:O | 38:SI:909:ASN:ND2 | 2.47 | 0.47 |
| 3:NB:555:ASN:OD1 | 3:NB:555:ASN:N | 2.48 | 0.47 |
| 7:L4:138:TYR:HA | 7:L4:148:ARG:HA | 1.96 | 0.47 |
| 9:L7:144:VAL:HG23 | 28:LU:181:ALA:HB3 | 1.95 | 0.47 |
| 13:LD:68:GLY:HA3 | 13:LD:127:GLN:HE21 | 1.79 | 0.47 |
| 13:LD:134:THR:OG1 | 53:8:325:G:OP1 | 2.32 | 0.47 |
| 23:LO:496:THR:HA | 23:LO:513:GLU:HA | 1.96 | 0.47 |
| 23:LO:713:ASP:OD1 | 23:LO:713:ASP:N | 2.40 | 0.47 |
| 27:LT:51:VAL:HG21 | 27:LT:90:VAL:HG21 | 1.97 | 0.47 |
| 51:NH:755:PRO:HA | 51:NH:782:VAL:HA | 1.95 | 0.47 |
| 57:LR:190:THR:OG1 | 57:LR:217:ASP:OD2 | 2.32 | 0.47 |
| 64:NF:114:ARG:O | 64:NF:118:ILE:N | 2.48 | 0.47 |
| 5:L2:115:G:O2' | 5:L2:257:A:N3 | 2.44 | 0.47 |
| 12:LC:42:GLU:HA | 12:LC:45:ARG:HH12 | 1.79 | 0.47 |
| 13:LD:65:SER:OG | 53:8:115:G:OP2 | 2.33 | 0.47 |
| 14:LE:41:MET:HB2 | 14:LE:46:TYR:HB2 | 1.96 | 0.47 |
| 17:LH:195:ASN:N | 17:LH:195:ASN:OD1 | 2.47 | 0.47 |
| 18:LJ:32:SER:O | 18:LJ:71:ARG:NH2 | 2.39 | 0.47 |
| 22:LN:149:ILE:HD12 | 22:LN:153:GLN:HG3 | 1.95 | 0.47 |
| 28:LU:308:VAL:HA | 28:LU:324:SER:HA | 1.94 | 0.47 |
| 36:SG:348:LEU:HD22 | 36:SG:357:LEU:HD12 | 1.95 | 0.47 |
| 38:SI:56:VAL:HG23 | 45:SR:52:ILE:HD11 | 1.97 | 0.47 |
| 42:SN:190:ILE:HD12 | 42:SN:191:PRO:HD2 | 1.96 | 0.47 |
| 51:NH:631:GLY:N | 51:NH:665:HIS:O | 2.46 | 0.47 |
| 53:8:1203:A:O2' | 53:8:1209:C:O2' | 2.27 | 0.47 |
| 55:LI:594:SER:HA | 55:LI:597:GLN:HE22 | 1.79 | 0.47 |
| 57:LR:344:ARG:HE | 57:LR:395:ASP:HA | 1.78 | 0.47 |
| 57:LR:746:TRP:O | 57:LR:752:THR:OG1 | 2.32 | 0.47 |
| 58:NE:323:LYS:HA | 58:NE:326:ILE:HD12 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:SB:160:ASP:N | 59:SB:160:ASP:OD1 | 2.43 | 0.47 |
| 3:NB:602:LEU:HG | 3:NB:604:ARG:HG2 | 1.96 | 0.47 |
| 7:L4:71:LYS:HB2 | 7:L4:76:VAL:HA | 1.97 | 0.47 |
| 18:LJ:398:SER:O | 18:LJ:434:ARG:NH2 | 2.39 | 0.47 |
| 20:LL:338:ASN:OD1 | 26:LS:337:ALA:N | 2.48 | 0.47 |
| 20:LL:513:LEU:HD21 | 20:LL:523:LEU:HD11 | 1.97 | 0.47 |
| 25:LQ:41:LEU:HD23 | 25:LQ:52:TRP:HE1 | 1.80 | 0.47 |
| 27:LT:458:THR:OG1 | 27:LT:497:LYS:NZ | 2.41 | 0.47 |
| 27:LT:849:ILE:HD12 | 27:LT:887:LEU:HD23 | 1.97 | 0.47 |
| 34:SD:145:ASN:OD1 | 34:SD:148:ARG:NH1 | 2.47 | 0.47 |
| 34:SD:308:PRO:HG3 | 48:SY:129:SER:HA | 1.96 | 0.47 |
| 38:SI:54:LEU:HD21 | 45:SR:77:ILE:HB | 1.95 | 0.47 |
| 38:SI:1024:LYS:O | 38:SI:1026:LYS:NZ | 2.45 | 0.47 |
| 53:8:9:U:O2' | 58:NE:239:ARG:NH1 | 2.47 | 0.47 |
| 53:8:300:A:H2' | 53:8:301:A:C8 | 2.49 | 0.47 |
| 53:8:897:C:OP2 | 53:8:914:G:N2 | 2.47 | 0.47 |
| 57:LR:290:ILE:HG22 | 57:LR:306:LEU:HG | 1.97 | 0.47 |
| 1:NA:464:SER:OG | 1:NA:465:LEU:N | 2.48 | 0.47 |
| 3:NB:540:ILE:HD13 | 38:SI:150:MET:HG3 | 1.97 | 0.47 |
| 4:L0:503:C:H2' | 4:L0:504:U:H6 | 1.79 | 0.47 |
| 7:L4:42:LEU:HD21 | 7:L4:47:PHE:HB2 | 1.96 | 0.47 |
| 8:L5:26:ALA:HB3 | 12:LC:28:LEU:HB3 | 1.97 | 0.47 |
| 10:L8:67:TRP:HE1 | 10:L8:69:SER:HG | 1.63 | 0.47 |
| 12:LC:55:VAL:HG21 | 12:LC:89:LEU:HD21 | 1.97 | 0.47 |
| 16:LG:62:GLU:HB3 | 16:LG:64:ARG:HH21 | 1.80 | 0.47 |
| 19:LK:475:THR:HA | 19:LK:478:ASN:HB2 | 1.97 | 0.47 |
| 22:LN:566:LEU:HD23 | 22:LN:570:ILE:HG12 | 1.96 | 0.47 |
| 22:LN:594:PHE:HA | 22:LN:611:LEU:HA | 1.95 | 0.47 |
| 23:LO:296:GLN:OE1 | 23:LO:330:TYR:OH | 2.32 | 0.47 |
| 23:LO:412:ARG:NH2 | 25:LQ:942:VAL:O | 2.48 | 0.47 |
| 23:LO:541:ILE:HD13 | 23:LO:606:VAL:HG13 | 1.97 | 0.47 |
| 25:LQ:476:ILE:HA | 25:LQ:492:SER:HA | 1.96 | 0.47 |
| 25:LQ:603:ASP:N | 25:LQ:603:ASP:OD1 | 2.44 | 0.47 |
| 27:LT:194:ARG:HD3 | 59:SB:436:ALA:HB2 | 1.96 | 0.47 |
| 28:LU:185:ILE:HD11 | 28:LU:194:PHE:HD2 | 1.79 | 0.47 |
| 29:LV:277:ILE:HG12 | 29:LV:291:THR:HG22 | 1.97 | 0.47 |
| 30:LW:329:LEU:HD11 | 30:LW:340:LEU:HB3 | 1.96 | 0.47 |
| 38:SI:978:ARG:NH1 | 53:8:1600:A:OP1 | 2.48 | 0.47 |
| 38:SI:1034:LEU:HB2 | 38:SI:1037:GLN:HG3 | 1.97 | 0.47 |
| 39:SJ:90:ASP:N | 39:SJ:90:ASP:OD1 | 2.47 | 0.47 |
| 41:SM:149:PRO:HG2 | 41:SM:170:VAL:HG21 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:SN:128:ASP:OD1 | 42:SN:128:ASP:N | 2.47 | 0.47 |
| 48:SY:135:ILE:HG23 | 56:ND:178:VAL:HG22 | 1.97 | 0.47 |
| 53:8:239:C:O2' | 53:8:241:U:OP1 | 2.32 | 0.47 |
| 57:LR:337:HIS:HB3 | 57:LR:340:ILE:HD11 | 1.96 | 0.47 |
| 59:SB:351:ALA:HB1 | 59:SB:355:ASN:HB3 | 1.97 | 0.47 |
| 4:L0:293:U:H2' | 23:LO:631:ASN:HA | 1.97 | 0.47 |
| 18:LJ:222:SER:HB3 | 18:LJ:225:GLN:HB2 | 1.96 | 0.47 |
| 18:LJ:258:LEU:HD21 | 18:LJ:272:LEU:HD11 | 1.97 | 0.47 |
| 20:LL:58:LEU:HB2 | 20:LL:80:MET:HE1 | 1.96 | 0.47 |
| 25:LQ:24:VAL:HG12 | 25:LQ:42:ILE:HB | 1.95 | 0.47 |
| 25:LQ:629:ASN:HD22 | 25:LQ:643:ASP:HA | 1.80 | 0.47 |
| 27:LT:510:LEU:HD21 | 27:LT:514:ASN:HA | 1.95 | 0.47 |
| 27:LT:601:VAL:HG12 | 27:LT:611:THR:HG22 | 1.96 | 0.47 |
| 29:LV:191:VAL:HG23 | 65:5:484:LYS:HB2 | 1.97 | 0.47 |
| 36:SG:333:MET:SD | 36:SG:334:GLU:N | 2.88 | 0.47 |
| 37:SH:327:ARG:NH2 | 38:SI:558:ILE:O | 2.36 | 0.47 |
| 38:SI:300:GLN:HG3 | 38:SI:792:VAL:HG22 | 1.96 | 0.47 |
| 38:SI:1042:MET:HG3 | 38:SI:1044:LEU:HD13 | 1.95 | 0.47 |
| 42:SN:153:MET:HG3 | 60:SV:191:LEU:HD22 | 1.96 | 0.47 |
| 54:SU:317:ILE:HG23 | 54:SU:358:PHE:HB2 | 1.97 | 0.47 |
| 62:LX:569:PRO:HD3 | 62:LX:583:LEU:HG | 1.97 | 0.47 |
| 1:NA:295:LYS:HB3 | 1:NA:296:ASN:H | 1.52 | 0.47 |
| 4:L0:267:U:H3 | 12:LC:21:HIS:CG | 2.32 | 0.47 |
| 7:L4:151:ASP:OD1 | 63:L6:215:ARG:NH2 | 2.48 | 0.47 |
| 14:LE:106:THR:HG23 | 14:LE:108:ALA:H | 1.79 | 0.47 |
| 20:LL:151:LEU:HD11 | 20:LL:163:LEU:HD22 | 1.97 | 0.47 |
| 22:LN:288:THR:HG22 | 22:LN:295:VAL:HG23 | 1.96 | 0.47 |
| 22:LN:620:ASP:OD1 | 22:LN:620:ASP:N | 2.48 | 0.47 |
| 23:LO:273:ARG:NH1 | 27:LT:763:SER:O | 2.45 | 0.47 |
| 27:LT:414:ILE:HA | 27:LT:434:HIS:HA | 1.97 | 0.47 |
| 29:LV:85:ASP:O | 29:LV:89:LEU:N | 2.42 | 0.47 |
| 36:SG:186:PHE:HE1 | 36:SG:211:LEU:HD13 | 1.79 | 0.47 |
| 38:SI:1135:ARG:NH1 | 53:8:495:C:OP2 | 2.48 | 0.47 |
| 51:NH:186:ILE:HA | 51:NH:190:ALA:HB2 | 1.96 | 0.47 |
| 54:SU:279:LEU:HA | 54:SU:357:ARG:HH12 | 1.79 | 0.47 |
| 59:SB:379:ASP:OD1 | 59:SB:379:ASP:N | 2.40 | 0.47 |
| 62:LX:45:MET:SD | 62:LX:45:MET:N | 2.88 | 0.47 |
| 62:LX:87:GLU:HB3 | 62:LX:90:GLU:HB2 | 1.96 | 0.47 |
| 1:NA:526:ASN:OD1 | 1:NA:529:ARG:NH2 | 2.47 | 0.47 |
| 8:L5:157:ARG:HB2 | 8:L5:224:ASN:HD21 | 1.80 | 0.47 |
| 9:L7:27:LEU:HG | 9:L7:38:LEU:HD11 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:LH:233:ASP:OD1 | 17:LH:236:ASN:ND2 | 2.47 | 0.47 |
| 17:LH:510:TYR:HE1 | 17:LH:527:HIS:HB3 | 1.80 | 0.47 |
| 20:LL:281:ILE:HB | 20:LL:291:ILE:HD11 | 1.97 | 0.47 |
| 22:LN:429:SER:OG | 22:LN:430:THR:N | 2.46 | 0.47 |
| 23:LO:159:ARG:NH1 | 23:LO:179:GLU:OE2 | 2.48 | 0.47 |
| 24:LP:278:MET:HB2 | 24:LP:312:LEU:HD13 | 1.96 | 0.47 |
| 30:LW:327:THR:OG1 | 30:LW:405:GLY:O | 2.32 | 0.47 |
| 53:8:894:U:O2' | 53:8:919:A:N6 | 2.48 | 0.47 |
| 53:8:1743:U:H2' | 53:8:1744:A:H8 | 1.79 | 0.47 |
| 54:SU:399:ILE:HG21 | 54:SU:480:LEU:HB3 | 1.96 | 0.47 |
| 62:LX:817:ASP:OD1 | 62:LX:817:ASP:N | 2.48 | 0.47 |
| 62:LX:894:ASN:O | 62:LX:897:THR:OG1 | 2.30 | 0.47 |
| 4:L0:145:A:H2' | 4:L0:146:G:H8 | 1.80 | 0.46 |
| 4:L0:413:C:H2' | 4:L0:414:G:H8 | 1.79 | 0.46 |
| 16:LG:10:ALA:HB1 | 16:LG:30:VAL:HB | 1.97 | 0.46 |
| 17:LH:408:THR:HG21 | 17:LH:488:LEU:HB2 | 1.97 | 0.46 |
| 18:LJ:376:ASN:OD1 | 18:LJ:376:ASN:N | 2.47 | 0.46 |
| 19:LK:462:LEU:HD11 | 20:LL:556:THR:HG21 | 1.96 | 0.46 |
| 22:LN:624:LYS:HD3 | 22:LN:624:LYS:HA | 1.72 | 0.46 |
| 24:LP:268:ASP:N | 24:LP:268:ASP:OD1 | 2.48 | 0.46 |
| 30:LW:178:ASP:OD2 | 40:SL:24:ARG:NH1 | 2.48 | 0.46 |
| 36:SG:488:ILE:HG12 | 36:SG:498:VAL:HG12 | 1.96 | 0.46 |
| 37:SH:105:TYR:HE2 | 37:SH:296:LEU:HA | 1.80 | 0.46 |
| 37:SH:298:ILE:HG13 | 37:SH:322:PHE:HE1 | 1.79 | 0.46 |
| 37:SH:366:ILE:HD11 | 38:SI:920:GLU:HA | 1.96 | 0.46 |
| 38:SI:248:ARG:HB3 | 38:SI:357:PRO:HG2 | 1.98 | 0.46 |
| 39:SJ:113:TYR:HB3 | 39:SJ:121:LEU:HD11 | 1.96 | 0.46 |
| 40:SL:101:CYS:SG | 40:SL:102:VAL:N | 2.89 | 0.46 |
| 53:8:239:C:O2 | 53:8:244:A:N6 | 2.49 | 0.46 |
| 57:LR:332:SER:OG | 57:LR:381:VAL:O | 2.32 | 0.46 |
| 57:LR:464:LYS:HA | 57:LR:487:ARG:H | 1.80 | 0.46 |
| 2:SA:203:PHE:HB3 | 2:SA:206:LEU:HD13 | 1.97 | 0.46 |
| 4:L0:125:G:H2' | 4:L0:126:A:H8 | 1.80 | 0.46 |
| 10:L8:6:ASP:HB2 | 10:L8:28:GLU:HG3 | 1.97 | 0.46 |
| 11:L9:34:PHE:HD2 | 11:L9:111:THR:HG21 | 1.80 | 0.46 |
| 11:L9:58:ASP:HA | 11:L9:61:THR:HG22 | 1.97 | 0.46 |
| 13:LD:130:PRO:HB3 | 13:LD:136:ARG:HA | 1.97 | 0.46 |
| 17:LH:215:VAL:HA | 17:LH:218:LYS:HB2 | 1.96 | 0.46 |
| 17:LH:367:SER:O | 17:LH:367:SER:OG | 2.34 | 0.46 |
| 18:LJ:172:ARG:HH12 | 54:SU:370:HIS:HA | 1.79 | 0.46 |
| 20:LL:191:VAL:HA | 20:LL:206:ALA:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:LN:82:ARG:NH1 | 22:LN:726:UNK:O | 2.48 | 0.46 |
| 22:LN:550:VAL:HG23 | 22:LN:563:LEU:HB2 | 1.98 | 0.46 |
| 23:LO:805:ALA:HA | 57:LR:815:LYS:HE2 | 1.97 | 0.46 |
| 26:LS:534:SER:HB3 | 26:LS:540:ALA:HB1 | 1.96 | 0.46 |
| 27:LT:416:ALA:HB3 | 27:LT:433:ALA:HB3 | 1.96 | 0.46 |
| 28:LU:439:ARG:O | 28:LU:443:ASN:ND2 | 2.48 | 0.46 |
| 32:NG:45:GLY:N | 53:8:900:A:OP1 | 2.47 | 0.46 |
| 37:SH:59:VAL:HG23 | 37:SH:60:THR:HG23 | 1.95 | 0.46 |
| 39:SK:100:LEU:HD11 | 39:SK:112:VAL:HG11 | 1.96 | 0.46 |
| 48:SY:5:VAL:HG21 | 48:SY:10:LYS:HE3 | 1.96 | 0.46 |
| 57:LR:97:ARG:HH22 | 57:LR:133:ASN:HA | 1.80 | 0.46 |
| 62:LX:725:VAL:HG22 | 62:LX:762:MET:HB2 | 1.97 | 0.46 |
| 62:LX:807:SER:HA | 62:LX:810:LYS:HE2 | 1.96 | 0.46 |
| 63:L6:48:TYR:OH | 63:L6:119:GLN:O | 2.33 | 0.46 |
| 3:NB:608:PHE:HE2 | 34:SC:303:GLN:HB3 | 1.79 | 0.46 |
| 4:L0:90:G:OP1 | 18:LJ:378:LYS:NZ | 2.42 | 0.46 |
| 4:L0:220:U:H5'' | 56:ND:200:ARG:HH21 | 1.80 | 0.46 |
| 22:LN:476:LYS:HG3 | 22:LN:491:CYS:HA | 1.96 | 0.46 |
| 24:LP:278:MET:SD | 24:LP:278:MET:N | 2.81 | 0.46 |
| 25:LQ:259:ILE:HG12 | 25:LQ:274:ILE:HG23 | 1.97 | 0.46 |
| 26:LS:454:GLY:O | 26:LS:487:GLU:N | 2.48 | 0.46 |
| 28:LU:2:LYS:HB2 | 30:LW:75:GLU:HB2 | 1.98 | 0.46 |
| 29:LV:333:ASN:OD1 | 29:LV:333:ASN:N | 2.43 | 0.46 |
| 38:SI:355:TYR:OH | 38:SI:788:TYR:OH | 2.29 | 0.46 |
| 38:SI:1148:GLU:HB3 | 38:SI:1152:ARG:HH12 | 1.80 | 0.46 |
| 39:SJ:228:SER:HB3 | 39:SJ:232:LEU:HD21 | 1.96 | 0.46 |
| 39:SK:100:LEU:HD13 | 39:SK:130:ILE:HD11 | 1.97 | 0.46 |
| 39:SK:178:VAL:HG23 | 39:SK:204:VAL:HG22 | 1.97 | 0.46 |
| 53:8:35:U:H1' | 53:8:474:A:H61 | 1.80 | 0.46 |
| 53:8:1695:G:H2' | 53:8:1696:G:C8 | 2.50 | 0.46 |
| 54:SU:196:GLN:OE1 | 54:SU:260:ASN:ND2 | 2.47 | 0.46 |
| 57:LR:510:SER:OG | 57:LR:514:THR:OG1 | 2.31 | 0.46 |
| 58:NE:268:LYS:HD2 | 58:NE:298:LYS:HZ1 | 1.79 | 0.46 |
| 4:L0:93:A:OP2 | 18:LJ:384:ARG:NH2 | 2.42 | 0.46 |
| 5:L2:254:A:C8 | 35:SF:35:LYS:HE2 | 2.50 | 0.46 |
| 12:LC:103:ASN:HD21 | 23:LO:554:ASP:HB2 | 1.80 | 0.46 |
| 25:LQ:489:VAL:HG21 | 25:LQ:546:LEU:HD11 | 1.96 | 0.46 |
| 32:NG:15:GLY:N | 32:NG:78:ALA:O | 2.48 | 0.46 |
| 34:SC:293:LEU:HD22 | 34:SC:298:ILE:HD12 | 1.98 | 0.46 |
| 39:SK:155:SER:O | 39:SK:155:SER:OG | 2.32 | 0.46 |
| 57:LR:738:LEU:HA | 57:LR:741:LYS:HE2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:SP:248:HIS:H | 61:SP:251:ALA:HB3 | 1.80 | 0.46 |
| 65:5:446:SER:HA | 65:5:449:LYS:HZ1 | 1.81 | 0.46 |
| 2:SA:6:TYR:HD2 | 2:SA:86:LEU:HD23 | 1.80 | 0.46 |
| 2:SA:283:ASP:OD1 | 2:SA:286:ARG:NH2 | 2.47 | 0.46 |
| 4:L0:348:U:N3 | 4:L0:376:U:O2 | 2.49 | 0.46 |
| 6:L3:82:PRO:HB3 | 42:SN:68:ARG:HB2 | 1.97 | 0.46 |
| 19:LK:505:MET:O | 19:LK:509:GLN:N | 2.34 | 0.46 |
| 22:LN:649:TRP:NE1 | 22:LN:744:VAL:O | 2.49 | 0.46 |
| 24:LP:67:ARG:NH2 | 24:LP:84:SER:OG | 2.49 | 0.46 |
| 26:LS:519:SER:HB3 | 26:LS:535:ARG:HG2 | 1.98 | 0.46 |
| 27:LT:918:LYS:O | 27:LT:921:ARG:NE | 2.45 | 0.46 |
| 29:LV:282:ASN:OD1 | 29:LV:325:GLY:N | 2.36 | 0.46 |
| 35:SE:32:GLN:NE2 | 35:SE:103:THR:O | 2.41 | 0.46 |
| 35:SF:35:LYS:HD2 | 35:SF:91:CYS:SG | 2.55 | 0.46 |
| 53:8:1684:U:H2' | 53:8:1685:G:H8 | 1.79 | 0.46 |
| 62:LX:871:MET:N | 62:LX:871:MET:SD | 2.89 | 0.46 |
| 63:L6:98:ARG:NH1 | 63:L6:101:ILE:O | 2.49 | 0.46 |
| 17:LH:508:ILE:HD11 | 17:LH:560:ILE:HG21 | 1.97 | 0.46 |
| 22:LN:251:ASP:OD1 | 22:LN:251:ASP:N | 2.48 | 0.46 |
| 22:LN:330:GLY:HA3 | 22:LN:353:GLU:HG3 | 1.98 | 0.46 |
| 25:LQ:392:THR:OG1 | 25:LQ:393:ASP:N | 2.48 | 0.46 |
| 34:SD:271:ILE:HG12 | 34:SD:289:GLU:HG3 | 1.97 | 0.46 |
| 36:SG:198:LYS:HD3 | 36:SG:268:LEU:HD13 | 1.97 | 0.46 |
| 39:SK:180:LEU:HD23 | 39:SK:237:ALA:HB1 | 1.97 | 0.46 |
| 53:8:329:G:H2' | 53:8:330:G:H8 | 1.80 | 0.46 |
| 56:ND:160:ARG:HA | 56:ND:163:LEU:HB3 | 1.97 | 0.46 |
| 57:LR:72:ASP:OD1 | 57:LR:72:ASP:N | 2.46 | 0.46 |
| 57:LR:299:ASN:HB2 | 57:LR:301:GLN:HG2 | 1.98 | 0.46 |
| 65:5:241:ARG:NH2 | 66:6:19:SER:O | 2.49 | 0.46 |
| 3:NB:559:ARG:HA | 53:8:545:A:H62 | 1.79 | 0.46 |
| 17:LH:334:LEU:HD22 | 18:LJ:2:SER:HB2 | 1.97 | 0.46 |
| 23:LO:530:VAL:HG23 | 23:LO:544:ILE:HG12 | 1.97 | 0.46 |
| 25:LQ:165:SER:HB3 | 25:LQ:182:LYS:HB2 | 1.98 | 0.46 |
| 25:LQ:198:GLU:OE1 | 25:LQ:200:HIS:ND1 | 2.42 | 0.46 |
| 25:LQ:592:SER:OG | 25:LQ:593:ALA:N | 2.47 | 0.46 |
| 26:LS:233:LEU:O | 26:LS:554:ASN:ND2 | 2.41 | 0.46 |
| 28:LU:387:THR:HG23 | 28:LU:390:GLU:H | 1.81 | 0.46 |
| 34:SD:228:GLN:HA | 34:SD:231:ARG:HB2 | 1.98 | 0.46 |
| 36:SG:131:ARG:HE | 36:SG:411:PHE:HE2 | 1.62 | 0.46 |
| 36:SG:447:SER:OG | 36:SG:449:ASN:OD1 | 2.34 | 0.46 |
| 37:SH:65:ILE:HG12 | 37:SH:76:TYR:HD1 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:SH:221:CYS:SG | 37:SH:222:GLU:N | 2.88 | 0.46 |
| 38:SI:861:THR:N | 38:SI:882:ASN:O | 2.44 | 0.46 |
| 38:SI:1051:ASP:OD1 | 38:SI:1051:ASP:N | 2.48 | 0.46 |
| 48:SY:207:ARG:NH1 | 48:SY:210:GLN:OE1 | 2.49 | 0.46 |
| 66:6:306:ARG:O | 66:6:310:GLN:NE2 | 2.49 | 0.46 |
| 4:L0:226:U:C2 | 22:LN:236:LYS:HE3 | 2.51 | 0.46 |
| 7:L4:233:LYS:HB3 | 7:L4:233:LYS:HE2 | 1.80 | 0.46 |
| 13:LD:125:VAL:HB | 13:LD:137:PHE:HB3 | 1.97 | 0.46 |
| 18:LJ:104:LEU:HB2 | 18:LJ:121:ASN:HA | 1.98 | 0.46 |
| 21:LM:387:LEU:HD12 | 21:LM:407:PHE:HE2 | 1.79 | 0.46 |
| 25:LQ:118:ASN:N | 25:LQ:118:ASN:OD1 | 2.48 | 0.46 |
| 27:LT:76:THR:OG1 | 27:LT:78:SER:O | 2.34 | 0.46 |
| 31:LZ:29:ASP:OD1 | 31:LZ:29:ASP:N | 2.45 | 0.46 |
| 34:SD:224:ALA:O | 34:SD:256:ASN:ND2 | 2.39 | 0.46 |
| 36:SG:263:TRP:HA | 36:SG:270:PRO:HA | 1.98 | 0.46 |
| 36:SG:417:SER:OG | 36:SG:418:ASP:N | 2.48 | 0.46 |
| 37:SH:183:ILE:HD13 | 37:SH:310:ARG:HH12 | 1.81 | 0.46 |
| 53:8:362:G:H2' | 53:8:363:G:H8 | 1.80 | 0.46 |
| 54:SU:366:LEU:HB3 | 54:SU:405:LEU:HD21 | 1.97 | 0.46 |
| 57:LR:216:ARG:NE | 57:LR:243:VAL:O | 2.43 | 0.46 |
| 65:5:205:LYS:HA | 65:5:349:PRO:HA | 1.98 | 0.46 |
| 4:L0:411:A:H2' | 4:L0:412:A:H8 | 1.81 | 0.46 |
| 10:L8:7:SER:OG | 53:8:336:G:N2 | 2.49 | 0.46 |
| 10:L8:36:THR:OG1 | 10:L8:37:LYS:N | 2.49 | 0.46 |
| 12:LC:36:ILE:HG23 | 12:LC:49:TYR:HE1 | 1.80 | 0.46 |
| 13:LD:35:TYR:OH | 53:8:247:A:O3' | 2.33 | 0.46 |
| 17:LH:200:ASN:HD22 | 17:LH:263:ALA:HA | 1.80 | 0.46 |
| 17:LH:720:ILE:HD11 | 17:LH:766:ILE:HG21 | 1.98 | 0.46 |
| 17:LH:868:ASN:O | 17:LH:871:SER:OG | 2.33 | 0.46 |
| 18:LJ:52:PRO:HB3 | 18:LJ:309:PRO:HD2 | 1.97 | 0.46 |
| 20:LL:333:ASN:OD1 | 20:LL:333:ASN:N | 2.49 | 0.46 |
| 20:LL:441:LEU:HB2 | 20:LL:456:VAL:HG11 | 1.98 | 0.46 |
| 25:LQ:331:THR:OG1 | 25:LQ:333:ARG:NH1 | 2.48 | 0.46 |
| 27:LT:163:GLN:O | 27:LT:187:ASN:ND2 | 2.44 | 0.46 |
| 27:LT:359:ALA:HA | 27:LT:419:ILE:HD13 | 1.98 | 0.46 |
| 35:SE:70:LEU:HD13 | 59:SB:311:LYS:HD2 | 1.98 | 0.46 |
| 36:SG:137:GLY:H | 36:SG:485:ASN:HD21 | 1.63 | 0.46 |
| 51:NH:268:LEU:H | 51:NH:294:LEU:H | 1.64 | 0.46 |
| 53:8:1576:A:H3' | 53:8:1577:A:H8 | 1.81 | 0.46 |
| 55:LI:537:THR:HB | 55:LI:560:ASN:HB2 | 1.97 | 0.46 |
| 56:ND:183:THR:OG1 | 56:ND:186:ASP:OD2 | 2.33 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:L5:218:GLU:O | 8:L5:222:LYS:N | 2.46 | 0.46 |
| 12:LC:58:ASP:O | 12:LC:61:SER:OG | 2.31 | 0.46 |
| 14:LE:106:THR:OG1 | 14:LE:107:SER:N | 2.49 | 0.46 |
| 17:LH:762:TYR:HB3 | 17:LH:779:ILE:HG12 | 1.98 | 0.46 |
| 18:LJ:273:ILE:HG22 | 18:LJ:283:VAL:HG23 | 1.98 | 0.46 |
| 20:LL:166:ALA:HB2 | 20:LL:170:ILE:HG23 | 1.98 | 0.46 |
| 25:LQ:145:ILE:HB | 25:LQ:159:LEU:HB2 | 1.98 | 0.46 |
| 27:LT:546:ILE:HG23 | 27:LT:560:LEU:HB3 | 1.98 | 0.46 |
| 31:LZ:173:TYR:OH | 38:SI:1082:GLN:OE1 | 2.33 | 0.46 |
| 34:SC:306:LEU:HD23 | 34:SC:315:ILE:HG12 | 1.96 | 0.46 |
| 35:SE:62:GLU:HG2 | 59:SB:373:TYR:HA | 1.97 | 0.46 |
| 37:SH:347:ASN:ND2 | 37:SH:349:ASP:OD2 | 2.49 | 0.46 |
| 38:SI:295:ASP:OD2 | 38:SI:852:ARG:NH2 | 2.49 | 0.46 |
| 42:SN:181:ARG:NH1 | 60:SV:201:ASP:O | 2.48 | 0.46 |
| 55:LI:55:TYR:HA | 55:LI:72:THR:HA | 1.98 | 0.46 |
| 55:LI:185:SER:HA | 55:LI:201:PHE:HA | 1.97 | 0.46 |
| 57:LR:302:MET:N | 57:LR:302:MET:SD | 2.89 | 0.46 |
| 62:LX:660:TYR:HB2 | 62:LX:712:LEU:HD21 | 1.97 | 0.46 |
| 66:6:235:ASP:OD1 | 66:6:235:ASP:N | 2.48 | 0.46 |
| 16:LG:10:ALA:N | 16:LG:54:LEU:O | 2.49 | 0.45 |
| 18:LJ:440:GLU:O | 18:LJ:444:ASN:ND2 | 2.45 | 0.45 |
| 25:LQ:124:ILE:HA | 25:LQ:140:SER:HA | 1.98 | 0.45 |
| 28:LU:58:PHE:HA | 28:LU:375:TRP:CD1 | 2.51 | 0.45 |
| 28:LU:359:ASP:OD1 | 28:LU:359:ASP:N | 2.49 | 0.45 |
| 34:SC:273:ALA:HA | 34:SC:285:VAL:HG11 | 1.97 | 0.45 |
| 40:SL:149:LYS:HG2 | 40:SL:170:ILE:HD11 | 1.97 | 0.45 |
| 41:SM:7:ARG:NH1 | 41:SM:11:GLU:OE2 | 2.49 | 0.45 |
| 41:SM:72:GLN:NE2 | 41:SM:73:VAL:O | 2.48 | 0.45 |
| 55:LI:257:SER:O | 55:LI:259:ILE:N | 2.49 | 0.45 |
| 9:L7:137:GLY:HA3 | 9:L7:153:LEU:HD23 | 1.97 | 0.45 |
| 17:LH:875:MET:N | 17:LH:875:MET:SD | 2.89 | 0.45 |
| 20:LL:252:SER:OG | 20:LL:253:LEU:N | 2.50 | 0.45 |
| 24:LP:44:ASN:OD1 | 24:LP:98:ARG:NH1 | 2.50 | 0.45 |
| 25:LQ:400:SER:OG | 25:LQ:401:ASP:N | 2.47 | 0.45 |
| 29:LV:207:TRP:CE2 | 29:LV:214:ARG:HB3 | 2.51 | 0.45 |
| 30:LW:340:LEU:O | 30:LW:368:TYR:N | 2.45 | 0.45 |
| 31:LZ:30:THR:HG23 | 31:LZ:34:ARG:HH21 | 1.82 | 0.45 |
| 36:SG:261:ILE:HG23 | 36:SG:273:VAL:HG12 | 1.99 | 0.45 |
| 38:SI:372:TYR:HD1 | 62:LX:5:ALA:HA | 1.80 | 0.45 |
| 39:SK:112:VAL:HG13 | 39:SK:124:VAL:HB | 1.98 | 0.45 |
| 53:8:1486:G:O6 | 53:8:1487:A:N6 | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:8:1662:G:H2' | 53:8:1663:G:H8 | 1.81 | 0.45 |
| 57:LR:340:ILE:HD12 | 57:LR:355:LEU:HD22 | 1.98 | 0.45 |
| 57:LR:786:ILE:O | 57:LR:789:THR:OG1 | 2.30 | 0.45 |
| 65:5:413:PHE:O | 65:5:417:LEU:N | 2.43 | 0.45 |
| 17:LH:96:ILE:H | 17:LH:108:THR:HG21 | 1.81 | 0.45 |
| 22:LN:55:SER:HB2 | 22:LN:290:THR:HB | 1.98 | 0.45 |
| 26:LS:426:VAL:HG23 | 26:LS:432:VAL:HG22 | 1.98 | 0.45 |
| 27:LT:49:TYR:OH | 27:LT:86:HIS:O | 2.30 | 0.45 |
| 27:LT:192:ASN:O | 27:LT:196:GLY:N | 2.49 | 0.45 |
| 27:LT:639:ASP:OD1 | 27:LT:639:ASP:N | 2.47 | 0.45 |
| 28:LU:321:VAL:HG23 | 28:LU:331:ILE:HG12 | 1.98 | 0.45 |
| 29:LV:63:LYS:HD2 | 29:LV:63:LYS:HA | 1.80 | 0.45 |
| 34:SC:268:VAL:HG22 | 34:SC:317:VAL:HG13 | 1.98 | 0.45 |
| 44:SQ:54:GLU:O | 44:SQ:58:ASN:ND2 | 2.49 | 0.45 |
| 45:SR:89:ASN:O | 45:SR:91:GLY:N | 2.49 | 0.45 |
| 54:SU:430:ASP:OD1 | 54:SU:430:ASP:N | 2.49 | 0.45 |
| 57:LR:191:SER:HB3 | 57:LR:216:ARG:H | 1.82 | 0.45 |
| 57:LR:281:THR:HG22 | 57:LR:327:ILE:HB | 1.97 | 0.45 |
| 58:NE:274:LYS:HA | 58:NE:274:LYS:HD3 | 1.79 | 0.45 |
| 4:L0:253:U:H3 | 42:SN:78:ASP:HB2 | 1.81 | 0.45 |
| 10:L8:57:ALA:HB2 | 10:L8:177:GLY:HA2 | 1.98 | 0.45 |
| 15:LF:78:SER:OG | 15:LF:81:GLU:OE2 | 2.34 | 0.45 |
| 22:LN:579:ARG:NH1 | 22:LN:593:GLU:OE2 | 2.41 | 0.45 |
| 28:LU:273:GLU:OE1 | 28:LU:288:TYR:OH | 2.34 | 0.45 |
| 38:SI:900:GLN:HG2 | 38:SI:914:ALA:HB2 | 1.97 | 0.45 |
| 42:SN:189:TYR:OH | 42:SN:231:GLN:O | 2.32 | 0.45 |
| 42:SN:228:LYS:HE3 | 42:SN:228:LYS:HB3 | 1.68 | 0.45 |
| 53:8:312:A:H62 | 53:8:352:A:H1' | 1.82 | 0.45 |
| 53:8:1511:U:H2' | 53:8:1512:G:C8 | 2.52 | 0.45 |
| 53:8:1541:G:N2 | 53:8:1569:A:N7 | 2.64 | 0.45 |
| 4:L0:487:A:H62 | 24:LP:3:LYS:HG3 | 1.80 | 0.45 |
| 5:L2:105:C:O2' | 5:L2:106:C:O4' | 2.32 | 0.45 |
| 11:L9:134:ILE:HA | 11:L9:158:PHE:HA | 1.98 | 0.45 |
| 17:LH:397:LYS:NZ | 17:LH:738:ASN:OD1 | 2.50 | 0.45 |
| 17:LH:719:ASN:OD1 | 17:LH:719:ASN:N | 2.50 | 0.45 |
| 22:LN:120:SER:OG | 22:LN:121:THR:N | 2.40 | 0.45 |
| 22:LN:298:ALA:HB2 | 22:LN:336:ILE:HG13 | 1.99 | 0.45 |
| 22:LN:495:VAL:HB | 22:LN:511:VAL:HB | 1.98 | 0.45 |
| 23:LO:221:THR:OG1 | 23:LO:222:LYS:N | 2.48 | 0.45 |
| 23:LO:356:ASP:OD1 | 23:LO:356:ASP:N | 2.39 | 0.45 |
| 23:LO:568:ARG:HD3 | 23:LO:568:ARG:HA | 1.71 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:777:ARG:HA | 23:LO:777:ARG:HD2 | 1.80 | 0.45 |
| 25:LQ:17:ILE:HB | 25:LQ:360:ASN:HB3 | 1.99 | 0.45 |
| 25:LQ:125:THR:N | 25:LQ:139:GLY:O | 2.50 | 0.45 |
| 27:LT:594:SER:HB2 | 27:LT:599:TRP:HB2 | 1.98 | 0.45 |
| 28:LU:329:ILE:HG13 | 28:LU:375:TRP:HZ3 | 1.80 | 0.45 |
| 29:LV:24:SER:O | 29:LV:44:GLN:NE2 | 2.50 | 0.45 |
| 29:LV:62:ILE:HG23 | 29:LV:321:GLU:HB2 | 1.97 | 0.45 |
| 34:SD:223:ASP:OD2 | 34:SD:226:HIS:ND1 | 2.47 | 0.45 |
| 39:SK:25:PRO:HB2 | 47:ST:708:VAL:HG23 | 1.99 | 0.45 |
| 39:SK:96:LEU:HB3 | 39:SK:130:ILE:HD13 | 1.99 | 0.45 |
| 47:ST:546:LEU:HD23 | 47:ST:549:ILE:HD12 | 1.99 | 0.45 |
| 49:SZ:347:VAL:N | 53:8:1220:C:OP1 | 2.50 | 0.45 |
| 53:8:327:U:H2' | 53:8:328:A:H8 | 1.82 | 0.45 |
| 53:8:590:C:H2' | 53:8:591:A:H8 | 1.82 | 0.45 |
| 59:SB:298:ARG:HB3 | 59:SB:341:LEU:HD21 | 1.98 | 0.45 |
| 62:LX:857:ASP:N | 62:LX:857:ASP:OD1 | 2.50 | 0.45 |
| 2:SA:81:ILE:O | 2:SA:85:ASN:ND2 | 2.50 | 0.45 |
| 2:SA:259:UNK:O | 2:SA:264:SER:N | 2.49 | 0.45 |
| 5:L2:8:U:H2' | 5:L2:9:A:H8 | 1.82 | 0.45 |
| 6:L3:28:ILE:HA | 6:L3:31:ALA:HB3 | 1.97 | 0.45 |
| 8:L5:224:ASN:OD1 | 8:L5:224:ASN:N | 2.48 | 0.45 |
| 9:L7:49:ILE:HG23 | 9:L7:175:LYS:HD3 | 1.98 | 0.45 |
| 18:LJ:165:THR:OG1 | 18:LJ:166:GLY:N | 2.49 | 0.45 |
| 18:LJ:378:LYS:HZ3 | 18:LJ:378:LYS:HG2 | 1.50 | 0.45 |
| 22:LN:240:LEU:H | 22:LN:258:SER:HB3 | 1.80 | 0.45 |
| 24:LP:40:GLU:OE2 | 24:LP:91:ARG:NH2 | 2.45 | 0.45 |
| 24:LP:92:ILE:HA | 24:LP:95:ILE:HD12 | 1.98 | 0.45 |
| 25:LQ:85:LEU:HB2 | 25:LQ:94:LEU:HD11 | 1.98 | 0.45 |
| 28:LU:225:LEU:HA | 28:LU:237:SER:HA | 1.98 | 0.45 |
| 28:LU:357:SER:OG | 28:LU:359:ASP:OD1 | 2.27 | 0.45 |
| 29:LV:117:LEU:HD12 | 29:LV:123:ILE:HD11 | 1.99 | 0.45 |
| 34:SC:242:ALA:HB2 | 34:SC:253:ILE:HD11 | 1.98 | 0.45 |
| 34:SD:236:MET:SD | 34:SD:236:MET:N | 2.90 | 0.45 |
| 36:SG:229:GLU:HB2 | 36:SG:231:THR:HG23 | 1.99 | 0.45 |
| 38:SI:306:ASP:OD1 | 38:SI:306:ASP:N | 2.42 | 0.45 |
| 51:NH:765:LEU:HA | 51:NH:914:ARG:HA | 1.99 | 0.45 |
| 53:8:319:U:H1' | 53:8:323:A:C8 | 2.51 | 0.45 |
| 53:8:396:G:H21 | 53:8:398:G:H3' | 1.81 | 0.45 |
| 53:8:1629:G:O2' | 53:8:1630:U:O4' | 2.33 | 0.45 |
| 57:LR:620:LEU:HA | 57:LR:636:ASP:HA | 1.99 | 0.45 |
| 57:LR:744:ARG:HG3 | 57:LR:785:ILE:HG12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:LY:58:ALA:HB3 | 62:LY:125:GLN:H | 1.82 | 0.45 |
| 62:LX:851:ASP:HB3 | 62:LX:854:VAL:HG23 | 1.99 | 0.45 |
| 65:5:216:ALA:HB1 | 66:6:4:LEU:HD22 | 1.99 | 0.45 |
| 9:L7:35:LYS:O | 9:L7:39:ARG:NH1 | 2.50 | 0.45 |
| 17:LH:592:SER:O | 17:LH:592:SER:OG | 2.31 | 0.45 |
| 22:LN:399:VAL:HB | 22:LN:420:LEU:HD12 | 1.98 | 0.45 |
| 23:LO:446:CYS:HB3 | 23:LO:457:VAL:HG12 | 1.98 | 0.45 |
| 23:LO:563:ARG:HH11 | 23:LO:630:LEU:HD12 | 1.82 | 0.45 |
| 25:LQ:614:HIS:HB2 | 25:LQ:618:ILE:HG12 | 1.98 | 0.45 |
| 27:LT:360:ASP:N | 27:LT:360:ASP:OD1 | 2.49 | 0.45 |
| 28:LU:46:ASN:ND2 | 30:LW:434:LEU:O | 2.45 | 0.45 |
| 28:LU:58:PHE:HD1 | 28:LU:375:TRP:HE1 | 1.65 | 0.45 |
| 30:LW:99:THR:HA | 30:LW:102:LYS:HB2 | 1.99 | 0.45 |
| 36:SG:292:SER:OG | 36:SG:293:ASP:N | 2.50 | 0.45 |
| 38:SI:996:LEU:HB3 | 38:SI:998:SER:H | 1.81 | 0.45 |
| 39:SK:124:VAL:HG22 | 39:SK:160:LEU:HD22 | 1.98 | 0.45 |
| 39:SK:181:SER:OG | 39:SK:182:PHE:N | 2.49 | 0.45 |
| 41:SM:144:GLU:OE1 | 41:SM:147:GLY:N | 2.47 | 0.45 |
| 51:NH:403:GLY:HA2 | 51:NH:411:ILE:H | 1.82 | 0.45 |
| 53:8:878:G:H2' | 53:8:879:G:H8 | 1.81 | 0.45 |
| 3:NB:533:SER:OG | 3:NB:534:GLY:N | 2.49 | 0.45 |
| 4:L0:472:A:OP1 | 30:LW:145:ARG:NH1 | 2.48 | 0.45 |
| 7:L4:26:CYS:SG | 7:L4:27:TYR:N | 2.89 | 0.45 |
| 25:LQ:80:ALA:HB1 | 25:LQ:98:TYR:HB3 | 1.99 | 0.45 |
| 28:LU:225:LEU:HD12 | 28:LU:235:LEU:HD11 | 1.99 | 0.45 |
| 31:LZ:113:VAL:HG22 | 31:LZ:124:ILE:HD11 | 1.99 | 0.45 |
| 37:SH:68:SER:OG | 37:SH:69:TYR:N | 2.49 | 0.45 |
| 37:SH:234:ASN:OD1 | 37:SH:234:ASN:N | 2.49 | 0.45 |
| 53:8:1157:A:O2' | 53:8:1159:C:OP2 | 2.30 | 0.45 |
| 53:8:1693:A:H2' | 53:8:1694:A:C4 | 2.52 | 0.45 |
| 57:LR:510:SER:OG | 57:LR:512:ASP:OD1 | 2.33 | 0.45 |
| 66:6:88:LYS:HA | 66:6:88:LYS:HD3 | 1.75 | 0.45 |
| 4:L0:100:G:N7 | 18:LJ:25:ARG:NH1 | 2.56 | 0.45 |
| 4:L0:548:A:H2' | 4:L0:549:G:C8 | 2.52 | 0.45 |
| 5:L2:114:A:H61 | 5:L2:256:G:H1' | 1.81 | 0.45 |
| 8:L5:95:ASN:O | 53:8:1611:A:O2' | 2.30 | 0.45 |
| 14:LE:11:LEU:O | 14:LE:15:ASN:ND2 | 2.49 | 0.45 |
| 17:LH:437:THR:HB | 17:LH:709:ARG:HD2 | 1.98 | 0.45 |
| 18:LJ:255:VAL:HG12 | 18:LJ:276:SER:HA | 1.99 | 0.45 |
| 21:LM:250:SER:OG | 21:LM:253:CYS:SG | 2.69 | 0.45 |
| 22:LN:303:LYS:HD3 | 22:LN:305:PHE:HE1 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LQ:81:GLU:OE1 | 25:LQ:657:GLN:NE2 | 2.50 | 0.45 |
| 28:LU:67:ARG:NH1 | 28:LU:89:ASP:OD2 | 2.41 | 0.45 |
| 28:LU:347:ARG:O | 28:LU:373:ARG:NH2 | 2.50 | 0.45 |
| 36:SG:235:HIS:HA | 36:SG:259:LYS:HZ1 | 1.81 | 0.45 |
| 38:SI:196:THR:HG23 | 38:SI:197:GLU:HG3 | 1.98 | 0.45 |
| 41:SM:285:ASN:HD22 | 47:ST:767:ILE:HD12 | 1.82 | 0.45 |
| 47:ST:511:SER:HA | 47:ST:557:SER:HB3 | 1.98 | 0.45 |
| 54:SU:252:LYS:O | 54:SU:256:ASN:ND2 | 2.50 | 0.45 |
| 63:L6:4:ASN:O | 63:L6:111:LEU:N | 2.46 | 0.45 |
| 4:L0:86:C:H5' | 17:LH:295:TRP:HZ2 | 1.82 | 0.45 |
| 5:L2:62:C:O2' | 27:LT:447:ASN:O | 2.35 | 0.45 |
| 9:L7:127:GLU:HA | 9:L7:130:VAL:HG22 | 1.98 | 0.45 |
| 17:LH:31:ASN:HD21 | 17:LH:201:ILE:HD12 | 1.81 | 0.45 |
| 17:LH:60:ARG:NH1 | 17:LH:381:SER:O | 2.45 | 0.45 |
| 17:LH:283:VAL:HB | 17:LH:290:ILE:HG22 | 1.98 | 0.45 |
| 17:LH:403:ILE:HG12 | 17:LH:417:LEU:HD21 | 1.99 | 0.45 |
| 26:LS:271:THR:OG1 | 26:LS:273:ARG:NH1 | 2.50 | 0.45 |
| 26:LS:351:THR:OG1 | 26:LS:352:GLN:N | 2.50 | 0.45 |
| 26:LS:514:LEU:O | 48:SY:248:ARG:NH2 | 2.50 | 0.45 |
| 30:LW:237:ALA:HB1 | 30:LW:280:ILE:HG12 | 1.99 | 0.45 |
| 7:L4:39:ARG:HA | 7:L4:39:ARG:HD3 | 1.87 | 0.44 |
| 13:LD:71:LEU:HD21 | 13:LD:88:ARG:HG3 | 1.99 | 0.44 |
| 17:LH:707:MET:N | 17:LH:707:MET:SD | 2.91 | 0.44 |
| 17:LH:729:THR:O | 17:LH:734:VAL:N | 2.50 | 0.44 |
| 18:LJ:13:ALA:HB2 | 18:LJ:454:ARG:HG3 | 1.99 | 0.44 |
| 27:LT:66:LEU:HD12 | 27:LT:344:ARG:HB3 | 1.98 | 0.44 |
| 28:LU:230:ASN:ND2 | 28:LU:271:PRO:O | 2.50 | 0.44 |
| 36:SG:206:LYS:HD2 | 36:SG:206:LYS:HA | 1.77 | 0.44 |
| 38:SI:826:LYS:HB2 | 38:SI:921:GLU:HB3 | 1.98 | 0.44 |
| 38:SI:906:ASP:OD1 | 38:SI:906:ASP:N | 2.43 | 0.44 |
| 41:SM:188:HIS:HB2 | 41:SM:221:VAL:HG12 | 1.99 | 0.44 |
| 53:8:29:U:H2' | 53:8:30:G:H8 | 1.82 | 0.44 |
| 53:8:1502:G:N2 | 53:8:1505:A:OP2 | 2.42 | 0.44 |
| 57:LR:312:GLN:HB3 | 57:LR:329:VAL:HG21 | 1.99 | 0.44 |
| 62:LX:55:VAL:HG13 | 62:LX:103:ILE:HG23 | 1.99 | 0.44 |
| 17:LH:876:PHE:HZ | 21:LM:180:ILE:HD11 | 1.82 | 0.44 |
| 19:LK:507:ARG:HB3 | 55:LI:655:LEU:HD23 | 1.99 | 0.44 |
| 23:LO:5:PHE:HA | 23:LO:706:THR:HG22 | 1.99 | 0.44 |
| 23:LO:7:PHE:HD2 | 23:LO:51:GLU:HA | 1.82 | 0.44 |
| 23:LO:825:GLN:HA | 23:LO:828:ILE:HG22 | 1.98 | 0.44 |
| 27:LT:139:ILE:HD11 | 27:LT:157:LEU:HD12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:LV:16:VAL:HG23 | 29:LV:340:THR:HG23 | 1.99 | 0.44 |
| 29:LV:106:ILE:HD11 | 29:LV:111:TRP:HA | 1.98 | 0.44 |
| 38:SI:195:TRP:NE1 | 38:SI:202:ALA:O | 2.38 | 0.44 |
| 39:SJ:232:LEU:HB3 | 39:SJ:237:ALA:HB2 | 2.00 | 0.44 |
| 41:SM:217:ASP:OD1 | 41:SM:217:ASP:N | 2.45 | 0.44 |
| 42:SN:223:LEU:HB3 | 42:SN:235:ILE:HD12 | 1.98 | 0.44 |
| 48:SY:6:HIS:H | 48:SY:9:GLN:HB3 | 1.82 | 0.44 |
| 54:SU:222:LEU:O | 54:SU:225:HIS:NE2 | 2.46 | 0.44 |
| 57:LR:113:THR:OG1 | 57:LR:114:SER:N | 2.49 | 0.44 |
| 57:LR:465:LYS:H | 57:LR:486:THR:HA | 1.82 | 0.44 |
| 59:SB:430:ASP:N | 59:SB:430:ASP:OD1 | 2.49 | 0.44 |
| 61:SP:1398:LEU:O | 61:SP:1402:ILE:N | 2.48 | 0.44 |
| 62:LY:567:LEU:O | 62:LY:583:LEU:N | 2.49 | 0.44 |
| 66:6:265:ASP:HB2 | 66:6:275:LYS:HB2 | 1.99 | 0.44 |
| 7:L4:212:ASP:OD1 | 7:L4:212:ASP:N | 2.45 | 0.44 |
| 8:L5:71:ALA:HB1 | 8:L5:91:GLU:HA | 2.00 | 0.44 |
| 13:LD:78:THR:HA | 13:LD:84:ILE:HG22 | 1.98 | 0.44 |
| 17:LH:550:PRO:HA | 20:LL:366:GLY:HA3 | 2.00 | 0.44 |
| 17:LH:561:LEU:HD21 | 17:LH:615:TRP:HB2 | 1.99 | 0.44 |
| 18:LJ:95:LEU:HD11 | 18:LJ:117:LEU:HD22 | 1.99 | 0.44 |
| 22:LN:258:SER:HA | 22:LN:282:ASP:HB3 | 1.98 | 0.44 |
| 22:LN:258:SER:HB2 | 56:ND:205:TRP:HZ2 | 1.83 | 0.44 |
| 23:LO:311:ASN:HD22 | 23:LO:316:TRP:HB2 | 1.81 | 0.44 |
| 26:LS:181:GLU:HB3 | 27:LT:281:ARG:HH21 | 1.82 | 0.44 |
| 27:LT:114:THR:HG22 | 27:LT:116:ALA:H | 1.82 | 0.44 |
| 34:SC:244:VAL:HG22 | 34:SC:246:GLN:HG2 | 1.99 | 0.44 |
| 38:SI:90:VAL:HG11 | 38:SI:105:ILE:HD12 | 2.00 | 0.44 |
| 38:SI:833:ARG:NH2 | 45:SR:141:GLU:OE2 | 2.51 | 0.44 |
| 42:SN:74:LEU:HD13 | 42:SN:154:ILE:HD11 | 2.00 | 0.44 |
| 53:8:473:A:H1' | 66:6:271:ARG:HD2 | 1.99 | 0.44 |
| 62:LX:36:GLN:HE21 | 62:LX:204:GLU:H | 1.64 | 0.44 |
| 62:LX:162:TYR:O | 62:LX:165:THR:OG1 | 2.32 | 0.44 |
| 66:6:266:ILE:HG22 | 66:6:274:ILE:HA | 1.99 | 0.44 |
| 15:LF:38:ASP:OD1 | 15:LF:41:ARG:NH1 | 2.50 | 0.44 |
| 17:LH:71:ASN:HB3 | 17:LH:74:LEU:HB2 | 1.99 | 0.44 |
| 17:LH:597:LYS:HA | 17:LH:597:LYS:HD3 | 1.71 | 0.44 |
| 17:LH:661:THR:HB | 17:LH:673:ALA:HB3 | 2.00 | 0.44 |
| 20:LL:370:LYS:H | 20:LL:372:VAL:HG23 | 1.82 | 0.44 |
| 21:LM:317:SER:OG | 21:LM:321:LYS:NZ | 2.50 | 0.44 |
| 22:LN:530:ARG:HD3 | 22:LN:530:ARG:HA | 1.76 | 0.44 |
| 23:LO:593:VAL:HG11 | 23:LO:684:VAL:HG11 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:760:ILE:HA | 23:LO:763:ILE:HD12 | 1.99 | 0.44 |
| 28:LU:158:LYS:HA | 28:LU:158:LYS:HD3 | 1.71 | 0.44 |
| 29:LV:143:SER:HB3 | 29:LV:186:VAL:HG12 | 1.98 | 0.44 |
| 34:SD:108:THR:OG1 | 34:SD:144:TRP:NE1 | 2.48 | 0.44 |
| 37:SH:323:ILE:HG12 | 38:SI:553:ILE:HG12 | 1.99 | 0.44 |
| 38:SI:843:ASP:OD1 | 38:SI:1035:THR:OG1 | 2.36 | 0.44 |
| 47:ST:731:ASP:HB3 | 47:ST:734:ARG:HB2 | 1.99 | 0.44 |
| 48:SY:3:LYS:HA | 48:SY:3:LYS:HD2 | 1.81 | 0.44 |
| 48:SY:29:GLU:OE2 | 48:SY:37:ARG:NH1 | 2.50 | 0.44 |
| 53:8:327:U:H2' | 53:8:328:A:C8 | 2.52 | 0.44 |
| 54:SU:277:ILE:HA | 54:SU:280:ILE:HD12 | 1.99 | 0.44 |
| 54:SU:340:LYS:HD2 | 54:SU:340:LYS:HA | 1.79 | 0.44 |
| 58:NE:234:VAL:HG23 | 58:NE:239:ARG:HB2 | 2.00 | 0.44 |
| 63:L6:54:GLY:O | 63:L6:110:ALA:N | 2.39 | 0.44 |
| 2:SA:101:SER:HB3 | 2:SA:128:ILE:HG21 | 1.99 | 0.44 |
| 4:L0:289:U:H2' | 4:L0:290:G:H8 | 1.81 | 0.44 |
| 11:L9:19:TYR:HH | 53:8:20:G:H1 | 1.64 | 0.44 |
| 13:LD:133:LYS:NZ | 53:8:324:U:OP1 | 2.45 | 0.44 |
| 23:LO:624:ASN:HB2 | 23:LO:678:GLU:HA | 1.99 | 0.44 |
| 30:LW:460:ARG:HB3 | 46:SS:847:VAL:HB | 1.99 | 0.44 |
| 30:LW:462:ASN:HB2 | 30:LW:465:ASP:H | 1.82 | 0.44 |
| 31:LZ:30:THR:HA | 31:LZ:33:MET:HB2 | 1.99 | 0.44 |
| 34:SD:241:PHE:HA | 34:SD:268:VAL:HB | 2.00 | 0.44 |
| 37:SH:42:ASN:OD1 | 37:SH:42:ASN:N | 2.50 | 0.44 |
| 53:8:468:A:H2 | 53:8:471:A:H62 | 1.64 | 0.44 |
| 53:8:1726:G:H2' | 53:8:1727:G:C8 | 2.53 | 0.44 |
| 57:LR:14:PRO:HG3 | 57:LR:639:GLY:HA3 | 2.00 | 0.44 |
| 60:SV:181:ASP:HB2 | 60:SV:187:LEU:HD22 | 2.00 | 0.44 |
| 62:LX:861:MET:HA | 62:LX:864:LEU:HD12 | 2.00 | 0.44 |
| 1:NA:364:SER:HB2 | 41:SM:227:ARG:HH22 | 1.82 | 0.44 |
| 2:SA:30:ARG:NH1 | 2:SA:122:GLU:OE2 | 2.50 | 0.44 |
| 4:L0:494:C:H2' | 4:L0:495:G:H8 | 1.81 | 0.44 |
| 6:L3:67:GLU:HA | 6:L3:70:VAL:HG12 | 2.00 | 0.44 |
| 14:LE:78:ARG:NH2 | 14:LE:125:ILE:O | 2.51 | 0.44 |
| 16:LG:60:GLU:N | 16:LG:60:GLU:OE2 | 2.50 | 0.44 |
| 21:LM:2:SER:OG | 21:LM:3:SER:N | 2.51 | 0.44 |
| 22:LN:116:SER:HB3 | 22:LN:126:TRP:HE1 | 1.82 | 0.44 |
| 23:LO:61:ILE:HG23 | 23:LO:70:LEU:HD11 | 2.00 | 0.44 |
| 23:LO:295:ILE:HG22 | 23:LO:296:GLN:HG3 | 2.00 | 0.44 |
| 30:LW:381:LEU:HD12 | 30:LW:390:LEU:HD12 | 2.00 | 0.44 |
| 35:SE:34:LYS:HD3 | 35:SE:34:LYS:HA | 1.84 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:SH:107:ALA:HB1 | 37:SH:170:VAL:HG21 | 2.00 | 0.44 |
| 38:SI:889:LEU:HD22 | 38:SI:922:ILE:HG23 | 1.98 | 0.44 |
| 41:SM:219:GLU:HB3 | 47:ST:6:LEU:HD13 | 2.00 | 0.44 |
| 47:ST:698:ILE:HG12 | 54:SU:439:LYS:HD2 | 2.00 | 0.44 |
| 53:8:101:U:O5' | 53:8:383:G:N2 | 2.51 | 0.44 |
| 57:LR:617:ASN:OD1 | 57:LR:617:ASN:N | 2.51 | 0.44 |
| 58:NE:225:GLN:HA | 58:NE:228:ILE:HG12 | 1.98 | 0.44 |
| 59:SB:245:THR:OG1 | 59:SB:246:GLU:N | 2.51 | 0.44 |
| 62:LX:16:ASN:HD21 | 62:LX:218:PRO:HA | 1.81 | 0.44 |
| 62:LX:771:SER:OG | 62:LX:772:ASN:N | 2.49 | 0.44 |
| 1:NA:342:THR:HG22 | 6:L3:119:ILE:HG21 | 1.99 | 0.44 |
| 4:L0:499:U:H2' | 4:L0:500:G:C8 | 2.52 | 0.44 |
| 5:L2:77:U:H2' | 5:L2:78:G:H8 | 1.83 | 0.44 |
| 7:L4:51:ARG:HH22 | 7:L4:110:ALA:HA | 1.82 | 0.44 |
| 7:L4:102:VAL:N | 7:L4:110:ALA:O | 2.47 | 0.44 |
| 17:LH:55:TYR:HA | 17:LH:62:CYS:HA | 1.98 | 0.44 |
| 17:LH:364:ASN:ND2 | 17:LH:410:ASN:OD1 | 2.46 | 0.44 |
| 17:LH:483:LYS:HD3 | 17:LH:488:LEU:HA | 1.98 | 0.44 |
| 18:LJ:38:GLU:N | 18:LJ:325:GLY:O | 2.45 | 0.44 |
| 18:LJ:449:GLY:O | 18:LJ:455:SER:OG | 2.36 | 0.44 |
| 21:LM:364:ASN:OD1 | 21:LM:364:ASN:N | 2.49 | 0.44 |
| 23:LO:266:VAL:HG12 | 23:LO:277:VAL:HA | 2.00 | 0.44 |
| 25:LQ:355:LEU:HB3 | 25:LQ:363:GLU:HB2 | 1.99 | 0.44 |
| 27:LT:305:ASN:ND2 | 59:SB:425:ARG:O | 2.46 | 0.44 |
| 28:LU:300:VAL:HG22 | 53:8:-1:G:C6 | 2.53 | 0.44 |
| 29:LV:20:ASN:N | 29:LV:20:ASN:OD1 | 2.50 | 0.44 |
| 29:LV:182:GLY:HA3 | 29:LV:199:THR:HA | 1.99 | 0.44 |
| 38:SI:893:ASN:HD21 | 45:SR:98:GLU:HB3 | 1.83 | 0.44 |
| 44:SQ:56:GLU:O | 44:SQ:60:LYS:NZ | 2.45 | 0.44 |
| 47:ST:776:ASP:OD1 | 47:ST:780:LYS:NZ | 2.48 | 0.44 |
| 51:NH:780:GLN:H | 51:NH:850:PHE:HA | 1.83 | 0.44 |
| 53:8:1592:A:H2' | 53:8:1593:A:H8 | 1.82 | 0.44 |
| 63:L6:115:LYS:HE3 | 63:L6:115:LYS:HB2 | 1.84 | 0.44 |
| 66:6:84:ASP:HB3 | 66:6:87:CYS:HB2 | 1.99 | 0.44 |
| 5:L2:17:G:H2' | 5:L2:18:G:C8 | 2.52 | 0.44 |
| 11:L9:139:GLN:HB3 | 66:6:266:ILE:HD11 | 2.00 | 0.44 |
| 12:LC:94:GLN:HB3 | 12:LC:102:LYS:HG3 | 2.00 | 0.44 |
| 16:LG:52:ASP:OD1 | 16:LG:52:ASP:N | 2.51 | 0.44 |
| 18:LJ:5:ARG:NH1 | 18:LJ:393:ASN:OD1 | 2.51 | 0.44 |
| 18:LJ:500:GLU:OE2 | 18:LJ:503:ARG:NH1 | 2.51 | 0.44 |
| 21:LM:122:VAL:HA | 21:LM:127:ILE:HG12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LN:57:ILE:HG22 | 22:LN:340:GLN:HB3 | 2.00 | 0.44 |
| 22:LN:561:LYS:HD3 | 22:LN:561:LYS:HA | 1.88 | 0.44 |
| 25:LQ:42:ILE:HG12 | 25:LQ:51:ILE:HB | 1.98 | 0.44 |
| 25:LQ:455:GLN:HG2 | 25:LQ:467:THR:HB | 2.00 | 0.44 |
| 29:LV:356:LEU:HD23 | 29:LV:359:ILE:HD11 | 1.99 | 0.44 |
| 34:SD:86:VAL:HG11 | 34:SD:123:ILE:HG21 | 2.00 | 0.44 |
| 37:SH:108:PRO:HB2 | 37:SH:174:ILE:HG12 | 2.00 | 0.44 |
| 37:SH:320:GLU:HA | 37:SH:323:ILE:HD12 | 2.00 | 0.44 |
| 53:8:148:A:N6 | 53:8:166:C:N3 | 2.66 | 0.44 |
| 53:8:225:A:H2' | 53:8:226:A:H4' | 1.99 | 0.44 |
| 53:8:1592:A:H2' | 53:8:1593:A:C8 | 2.53 | 0.44 |
| 53:8:1702:A:N6 | 53:8:1703:C:O2 | 2.51 | 0.44 |
| 54:SU:309:ASN:HB3 | 54:SU:312:ALA:HB3 | 1.98 | 0.44 |
| 54:SU:504:ASP:N | 54:SU:504:ASP:OD1 | 2.51 | 0.44 |
| 55:LI:228:GLU:O | 55:LI:242:CYS:N | 2.51 | 0.44 |
| 57:LR:293:VAL:HG12 | 57:LR:304:LEU:HG | 2.00 | 0.44 |
| 62:LX:779:LYS:HA | 62:LX:782:ARG:HE | 1.83 | 0.44 |
| 65:5:193:ARG:O | 65:5:193:ARG:NE | 2.49 | 0.44 |
| 5:L2:1:G:N2 | 53:8:1124:A:H1' | 2.33 | 0.44 |
| 8:L5:89:ILE:HD12 | 8:L5:137:ILE:HD12 | 2.00 | 0.44 |
| 9:L7:75:THR:O | 9:L7:79:ARG:NH1 | 2.51 | 0.44 |
| 11:L9:78:ARG:HH12 | 66:6:251:GLU:HG2 | 1.82 | 0.44 |
| 12:LC:99:GLU:HB2 | 12:LC:102:LYS:HE3 | 2.00 | 0.44 |
| 20:LL:253:LEU:HD21 | 20:LL:301:LEU:HD11 | 2.00 | 0.44 |
| 25:LQ:452:GLY:O | 25:LQ:471:ALA:N | 2.51 | 0.44 |
| 25:LQ:588:ILE:O | 25:LQ:600:TRP:N | 2.46 | 0.44 |
| 29:LV:71:CYS:SG | 29:LV:72:MET:N | 2.91 | 0.44 |
| 29:LV:250:GLY:HA3 | 29:LV:271:GLY:HA2 | 2.00 | 0.44 |
| 47:ST:604:VAL:HG13 | 47:ST:606:PHE:H | 1.82 | 0.44 |
| 53:8:153:G:OP1 | 63:L6:15:THR:OG1 | 2.33 | 0.44 |
| 53:8:933:A:H4' | 53:8:934:C:H5' | 1.99 | 0.44 |
| 53:8:1506:G:H2' | 53:8:1507:G:C8 | 2.53 | 0.44 |
| 57:LR:242:GLN:HE21 | 57:LR:263:GLY:HA3 | 1.83 | 0.44 |
| 6:L3:2:SER:OG | 54:SU:370:HIS:O | 2.36 | 0.43 |
| 7:L4:201:HIS:HB2 | 7:L4:207:LEU:HG | 2.00 | 0.43 |
| 10:L8:7:SER:O | 10:L8:10:LYS:NZ | 2.38 | 0.43 |
| 14:LE:30:SER:HA | 14:LE:34:ILE:HD11 | 2.00 | 0.43 |
| 18:LJ:426:LYS:HB2 | 18:LJ:429:VAL:HG23 | 1.99 | 0.43 |
| 20:LL:494:ARG:HE | 20:LL:498:LEU:HD11 | 1.83 | 0.43 |
| 21:LM:249:LYS:HE3 | 21:LM:249:LYS:HB3 | 1.87 | 0.43 |
| 21:LM:336:LEU:HD22 | 21:LM:373:ILE:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LN:67:LEU:HD23 | 22:LN:81:PRO:HG3 | 1.99 | 0.43 |
| 22:LN:313:LYS:HD2 | 22:LN:313:LYS:HA | 1.78 | 0.43 |
| 23:LO:261:ALA:HB1 | 23:LO:279:PHE:HB3 | 2.00 | 0.43 |
| 24:LP:279:LYS:HA | 24:LP:279:LYS:HD2 | 1.86 | 0.43 |
| 25:LQ:937:ARG:HD2 | 25:LQ:937:ARG:HA | 1.78 | 0.43 |
| 26:LS:512:ASP:N | 26:LS:512:ASP:OD1 | 2.51 | 0.43 |
| 27:LT:931:GLY:N | 57:LR:801:GLU:OE2 | 2.51 | 0.43 |
| 37:SH:290:GLY:HA3 | 37:SH:293:GLN:HG3 | 2.00 | 0.43 |
| 38:SI:992:GLU:OE1 | 53:8:564:G:O2' | 2.32 | 0.43 |
| 51:NH:675:GLU:HA | 51:NH:702:LYS:HA | 1.99 | 0.43 |
| 57:LR:513:LYS:HE2 | 57:LR:513:LYS:HB3 | 1.83 | 0.43 |
| 4:L0:189:U:H3 | 4:L0:209:G:H22 | 1.66 | 0.43 |
| 4:L0:331:U:H3 | 23:LO:656:ARG:HH12 | 1.64 | 0.43 |
| 21:LM:218:ILE:HD12 | 21:LM:263:VAL:HB | 2.00 | 0.43 |
| 21:LM:276:LEU:HD23 | 21:LM:276:LEU:HA | 1.90 | 0.43 |
| 23:LO:516:SER:HB3 | 23:LO:536:LYS:HD3 | 1.99 | 0.43 |
| 34:SD:242:ALA:HB3 | 34:SD:269:ILE:HA | 1.99 | 0.43 |
| 37:SH:156:ARG:HD2 | 37:SH:198:THR:HG21 | 2.00 | 0.43 |
| 38:SI:179:SER:OG | 38:SI:182:THR:OG1 | 2.35 | 0.43 |
| 42:SN:41:ASN:OD1 | 42:SN:41:ASN:N | 2.51 | 0.43 |
| 49:SZ:380:TYR:HA | 53:8:1220:C:H4' | 1.99 | 0.43 |
| 53:8:52:U:H2' | 53:8:53:G:C8 | 2.52 | 0.43 |
| 53:8:154:G:N3 | 63:L6:56:ASN:ND2 | 2.67 | 0.43 |
| 53:8:262:U:H2' | 53:8:263:C:H4' | 2.00 | 0.43 |
| 53:8:406:U:H2' | 53:8:407:A:C8 | 2.53 | 0.43 |
| 53:8:1655:A:H2 | 53:8:1745:G:H22 | 1.66 | 0.43 |
| 57:LR:548:LEU:N | 57:LR:560:TRP:O | 2.49 | 0.43 |
| 57:LR:655:GLU:HA | 57:LR:658:LYS:HB2 | 2.00 | 0.43 |
| 4:L0:82:A:N7 | 17:LH:256:THR:OG1 | 2.46 | 0.43 |
| 4:L0:114:G:H2' | 4:L0:115:G:H8 | 1.82 | 0.43 |
| 4:L0:529:A:H2' | 4:L0:530:A:C8 | 2.53 | 0.43 |
| 7:L4:57:ASN:N | 7:L4:60:GLU:OE2 | 2.51 | 0.43 |
| 8:L5:185:ARG:NH2 | 53:8:1472:C:OP1 | 2.50 | 0.43 |
| 9:L7:35:LYS:HA | 9:L7:38:LEU:HB2 | 1.98 | 0.43 |
| 12:LC:14:LYS:NZ | 53:8:1610:G:N7 | 2.66 | 0.43 |
| 22:LN:130:THR:HG23 | 22:LN:132:LEU:H | 1.81 | 0.43 |
| 27:LT:30:ILE:HG13 | 27:LT:380:LEU:HD23 | 1.99 | 0.43 |
| 28:LU:85:THR:HG21 | 28:LU:372:VAL:HG21 | 2.01 | 0.43 |
| 28:LU:114:THR:OG1 | 28:LU:139:CYS:SG | 2.66 | 0.43 |
| 34:SC:253:ILE:HD13 | 34:SC:253:ILE:HA | 1.89 | 0.43 |
| 53:8:164:A:H2' | 53:8:165:G:C8 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:LR:433:HIS:HE1 | 57:LR:437:VAL:HB | 1.83 | 0.43 |
| 62:LX:9:ARG:HH21 | 62:LX:199:LEU:HD21 | 1.83 | 0.43 |
| 62:LX:748:ARG:HD3 | 62:LX:748:ARG:HA | 1.80 | 0.43 |
| 65:5:332:ASP:OD1 | 65:5:332:ASP:N | 2.46 | 0.43 |
| 65:5:418:LEU:HD13 | 65:5:441:SER:HB2 | 2.01 | 0.43 |
| 5:L2:1:G:H2' | 5:L2:2:U:C6 | 2.53 | 0.43 |
| 11:L9:26:ALA:HA | 40:SL:55:TYR:HE2 | 1.83 | 0.43 |
| 13:LD:59:PRO:HA | 13:LD:64:VAL:HG23 | 2.00 | 0.43 |
| 17:LH:212:CYS:SG | 17:LH:224:SER:OG | 2.74 | 0.43 |
| 22:LN:249:ARG:NH2 | 22:LN:309:GLN:OE1 | 2.51 | 0.43 |
| 22:LN:635:GLY:HA3 | 22:LN:649:TRP:CE2 | 2.53 | 0.43 |
| 23:LO:147:GLN:HB3 | 23:LO:166:LYS:HB2 | 2.00 | 0.43 |
| 25:LQ:668:ASP:OD1 | 25:LQ:668:ASP:N | 2.52 | 0.43 |
| 35:SF:21:LEU:HA | 35:SF:24:VAL:HG22 | 1.99 | 0.43 |
| 36:SG:457:GLU:OE2 | 36:SG:461:LYS:NZ | 2.51 | 0.43 |
| 37:SH:17:PHE:N | 38:SI:609:GLU:OE2 | 2.52 | 0.43 |
| 38:SI:751:TYR:HB2 | 45:SR:77:ILE:HG22 | 2.00 | 0.43 |
| 48:SY:229:SER:HB2 | 48:SY:245:LYS:HB2 | 1.99 | 0.43 |
| 53:8:1049:U:H2' | 53:8:1050:G:C8 | 2.53 | 0.43 |
| 53:8:1274:C:H2' | 53:8:1275:A:C8 | 2.53 | 0.43 |
| 57:LR:554:ASP:OD1 | 57:LR:554:ASP:N | 2.49 | 0.43 |
| 62:LX:73:ARG:HH22 | 62:LX:99:SER:HA | 1.83 | 0.43 |
| 62:LX:587:GLN:O | 62:LX:636:VAL:N | 2.48 | 0.43 |
| 66:6:98:ARG:HH22 | 66:6:101:GLN:HG2 | 1.83 | 0.43 |
| 66:6:339:SER:O | 66:6:345:LYS:NZ | 2.51 | 0.43 |
| 2:SA:171:ASP:N | 2:SA:171:ASP:OD1 | 2.49 | 0.43 |
| 7:L4:112:HIS:CD2 | 7:L4:239:PRO:HG3 | 2.53 | 0.43 |
| 10:L8:184:LEU:HG | 10:L8:189:LEU:HG | 1.99 | 0.43 |
| 11:L9:82:ARG:NH1 | 66:6:323:GLU:OE1 | 2.49 | 0.43 |
| 15:LF:45:ALA:HA | 15:LF:50:ALA:HB3 | 1.99 | 0.43 |
| 18:LJ:117:LEU:HD23 | 18:LJ:118:LEU:HB2 | 2.00 | 0.43 |
| 20:LL:518:ASN:OD1 | 20:LL:518:ASN:N | 2.50 | 0.43 |
| 21:LM:166:ASN:HD21 | 59:SB:409:THR:HG22 | 1.83 | 0.43 |
| 21:LM:304:GLN:HA | 21:LM:346:LYS:HD2 | 2.01 | 0.43 |
| 25:LQ:392:THR:HG23 | 25:LQ:409:ALA:HB1 | 2.01 | 0.43 |
| 25:LQ:539:VAL:HG22 | 25:LQ:546:LEU:HD12 | 2.00 | 0.43 |
| 30:LW:109:LYS:HD3 | 30:LW:396:THR:HB | 2.00 | 0.43 |
| 30:LW:312:VAL:HG21 | 30:LW:353:PRO:HG2 | 2.00 | 0.43 |
| 42:SN:180:LEU:HA | 42:SN:183:ILE:HG22 | 2.01 | 0.43 |
| 4:L0:133:U:H2' | 4:L0:134:A:H8 | 1.84 | 0.43 |
| 7:L4:148:ARG:HH12 | 53:8:125:U:H5' | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:LE:12:ASN:OD1 | 14:LE:12:ASN:N | 2.51 | 0.43 |
| 17:LH:363:ASN:ND2 | 17:LH:390:PRO:O | 2.50 | 0.43 |
| 19:LK:439:LYS:HA | 19:LK:439:LYS:HD2 | 1.83 | 0.43 |
| 20:LL:104:SER:O | 20:LL:104:SER:OG | 2.33 | 0.43 |
| 21:LM:201:LYS:HE2 | 21:LM:201:LYS:HB3 | 1.85 | 0.43 |
| 22:LN:382:VAL:HG11 | 22:LN:755:ILE:HD13 | 2.00 | 0.43 |
| 28:LU:174:ARG:HD2 | 28:LU:209:LEU:HD21 | 2.00 | 0.43 |
| 40:SL:16:THR:OG1 | 40:SL:17:LEU:N | 2.49 | 0.43 |
| 53:8:109:G:O3' | 66:6:227:ARG:NH2 | 2.51 | 0.43 |
| 53:8:878:G:H2' | 53:8:879:G:C8 | 2.53 | 0.43 |
| 62:LX:92:ASP:HB3 | 62:LX:95:GLU:H | 1.83 | 0.43 |
| 62:LX:139:ILE:HG13 | 62:LX:486:LEU:HD13 | 2.00 | 0.43 |
| 1:NA:315:GLU:HG2 | 38:SI:1038:ILE:HG21 | 2.01 | 0.43 |
| 4:L0:423:C:H2' | 4:L0:424:G:H8 | 1.83 | 0.43 |
| 5:L2:8:U:H2' | 5:L2:9:A:C8 | 2.54 | 0.43 |
| 7:L4:193:GLY:H | 7:L4:194:THR:HG23 | 1.84 | 0.43 |
| 17:LH:43:ASN:N | 17:LH:43:ASN:OD1 | 2.52 | 0.43 |
| 20:LL:80:MET:SD | 20:LL:86:TRP:NE1 | 2.91 | 0.43 |
| 20:LL:302:ASN:HD21 | 20:LL:314:PHE:HB3 | 1.84 | 0.43 |
| 25:LQ:175:ASP:HA | 25:LQ:191:LEU:HB2 | 1.99 | 0.43 |
| 25:LQ:189:TRP:HA | 25:LQ:196:CYS:HA | 2.01 | 0.43 |
| 26:LS:444:ILE:HG22 | 26:LS:445:ARG:HG2 | 2.01 | 0.43 |
| 27:LT:432:THR:OG1 | 27:LT:443:TRP:NE1 | 2.37 | 0.43 |
| 29:LV:104:PHE:HE1 | 29:LV:114:SER:HB2 | 1.84 | 0.43 |
| 33:NK:44:LEU:HA | 33:NK:79:SER:HA | 2.01 | 0.43 |
| 34:SC:242:ALA:HB3 | 34:SC:269:ILE:HA | 1.99 | 0.43 |
| 36:SG:476:THR:HG22 | 36:SG:491:SER:HA | 2.00 | 0.43 |
| 37:SH:292:ASN:OD1 | 37:SH:292:ASN:N | 2.51 | 0.43 |
| 38:SI:108:VAL:HA | 38:SI:114:ARG:HB3 | 2.00 | 0.43 |
| 38:SI:373:ILE:HB | 62:LX:6:ILE:HD11 | 2.01 | 0.43 |
| 41:SM:60:GLN:OE1 | 58:NE:207:ARG:NH2 | 2.51 | 0.43 |
| 41:SM:190:ILE:HB | 41:SM:223:THR:HA | 2.01 | 0.43 |
| 42:SN:231:GLN:N | 42:SN:231:GLN:OE1 | 2.51 | 0.43 |
| 47:ST:444:ASN:OD1 | 47:ST:444:ASN:N | 2.52 | 0.43 |
| 53:8:590:C:H2' | 53:8:591:A:C8 | 2.54 | 0.43 |
| 57:LR:314:ILE:HD13 | 57:LR:329:VAL:HA | 2.00 | 0.43 |
| 57:LR:437:VAL:HA | 57:LR:458:SER:HA | 2.01 | 0.43 |
| 57:LR:733:ASP:OD1 | 57:LR:733:ASP:N | 2.43 | 0.43 |
| 58:NE:248:LYS:HE2 | 58:NE:248:LYS:HB2 | 1.93 | 0.43 |
| 1:NA:341:LEU:HD22 | 6:L3:116:LEU:HD11 | 2.00 | 0.43 |
| 1:NA:354:VAL:HG21 | 41:SM:168:HIS:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:NA:362:THR:HG22 | 41:SM:234:ARG:HH12 | 1.84 | 0.43 |
| 4:L0:486:U:H4' | 4:L0:487:A:H5'' | 2.01 | 0.43 |
| 7:L4:202:ASP:OD1 | 7:L4:202:ASP:N | 2.52 | 0.43 |
| 12:LC:39:VAL:HG12 | 12:LC:41:PRO:HD2 | 2.00 | 0.43 |
| 12:LC:98:ASP:HA | 27:LT:490:GLN:HG3 | 2.00 | 0.43 |
| 15:LF:20:ARG:HG2 | 15:LF:76:TYR:HE2 | 1.84 | 0.43 |
| 18:LJ:226:ILE:HG23 | 18:LJ:239:LEU:HD11 | 1.99 | 0.43 |
| 18:LJ:494:GLU:HG3 | 20:LL:540:LEU:HD13 | 2.01 | 0.43 |
| 21:LM:382:LEU:HD23 | 21:LM:382:LEU:HA | 1.90 | 0.43 |
| 23:LO:192:ASP:HB2 | 23:LO:212:ASP:HB3 | 2.00 | 0.43 |
| 25:LQ:449:THR:OG1 | 25:LQ:451:ASN:O | 2.37 | 0.43 |
| 29:LV:171:ARG:HG2 | 65:5:468:VAL:HA | 2.00 | 0.43 |
| 36:SG:495:SER:HB2 | 36:SG:513:GLU:HG3 | 2.00 | 0.43 |
| 37:SH:70:THR:HG23 | 37:SH:72:THR:H | 1.84 | 0.43 |
| 39:SK:169:ASP:OD1 | 39:SK:169:ASP:N | 2.51 | 0.43 |
| 57:LR:77:THR:HG21 | 57:LR:117:LEU:HG | 2.00 | 0.43 |
| 58:NE:247:VAL:HA | 58:NE:250:ILE:HB | 2.01 | 0.43 |
| 62:LX:392:ILE:O | 62:LX:546:TYR:OH | 2.34 | 0.43 |
| 5:L2:17:G:H2' | 5:L2:18:G:H8 | 1.84 | 0.43 |
| 5:L2:47:G:O2' | 40:SL:15:ARG:NH2 | 2.52 | 0.43 |
| 22:LN:744:VAL:HG13 | 22:LN:752:LEU:HD11 | 2.00 | 0.43 |
| 23:LO:211:LYS:HE3 | 23:LO:262:LYS:HD3 | 1.99 | 0.43 |
| 38:SI:1021:LEU:HA | 38:SI:1026:LYS:HG2 | 2.01 | 0.43 |
| 40:SL:78:LYS:HE3 | 40:SL:177:GLY:H | 1.83 | 0.43 |
| 41:SM:107:ILE:HD13 | 41:SM:107:ILE:HA | 1.90 | 0.43 |
| 53:8:1499:G:H1 | 53:8:1508:U:H3 | 1.66 | 0.43 |
| 53:8:1694:A:H2' | 53:8:1695:G:C5 | 2.54 | 0.43 |
| 62:LY:506:GLY:HA3 | 65:5:489:GLN:HB2 | 2.01 | 0.43 |
| 63:L6:1:MET:HG2 | 63:L6:24:ILE:HD13 | 2.00 | 0.43 |
| 65:5:497:LEU:HB3 | 65:5:500:GLN:HB3 | 1.99 | 0.43 |
| 2:SA:194:ARG:HD2 | 59:SB:169:LEU:HD12 | 2.01 | 0.43 |
| 4:L0:397:A:H2' | 4:L0:398:A:C8 | 2.54 | 0.43 |
| 12:LC:8:GLN:HE21 | 12:LC:10:PHE:HE1 | 1.67 | 0.43 |
| 23:LO:3:SER:HB2 | 23:LO:612:LEU:HD13 | 2.01 | 0.43 |
| 23:LO:559:ILE:HG23 | 23:LO:598:ASN:HD22 | 1.83 | 0.43 |
| 25:LQ:7:ARG:HH21 | 25:LQ:71:ALA:HA | 1.84 | 0.43 |
| 30:LW:109:LYS:HB2 | 30:LW:109:LYS:HE2 | 1.79 | 0.43 |
| 35:SF:17:THR:HG23 | 35:SF:81:VAL:HG12 | 2.01 | 0.43 |
| 47:ST:577:VAL:HG23 | 47:ST:585:PRO:HG3 | 2.00 | 0.43 |
| 53:8:868:G:H21 | 64:NF:90:TYR:H | 1.66 | 0.43 |
| 62:LX:529:VAL:O | 62:LX:533:PHE:N | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:L0:295:A:OP2 | 27:LT:385:GLN:NE2 | 2.45 | 0.42 |
| 6:L3:63:GLN:HA | 6:L3:66:LEU:HB2 | 2.01 | 0.42 |
| 17:LH:437:THR:HG21 | 17:LH:706:HIS:HB3 | 2.00 | 0.42 |
| 17:LH:451:PHE:HB2 | 17:LH:458:GLN:HB3 | 2.01 | 0.42 |
| 18:LJ:34:GLN:HE21 | 18:LJ:329:ILE:HD12 | 1.83 | 0.42 |
| 21:LM:103:LEU:HD23 | 21:LM:103:LEU:HA | 1.92 | 0.42 |
| 23:LO:477:SER:N | 23:LO:491:ALA:O | 2.41 | 0.42 |
| 23:LO:746:ASN:OD1 | 23:LO:777:ARG:NE | 2.49 | 0.42 |
| 25:LQ:270:SER:OG | 25:LQ:286:ILE:O | 2.34 | 0.42 |
| 25:LQ:287:ARG:NH1 | 25:LQ:323:SER:O | 2.51 | 0.42 |
| 25:LQ:673:VAL:HG22 | 25:LQ:683:ILE:HG12 | 2.00 | 0.42 |
| 26:LS:429:TYR:CD1 | 26:LS:448:LYS:HE2 | 2.54 | 0.42 |
| 26:LS:431:GLU:HB3 | 26:LS:446:ARG:HH21 | 1.83 | 0.42 |
| 27:LT:100:ILE:HD13 | 27:LT:149:TYR:HB2 | 2.01 | 0.42 |
| 31:LZ:75:GLU:HG3 | 31:LZ:94:ILE:HG12 | 2.00 | 0.42 |
| 33:NK:166:VAL:HA | 33:NK:171:VAL:HA | 2.01 | 0.42 |
| 34:SD:121:LYS:HG2 | 34:SD:143:VAL:HG11 | 2.01 | 0.42 |
| 35:SF:73:ASP:OD1 | 35:SF:73:ASP:N | 2.52 | 0.42 |
| 36:SG:363:ASP:N | 36:SG:363:ASP:OD1 | 2.43 | 0.42 |
| 36:SG:501:ILE:HG22 | 36:SG:508:PHE:HB3 | 2.01 | 0.42 |
| 47:ST:444:ASN:O | 47:ST:447:SER:OG | 2.37 | 0.42 |
| 53:8:22:A:O2' | 53:8:23:G:O4' | 2.37 | 0.42 |
| 55:LI:69:ILE:HA | 55:LI:79:ASN:HA | 2.01 | 0.42 |
| 57:LR:175:TRP:HA | 57:LR:182:CYS:HA | 2.01 | 0.42 |
| 57:LR:403:ILE:HD12 | 57:LR:415:TRP:HB2 | 2.00 | 0.42 |
| 57:LR:589:GLN:HA | 57:LR:603:ASP:HA | 2.01 | 0.42 |
| 58:NE:230:LYS:HD3 | 58:NE:230:LYS:HA | 1.79 | 0.42 |
| 62:LX:21:LYS:HB3 | 62:LX:477:ALA:HB2 | 2.01 | 0.42 |
| 2:SA:146:ASP:N | 2:SA:146:ASP:OD1 | 2.48 | 0.42 |
| 5:L2:30:A:C5 | 28:LU:57:PRO:HG2 | 2.55 | 0.42 |
| 9:L7:85:PHE:HB3 | 9:L7:88:ARG:HB2 | 2.00 | 0.42 |
| 17:LH:868:ASN:OD1 | 17:LH:868:ASN:N | 2.49 | 0.42 |
| 22:LN:262:ILE:HD11 | 22:LN:283:VAL:HG11 | 2.00 | 0.42 |
| 22:LN:580:LYS:HG3 | 22:LN:596:MET:HB2 | 2.00 | 0.42 |
| 23:LO:336:SER:HA | 27:LT:745:LYS:HA | 2.00 | 0.42 |
| 24:LP:286:ILE:HD13 | 24:LP:286:ILE:HA | 1.93 | 0.42 |
| 28:LU:143:LYS:HE2 | 28:LU:143:LYS:HB2 | 1.84 | 0.42 |
| 34:SC:272:LYS:HA | 34:SC:313:HIS:HD2 | 1.84 | 0.42 |
| 37:SH:143:LYS:HD2 | 37:SH:143:LYS:HA | 1.82 | 0.42 |
| 44:SQ:79:LYS:HA | 44:SQ:79:LYS:HD2 | 1.80 | 0.42 |
| 47:ST:102:ARG:O | 47:ST:106:LYS:NZ | 2.41 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:ST:607:THR:OG1 | 47:ST:608:LYS:N | 2.53 | 0.42 |
| 53:8:487:G:H2' | 53:8:488:G:C8 | 2.54 | 0.42 |
| 53:8:939:A:H61 | 53:8:975:C:H1' | 1.84 | 0.42 |
| 53:8:1130:G:H3' | 53:8:1131:A:H4' | 2.00 | 0.42 |
| 54:SU:130:GLU:HG2 | 54:SU:134:PHE:HB2 | 2.01 | 0.42 |
| 55:LI:563:LEU:HD13 | 55:LI:598:GLU:HG3 | 2.02 | 0.42 |
| 57:LR:24:THR:HG21 | 57:LR:68:LYS:HD3 | 2.01 | 0.42 |
| 57:LR:294:LEU:HB2 | 57:LR:303:PHE:HB2 | 2.01 | 0.42 |
| 62:LX:86:ARG:HH21 | 62:LX:91:MET:HA | 1.84 | 0.42 |
| 62:LX:653:ALA:HA | 62:LX:656:LEU:HB2 | 2.00 | 0.42 |
| 2:SA:393:SER:N | 35:SF:62:GLU:OE2 | 2.52 | 0.42 |
| 3:NB:509:ARG:NE | 53:8:1504:G:OP1 | 2.52 | 0.42 |
| 4:L0:409:C:H5'' | 38:SI:1089:GLN:HE21 | 1.85 | 0.42 |
| 13:LD:84:ILE:HG12 | 13:LD:111:VAL:HB | 2.01 | 0.42 |
| 17:LH:449:LEU:N | 17:LH:460:PHE:O | 2.52 | 0.42 |
| 26:LS:229:PRO:HA | 26:LS:230:PRO:HD3 | 1.91 | 0.42 |
| 26:LS:571:SER:OG | 26:LS:575:GLY:N | 2.52 | 0.42 |
| 28:LU:230:ASN:HB2 | 28:LU:274:ALA:HB2 | 2.01 | 0.42 |
| 29:LV:6:THR:HG22 | 29:LV:12:SER:HA | 2.00 | 0.42 |
| 29:LV:101:ASN:HA | 29:LV:118:GLN:HG3 | 2.00 | 0.42 |
| 44:SQ:119:ARG:HG2 | 44:SQ:174:LEU:HD22 | 2.01 | 0.42 |
| 57:LR:228:LYS:HD2 | 57:LR:228:LYS:HA | 1.78 | 0.42 |
| 1:NA:480:GLN:HG3 | 1:NA:482:LEU:H | 1.83 | 0.42 |
| 4:L0:210:U:H2' | 4:L0:211:G:C8 | 2.54 | 0.42 |
| 11:L9:120:LYS:HB2 | 11:L9:120:LYS:HE3 | 1.80 | 0.42 |
| 22:LN:116:SER:OG | 22:LN:117:ILE:N | 2.53 | 0.42 |
| 23:LO:522:SER:HB3 | 23:LO:583:ILE:HG22 | 2.02 | 0.42 |
| 27:LT:428:GLU:OE2 | 27:LT:452:ARG:NH1 | 2.52 | 0.42 |
| 29:LV:101:ASN:OD1 | 29:LV:118:GLN:NE2 | 2.51 | 0.42 |
| 38:SI:284:PRO:HD3 | 38:SI:779:ARG:HH22 | 1.84 | 0.42 |
| 38:SI:371:VAL:HG13 | 62:LX:6:ILE:HD12 | 2.01 | 0.42 |
| 41:SM:268:ASN:HD22 | 41:SM:271:ALA:HB2 | 1.83 | 0.42 |
| 44:SQ:75:LYS:NZ | 44:SQ:76:LYS:O | 2.51 | 0.42 |
| 44:SQ:130:LEU:HA | 44:SQ:187:PHE:HZ | 1.84 | 0.42 |
| 47:ST:419:LYS:HE3 | 47:ST:419:LYS:HB2 | 1.75 | 0.42 |
| 62:LX:69:HIS:CE1 | 62:LX:71:LYS:HB2 | 2.53 | 0.42 |
| 14:LE:117:ARG:O | 14:LE:120:HIS:ND1 | 2.51 | 0.42 |
| 21:LM:175:THR:OG1 | 21:LM:176:ALA:N | 2.52 | 0.42 |
| 22:LN:111:SER:HA | 22:LN:524:LYS:HA | 2.01 | 0.42 |
| 22:LN:325:ASN:OD1 | 22:LN:325:ASN:N | 2.50 | 0.42 |
| 23:LO:99:CYS:HA | 23:LO:115:SER:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:335:GLU:O | 25:LQ:924:TYR:OH | 2.37 | 0.42 |
| 23:LO:478:CYS:SG | 23:LO:479:LEU:N | 2.93 | 0.42 |
| 24:LP:169:GLN:HE22 | 46:SS:338:LEU:HD22 | 1.83 | 0.42 |
| 27:LT:482:GLY:HA2 | 27:LT:505:VAL:HG23 | 2.01 | 0.42 |
| 27:LT:930:MET:HA | 27:LT:933:ALA:HB3 | 2.02 | 0.42 |
| 29:LV:59:SER:OG | 29:LV:74:THR:OG1 | 2.28 | 0.42 |
| 37:SH:53:LEU:HD22 | 37:SH:65:ILE:HD13 | 2.02 | 0.42 |
| 48:SY:223:GLU:HA | 48:SY:226:LYS:HE3 | 2.02 | 0.42 |
| 59:SB:201:ASP:HB3 | 59:SB:204:ALA:HB3 | 2.02 | 0.42 |
| 62:LX:202:ASP:OD2 | 62:LX:206:ASN:ND2 | 2.53 | 0.42 |
| 65:5:290:ARG:NH1 | 66:6:101:GLN:HE21 | 2.17 | 0.42 |
| 11:L9:25:ASP:HA | 11:L9:28:LEU:HB3 | 2.00 | 0.42 |
| 11:L9:80:LEU:HA | 11:L9:83:VAL:HG22 | 2.00 | 0.42 |
| 22:LN:207:ASP:HB3 | 22:LN:209:ARG:HE | 1.84 | 0.42 |
| 22:LN:481:ILE:HB | 22:LN:485:LYS:HB3 | 2.00 | 0.42 |
| 24:LP:115:ASN:ND2 | 44:SQ:70:ASP:OD1 | 2.53 | 0.42 |
| 26:LS:234:ASP:OD2 | 26:LS:234:ASP:N | 2.41 | 0.42 |
| 27:LT:579:ARG:NE | 27:LT:614:LEU:O | 2.52 | 0.42 |
| 34:SD:177:SER:OG | 34:SD:202:ARG:NH1 | 2.53 | 0.42 |
| 38:SI:853:ARG:HH21 | 38:SI:1020:SER:HB3 | 1.85 | 0.42 |
| 39:SJ:136:ARG:NH2 | 53:8:1196:A:N3 | 2.58 | 0.42 |
| 39:SK:51:GLU:OE2 | 39:SK:51:GLU:N | 2.52 | 0.42 |
| 53:8:1049:U:H2' | 53:8:1050:G:H8 | 1.84 | 0.42 |
| 62:LX:516:PHE:HD1 | 62:LX:711:LYS:HA | 1.85 | 0.42 |
| 2:SA:218:LYS:HA | 2:SA:218:LYS:HD2 | 1.65 | 0.42 |
| 2:SA:224:LYS:HB3 | 2:SA:268:MET:HE3 | 2.01 | 0.42 |
| 9:L7:8:ILE:HD12 | 9:L7:8:ILE:HG23 | 1.85 | 0.42 |
| 10:L8:26:LYS:HE3 | 10:L8:26:LYS:HB3 | 1.82 | 0.42 |
| 11:L9:68:LYS:HB2 | 11:L9:68:LYS:HE2 | 1.84 | 0.42 |
| 20:LL:85:ILE:HB | 20:LL:99:PHE:HB2 | 2.01 | 0.42 |
| 22:LN:422:LEU:HD13 | 22:LN:444:ARG:HH22 | 1.83 | 0.42 |
| 23:LO:397:LYS:HZ2 | 23:LO:442:GLY:H | 1.67 | 0.42 |
| 25:LQ:332:ILE:HG12 | 25:LQ:379:PRO:HG3 | 2.01 | 0.42 |
| 25:LQ:931:SER:O | 25:LQ:936:LYS:NZ | 2.45 | 0.42 |
| 26:LS:496:ARG:HA | 26:LS:496:ARG:HD2 | 1.86 | 0.42 |
| 36:SG:310:ASN:N | 36:SG:310:ASN:OD1 | 2.52 | 0.42 |
| 36:SG:481:ILE:H | 36:SG:481:ILE:HD12 | 1.84 | 0.42 |
| 39:SK:148:LEU:HD11 | 53:8:1575:G:H21 | 1.84 | 0.42 |
| 41:SM:285:ASN:OD1 | 41:SM:285:ASN:N | 2.48 | 0.42 |
| 44:SQ:177:LEU:HD12 | 44:SQ:177:LEU:HA | 1.93 | 0.42 |
| 53:8:126:A:N6 | 53:8:290:G:H1 | 2.17 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:8:399:A:H1' | 53:8:401:A:H5' | 2.02 | 0.42 |
| 57:LR:453:PHE:HB2 | 57:LR:465:LYS:HD2 | 2.01 | 0.42 |
| 62:LX:69:HIS:HE1 | 62:LX:71:LYS:HB2 | 1.84 | 0.42 |
| 14:LE:55:ASP:OD2 | 14:LE:57:ARG:NH1 | 2.53 | 0.42 |
| 17:LH:308:ASP:OD1 | 17:LH:308:ASP:N | 2.46 | 0.42 |
| 17:LH:603:ASN:O | 55:LI:592:ARG:NH2 | 2.52 | 0.42 |
| 23:LO:172:ILE:HD11 | 23:LO:206:ILE:HG12 | 2.01 | 0.42 |
| 23:LO:431:ILE:HG21 | 23:LO:452:ASN:HB2 | 2.02 | 0.42 |
| 24:LP:388:UNK:O | 24:LP:392:UNK:N | 2.53 | 0.42 |
| 25:LQ:626:GLN:NE2 | 25:LQ:668:ASP:O | 2.44 | 0.42 |
| 34:SC:165:ALA:HB3 | 34:SC:168:LYS:HB2 | 2.01 | 0.42 |
| 36:SG:442:ILE:HD12 | 36:SG:470:LEU:HD22 | 2.01 | 0.42 |
| 38:SI:943:LYS:NZ | 53:8:1595:U:O2 | 2.40 | 0.42 |
| 38:SI:966:ILE:HD11 | 38:SI:1001:VAL:HB | 2.01 | 0.42 |
| 38:SI:1153:ASP:HA | 38:SI:1156:LYS:HE3 | 2.00 | 0.42 |
| 42:SN:35:ASP:OD1 | 42:SN:35:ASP:N | 2.43 | 0.42 |
| 53:8:199:G:N3 | 53:8:201:G:N2 | 2.68 | 0.42 |
| 53:8:362:G:H2' | 53:8:363:G:C8 | 2.55 | 0.42 |
| 56:ND:181:LEU:HD23 | 56:ND:181:LEU:HA | 1.89 | 0.42 |
| 57:LR:63:GLU:O | 57:LR:81:GLN:N | 2.53 | 0.42 |
| 59:SB:157:ASP:HA | 59:SB:279:ARG:HH21 | 1.85 | 0.42 |
| 62:LX:185:ASN:OD1 | 62:LX:185:ASN:N | 2.53 | 0.42 |
| 2:SA:389:ILE:HG22 | 35:SF:62:GLU:HB3 | 2.02 | 0.42 |
| 18:LJ:499:LYS:HB3 | 18:LJ:503:ARG:HH12 | 1.84 | 0.42 |
| 22:LN:645:ARG:HD3 | 22:LN:656:ARG:HH22 | 1.84 | 0.42 |
| 23:LO:69:LEU:HD23 | 23:LO:69:LEU:HA | 1.92 | 0.42 |
| 23:LO:317:LEU:HD12 | 23:LO:332:TRP:HB3 | 2.02 | 0.42 |
| 25:LQ:279:LYS:HE2 | 25:LQ:279:LYS:HB2 | 1.91 | 0.42 |
| 27:LT:90:VAL:HG13 | 27:LT:101:TYR:HB2 | 2.01 | 0.42 |
| 27:LT:316:ASP:OD1 | 27:LT:316:ASP:N | 2.51 | 0.42 |
| 38:SI:150:MET:HA | 38:SI:153:MET:HB3 | 2.00 | 0.42 |
| 39:SJ:52:THR:HG21 | 39:SJ:146:HIS:CE1 | 2.55 | 0.42 |
| 39:SK:72:ASP:OD2 | 39:SK:73:HIS:ND1 | 2.41 | 0.42 |
| 41:SM:109:LEU:HD12 | 41:SM:109:LEU:HA | 1.90 | 0.42 |
| 53:8:322:G:C8 | 65:5:460:LYS:HE3 | 2.54 | 0.42 |
| 55:LI:562:PRO:HB2 | 55:LI:565:GLU:HB2 | 2.01 | 0.42 |
| 57:LR:16:TYR:OH | 57:LR:21:ALA:O | 2.31 | 0.42 |
| 57:LR:43:ILE:HG22 | 57:LR:52:ILE:HA | 2.02 | 0.42 |
| 4:L0:415:U:H2' | 4:L0:416:A:H8 | 1.85 | 0.42 |
| 15:LF:20:ARG:HG2 | 15:LF:76:TYR:CE2 | 2.55 | 0.42 |
| 17:LH:378:ASP:O | 26:LS:344:ARG:NH1 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:LJ:492:ARG:HH21 | 18:LJ:495:ILE:HD12 | 1.85 | 0.42 |
| 22:LN:631:GLU:HG2 | 22:LN:651:ALA:HB3 | 2.02 | 0.42 |
| 25:LQ:590:THR:HG1 | 25:LQ:600:TRP:HE1 | 1.66 | 0.42 |
| 28:LU:174:ARG:NH2 | 28:LU:206:VAL:O | 2.49 | 0.42 |
| 28:LU:448:ARG:HE | 53:8:1050:G:H21 | 1.68 | 0.42 |
| 30:LW:254:GLY:HA2 | 30:LW:277:VAL:HG23 | 2.02 | 0.42 |
| 35:SE:111:LYS:HA | 35:SE:111:LYS:HD2 | 1.78 | 0.42 |
| 36:SG:257:ASP:HB2 | 36:SG:259:LYS:HE2 | 2.02 | 0.42 |
| 37:SH:231:ARG:HA | 37:SH:231:ARG:HD3 | 1.90 | 0.42 |
| 42:SN:44:LYS:HD2 | 42:SN:236:LYS:HB2 | 2.00 | 0.42 |
| 44:SQ:117:VAL:HG23 | 44:SQ:149:ILE:HD11 | 2.01 | 0.42 |
| 53:8:243:G:H2' | 53:8:244:A:H8 | 1.84 | 0.42 |
| 53:8:591:A:H2' | 53:8:592:A:C8 | 2.55 | 0.42 |
| 53:8:1659:A:H2' | 53:8:1660:A:C8 | 2.54 | 0.42 |
| 53:8:1661:U:H2' | 53:8:1662:G:H8 | 1.85 | 0.42 |
| 54:SU:227:LYS:HA | 54:SU:227:LYS:HD2 | 1.75 | 0.42 |
| 58:NE:199:ASP:N | 58:NE:199:ASP:OD1 | 2.48 | 0.42 |
| 62:LX:18:VAL:HG11 | 62:LX:44:MET:HB2 | 2.00 | 0.42 |
| 62:LX:906:SER:OG | 62:LX:907:ASN:N | 2.53 | 0.42 |
| 66:6:249:ILE:O | 66:6:253:SER:OG | 2.31 | 0.42 |
| 4:L0:264:C:H2' | 4:L0:265:A:C8 | 2.55 | 0.41 |
| 5:L2:18:G:H2' | 5:L2:19:A:H8 | 1.85 | 0.41 |
| 9:L7:49:ILE:HG12 | 9:L7:172:VAL:HG12 | 2.01 | 0.41 |
| 17:LH:60:ARG:HB2 | 20:LL:341:ALA:HB1 | 2.02 | 0.41 |
| 18:LJ:109:ASP:OD1 | 18:LJ:109:ASP:N | 2.51 | 0.41 |
| 19:LK:447:ASN:O | 55:LI:671:ARG:NH2 | 2.51 | 0.41 |
| 20:LL:110:ILE:HD11 | 20:LL:117:LEU:HD21 | 2.02 | 0.41 |
| 20:LL:212:LEU:HB2 | 20:LL:226:LEU:HB2 | 2.02 | 0.41 |
| 23:LO:30:LEU:HD22 | 23:LO:39:VAL:HG22 | 2.02 | 0.41 |
| 25:LQ:553:ASN:HD22 | 25:LQ:573:LYS:H | 1.66 | 0.41 |
| 25:LQ:659:GLU:O | 25:LQ:677:HIS:N | 2.49 | 0.41 |
| 28:LU:75:LYS:H | 28:LU:75:LYS:HG2 | 1.70 | 0.41 |
| 29:LV:144:LEU:HB2 | 29:LV:155:VAL:HG22 | 2.02 | 0.41 |
| 36:SG:430:LYS:H | 66:6:254:ASP:HB2 | 1.85 | 0.41 |
| 36:SG:523:LYS:HD2 | 36:SG:523:LYS:HA | 1.85 | 0.41 |
| 38:SI:137:LEU:HD22 | 38:SI:232:PHE:HE1 | 1.84 | 0.41 |
| 38:SI:257:LEU:HA | 38:SI:260:THR:HG22 | 2.01 | 0.41 |
| 41:SM:287:LYS:NZ | 53:8:562:G:OP1 | 2.39 | 0.41 |
| 42:SN:227:SER:OG | 42:SN:228:LYS:N | 2.52 | 0.41 |
| 47:ST:753:LYS:HA | 47:ST:753:LYS:HD2 | 1.79 | 0.41 |
| 53:8:329:G:H2' | 53:8:330:G:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 53:8:523:G:N2 | 53:8:529:A:H62 | 2.17 | 0.41 |
| 53:8:1690:G:H2' | 53:8:1691:A:H8 | 1.84 | 0.41 |
| 62:LX:197:ASN:OD1 | 62:LX:197:ASN:N | 2.52 | 0.41 |
| 65:5:297:TRP:HE1 | 66:6:59:SER:HG | 1.68 | 0.41 |
| 3:NB:560:ASN:ND2 | 53:8:477:A:OP1 | 2.53 | 0.41 |
| 8:L5:133:VAL:HG22 | 8:L5:198:LEU:HD13 | 2.01 | 0.41 |
| 12:LC:94:GLN:HE22 | 31:LZ:182:PHE:HB3 | 1.84 | 0.41 |
| 14:LE:39:GLN:O | 14:LE:43:LYS:N | 2.46 | 0.41 |
| 17:LH:491:GLN:H | 17:LH:491:GLN:HG2 | 1.65 | 0.41 |
| 17:LH:698:VAL:HA | 17:LH:701:VAL:HG22 | 2.01 | 0.41 |
| 19:LK:506:LEU:HB3 | 55:LI:655:LEU:HD21 | 2.02 | 0.41 |
| 20:LL:150:LYS:HD2 | 20:LL:150:LYS:HA | 1.89 | 0.41 |
| 22:LN:741:LEU:HA | 22:LN:756:GLU:HA | 2.02 | 0.41 |
| 27:LT:169:SER:HG | 27:LT:171:GLN:HE21 | 1.66 | 0.41 |
| 27:LT:932:VAL:HG22 | 57:LR:808:TYR:HB2 | 2.02 | 0.41 |
| 28:LU:195:ALA:HB2 | 28:LU:203:LEU:HD12 | 2.01 | 0.41 |
| 30:LW:46:LEU:HD13 | 46:SS:859:ARG:HH12 | 1.84 | 0.41 |
| 30:LW:123:THR:OG1 | 30:LW:140:ARG:NH2 | 2.53 | 0.41 |
| 37:SH:125:HIS:NE2 | 37:SH:263:ASP:OD1 | 2.45 | 0.41 |
| 38:SI:140:LEU:HD11 | 38:SI:152:THR:HB | 2.01 | 0.41 |
| 38:SI:1135:ARG:HH11 | 53:8:494:U:H3' | 1.85 | 0.41 |
| 40:SL:18:ASN:HD22 | 40:SL:21:LYS:HD2 | 1.84 | 0.41 |
| 40:SL:67:ILE:HG23 | 40:SL:71:PHE:HD2 | 1.85 | 0.41 |
| 41:SM:288:ASP:OD1 | 41:SM:288:ASP:N | 2.51 | 0.41 |
| 53:8:972:G:H2' | 53:8:973:A:H8 | 1.85 | 0.41 |
| 53:8:1672:G:H2' | 53:8:1673:G:C8 | 2.55 | 0.41 |
| 54:SU:341:LEU:HD23 | 54:SU:341:LEU:HA | 1.93 | 0.41 |
| 55:LI:68:PRO:O | 55:LI:80:ALA:N | 2.50 | 0.41 |
| 62:LX:916:ILE:HA | 62:LX:919:LYS:HD2 | 2.02 | 0.41 |
| 65:5:458:ALA:HB2 | 65:5:463:LYS:HE3 | 2.02 | 0.41 |
| 1:NA:345:LEU:HD11 | 38:SI:961:PHE:HZ | 1.85 | 0.41 |
| 5:L2:63:C:H2' | 5:L2:64:A:H8 | 1.85 | 0.41 |
| 7:L4:62:LYS:NZ | 53:8:454:U:OP2 | 2.44 | 0.41 |
| 7:L4:178:GLY:O | 7:L4:231:GLN:NE2 | 2.49 | 0.41 |
| 8:L5:79:ASN:OD1 | 53:8:1583:A:O2' | 2.36 | 0.41 |
| 9:L7:123:ASP:HA | 9:L7:126:LEU:HG | 2.02 | 0.41 |
| 9:L7:163:ASP:HA | 9:L7:166:LEU:HD23 | 2.02 | 0.41 |
| 10:L8:195:ARG:NH2 | 13:LD:10:GLU:O | 2.54 | 0.41 |
| 12:LC:13:LYS:HD2 | 12:LC:13:LYS:HA | 1.89 | 0.41 |
| 17:LH:168:LEU:HD23 | 17:LH:168:LEU:HA | 1.94 | 0.41 |
| 22:LN:71:ARG:HB2 | 22:LN:75:ASN:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LO:538:GLN:HG3 | 23:LO:554:ASP:HA | 2.01 | 0.41 |
| 25:LQ:656:HIS:CE1 | 25:LQ:660:VAL:HG22 | 2.55 | 0.41 |
| 27:LT:293:GLU:OE1 | 27:LT:293:GLU:N | 2.52 | 0.41 |
| 28:LU:2:LYS:HZ2 | 30:LW:77:GLU:HG3 | 1.84 | 0.41 |
| 28:LU:48:THR:HA | 28:LU:51:GLU:HG2 | 2.02 | 0.41 |
| 29:LV:158:SER:H | 29:LV:183:VAL:HG12 | 1.86 | 0.41 |
| 34:SC:272:LYS:HG2 | 34:SC:275:CYS:H | 1.85 | 0.41 |
| 39:SJ:97:LEU:HD23 | 39:SJ:97:LEU:HA | 1.94 | 0.41 |
| 39:SJ:115:GLN:HB3 | 39:SJ:121:LEU:HD13 | 2.02 | 0.41 |
| 39:SJ:229:ASN:OD1 | 39:SJ:229:ASN:N | 2.53 | 0.41 |
| 51:NH:1098:PHE:H | 51:NH:1184:GLY:HA3 | 1.84 | 0.41 |
| 53:8:1208:A:N6 | 53:8:1454:G:C6 | 2.88 | 0.41 |
| 57:LR:548:LEU:O | 57:LR:560:TRP:N | 2.44 | 0.41 |
| 63:L6:102:VAL:HG23 | 63:L6:106:LEU:HG | 2.02 | 0.41 |
| 4:L0:145:A:H2' | 4:L0:146:G:C8 | 2.54 | 0.41 |
| 12:LC:26:LYS:H | 12:LC:26:LYS:HG2 | 1.73 | 0.41 |
| 17:LH:730:ASP:HB3 | 17:LH:734:VAL:HG22 | 2.02 | 0.41 |
| 17:LH:847:ASP:N | 17:LH:847:ASP:OD1 | 2.53 | 0.41 |
| 21:LM:160:LEU:HD23 | 59:SB:412:VAL:HG11 | 2.02 | 0.41 |
| 22:LN:474:SER:OG | 22:LN:475:THR:N | 2.52 | 0.41 |
| 23:LO:11:LEU:HD11 | 23:LO:372:TRP:HB3 | 2.03 | 0.41 |
| 25:LQ:220:THR:HB | 25:LQ:259:ILE:HD11 | 2.02 | 0.41 |
| 27:LT:417:LEU:HG | 27:LT:432:THR:HG22 | 2.01 | 0.41 |
| 29:LV:80:GLN:HB3 | 29:LV:82:HIS:CD2 | 2.56 | 0.41 |
| 31:LZ:135:HIS:HB3 | 31:LZ:166:ILE:HG21 | 2.02 | 0.41 |
| 34:SD:244:VAL:HG11 | 34:SD:252:ILE:HG21 | 2.02 | 0.41 |
| 35:SF:24:VAL:HG12 | 35:SF:102:ILE:HD11 | 2.03 | 0.41 |
| 36:SG:410:ASP:OD1 | 36:SG:410:ASP:N | 2.53 | 0.41 |
| 37:SH:133:ILE:HG23 | 37:SH:137:LEU:HD12 | 2.03 | 0.41 |
| 53:8:202:A:O2' | 53:8:203:U:O4' | 2.38 | 0.41 |
| 63:L6:3:LEU:HD12 | 63:L6:111:LEU:HD11 | 2.01 | 0.41 |
| 2:SA:6:TYR:HE1 | 2:SA:19:LYS:HD2 | 1.86 | 0.41 |
| 2:SA:302:ASN:OD1 | 2:SA:401:GLY:N | 2.53 | 0.41 |
| 4:L0:89:C:H5'' | 4:L0:90:G:H5' | 2.02 | 0.41 |
| 4:L0:192:G:H2' | 4:L0:193:G:C8 | 2.56 | 0.41 |
| 9:L7:45:SER:OG | 9:L7:47:ARG:NH1 | 2.53 | 0.41 |
| 9:L7:165:LYS:HE2 | 9:L7:169:PHE:HZ | 1.85 | 0.41 |
| 13:LD:90:TYR:O | 13:LD:92:HIS:ND1 | 2.54 | 0.41 |
| 17:LH:648:LYS:HE2 | 17:LH:648:LYS:HB2 | 1.88 | 0.41 |
| 18:LJ:262:GLU:HG3 | 18:LJ:270:SER:HB3 | 2.02 | 0.41 |
| 21:LM:316:PRO:HD2 | 21:LM:319:ILE:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LN:143:VAL:HB | 56:ND:198:ILE:HD13 | 2.02 | 0.41 |
| 23:LO:641:LEU:HD12 | 23:LO:641:LEU:HA | 1.93 | 0.41 |
| 23:LO:728:GLU:HA | 23:LO:731:ARG:HD2 | 2.01 | 0.41 |
| 25:LQ:142:ASP:OD1 | 25:LQ:142:ASP:N | 2.39 | 0.41 |
| 25:LQ:676:SER:OG | 25:LQ:678:ASP:OD1 | 2.27 | 0.41 |
| 26:LS:251:ILE:HG12 | 26:LS:584:GLY:HA2 | 2.03 | 0.41 |
| 28:LU:233:ASP:HB3 | 28:LU:249:LEU:HB2 | 2.01 | 0.41 |
| 28:LU:267:ILE:HG22 | 28:LU:279:THR:HG22 | 2.03 | 0.41 |
| 29:LV:80:GLN:HB3 | 29:LV:82:HIS:HD2 | 1.85 | 0.41 |
| 30:LW:203:TYR:HE2 | 30:LW:433:LEU:HA | 1.85 | 0.41 |
| 34:SC:291:GLN:HE21 | 40:SL:128:LEU:HB2 | 1.85 | 0.41 |
| 38:SI:98:LEU:HB2 | 38:SI:101:ILE:HD11 | 2.02 | 0.41 |
| 38:SI:841:THR:HG22 | 38:SI:860:TYR:H | 1.84 | 0.41 |
| 39:SJ:46:ALA:HA | 39:SJ:115:GLN:HG2 | 2.01 | 0.41 |
| 40:SL:185:LEU:HD23 | 40:SL:186:PRO:HD2 | 2.02 | 0.41 |
| 46:SS:837:LYS:HD3 | 46:SS:837:LYS:HA | 1.89 | 0.41 |
| 53:8:415:C:OP1 | 62:LX:70:ARG:NH1 | 2.52 | 0.41 |
| 53:8:1131:A:O2' | 53:8:1136:U:O4 | 2.34 | 0.41 |
| 54:SU:130:GLU:HB3 | 54:SU:144:PRO:HG3 | 2.02 | 0.41 |
| 54:SU:136:SER:O | 54:SU:136:SER:OG | 2.36 | 0.41 |
| 55:LI:608:GLN:HA | 55:LI:611:ILE:HG12 | 2.03 | 0.41 |
| 62:LX:15:ARG:HH21 | 62:LX:47:ALA:HB2 | 1.84 | 0.41 |
| 1:NA:437:ILE:HD11 | 31:LZ:61:LEU:HG | 2.03 | 0.41 |
| 4:L0:68:U:O4 | 17:LH:422:LYS:NZ | 2.53 | 0.41 |
| 7:L4:69:HIS:HD2 | 15:LF:17:LEU:HB2 | 1.85 | 0.41 |
| 9:L7:81:LEU:HD23 | 9:L7:81:LEU:HA | 1.87 | 0.41 |
| 17:LH:96:ILE:HG12 | 17:LH:108:THR:HG21 | 2.02 | 0.41 |
| 22:LN:497:ILE:HD11 | 22:LN:555:LEU:HD13 | 2.02 | 0.41 |
| 26:LS:154:LYS:HB3 | 26:LS:154:LYS:HE2 | 1.83 | 0.41 |
| 26:LS:247:SER:OG | 26:LS:248:HIS:N | 2.54 | 0.41 |
| 27:LT:474:PHE:HE1 | 27:LT:495:ARG:HG3 | 1.86 | 0.41 |
| 38:SI:54:LEU:HD23 | 45:SR:50:LYS:HB2 | 2.03 | 0.41 |
| 38:SI:568:ARG:HA | 38:SI:568:ARG:HD3 | 1.80 | 0.41 |
| 38:SI:1123:LYS:HE2 | 38:SI:1123:LYS:HB2 | 1.91 | 0.41 |
| 39:SJ:152:SER:O | 39:SJ:155:SER:OG | 2.28 | 0.41 |
| 44:SQ:60:LYS:H | 44:SQ:60:LYS:HG2 | 1.70 | 0.41 |
| 45:SR:58:GLY:HA3 | 45:SR:69:ARG:HA | 2.02 | 0.41 |
| 47:ST:267:UNK:O | 47:ST:271:UNK:N | 2.53 | 0.41 |
| 53:8:140:A:N9 | 63:L6:184:LEU:N | 2.69 | 0.41 |
| 53:8:144:U:H2' | 53:8:145:A:H4' | 2.02 | 0.41 |
| 53:8:890:C:H2' | 53:8:891:A:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:LI:170:LYS:HA | 55:LI:177:SER:HA | 2.03 | 0.41 |
| 55:LI:248:LEU:HA | 55:LI:264:SER:HA | 2.02 | 0.41 |
| 59:SB:153:LYS:HE3 | 59:SB:378:GLU:HB2 | 2.02 | 0.41 |
| 1:NA:357:ILE:HD13 | 41:SM:234:ARG:HH21 | 1.86 | 0.41 |
| 2:SA:180:LEU:HD13 | 59:SB:183:ARG:HG2 | 2.03 | 0.41 |
| 2:SA:388:ARG:HB3 | 35:SF:63:ILE:HA | 2.02 | 0.41 |
| 4:L0:411:A:H2' | 4:L0:412:A:C8 | 2.56 | 0.41 |
| 4:L0:489:G:H22 | 24:LP:125:SER:H | 1.69 | 0.41 |
| 10:L8:32:GLN:HE22 | 10:L8:34:ALA:HB2 | 1.84 | 0.41 |
| 17:LH:31:ASN:OD1 | 17:LH:31:ASN:N | 2.53 | 0.41 |
| 20:LL:20:VAL:HG12 | 20:LL:29:VAL:HG22 | 2.03 | 0.41 |
| 22:LN:287:THR:HG21 | 22:LN:337:CYS:HA | 2.03 | 0.41 |
| 23:LO:557:LYS:HD3 | 23:LO:557:LYS:HA | 1.88 | 0.41 |
| 26:LS:150:TYR:HE1 | 30:LW:80:LEU:HA | 1.86 | 0.41 |
| 26:LS:529:ILE:HD12 | 26:LS:591:LEU:HD13 | 2.02 | 0.41 |
| 27:LT:184:THR:OG1 | 27:LT:187:ASN:OD1 | 2.32 | 0.41 |
| 28:LU:255:THR:OG1 | 28:LU:256:GLN:N | 2.53 | 0.41 |
| 28:LU:401:LYS:HE3 | 28:LU:401:LYS:HB2 | 1.79 | 0.41 |
| 29:LV:81:ILE:HD12 | 29:LV:81:ILE:HA | 1.96 | 0.41 |
| 30:LW:148:LEU:HD23 | 30:LW:148:LEU:HA | 1.96 | 0.41 |
| 30:LW:182:THR:HG22 | 40:SL:15:ARG:HG2 | 2.02 | 0.41 |
| 30:LW:204:LEU:HD12 | 30:LW:204:LEU:HA | 1.93 | 0.41 |
| 30:LW:384:VAL:HA | 30:LW:385:PRO:HD3 | 1.92 | 0.41 |
| 38:SI:776:GLN:HA | 38:SI:780:ILE:HG22 | 2.01 | 0.41 |
| 46:SS:277:ARG:HA | 46:SS:280:GLN:HG2 | 2.03 | 0.41 |
| 48:SY:125:LEU:HD12 | 48:SY:125:LEU:HA | 1.93 | 0.41 |
| 53:8:999:U:N3 | 53:8:1002:G:OP1 | 2.42 | 0.41 |
| 54:SU:383:LEU:O | 54:SU:387:THR:OG1 | 2.28 | 0.41 |
| 62:LY:744:PRO:HA | 62:LY:762:MET:HA | 2.03 | 0.41 |
| 62:LX:132:PRO:HA | 62:LX:135:LEU:HD12 | 2.02 | 0.41 |
| 65:5:406:TYR:O | 66:6:82:ARG:NH2 | 2.54 | 0.41 |
| 65:5:470:ASP:OD1 | 65:5:471:PRO:HD3 | 2.20 | 0.41 |
| 2:SA:324:ASN:HA | 2:SA:327:LYS:HB2 | 2.03 | 0.41 |
| 4:L0:289:U:H2' | 4:L0:290:G:C8 | 2.56 | 0.41 |
| 4:L0:409:C:H2' | 4:L0:410:A:C8 | 2.56 | 0.41 |
| 10:L8:32:GLN:H | 10:L8:32:GLN:HG3 | 1.70 | 0.41 |
| 13:LD:32:LYS:HE2 | 13:LD:32:LYS:HB2 | 1.82 | 0.41 |
| 17:LH:690:ASN:ND2 | 17:LH:750:LEU:O | 2.54 | 0.41 |
| 18:LJ:507:MET:HE2 | 18:LJ:507:MET:HB3 | 1.96 | 0.41 |
| 22:LN:105:SER:O | 22:LN:105:SER:OG | 2.34 | 0.41 |
| 24:LP:410:UNK:O | 24:LP:414:UNK:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LQ:400:SER:HB3 | 25:LQ:404:LYS:HB3 | 2.03 | 0.41 |
| 25:LQ:824:MET:HA | 25:LQ:825:PRO:HD3 | 1.94 | 0.41 |
| 27:LT:187:ASN:OD1 | 27:LT:187:ASN:N | 2.51 | 0.41 |
| 28:LU:26:ARG:NH2 | 46:SS:867:GLN:O | 2.54 | 0.41 |
| 28:LU:142:ASP:OD1 | 28:LU:142:ASP:N | 2.48 | 0.41 |
| 28:LU:254:PRO:HG2 | 46:SS:284:ARG:NE | 2.36 | 0.41 |
| 29:LV:126:GLN:HE21 | 29:LV:130:GLY:HA2 | 1.86 | 0.41 |
| 31:LZ:57:LEU:HA | 31:LZ:57:LEU:HD12 | 1.85 | 0.41 |
| 36:SG:553:ILE:HD12 | 36:SG:553:ILE:HA | 1.99 | 0.41 |
| 38:SI:838:ILE:HD11 | 53:8:578:U:C4 | 2.56 | 0.41 |
| 38:SI:969:VAL:HG12 | 38:SI:1000:ILE:H | 1.85 | 0.41 |
| 52:NI:41:ARG:HA | 52:NI:53:LEU:HA | 2.02 | 0.41 |
| 53:8:600:U:H2' | 53:8:601:A:C8 | 2.55 | 0.41 |
| 53:8:1110:G:O2' | 53:8:1111:G:O4' | 2.37 | 0.41 |
| 53:8:1661:U:H2' | 53:8:1662:G:C8 | 2.56 | 0.41 |
| 2:SA:15:TYR:CZ | 2:SA:78:LEU:HB2 | 2.55 | 0.41 |
| 4:L0:114:G:H2' | 4:L0:115:G:C8 | 2.56 | 0.41 |
| 4:L0:223:C:H2' | 4:L0:224:G:C8 | 2.56 | 0.41 |
| 7:L4:36:HIS:CE1 | 7:L4:85:GLY:HA3 | 2.56 | 0.41 |
| 7:L4:125:LYS:HB3 | 7:L4:142:HIS:HD2 | 1.85 | 0.41 |
| 8:L5:196:GLU:OE2 | 8:L5:200:ASN:ND2 | 2.45 | 0.41 |
| 9:L7:56:LYS:HB2 | 9:L7:88:ARG:HH12 | 1.86 | 0.41 |
| 9:L7:91:ILE:HG21 | 9:L7:129:LEU:HD12 | 2.03 | 0.41 |
| 11:L9:173:ALA:HB2 | 53:8:511:A:H5' | 2.03 | 0.41 |
| 14:LE:19:LYS:HD3 | 14:LE:19:LYS:HA | 1.83 | 0.41 |
| 17:LH:780:GLU:O | 17:LH:782:THR:N | 2.54 | 0.41 |
| 18:LJ:90:ARG:HG3 | 18:LJ:92:ASP:H | 1.85 | 0.41 |
| 21:LM:284:SER:OG | 21:LM:285:ASN:N | 2.53 | 0.41 |
| 23:LO:482:SER:OG | 23:LO:486:SER:N | 2.53 | 0.41 |
| 23:LO:791:HIS:O | 23:LO:795:ASN:ND2 | 2.54 | 0.41 |
| 26:LS:156:ASN:OD1 | 26:LS:156:ASN:N | 2.54 | 0.41 |
| 27:LT:59:GLN:HG2 | 27:LT:71:VAL:HG12 | 2.02 | 0.41 |
| 27:LT:173:LEU:HD23 | 27:LT:173:LEU:HA | 1.90 | 0.41 |
| 28:LU:247:TYR:HD1 | 28:LU:254:PRO:HB3 | 1.86 | 0.41 |
| 29:LV:102:VAL:HG23 | 29:LV:117:LEU:HD23 | 2.03 | 0.41 |
| 35:SE:21:LEU:HA | 35:SE:24:VAL:HG22 | 2.02 | 0.41 |
| 35:SE:37:ALA:HA | 35:SE:99:ALA:HB3 | 2.03 | 0.41 |
| 36:SG:274:ILE:HA | 36:SG:275:PRO:HD3 | 1.89 | 0.41 |
| 36:SG:343:ASP:OD1 | 36:SG:343:ASP:N | 2.47 | 0.41 |
| 36:SG:523:LYS:NZ | 36:SG:525:GLN:OE1 | 2.41 | 0.41 |
| 37:SH:24:ALA:HA | 37:SH:27:SER:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:SH:134:LYS:HB3 | 37:SH:134:LYS:HE2 | 1.90 | 0.41 |
| 37:SH:298:ILE:HD13 | 37:SH:298:ILE:HA | 1.95 | 0.41 |
| 38:SI:780:ILE:HD12 | 38:SI:780:ILE:HA | 1.92 | 0.41 |
| 39:SK:88:ARG:HE | 39:SK:88:ARG:HB3 | 1.64 | 0.41 |
| 39:SK:188:ARG:HG2 | 39:SK:190:GLN:HB2 | 2.03 | 0.41 |
| 42:SN:242:ILE:HG12 | 42:SN:255:TYR:HB3 | 2.03 | 0.41 |
| 45:SR:104:LEU:HD13 | 45:SR:104:LEU:HA | 1.92 | 0.41 |
| 47:ST:495:ASN:ND2 | 47:ST:617:HIS:O | 2.53 | 0.41 |
| 47:ST:575:PHE:HD1 | 47:ST:600:LEU:HB2 | 1.84 | 0.41 |
| 52:NI:40:LYS:O | 52:NI:54:PHE:N | 2.53 | 0.41 |
| 53:8:9:U:H5' | 58:NE:292:LYS:HE2 | 2.01 | 0.41 |
| 53:8:107:C:H2' | 53:8:108:A:H8 | 1.86 | 0.41 |
| 53:8:116:U:H2' | 53:8:117:U:C6 | 2.56 | 0.41 |
| 53:8:222:A:H5' | 53:8:246:G:C2 | 2.56 | 0.41 |
| 53:8:312:A:H4' | 53:8:313:U:H5' | 2.03 | 0.41 |
| 53:8:477:A:H2' | 53:8:478:A:H8 | 1.85 | 0.41 |
| 53:8:911:U:H5' | 57:LR:534:ARG:HB2 | 2.02 | 0.41 |
| 53:8:1783:C:H2' | 53:8:1784:C:C6 | 2.56 | 0.41 |
| 55:LI:572:SER:HB3 | 55:LI:574:ARG:NH1 | 2.36 | 0.41 |
| 55:LI:604:LYS:HB2 | 55:LI:604:LYS:HE2 | 1.86 | 0.41 |
| 57:LR:87:ILE:HG12 | 57:LR:97:ARG:HB2 | 2.03 | 0.41 |
| 57:LR:284:PRO:HB2 | 57:LR:288:LEU:HD23 | 2.03 | 0.41 |
| 63:L6:201:GLN:O | 63:L6:205:ALA:N | 2.50 | 0.41 |
| 2:SA:18:PHE:HD1 | 2:SA:50:LEU:HA | 1.86 | 0.41 |
| 2:SA:411:ARG:HA | 2:SA:411:ARG:HD3 | 1.94 | 0.41 |
| 3:NB:559:ARG:HE | 53:8:545:A:H8 | 1.67 | 0.41 |
| 3:NB:604:ARG:NH1 | 53:8:498:G:O3' | 2.50 | 0.41 |
| 4:L0:467:A:N1 | 4:L0:468:A:N6 | 2.69 | 0.41 |
| 11:L9:77:ILE:HG23 | 11:L9:86:LEU:HD23 | 2.03 | 0.41 |
| 12:LC:39:VAL:O | 12:LC:45:ARG:NH2 | 2.54 | 0.41 |
| 14:LE:40:VAL:O | 14:LE:44:HIS:ND1 | 2.40 | 0.41 |
| 16:LG:21:SER:OG | 16:LG:25:VAL:O | 2.28 | 0.41 |
| 18:LJ:101:ALA:HA | 18:LJ:126:PRO:HB3 | 2.03 | 0.41 |
| 20:LL:198:THR:HG23 | 20:LL:200:GLU:H | 1.86 | 0.41 |
| 22:LN:112:LEU:HD11 | 22:LN:525:VAL:HG22 | 2.02 | 0.41 |
| 22:LN:197:LYS:HA | 22:LN:197:LYS:HD3 | 1.76 | 0.41 |
| 22:LN:393:SER:OG | 22:LN:394:TRP:N | 2.54 | 0.41 |
| 23:LO:539:ILE:HB | 23:LO:553:ILE:HG13 | 2.02 | 0.41 |
| 26:LS:541:LEU:O | 26:LS:542:ARG:NH1 | 2.42 | 0.41 |
| 28:LU:186:ASP:HB2 | 28:LU:225:LEU:HG | 2.03 | 0.41 |
| 35:SE:106:ASP:OD1 | 35:SE:106:ASP:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:SG:461:LYS:HA | 36:SG:461:LYS:HD3 | 1.92 | 0.41 |
| 38:SI:118:LEU:HD23 | 38:SI:131:ILE:HD11 | 2.01 | 0.41 |
| 47:ST:426:THR:HG22 | 47:ST:462:LEU:HD13 | 2.02 | 0.41 |
| 57:LR:768:ASN:HB3 | 57:LR:771:LYS:HE3 | 2.03 | 0.41 |
| 65:5:486:SER:OG | 65:5:488:ASP:OD1 | 2.29 | 0.41 |
| 3:NB:518:ILE:HD13 | 3:NB:518:ILE:HA | 1.91 | 0.40 |
| 4:L0:409:C:H2' | 4:L0:410:A:H8 | 1.87 | 0.40 |
| 7:L4:75:LYS:HB2 | 7:L4:77:ARG:HG2 | 2.02 | 0.40 |
| 9:L7:76:LYS:HA | 9:L7:76:LYS:HD2 | 1.89 | 0.40 |
| 13:LD:74:THR:O | 13:LD:87:ARG:N | 2.54 | 0.40 |
| 17:LH:75:SER:HA | 17:LH:79:LEU:HB2 | 2.02 | 0.40 |
| 17:LH:600:SER:HB2 | 17:LH:638:PHE:HB3 | 2.03 | 0.40 |
| 23:LO:188:ASN:N | 23:LO:188:ASN:OD1 | 2.52 | 0.40 |
| 29:LV:24:SER:H | 29:LV:49:LEU:HD21 | 1.86 | 0.40 |
| 29:LV:177:LYS:HA | 29:LV:177:LYS:HD2 | 1.81 | 0.40 |
| 34:SC:104:ASP:OD1 | 44:SQ:127:ARG:NH1 | 2.54 | 0.40 |
| 34:SD:304:LEU:HD23 | 34:SD:306:LEU:HD12 | 2.04 | 0.40 |
| 38:SI:129:ILE:HD11 | 38:SI:853:ARG:HD2 | 2.03 | 0.40 |
| 39:SJ:174:LYS:HG2 | 39:SJ:199:ASP:HB3 | 2.03 | 0.40 |
| 39:SJ:175:CYS:SG | 39:SJ:176:ARG:N | 2.94 | 0.40 |
| 41:SM:263:LEU:HD12 | 41:SM:263:LEU:HA | 1.91 | 0.40 |
| 42:SN:125:VAL:HG13 | 42:SN:151:PRO:HA | 2.02 | 0.40 |
| 53:8:340:U:H2' | 53:8:341:A:H8 | 1.86 | 0.40 |
| 53:8:922:G:H2' | 53:8:923:A:C8 | 2.56 | 0.40 |
| 53:8:1695:G:C2 | 53:8:1706:C:C2 | 3.08 | 0.40 |
| 59:SB:53:ALA:HB3 | 59:SB:56:ALA:HB3 | 2.03 | 0.40 |
| 59:SB:210:LEU:HD11 | 59:SB:260:GLU:HB3 | 2.03 | 0.40 |
| 59:SB:299:LEU:HD23 | 59:SB:341:LEU:HD23 | 2.03 | 0.40 |
| 2:SA:82:LEU:HD23 | 2:SA:82:LEU:HA | 1.81 | 0.40 |
| 4:L0:250:G:H1 | 4:L0:262:U:H3 | 1.70 | 0.40 |
| 4:L0:523:U:H5'' | 28:LU:126:LYS:HA | 2.02 | 0.40 |
| 9:L7:166:LEU:HA | 9:L7:169:PHE:CD1 | 2.56 | 0.40 |
| 15:LF:59:GLY:HA3 | 15:LF:72:PHE:HB3 | 2.03 | 0.40 |
| 20:LL:516:ILE:HG23 | 20:LL:519:LEU:HD21 | 2.04 | 0.40 |
| 23:LO:526:ASP:HA | 23:LO:815:TYR:CZ | 2.57 | 0.40 |
| 25:LQ:292:UNK:O | 25:LQ:296:UNK:N | 2.54 | 0.40 |
| 27:LT:847:LEU:O | 27:LT:851:SER:OG | 2.31 | 0.40 |
| 28:LU:58:PHE:HE1 | 28:LU:373:ARG:HG2 | 1.86 | 0.40 |
| 28:LU:92:ILE:HG13 | 28:LU:106:PHE:HB2 | 2.02 | 0.40 |
| 28:LU:109:HIS:CG | 28:LU:140:SER:HB2 | 2.55 | 0.40 |
| 28:LU:263:ARG:O | 28:LU:281:ASN:ND2 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:LW:458:THR:HA | 46:SS:854:ARG:HD3 | 2.02 | 0.40 |
| 32:NG:21:ALA:HA | 32:NG:26:THR:HA | 2.02 | 0.40 |
| 36:SG:225:LYS:HE3 | 36:SG:225:LYS:HB3 | 1.92 | 0.40 |
| 37:SH:244:THR:HG23 | 37:SH:259:GLU:HB3 | 2.02 | 0.40 |
| 37:SH:307:ASP:OD1 | 38:SI:765:ASN:ND2 | 2.46 | 0.40 |
| 43:SO:263:LEU:HA | 43:SO:266:VAL:HG22 | 2.02 | 0.40 |
| 45:SR:130:VAL:HG13 | 45:SR:135:LEU:HD21 | 2.02 | 0.40 |
| 46:SS:278:ILE:H | 46:SS:278:ILE:HD12 | 1.86 | 0.40 |
| 53:8:1733:C:H2' | 53:8:1734:U:H6 | 1.87 | 0.40 |
| 57:LR:200:GLU:O | 57:LR:256:ARG:NH2 | 2.54 | 0.40 |
| 62:LX:658:ARG:HD3 | 62:LX:766:LEU:HD13 | 2.04 | 0.40 |
| 65:5:416:VAL:O | 65:5:420:ASP:N | 2.45 | 0.40 |
| 3:NB:591:TYR:OH | 3:NB:594:GLU:O | 2.32 | 0.40 |
| 4:L0:286:U:H2' | 4:L0:287:G:H8 | 1.86 | 0.40 |
| 4:L0:494:C:H2' | 4:L0:495:G:C8 | 2.56 | 0.40 |
| 5:L2:45:U:O2' | 40:SL:23:GLN:OE1 | 2.28 | 0.40 |
| 5:L2:310:G:H2' | 5:L2:311:G:C8 | 2.55 | 0.40 |
| 9:L7:154:LEU:HD12 | 9:L7:185:ILE:HG22 | 2.03 | 0.40 |
| 10:L8:78:ILE:HA | 10:L8:104:ILE:HG22 | 2.02 | 0.40 |
| 17:LH:546:LYS:HE2 | 17:LH:548:ILE:HD11 | 2.02 | 0.40 |
| 18:LJ:256:THR:HG21 | 18:LJ:277:LEU:HD13 | 2.03 | 0.40 |
| 21:LM:31:ALA:HB1 | 21:LM:154:ILE:HG23 | 2.03 | 0.40 |
| 21:LM:83:ARG:HE | 21:LM:91:ILE:HD11 | 1.86 | 0.40 |
| 21:LM:124:ARG:HA | 21:LM:124:ARG:HD2 | 1.87 | 0.40 |
| 23:LO:425:PHE:HB3 | 23:LO:458:TRP:CD1 | 2.56 | 0.40 |
| 23:LO:496:THR:HG22 | 23:LO:513:GLU:HB3 | 2.03 | 0.40 |
| 23:LO:612:LEU:HD23 | 23:LO:612:LEU:HA | 1.90 | 0.40 |
| 27:LT:814:GLU:OE1 | 27:LT:822:ARG:NH1 | 2.55 | 0.40 |
| 27:LT:856:GLU:HB2 | 43:SO:252:LEU:HD11 | 2.03 | 0.40 |
| 31:LZ:55:ARG:HG2 | 31:LZ:98:GLU:HG2 | 2.03 | 0.40 |
| 34:SD:163:PHE:CG | 34:SD:266:GLY:HA3 | 2.56 | 0.40 |
| 35:SE:68:PRO:HA | 35:SE:71:CYS:HB2 | 2.02 | 0.40 |
| 37:SH:113:LYS:HE3 | 37:SH:113:LYS:HB3 | 1.94 | 0.40 |
| 38:SI:180:GLN:HA | 38:SI:183:LEU:HB3 | 2.03 | 0.40 |
| 38:SI:310:THR:HA | 38:SI:311:PRO:HD3 | 1.96 | 0.40 |
| 38:SI:832:HIS:CD2 | 38:SI:834:TRP:HB2 | 2.56 | 0.40 |
| 39:SJ:150:ILE:HD12 | 39:SJ:160:LEU:HD12 | 2.02 | 0.40 |
| 47:ST:643:LEU:HD23 | 47:ST:684:ILE:HD13 | 2.03 | 0.40 |
| 53:8:1210:C:H2' | 53:8:1211:A:C8 | 2.56 | 0.40 |
| 59:SB:226:ILE:HG13 | 59:SB:227:LEU:HD12 | 2.03 | 0.40 |
| 62:LX:62:LYS:HA | 62:LX:62:LYS:HD3 | 1.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:LX:200:VAL:HG22 | 62:LX:208:LEU:HD12 | 2.03 | 0.40 |
| 62:LX:881:GLN:H | 62:LX:881:GLN:HG2 | 1.67 | 0.40 |
| 65:5:194:ILE:HD11 | 65:5:421:LEU:HD11 | 2.03 | 0.40 |
| 4:L0:192:G:H2' | 4:L0:193:G:H8 | 1.85 | 0.40 |
| 4:L0:305:A:H2' | 4:L0:306:G:C8 | 2.57 | 0.40 |
| 4:L0:480:C:O2 | 24:LP:46:ARG:NH1 | 2.54 | 0.40 |
| 7:L4:112:HIS:NE2 | 7:L4:237:SER:O | 2.55 | 0.40 |
| 18:LJ:62:ARG:HE | 18:LJ:62:ARG:HB3 | 1.76 | 0.40 |
| 18:LJ:128:HIS:CE1 | 18:LJ:172:ARG:HH21 | 2.40 | 0.40 |
| 21:LM:131:ASN:OD1 | 21:LM:131:ASN:N | 2.48 | 0.40 |
| 21:LM:218:ILE:HG23 | 21:LM:263:VAL:HG11 | 2.02 | 0.40 |
| 22:LN:394:TRP:HB3 | 22:LN:399:VAL:HG13 | 2.02 | 0.40 |
| 22:LN:639:ASP:OD2 | 22:LN:647:TRP:NE1 | 2.52 | 0.40 |
| 25:LQ:589:ILE:HG12 | 25:LQ:599:ILE:HG12 | 2.03 | 0.40 |
| 28:LU:326:ASP:OD1 | 28:LU:326:ASP:N | 2.46 | 0.40 |
| 29:LV:195:LEU:HD13 | 29:LV:207:TRP:HB2 | 2.04 | 0.40 |
| 29:LV:238:ASN:N | 29:LV:238:ASN:OD1 | 2.55 | 0.40 |
| 35:SE:20:ILE:HD13 | 35:SE:79:VAL:HG21 | 2.04 | 0.40 |
| 47:ST:571:ILE:HD13 | 47:ST:571:ILE:HA | 1.89 | 0.40 |
| 47:ST:573:LEU:HD23 | 47:ST:573:LEU:HA | 1.93 | 0.40 |
| 53:8:631:G:O6 | 53:8:968:U:O4 | 2.39 | 0.40 |
| 53:8:1512:G:H2' | 53:8:1513:G:C8 | 2.56 | 0.40 |
| 57:LR:299:ASN:O | 57:LR:301:GLN:NE2 | 2.41 | 0.40 |
| 57:LR:536:LEU:HA | 57:LR:552:SER:HA | 2.04 | 0.40 |
| 4:L0:505:G:H2' | 4:L0:506:G:C8 | 2.56 | 0.40 |
| 20:LL:58:LEU:HD13 | 20:LL:80:MET:HE1 | 2.04 | 0.40 |
| 20:LL:469:ILE:HB | 20:LL:508:ILE:HD12 | 2.04 | 0.40 |
| 21:LM:6:ASP:OD1 | 21:LM:6:ASP:N | 2.54 | 0.40 |
| 22:LN:758:ASN:HB2 | 22:LN:763:HIS:CD2 | 2.57 | 0.40 |
| 23:LO:162:LEU:HD13 | 23:LO:197:ALA:HB3 | 2.04 | 0.40 |
| 23:LO:750:LEU:HD23 | 23:LO:750:LEU:HA | 1.84 | 0.40 |
| 25:LQ:341:ALA:HB1 | 25:LQ:353:LEU:HD11 | 2.03 | 0.40 |
| 25:LQ:395:ARG:HA | 25:LQ:395:ARG:HD3 | 1.85 | 0.40 |
| 27:LT:544:ALA:HB3 | 27:LT:562:LEU:HD22 | 2.02 | 0.40 |
| 34:SC:178:GLY:HA2 | 34:SC:181:VAL:HG12 | 2.02 | 0.40 |
| 34:SD:253:ILE:HD13 | 34:SD:253:ILE:HA | 1.94 | 0.40 |
| 38:SI:241:HIS:HB3 | 38:SI:851:TRP:HE1 | 1.86 | 0.40 |
| 38:SI:833:ARG:HH12 | 45:SR:141:GLU:HG3 | 1.86 | 0.40 |
| 39:SJ:136:ARG:HD3 | 53:8:1195:C:C2 | 2.56 | 0.40 |
| 41:SM:16:LYS:HE2 | 41:SM:16:LYS:HB2 | 1.95 | 0.40 |
| 42:SN:223:LEU:HD12 | 42:SN:235:ILE:HG13 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:ST:418:UNK:O | 47:ST:420:GLU:N | 2.53 | 0.40 |
| 47:ST:644:ASP:HB3 | 47:ST:684:ILE:HG12 | 2.04 | 0.40 |
| 53:8:33:U:H2' | 53:8:34:G:C2 | 2.57 | 0.40 |
| 53:8:1670:G:HO2' | 53:8:1671:A:H8 | 1.67 | 0.40 |
| 54:SU:381:LYS:HE3 | 54:SU:385:ARG:HH21 | 1.85 | 0.40 |
| 57:LR:192:ALA:O | 57:LR:216:ARG:NH1 | 2.54 | 0.40 |
| 62:LX:185:ASN:HA | 62:LX:188:PHE:HB3 | 2.04 | 0.40 |
| 62:LX:319:LYS:O | 62:LX:323:GLU:N | 2.53 | 0.40 |
| 62:LX:862:LEU:O | 62:LX:866:TYR:N | 2.54 | 0.40 |
| 63:L6:183:ARG:O | 63:L6:187:LYS:N | 2.52 | 0.40 |
| 65:5:247:ILE:HG23 | 65:5:262:ALA:HB1 | 2.03 | 0.40 |
| 66:6:242:MET:HG3 | 66:6:245:MET:HG2 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | NA | 203/245 (83%) | 194 (96%) | 8 (4%) | 1 (0%) | 29 | 67 |
| 2 | SA | 338/413 (82%) | 332 (98%) | 6 (2%) | 0 | 100 | 100 |
| 3 | NB | 126/180 (70%) | 118 (94%) | 7 (6%) | 1 (1%) | 19 | 58 |
| 6 | L3 | 100/127 (79%) | 91 (91%) | 9 (9%) | 0 | 100 | 100 |
| 7 | L4 | 226/228 (99%) | 202 (89%) | 24 (11%) | 0 | 100 | 100 |
| 8 | L5 | 211/213 (99%) | 194 (92%) | 17 (8%) | 0 | 100 | 100 |
| 9 | L7 | 161/190 (85%) | 142 (88%) | 19 (12%) | 0 | 100 | 100 |
| 10 | L8 | 166/200 (83%) | 156 (94%) | 10 (6%) | 0 | 100 | 100 |
| 11 | L9 | 173/175 (99%) | 159 (92%) | 14 (8%) | 0 | 100 | 100 |
| 12 | LC | 123/125 (98%) | 113 (92%) | 10 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 13 | LD | 123/156 (79%) | 109 (89%) | 14 (11%) | 0 | 100 | 100 |
| 14 | LE | 125/127 (98%) | 115 (92%) | 10 (8%) | 0 | 100 | 100 |
| 15 | LF | 88/90 (98%) | 74 (84%) | 13 (15%) | 1 (1%) | 14 | 51 |
| 16 | LG | 61/63 (97%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 17 | LH | 810/896 (90%) | 754 (93%) | 56 (7%) | 0 | 100 | 100 |
| 18 | LJ | 489/513 (95%) | 461 (94%) | 28 (6%) | 0 | 100 | 100 |
| 19 | LK | 86/123 (70%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | LL | 465/555 (84%) | 435 (94%) | 30 (6%) | 0 | 100 | 100 |
| 21 | LM | 424/431 (98%) | 407 (96%) | 17 (4%) | 0 | 100 | 100 |
| 22 | LN | 654/748 (87%) | 610 (93%) | 43 (7%) | 1 (0%) | 47 | 79 |
| 23 | LO | 830/855 (97%) | 777 (94%) | 53 (6%) | 0 | 100 | 100 |
| 24 | LP | 259/420 (62%) | 257 (99%) | 2 (1%) | 0 | 100 | 100 |
| 25 | LQ | 798/939 (85%) | 739 (93%) | 58 (7%) | 1 (0%) | 51 | 84 |
| 26 | LS | 473/594 (80%) | 448 (95%) | 25 (5%) | 0 | 100 | 100 |
| 27 | LT | 844/921 (92%) | 805 (95%) | 39 (5%) | 0 | 100 | 100 |
| 28 | LU | 453/465 (97%) | 415 (92%) | 38 (8%) | 0 | 100 | 100 |
| 29 | LV | 360/362 (99%) | 324 (90%) | 36 (10%) | 0 | 100 | 100 |
| 30 | LW | 436/438 (100%) | 409 (94%) | 27 (6%) | 0 | 100 | 100 |
| 31 | LZ | 180/182 (99%) | 170 (94%) | 10 (6%) | 0 | 100 | 100 |
| 32 | NG | 109/111 (98%) | 97 (89%) | 12 (11%) | 0 | 100 | 100 |
| 33 | NK | 173/175 (99%) | 165 (95%) | 8 (5%) | 0 | 100 | 100 |
| 34 | SC | 238/247 (96%) | 227 (95%) | 11 (5%) | 0 | 100 | 100 |
| 34 | SD | 224/247 (91%) | 207 (92%) | 17 (8%) | 0 | 100 | 100 |
| 35 | SE | 119/121 (98%) | 110 (92%) | 9 (8%) | 0 | 100 | 100 |
| 35 | SF | 119/121 (98%) | 107 (90%) | 12 (10%) | 0 | 100 | 100 |
| 36 | SG | 423/464 (91%) | 401 (95%) | 22 (5%) | 0 | 100 | 100 |
| 37 | SH | 358/360 (99%) | 342 (96%) | 16 (4%) | 0 | 100 | 100 |
| 38 | SI | 763/1123 (68%) | 727 (95%) | 36 (5%) | 0 | 100 | 100 |
| 39 | SJ | 212/236 (90%) | 205 (97%) | 7 (3%) | 0 | 100 | 100 |
| 39 | SK | 226/236 (96%) | 221 (98%) | 5 (2%) | 0 | 100 | 100 |
| 40 | SL | 170/183 (93%) | 160 (94%) | 10 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 41 | SM | 278/290 (96%) | 260 (94%) | 18 (6%) | 0 | 100 | 100 |
| 42 | SN | 245/247 (99%) | 232 (95%) | 13 (5%) | 0 | 100 | 100 |
| 43 | SO | 177/179 (99%) | 163 (92%) | 14 (8%) | 0 | 100 | 100 |
| 44 | SQ | 129/167 (77%) | 124 (96%) | 5 (4%) | 0 | 100 | 100 |
| 45 | SR | 102/104 (98%) | 91 (89%) | 10 (10%) | 1 (1%) | 15 | 53 |
| 46 | SS | 142/197 (72%) | 132 (93%) | 10 (7%) | 0 | 100 | 100 |
| 47 | ST | 448/806 (56%) | 425 (95%) | 22 (5%) | 1 (0%) | 47 | 79 |
| 48 | SY | 237/248 (96%) | 222 (94%) | 15 (6%) | 0 | 100 | 100 |
| 49 | SZ | 259/261 (99%) | 237 (92%) | 22 (8%) | 0 | 100 | 100 |
| 50 | NJ | 263/265 (99%) | 259 (98%) | 4 (2%) | 0 | 100 | 100 |
| 51 | NH | 1072/1141 (94%) | 1025 (96%) | 47 (4%) | 0 | 100 | 100 |
| 52 | NI | 163/187 (87%) | 157 (96%) | 6 (4%) | 0 | 100 | 100 |
| 54 | SU | 471/513 (92%) | 447 (95%) | 24 (5%) | 0 | 100 | 100 |
| 55 | LI | 423/687 (62%) | 376 (89%) | 45 (11%) | 2 (0%) | 29 | 67 |
| 56 | ND | 58/60 (97%) | 58 (100%) | 0 | 0 | 100 | 100 |
| 57 | LR | 750/811 (92%) | 693 (92%) | 57 (8%) | 0 | 100 | 100 |
| 58 | NE | 157/240 (65%) | 139 (88%) | 18 (12%) | 0 | 100 | 100 |
| 59 | SB | 431/436 (99%) | 401 (93%) | 30 (7%) | 0 | 100 | 100 |
| 60 | SV | 59/92 (64%) | 56 (95%) | 3 (5%) | 0 | 100 | 100 |
| 61 | SP | 2189/2418 (90%) | 2132 (97%) | 57 (3%) | 0 | 100 | 100 |
| 62 | LX | 802/923 (87%) | 745 (93%) | 57 (7%) | 0 | 100 | 100 |
| 62 | LY | 827/923 (90%) | 774 (94%) | 53 (6%) | 0 | 100 | 100 |
| 63 | L6 | 161/219 (74%) | 150 (93%) | 11 (7%) | 0 | 100 | 100 |
| 64 | NF | 122/124 (98%) | 112 (92%) | 10 (8%) | 0 | 100 | 100 |
| 65 | 5 | 292/534 (55%) | 269 (92%) | 22 (8%) | 1 (0%) | 41 | 75 |
| 66 | 6 | 273/357 (76%) | 259 (95%) | 14 (5%) | 0 | 100 | 100 |
| All | All | 23449/27027 (87%) | 22060 (94%) | 1379 (6%) | 10 (0%) | 100 | 100 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | NA | 454 | VAL |
| 3 | NB | 441 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | SR | 90 | ASP |
| 65 | 5 | 451 | LYS |
| 22 | LN | 666 | ASN |
| 47 | ST | 419 | LYS |
| 55 | LI | 533 | PRO |
| 55 | LI | 258 | PRO |
| 15 | LF | 32 | ARG |
| 25 | LQ | 787 | LYS |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | NA | 187/223 (84%) | 183 (98%) | 4 (2%) | 53 | 72 |
| 2 | SA | 296/328 (90%) | 293 (99%) | 3 (1%) | 76 | 86 |
| 3 | NB | 108/139 (78%) | 106 (98%) | 2 (2%) | 57 | 75 |
| 6 | L3 | 96/108 (89%) | 95 (99%) | 1 (1%) | 76 | 86 |
| 7 | L4 | 196/196 (100%) | 182 (93%) | 14 (7%) | 14 | 42 |
| 8 | L5 | 180/180 (100%) | 177 (98%) | 3 (2%) | 60 | 78 |
| 9 | L7 | 146/170 (86%) | 139 (95%) | 7 (5%) | 25 | 53 |
| 10 | L8 | 138/161 (86%) | 132 (96%) | 6 (4%) | 29 | 56 |
| 11 | L9 | 150/150 (100%) | 142 (95%) | 8 (5%) | 22 | 51 |
| 12 | LC | 105/105 (100%) | 105 (100%) | 0 | 100 | 100 |
| 13 | LD | 114/137 (83%) | 108 (95%) | 6 (5%) | 22 | 51 |
| 14 | LE | 108/108 (100%) | 105 (97%) | 3 (3%) | 43 | 65 |
| 15 | LF | 76/76 (100%) | 71 (93%) | 5 (7%) | 16 | 45 |
| 16 | LG | 56/56 (100%) | 56 (100%) | 0 | 100 | 100 |
| 17 | LH | 758/813 (93%) | 746 (98%) | 12 (2%) | 62 | 79 |
| 18 | LJ | 437/454 (96%) | 432 (99%) | 5 (1%) | 73 | 85 |
| 19 | LK | 83/83 (100%) | 80 (96%) | 3 (4%) | 35 | 61 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 20 | LL | 428/497 (86%) | 422 (99%) | 6 (1%) | 67 | 81 |
| 21 | LM | 391/391 (100%) | 390 (100%) | 1 (0%) | 92 | 95 |
| 22 | LN | 604/671 (90%) | 595 (98%) | 9 (2%) | 65 | 80 |
| 23 | LO | 730/751 (97%) | 717 (98%) | 13 (2%) | 59 | 77 |
| 24 | LP | 248/302 (82%) | 242 (98%) | 6 (2%) | 49 | 69 |
| 25 | LQ | 717/794 (90%) | 708 (99%) | 9 (1%) | 69 | 82 |
| 26 | LS | 424/529 (80%) | 422 (100%) | 2 (0%) | 88 | 93 |
| 27 | LT | 745/802 (93%) | 741 (100%) | 4 (0%) | 88 | 93 |
| 28 | LU | 412/420 (98%) | 405 (98%) | 7 (2%) | 60 | 78 |
| 29 | LV | 307/326 (94%) | 302 (98%) | 5 (2%) | 62 | 79 |
| 30 | LW | 373/373 (100%) | 371 (100%) | 2 (0%) | 88 | 93 |
| 31 | LZ | 171/171 (100%) | 169 (99%) | 2 (1%) | 71 | 84 |
| 34 | SC | 202/206 (98%) | 200 (99%) | 2 (1%) | 76 | 86 |
| 34 | SD | 192/206 (93%) | 185 (96%) | 7 (4%) | 35 | 61 |
| 35 | SE | 100/100 (100%) | 95 (95%) | 5 (5%) | 24 | 52 |
| 35 | SF | 100/100 (100%) | 97 (97%) | 3 (3%) | 41 | 64 |
| 36 | SG | 373/402 (93%) | 371 (100%) | 2 (0%) | 88 | 93 |
| 37 | SH | 307/307 (100%) | 303 (99%) | 4 (1%) | 69 | 82 |
| 38 | SI | 684/965 (71%) | 666 (97%) | 18 (3%) | 46 | 67 |
| 39 | SJ | 195/209 (93%) | 190 (97%) | 5 (3%) | 46 | 67 |
| 39 | SK | 206/209 (99%) | 202 (98%) | 4 (2%) | 57 | 75 |
| 40 | SL | 156/165 (94%) | 146 (94%) | 10 (6%) | 17 | 45 |
| 41 | SM | 251/258 (97%) | 251 (100%) | 0 | 100 | 100 |
| 42 | SN | 230/230 (100%) | 222 (96%) | 8 (4%) | 36 | 61 |
| 43 | SO | 33/156 (21%) | 33 (100%) | 0 | 100 | 100 |
| 44 | SQ | 124/156 (80%) | 120 (97%) | 4 (3%) | 39 | 62 |
| 45 | SR | 86/86 (100%) | 85 (99%) | 1 (1%) | 71 | 84 |
| 46 | SS | 135/135 (100%) | 130 (96%) | 5 (4%) | 34 | 60 |
| 47 | ST | 417/604 (69%) | 409 (98%) | 8 (2%) | 57 | 75 |
| 48 | SY | 226/233 (97%) | 223 (99%) | 3 (1%) | 69 | 82 |
| 54 | SU | 360/473 (76%) | 354 (98%) | 6 (2%) | 60 | 78 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 55 | LI | 150/634 (24%) | 149 (99%) | 1 (1%) | 84 | 90 |
| 56 | ND | 57/57 (100%) | 54 (95%) | 3 (5%) | 22 | 51 |
| 57 | LR | 665/713 (93%) | 653 (98%) | 12 (2%) | 59 | 77 |
| 58 | NE | 119/210 (57%) | 116 (98%) | 3 (2%) | 47 | 68 |
| 59 | SB | 244/359 (68%) | 239 (98%) | 5 (2%) | 55 | 73 |
| 60 | SV | 22/87 (25%) | 20 (91%) | 2 (9%) | 9 | 33 |
| 62 | LX | 549/822 (67%) | 531 (97%) | 18 (3%) | 38 | 62 |
| 63 | L6 | 139/188 (74%) | 131 (94%) | 8 (6%) | 20 | 48 |
| 65 | 5 | 267/482 (55%) | 262 (98%) | 5 (2%) | 57 | 75 |
| 66 | 6 | 244/315 (78%) | 236 (97%) | 8 (3%) | 38 | 62 |
| All | All | 15617/18581 (84%) | 15309 (98%) | 308 (2%) | 57 | 73 |

All (308) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | NA | 304 | GLN |
| 1 | NA | 455 | HIS |
| 1 | NA | 456 | PHE |
| 1 | NA | 496 | TYR |
| 2 | SA | 193 | MET |
| 2 | SA | 268 | MET |
| 2 | SA | 388 | ARG |
| 3 | NB | 434 | PHE |
| 3 | NB | 495 | TYR |
| 6 | L3 | 78 | HIS |
| 7 | L4 | 16 | HIS |
| 7 | L4 | 24 | SER |
| 7 | L4 | 27 | TYR |
| 7 | L4 | 47 | PHE |
| 7 | L4 | 82 | TYR |
| 7 | L4 | 87 | MET |
| 7 | L4 | 103 | TYR |
| 7 | L4 | 113 | ARG |
| 7 | L4 | 138 | TYR |
| 7 | L4 | 149 | TYR |
| 7 | L4 | 153 | ASN |
| 7 | L4 | 205 | PHE |
| 7 | L4 | 218 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | L4 | 226 | PHE |
| 8 | L5 | 65 | ARG |
| 8 | L5 | 135 | ASP |
| 8 | L5 | 209 | TYR |
| 9 | L7 | 79 | ARG |
| 9 | L7 | 83 | LYS |
| 9 | L7 | 86 | GLN |
| 9 | L7 | 141 | ARG |
| 9 | L7 | 150 | GLN |
| 9 | L7 | 163 | ASP |
| 9 | L7 | 169 | PHE |
| 10 | L8 | 27 | PHE |
| 10 | L8 | 58 | LEU |
| 10 | L8 | 75 | LYS |
| 10 | L8 | 77 | ARG |
| 10 | L8 | 113 | PHE |
| 10 | L8 | 182 | TYR |
| 11 | L9 | 16 | LYS |
| 11 | L9 | 63 | ASP |
| 11 | L9 | 74 | ASN |
| 11 | L9 | 102 | GLU |
| 11 | L9 | 103 | ASP |
| 11 | L9 | 114 | TYR |
| 11 | L9 | 121 | SER |
| 11 | L9 | 180 | LYS |
| 13 | LD | 58 | CYS |
| 13 | LD | 67 | ARG |
| 13 | LD | 80 | MET |
| 13 | LD | 88 | ARG |
| 13 | LD | 98 | ASN |
| 13 | LD | 136 | ARG |
| 14 | LE | 41 | MET |
| 14 | LE | 104 | LEU |
| 14 | LE | 111 | MET |
| 15 | LF | 23 | PHE |
| 15 | LF | 40 | LEU |
| 15 | LF | 53 | ASP |
| 15 | LF | 84 | LYS |
| 15 | LF | 89 | TYR |
| 17 | LH | 145 | PHE |
| 17 | LH | 152 | ARG |
| 17 | LH | 267 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | LH | 336 | ARG |
| 17 | LH | 360 | MET |
| 17 | LH | 432 | ARG |
| 17 | LH | 478 | ASN |
| 17 | LH | 590 | HIS |
| 17 | LH | 605 | ASN |
| 17 | LH | 617 | GLN |
| 17 | LH | 626 | PHE |
| 17 | LH | 875 | MET |
| 18 | LJ | 69 | ARG |
| 18 | LJ | 112 | ASN |
| 18 | LJ | 158 | TYR |
| 18 | LJ | 194 | ARG |
| 18 | LJ | 305 | CYS |
| 19 | LK | 472 | ASP |
| 19 | LK | 481 | HIS |
| 19 | LK | 507 | ARG |
| 20 | LL | 222 | THR |
| 20 | LL | 350 | LEU |
| 20 | LL | 441 | LEU |
| 20 | LL | 450 | HIS |
| 20 | LL | 470 | PHE |
| 20 | LL | 554 | PHE |
| 21 | LM | 382 | LEU |
| 22 | LN | 31 | MET |
| 22 | LN | 113 | ARG |
| 22 | LN | 197 | LYS |
| 22 | LN | 258 | SER |
| 22 | LN | 302 | ARG |
| 22 | LN | 347 | LEU |
| 22 | LN | 369 | TYR |
| 22 | LN | 414 | TYR |
| 22 | LN | 663 | PHE |
| 23 | LO | 193 | TYR |
| 23 | LO | 264 | LYS |
| 23 | LO | 265 | CYS |
| 23 | LO | 293 | THR |
| 23 | LO | 339 | LEU |
| 23 | LO | 353 | TYR |
| 23 | LO | 398 | ARG |
| 23 | LO | 488 | LEU |
| 23 | LO | 505 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | LO | 513 | GLU |
| 23 | LO | 680 | ARG |
| 23 | LO | 821 | MET |
| 23 | LO | 826 | ARG |
| 24 | LP | 31 | LEU |
| 24 | LP | 133 | TYR |
| 24 | LP | 174 | PHE |
| 24 | LP | 195 | LYS |
| 24 | LP | 278 | MET |
| 24 | LP | 301 | ASN |
| 25 | LQ | 100 | ASP |
| 25 | LQ | 164 | ASP |
| 25 | LQ | 169 | PHE |
| 25 | LQ | 185 | MET |
| 25 | LQ | 255 | ARG |
| 25 | LQ | 333 | ARG |
| 25 | LQ | 391 | ARG |
| 25 | LQ | 607 | CYS |
| 25 | LQ | 623 | PHE |
| 26 | LS | 176 | LYS |
| 26 | LS | 319 | ARG |
| 27 | LT | 344 | ARG |
| 27 | LT | 510 | LEU |
| 27 | LT | 755 | LYS |
| 27 | LT | 840 | PHE |
| 28 | LU | 89 | ASP |
| 28 | LU | 139 | CYS |
| 28 | LU | 247 | TYR |
| 28 | LU | 268 | CYS |
| 28 | LU | 332 | TYR |
| 28 | LU | 356 | TYR |
| 28 | LU | 407 | MET |
| 29 | LV | 51 | GLN |
| 29 | LV | 85 | ASP |
| 29 | LV | 237 | ARG |
| 29 | LV | 263 | SER |
| 29 | LV | 328 | MET |
| 30 | LW | 105 | ASP |
| 30 | LW | 150 | LEU |
| 31 | LZ | 80 | ASP |
| 31 | LZ | 132 | GLU |
| 34 | SC | 172 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | SC | 275 | CYS |
| 34 | SD | 145 | ASN |
| 34 | SD | 148 | ARG |
| 34 | SD | 231 | ARG |
| 34 | SD | 241 | PHE |
| 34 | SD | 259 | MET |
| 34 | SD | 275 | CYS |
| 34 | SD | 303 | GLN |
| 35 | SE | 29 | ASN |
| 35 | SE | 83 | SER |
| 35 | SE | 91 | CYS |
| 35 | SE | 108 | SER |
| 35 | SE | 115 | TYR |
| 35 | SF | 54 | MET |
| 35 | SF | 91 | CYS |
| 35 | SF | 119 | ASP |
| 36 | SG | 114 | LYS |
| 36 | SG | 258 | ARG |
| 37 | SH | 48 | TYR |
| 37 | SH | 69 | TYR |
| 37 | SH | 141 | MET |
| 37 | SH | 301 | MET |
| 38 | SI | 92 | ARG |
| 38 | SI | 100 | ASP |
| 38 | SI | 150 | MET |
| 38 | SI | 177 | PHE |
| 38 | SI | 230 | MET |
| 38 | SI | 308 | CYS |
| 38 | SI | 348 | ASP |
| 38 | SI | 366 | MET |
| 38 | SI | 555 | MET |
| 38 | SI | 772 | MET |
| 38 | SI | 795 | LYS |
| 38 | SI | 833 | ARG |
| 38 | SI | 847 | LEU |
| 38 | SI | 944 | ASN |
| 38 | SI | 960 | ARG |
| 38 | SI | 973 | ARG |
| 38 | SI | 988 | ARG |
| 38 | SI | 997 | MET |
| 39 | SJ | 70 | CYS |
| 39 | SJ | 76 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | SJ | 80 | MET |
| 39 | SJ | 209 | MET |
| 39 | SJ | 242 | CYS |
| 39 | SK | 182 | PHE |
| 39 | SK | 194 | GLU |
| 39 | SK | 241 | PHE |
| 39 | SK | 250 | ASN |
| 40 | SL | 12 | LEU |
| 40 | SL | 55 | TYR |
| 40 | SL | 84 | ARG |
| 40 | SL | 88 | ASP |
| 40 | SL | 100 | ASP |
| 40 | SL | 107 | GLU |
| 40 | SL | 139 | ASP |
| 40 | SL | 150 | CYS |
| 40 | SL | 173 | MET |
| 40 | SL | 178 | HIS |
| 42 | SN | 46 | MET |
| 42 | SN | 73 | LEU |
| 42 | SN | 117 | GLN |
| 42 | SN | 134 | LEU |
| 42 | SN | 139 | LEU |
| 42 | SN | 167 | MET |
| 42 | SN | 175 | TYR |
| 42 | SN | 203 | TYR |
| 44 | SQ | 103 | TRP |
| 44 | SQ | 186 | TYR |
| 44 | SQ | 212 | MET |
| 44 | SQ | 216 | ARG |
| 45 | SR | 131 | SER |
| 46 | SS | 281 | ARG |
| 46 | SS | 314 | PRO |
| 46 | SS | 316 | ASN |
| 46 | SS | 841 | LYS |
| 46 | SS | 878 | LEU |
| 47 | ST | 16 | ARG |
| 47 | ST | 104 | MET |
| 47 | ST | 602 | LEU |
| 47 | ST | 693 | LYS |
| 47 | ST | 713 | HIS |
| 47 | ST | 716 | LYS |
| 47 | ST | 777 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | ST | 796 | LYS |
| 48 | SY | 27 | PHE |
| 48 | SY | 63 | TYR |
| 48 | SY | 82 | ARG |
| 54 | SU | 123 | TYR |
| 54 | SU | 174 | ASN |
| 54 | SU | 199 | PHE |
| 54 | SU | 413 | MET |
| 54 | SU | 417 | HIS |
| 54 | SU | 495 | MET |
| 55 | LI | 525 | PHE |
| 56 | ND | 160 | ARG |
| 56 | ND | 195 | GLU |
| 56 | ND | 208 | ARG |
| 57 | LR | 8 | LYS |
| 57 | LR | 50 | ARG |
| 57 | LR | 106 | TYR |
| 57 | LR | 171 | MET |
| 57 | LR | 176 | ASP |
| 57 | LR | 182 | CYS |
| 57 | LR | 217 | ASP |
| 57 | LR | 343 | MET |
| 57 | LR | 464 | LYS |
| 57 | LR | 596 | ASP |
| 57 | LR | 619 | ARG |
| 57 | LR | 626 | MET |
| 58 | NE | 201 | GLN |
| 58 | NE | 255 | GLN |
| 58 | NE | 272 | PHE |
| 59 | SB | 175 | LYS |
| 59 | SB | 178 | ASN |
| 59 | SB | 404 | ARG |
| 59 | SB | 406 | LEU |
| 59 | SB | 407 | ARG |
| 60 | SV | 182 | HIS |
| 60 | SV | 183 | ARG |
| 62 | LX | 32 | ARG |
| 62 | LX | 39 | ASN |
| 62 | LX | 44 | MET |
| 62 | LX | 51 | MET |
| 62 | LX | 91 | MET |
| 62 | LX | 122 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62 | LX | 137 | ARG |
| 62 | LX | 184 | PHE |
| 62 | LX | 185 | ASN |
| 62 | LX | 501 | ARG |
| 62 | LX | 537 | MET |
| 62 | LX | 649 | TYR |
| 62 | LX | 652 | ARG |
| 62 | LX | 785 | PHE |
| 62 | LX | 858 | MET |
| 62 | LX | 896 | ASP |
| 62 | LX | 917 | MET |
| 62 | LX | 920 | MET |
| 63 | L6 | 7 | TYR |
| 63 | L6 | 27 | PHE |
| 63 | L6 | 29 | ASP |
| 63 | L6 | 37 | ASP |
| 63 | L6 | 92 | ARG |
| 63 | L6 | 105 | ASP |
| 63 | L6 | 126 | ASP |
| 63 | L6 | 208 | TYR |
| 65 | 5 | 239 | PHE |
| 65 | 5 | 417 | LEU |
| 65 | 5 | 445 | ARG |
| 65 | 5 | 475 | TYR |
| 65 | 5 | 485 | TRP |
| 66 | 6 | 49 | TYR |
| 66 | 6 | 77 | MET |
| 66 | 6 | 93 | MET |
| 66 | 6 | 135 | TYR |
| 66 | 6 | 234 | LYS |
| 66 | 6 | 271 | ARG |
| 66 | 6 | 317 | MET |
| 66 | 6 | 356 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | L5 | 66 | GLN |
| 10 | L8 | 32 | GLN |
| 14 | LE | 15 | ASN |
| 17 | LH | 690 | ASN |
| 22 | LN | 632 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | LO | 598 | ASN |
| 26 | LS | 352 | GLN |
| 28 | LU | 133 | GLN |
| 28 | LU | 443 | ASN |
| 29 | LV | 116 | HIS |
| 29 | LV | 126 | GLN |
| 35 | SF | 38 | ASN |
| 38 | SI | 239 | ASN |
| 38 | SI | 1016 | ASN |
| 38 | SI | 1114 | GLN |
| 39 | SK | 190 | GLN |
| 42 | SN | 117 | GLN |
| 45 | SR | 99 | ASN |
| 47 | ST | 738 | ASN |
| 55 | LI | 608 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 4 | L0 | 483/700 (69%) | 164 (33%) | 3 (0%) |
| 5 | L2 | 163/333 (48%) | 56 (34%) | 0 |
| 53 | 8 | 1169/1807 (64%) | 527 (45%) | 17 (1%) |
| All | All | 1815/2840 (63%) | 747 (41%) | 20 (1%) |

All (747) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L0 | 18 | G |
| 4 | L0 | 20 | C |
| 4 | L0 | 22 | A |
| 4 | L0 | 59 | U |
| 4 | L0 | 60 | G |
| 4 | L0 | 63 | G |
| 4 | L0 | 69 | U |
| 4 | L0 | 82 | A |
| 4 | L0 | 86 | C |
| 4 | L0 | 87 | C |
| 4 | L0 | 90 | G |
| 4 | L0 | 98 | G |
| 4 | L0 | 103 | G |
| 4 | L0 | 104 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L0 | 107 | G |
| 4 | L0 | 117 | G |
| 4 | L0 | 123 | C |
| 4 | L0 | 124 | A |
| 4 | L0 | 125 | G |
| 4 | L0 | 129 | U |
| 4 | L0 | 130 | G |
| 4 | L0 | 131 | C |
| 4 | L0 | 141 | A |
| 4 | L0 | 142 | U |
| 4 | L0 | 143 | A |
| 4 | L0 | 144 | C |
| 4 | L0 | 150 | G |
| 4 | L0 | 151 | U |
| 4 | L0 | 152 | U |
| 4 | L0 | 155 | A |
| 4 | L0 | 161 | A |
| 4 | L0 | 163 | G |
| 4 | L0 | 169 | A |
| 4 | L0 | 173 | G |
| 4 | L0 | 175 | A |
| 4 | L0 | 176 | U |
| 4 | L0 | 177 | U |
| 4 | L0 | 178 | G |
| 4 | L0 | 184 | U |
| 4 | L0 | 185 | A |
| 4 | L0 | 187 | A |
| 4 | L0 | 188 | A |
| 4 | L0 | 189 | U |
| 4 | L0 | 190 | U |
| 4 | L0 | 191 | U |
| 4 | L0 | 197 | G |
| 4 | L0 | 198 | A |
| 4 | L0 | 199 | A |
| 4 | L0 | 200 | A |
| 4 | L0 | 201 | U |
| 4 | L0 | 205 | C |
| 4 | L0 | 213 | G |
| 4 | L0 | 215 | U |
| 4 | L0 | 216 | U |
| 4 | L0 | 218 | U |
| 4 | L0 | 219 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L0 | 220 | U |
| 4 | L0 | 227 | U |
| 4 | L0 | 233 | G |
| 4 | L0 | 234 | A |
| 4 | L0 | 235 | A |
| 4 | L0 | 236 | C |
| 4 | L0 | 238 | G |
| 4 | L0 | 239 | U |
| 4 | L0 | 240 | C |
| 4 | L0 | 243 | A |
| 4 | L0 | 252 | A |
| 4 | L0 | 253 | U |
| 4 | L0 | 254 | C |
| 4 | L0 | 255 | U |
| 4 | L0 | 256 | U |
| 4 | L0 | 259 | G |
| 4 | L0 | 261 | U |
| 4 | L0 | 262 | U |
| 4 | L0 | 267 | U |
| 4 | L0 | 268 | G |
| 4 | L0 | 279 | A |
| 4 | L0 | 280 | A |
| 4 | L0 | 281 | G |
| 4 | L0 | 284 | U |
| 4 | L0 | 304 | U |
| 4 | L0 | 305 | A |
| 4 | L0 | 309 | A |
| 4 | L0 | 310 | U |
| 4 | L0 | 311 | C |
| 4 | L0 | 312 | U |
| 4 | L0 | 313 | A |
| 4 | L0 | 314 | U |
| 4 | L0 | 315 | U |
| 4 | L0 | 316 | U |
| 4 | L0 | 322 | A |
| 4 | L0 | 323 | A |
| 4 | L0 | 324 | U |
| 4 | L0 | 325 | U |
| 4 | L0 | 326 | C |
| 4 | L0 | 331 | U |
| 4 | L0 | 332 | U |
| 4 | L0 | 337 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L0 | 338 | A |
| 4 | L0 | 339 | A |
| 4 | L0 | 340 | U |
| 4 | L0 | 341 | G |
| 4 | L0 | 347 | U |
| 4 | L0 | 348 | U |
| 4 | L0 | 352 | U |
| 4 | L0 | 373 | U |
| 4 | L0 | 374 | U |
| 4 | L0 | 375 | C |
| 4 | L0 | 382 | U |
| 4 | L0 | 385 | A |
| 4 | L0 | 386 | A |
| 4 | L0 | 395 | C |
| 4 | L0 | 396 | A |
| 4 | L0 | 397 | A |
| 4 | L0 | 398 | A |
| 4 | L0 | 399 | U |
| 4 | L0 | 404 | G |
| 4 | L0 | 407 | A |
| 4 | L0 | 427 | A |
| 4 | L0 | 430 | C |
| 4 | L0 | 431 | A |
| 4 | L0 | 433 | C |
| 4 | L0 | 440 | U |
| 4 | L0 | 451 | G |
| 4 | L0 | 461 | A |
| 4 | L0 | 468 | A |
| 4 | L0 | 470 | U |
| 4 | L0 | 474 | A |
| 4 | L0 | 481 | U |
| 4 | L0 | 482 | A |
| 4 | L0 | 483 | U |
| 4 | L0 | 485 | G |
| 4 | L0 | 486 | U |
| 4 | L0 | 487 | A |
| 4 | L0 | 488 | U |
| 4 | L0 | 489 | G |
| 4 | L0 | 491 | U |
| 4 | L0 | 492 | G |
| 4 | L0 | 493 | A |
| 4 | L0 | 494 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L0 | 497 | A |
| 4 | L0 | 502 | G |
| 4 | L0 | 512 | A |
| 4 | L0 | 513 | G |
| 4 | L0 | 517 | A |
| 4 | L0 | 518 | A |
| 4 | L0 | 519 | A |
| 4 | L0 | 521 | G |
| 4 | L0 | 522 | C |
| 4 | L0 | 523 | U |
| 4 | L0 | 524 | U |
| 4 | L0 | 526 | U |
| 4 | L0 | 530 | A |
| 4 | L0 | 531 | C |
| 4 | L0 | 535 | G |
| 4 | L0 | 536 | A |
| 4 | L0 | 540 | U |
| 4 | L0 | 543 | C |
| 4 | L0 | 554 | G |
| 4 | L0 | 583 | U |
| 4 | L0 | 584 | U |
| 4 | L0 | 585 | C |
| 4 | L0 | 586 | A |
| 4 | L0 | 591 | U |
| 5 | L2 | 2 | U |
| 5 | L2 | 3 | C |
| 5 | L2 | 14 | A |
| 5 | L2 | 15 | U |
| 5 | L2 | 16 | A |
| 5 | L2 | 24 | U |
| 5 | L2 | 25 | U |
| 5 | L2 | 28 | A |
| 5 | L2 | 30 | A |
| 5 | L2 | 32 | G |
| 5 | L2 | 33 | A |
| 5 | L2 | 35 | U |
| 5 | L2 | 37 | G |
| 5 | L2 | 38 | U |
| 5 | L2 | 44 | U |
| 5 | L2 | 55 | A |
| 5 | L2 | 56 | A |
| 5 | L2 | 60 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | L2 | 61 | G |
| 5 | L2 | 85 | G |
| 5 | L2 | 88 | U |
| 5 | L2 | 89 | C |
| 5 | L2 | 90 | C |
| 5 | L2 | 91 | C |
| 5 | L2 | 92 | A |
| 5 | L2 | 93 | U |
| 5 | L2 | 94 | A |
| 5 | L2 | 105 | C |
| 5 | L2 | 111 | G |
| 5 | L2 | 114 | A |
| 5 | L2 | 115 | G |
| 5 | L2 | 116 | A |
| 5 | L2 | 118 | A |
| 5 | L2 | 201 | C |
| 5 | L2 | 202 | G |
| 5 | L2 | 247 | U |
| 5 | L2 | 248 | G |
| 5 | L2 | 249 | G |
| 5 | L2 | 251 | G |
| 5 | L2 | 252 | C |
| 5 | L2 | 254 | A |
| 5 | L2 | 256 | G |
| 5 | L2 | 257 | A |
| 5 | L2 | 260 | U |
| 5 | L2 | 264 | C |
| 5 | L2 | 267 | A |
| 5 | L2 | 306 | G |
| 5 | L2 | 307 | G |
| 5 | L2 | 310 | G |
| 5 | L2 | 312 | U |
| 5 | L2 | 316 | A |
| 5 | L2 | 321 | C |
| 5 | L2 | 322 | A |
| 5 | L2 | 324 | U |
| 5 | L2 | 325 | C |
| 5 | L2 | 329 | C |
| 53 | 8 | -5 | G |
| 53 | 8 | -4 | A |
| 53 | 8 | -3 | U |
| 53 | 8 | -2 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | -1 | G |
| 53 | 8 | 0 | U |
| 53 | 8 | 1 | U |
| 53 | 8 | 8 | U |
| 53 | 8 | 9 | U |
| 53 | 8 | 16 | G |
| 53 | 8 | 18 | C |
| 53 | 8 | 19 | A |
| 53 | 8 | 20 | G |
| 53 | 8 | 21 | U |
| 53 | 8 | 22 | A |
| 53 | 8 | 23 | G |
| 53 | 8 | 26 | A |
| 53 | 8 | 28 | A |
| 53 | 8 | 33 | U |
| 53 | 8 | 34 | G |
| 53 | 8 | 35 | U |
| 53 | 8 | 36 | C |
| 53 | 8 | 37 | U |
| 53 | 8 | 39 | A |
| 53 | 8 | 50 | C |
| 53 | 8 | 51 | A |
| 53 | 8 | 53 | G |
| 53 | 8 | 55 | A |
| 53 | 8 | 99 | C |
| 53 | 8 | 102 | U |
| 53 | 8 | 103 | A |
| 53 | 8 | 104 | A |
| 53 | 8 | 109 | G |
| 53 | 8 | 110 | U |
| 53 | 8 | 111 | U |
| 53 | 8 | 112 | A |
| 53 | 8 | 113 | U |
| 53 | 8 | 114 | C |
| 53 | 8 | 115 | G |
| 53 | 8 | 116 | U |
| 53 | 8 | 119 | A |
| 53 | 8 | 122 | U |
| 53 | 8 | 126 | A |
| 53 | 8 | 127 | G |
| 53 | 8 | 140 | A |
| 53 | 8 | 141 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 142 | G |
| 53 | 8 | 143 | G |
| 53 | 8 | 144 | U |
| 53 | 8 | 145 | A |
| 53 | 8 | 146 | U |
| 53 | 8 | 147 | A |
| 53 | 8 | 150 | U |
| 53 | 8 | 153 | G |
| 53 | 8 | 159 | U |
| 53 | 8 | 160 | C |
| 53 | 8 | 161 | U |
| 53 | 8 | 162 | A |
| 53 | 8 | 180 | A |
| 53 | 8 | 181 | A |
| 53 | 8 | 185 | U |
| 53 | 8 | 186 | C |
| 53 | 8 | 188 | A |
| 53 | 8 | 190 | C |
| 53 | 8 | 191 | C |
| 53 | 8 | 192 | U |
| 53 | 8 | 194 | U |
| 53 | 8 | 195 | G |
| 53 | 8 | 196 | G |
| 53 | 8 | 197 | A |
| 53 | 8 | 199 | G |
| 53 | 8 | 200 | A |
| 53 | 8 | 201 | G |
| 53 | 8 | 204 | G |
| 53 | 8 | 205 | U |
| 53 | 8 | 207 | U |
| 53 | 8 | 210 | A |
| 53 | 8 | 211 | U |
| 53 | 8 | 212 | U |
| 53 | 8 | 213 | A |
| 53 | 8 | 214 | G |
| 53 | 8 | 223 | U |
| 53 | 8 | 226 | A |
| 53 | 8 | 227 | U |
| 53 | 8 | 228 | G |
| 53 | 8 | 233 | C |
| 53 | 8 | 234 | G |
| 53 | 8 | 235 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 236 | A |
| 53 | 8 | 237 | C |
| 53 | 8 | 239 | C |
| 53 | 8 | 240 | U |
| 53 | 8 | 241 | U |
| 53 | 8 | 242 | U |
| 53 | 8 | 245 | U |
| 53 | 8 | 246 | G |
| 53 | 8 | 257 | A |
| 53 | 8 | 258 | C |
| 53 | 8 | 261 | U |
| 53 | 8 | 262 | U |
| 53 | 8 | 263 | C |
| 53 | 8 | 264 | G |
| 53 | 8 | 265 | A |
| 53 | 8 | 266 | A |
| 53 | 8 | 267 | U |
| 53 | 8 | 269 | G |
| 53 | 8 | 271 | A |
| 53 | 8 | 273 | G |
| 53 | 8 | 278 | U |
| 53 | 8 | 280 | U |
| 53 | 8 | 281 | G |
| 53 | 8 | 282 | C |
| 53 | 8 | 283 | U |
| 53 | 8 | 284 | G |
| 53 | 8 | 285 | G |
| 53 | 8 | 286 | C |
| 53 | 8 | 287 | G |
| 53 | 8 | 289 | U |
| 53 | 8 | 298 | C |
| 53 | 8 | 300 | A |
| 53 | 8 | 301 | A |
| 53 | 8 | 305 | C |
| 53 | 8 | 306 | U |
| 53 | 8 | 307 | G |
| 53 | 8 | 308 | C |
| 53 | 8 | 312 | A |
| 53 | 8 | 313 | U |
| 53 | 8 | 315 | A |
| 53 | 8 | 316 | A |
| 53 | 8 | 319 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 320 | U |
| 53 | 8 | 321 | C |
| 53 | 8 | 322 | G |
| 53 | 8 | 323 | A |
| 53 | 8 | 325 | G |
| 53 | 8 | 336 | G |
| 53 | 8 | 337 | G |
| 53 | 8 | 338 | C |
| 53 | 8 | 345 | U |
| 53 | 8 | 346 | G |
| 53 | 8 | 347 | G |
| 53 | 8 | 348 | U |
| 53 | 8 | 351 | C |
| 53 | 8 | 352 | A |
| 53 | 8 | 355 | G |
| 53 | 8 | 359 | A |
| 53 | 8 | 360 | A |
| 53 | 8 | 361 | C |
| 53 | 8 | 362 | G |
| 53 | 8 | 366 | A |
| 53 | 8 | 368 | U |
| 53 | 8 | 369 | A |
| 53 | 8 | 371 | G |
| 53 | 8 | 372 | G |
| 53 | 8 | 373 | G |
| 53 | 8 | 374 | U |
| 53 | 8 | 376 | C |
| 53 | 8 | 377 | G |
| 53 | 8 | 378 | A |
| 53 | 8 | 379 | U |
| 53 | 8 | 382 | C |
| 53 | 8 | 383 | G |
| 53 | 8 | 390 | G |
| 53 | 8 | 396 | G |
| 53 | 8 | 398 | G |
| 53 | 8 | 400 | A |
| 53 | 8 | 401 | A |
| 53 | 8 | 402 | C |
| 53 | 8 | 404 | G |
| 53 | 8 | 407 | A |
| 53 | 8 | 412 | A |
| 53 | 8 | 414 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 417 | A |
| 53 | 8 | 418 | G |
| 53 | 8 | 420 | A |
| 53 | 8 | 421 | A |
| 53 | 8 | 423 | G |
| 53 | 8 | 431 | C |
| 53 | 8 | 440 | U |
| 53 | 8 | 442 | C |
| 53 | 8 | 444 | C |
| 53 | 8 | 448 | C |
| 53 | 8 | 449 | C |
| 53 | 8 | 452 | A |
| 53 | 8 | 453 | U |
| 53 | 8 | 454 | U |
| 53 | 8 | 455 | C |
| 53 | 8 | 456 | A |
| 53 | 8 | 459 | G |
| 53 | 8 | 460 | A |
| 53 | 8 | 461 | G |
| 53 | 8 | 465 | G |
| 53 | 8 | 466 | U |
| 53 | 8 | 468 | A |
| 53 | 8 | 469 | C |
| 53 | 8 | 470 | A |
| 53 | 8 | 471 | A |
| 53 | 8 | 477 | A |
| 53 | 8 | 480 | G |
| 53 | 8 | 485 | A |
| 53 | 8 | 486 | G |
| 53 | 8 | 487 | G |
| 53 | 8 | 493 | U |
| 53 | 8 | 495 | C |
| 53 | 8 | 496 | G |
| 53 | 8 | 501 | U |
| 53 | 8 | 502 | U |
| 53 | 8 | 504 | U |
| 53 | 8 | 505 | A |
| 53 | 8 | 506 | A |
| 53 | 8 | 507 | U |
| 53 | 8 | 511 | A |
| 53 | 8 | 514 | G |
| 53 | 8 | 515 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 520 | A |
| 53 | 8 | 527 | A |
| 53 | 8 | 529 | A |
| 53 | 8 | 530 | C |
| 53 | 8 | 532 | U |
| 53 | 8 | 533 | U |
| 53 | 8 | 534 | A |
| 53 | 8 | 535 | A |
| 53 | 8 | 536 | C |
| 53 | 8 | 538 | A |
| 53 | 8 | 539 | G |
| 53 | 8 | 540 | G |
| 53 | 8 | 542 | A |
| 53 | 8 | 543 | C |
| 53 | 8 | 544 | A |
| 53 | 8 | 545 | A |
| 53 | 8 | 546 | U |
| 53 | 8 | 553 | G |
| 53 | 8 | 562 | G |
| 53 | 8 | 563 | U |
| 53 | 8 | 565 | C |
| 53 | 8 | 570 | A |
| 53 | 8 | 572 | C |
| 53 | 8 | 573 | C |
| 53 | 8 | 574 | G |
| 53 | 8 | 576 | G |
| 53 | 8 | 579 | A |
| 53 | 8 | 580 | A |
| 53 | 8 | 581 | U |
| 53 | 8 | 582 | U |
| 53 | 8 | 584 | C |
| 53 | 8 | 585 | A |
| 53 | 8 | 586 | G |
| 53 | 8 | 587 | C |
| 53 | 8 | 594 | A |
| 53 | 8 | 595 | G |
| 53 | 8 | 600 | U |
| 53 | 8 | 603 | U |
| 53 | 8 | 624 | G |
| 53 | 8 | 627 | C |
| 53 | 8 | 629 | U |
| 53 | 8 | 630 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 632 | U |
| 53 | 8 | 633 | U |
| 53 | 8 | 636 | A |
| 53 | 8 | 637 | C |
| 53 | 8 | 638 | U |
| 53 | 8 | 860 | U |
| 53 | 8 | 861 | U |
| 53 | 8 | 862 | A |
| 53 | 8 | 863 | A |
| 53 | 8 | 864 | U |
| 53 | 8 | 865 | A |
| 53 | 8 | 866 | G |
| 53 | 8 | 870 | C |
| 53 | 8 | 871 | G |
| 53 | 8 | 872 | G |
| 53 | 8 | 877 | G |
| 53 | 8 | 880 | C |
| 53 | 8 | 881 | A |
| 53 | 8 | 882 | U |
| 53 | 8 | 886 | U |
| 53 | 8 | 887 | A |
| 53 | 8 | 892 | A |
| 53 | 8 | 894 | U |
| 53 | 8 | 895 | G |
| 53 | 8 | 896 | U |
| 53 | 8 | 897 | C |
| 53 | 8 | 898 | A |
| 53 | 8 | 899 | G |
| 53 | 8 | 900 | A |
| 53 | 8 | 904 | G |
| 53 | 8 | 905 | A |
| 53 | 8 | 906 | A |
| 53 | 8 | 908 | U |
| 53 | 8 | 911 | U |
| 53 | 8 | 912 | U |
| 53 | 8 | 913 | G |
| 53 | 8 | 914 | G |
| 53 | 8 | 916 | U |
| 53 | 8 | 917 | U |
| 53 | 8 | 918 | U |
| 53 | 8 | 919 | A |
| 53 | 8 | 920 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 8 | 921 | U |
| 53 | 8 | 924 | A |
| 53 | 8 | 925 | G |
| 53 | 8 | 929 | A |
| 53 | 8 | 931 | C |
| 53 | 8 | 932 | U |
| 53 | 8 | 933 | A |
| 53 | 8 | 934 | C |
| 53 | 8 | 935 | U |
| 53 | 8 | 939 | A |
| 53 | 8 | 940 | A |
| 53 | 8 | 942 | G |
| 53 | 8 | 945 | U |
| 53 | 8 | 947 | U |
| 53 | 8 | 948 | G |
| 53 | 8 | 950 | C |
| 53 | 8 | 952 | A |
| 53 | 8 | 955 | A |
| 53 | 8 | 959 | U |
| 53 | 8 | 961 | U |
| 53 | 8 | 962 | C |
| 53 | 8 | 963 | A |
| 53 | 8 | 964 | U |
| 53 | 8 | 965 | U |
| 53 | 8 | 966 | A |
| 53 | 8 | 967 | A |
| 53 | 8 | 969 | C |
| 53 | 8 | 972 | G |
| 53 | 8 | 975 | C |
| 53 | 8 | 976 | G |
| 53 | 8 | 978 | A |
| 53 | 8 | 979 | A |
| 53 | 8 | 980 | G |
| 53 | 8 | 981 | U |
| 53 | 8 | 983 | A |
| 53 | 8 | 984 | G |
| 53 | 8 | 988 | A |
| 53 | 8 | 992 | A |
| 53 | 8 | 993 | A |
| 53 | 8 | 994 | G |
| 53 | 8 | 995 | A |
| 53 | 8 | 996 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | 8 | 997 | G |
| 53 | 8 | 998 | A |
| 53 | 8 | 999 | U |
| 53 | 8 | 1001 | A |
| 53 | 8 | 1002 | G |
| 53 | 8 | 1003 | A |
| 53 | 8 | 1004 | U |
| 53 | 8 | 1005 | A |
| 53 | 8 | 1006 | C |
| 53 | 8 | 1007 | C |
| 53 | 8 | 1009 | U |
| 53 | 8 | 1010 | C |
| 53 | 8 | 1011 | G |
| 53 | 8 | 1012 | U |
| 53 | 8 | 1014 | G |
| 53 | 8 | 1015 | U |
| 53 | 8 | 1016 | C |
| 53 | 8 | 1017 | U |
| 53 | 8 | 1019 | A |
| 53 | 8 | 1036 | A |
| 53 | 8 | 1038 | U |
| 53 | 8 | 1039 | A |
| 53 | 8 | 1040 | G |
| 53 | 8 | 1042 | G |
| 53 | 8 | 1043 | A |
| 53 | 8 | 1053 | G |
| 53 | 8 | 1054 | U |
| 53 | 8 | 1057 | U |
| 53 | 8 | 1058 | U |
| 53 | 8 | 1060 | U |
| 53 | 8 | 1061 | A |
| 53 | 8 | 1062 | A |
| 53 | 8 | 1063 | U |
| 53 | 8 | 1064 | G |
| 53 | 8 | 1072 | C |
| 53 | 8 | 1076 | A |
| 53 | 8 | 1083 | G |
| 53 | 8 | 1084 | A |
| 53 | 8 | 1085 | G |
| 53 | 8 | 1086 | A |
| 53 | 8 | 1088 | A |
| 53 | 8 | 1089 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | 8 | 1090 | C |
| 53 | 8 | 1091 | A |
| 53 | 8 | 1092 | A |
| 53 | 8 | 1093 | A |
| 53 | 8 | 1094 | G |
| 53 | 8 | 1095 | U |
| 53 | 8 | 1096 | C |
| 53 | 8 | 1097 | U |
| 53 | 8 | 1098 | U |
| 53 | 8 | 1099 | U |
| 53 | 8 | 1100 | G |
| 53 | 8 | 1104 | U |
| 53 | 8 | 1106 | U |
| 53 | 8 | 1107 | G |
| 53 | 8 | 1108 | G |
| 53 | 8 | 1109 | G |
| 53 | 8 | 1110 | G |
| 53 | 8 | 1112 | G |
| 53 | 8 | 1113 | A |
| 53 | 8 | 1116 | A |
| 53 | 8 | 1118 | G |
| 53 | 8 | 1119 | G |
| 53 | 8 | 1126 | G |
| 53 | 8 | 1127 | G |
| 53 | 8 | 1131 | A |
| 53 | 8 | 1132 | A |
| 53 | 8 | 1134 | C |
| 53 | 8 | 1135 | U |
| 53 | 8 | 1144 | U |
| 53 | 8 | 1146 | G |
| 53 | 8 | 1149 | G |
| 53 | 8 | 1158 | C |
| 53 | 8 | 1159 | C |
| 53 | 8 | 1160 | A |
| 53 | 8 | 1164 | G |
| 53 | 8 | 1174 | C |
| 53 | 8 | 1191 | U |
| 53 | 8 | 1192 | C |
| 53 | 8 | 1193 | A |
| 53 | 8 | 1197 | C |
| 53 | 8 | 1198 | G |
| 53 | 8 | 1200 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | 8 | 1202 | A |
| 53 | 8 | 1204 | A |
| 53 | 8 | 1206 | U |
| 53 | 8 | 1212 | G |
| 53 | 8 | 1213 | G |
| 53 | 8 | 1214 | U |
| 53 | 8 | 1216 | C |
| 53 | 8 | 1218 | G |
| 53 | 8 | 1223 | A |
| 53 | 8 | 1224 | A |
| 53 | 8 | 1226 | A |
| 53 | 8 | 1259 | U |
| 53 | 8 | 1262 | U |
| 53 | 8 | 1266 | U |
| 53 | 8 | 1267 | G |
| 53 | 8 | 1268 | G |
| 53 | 8 | 1270 | G |
| 53 | 8 | 1272 | U |
| 53 | 8 | 1273 | G |
| 53 | 8 | 1276 | U |
| 53 | 8 | 1434 | U |
| 53 | 8 | 1436 | A |
| 53 | 8 | 1437 | U |
| 53 | 8 | 1438 | G |
| 53 | 8 | 1443 | U |
| 53 | 8 | 1449 | U |
| 53 | 8 | 1471 | A |
| 53 | 8 | 1473 | U |
| 53 | 8 | 1474 | G |
| 53 | 8 | 1477 | G |
| 53 | 8 | 1479 | A |
| 53 | 8 | 1483 | A |
| 53 | 8 | 1484 | G |
| 53 | 8 | 1486 | G |
| 53 | 8 | 1488 | G |
| 53 | 8 | 1489 | U |
| 53 | 8 | 1492 | A |
| 53 | 8 | 1493 | A |
| 53 | 8 | 1498 | G |
| 53 | 8 | 1504 | G |
| 53 | 8 | 1506 | G |
| 53 | 8 | 1509 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | 8 | 1531 | G |
| 53 | 8 | 1533 | C |
| 53 | 8 | 1534 | G |
| 53 | 8 | 1573 | A |
| 53 | 8 | 1574 | G |
| 53 | 8 | 1575 | G |
| 53 | 8 | 1576 | A |
| 53 | 8 | 1583 | A |
| 53 | 8 | 1584 | G |
| 53 | 8 | 1590 | G |
| 53 | 8 | 1595 | U |
| 53 | 8 | 1596 | C |
| 53 | 8 | 1597 | A |
| 53 | 8 | 1600 | A |
| 53 | 8 | 1602 | C |
| 53 | 8 | 1614 | A |
| 53 | 8 | 1618 | C |
| 53 | 8 | 1628 | U |
| 53 | 8 | 1629 | G |
| 53 | 8 | 1630 | U |
| 53 | 8 | 1632 | C |
| 53 | 8 | 1639 | C |
| 53 | 8 | 1640 | C |
| 53 | 8 | 1645 | G |
| 53 | 8 | 1652 | C |
| 53 | 8 | 1653 | C |
| 53 | 8 | 1657 | U |
| 53 | 8 | 1658 | G |
| 53 | 8 | 1666 | U |
| 53 | 8 | 1670 | G |
| 53 | 8 | 1678 | A |
| 53 | 8 | 1680 | G |
| 53 | 8 | 1681 | A |
| 53 | 8 | 1682 | U |
| 53 | 8 | 1683 | C |
| 53 | 8 | 1684 | U |
| 53 | 8 | 1693 | A |
| 53 | 8 | 1697 | G |
| 53 | 8 | 1703 | C |
| 53 | 8 | 1704 | U |
| 53 | 8 | 1711 | C |
| 53 | 8 | 1712 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | 8 | 1713 | G |
| 53 | 8 | 1717 | G |
| 53 | 8 | 1726 | G |
| 53 | 8 | 1727 | G |
| 53 | 8 | 1730 | A |
| 53 | 8 | 1736 | G |
| 53 | 8 | 1742 | U |
| 53 | 8 | 1744 | A |
| 53 | 8 | 1747 | G |
| 53 | 8 | 1748 | G |
| 53 | 8 | 1771 | U |
| 53 | 8 | 1773 | C |
| 53 | 8 | 1774 | G |
| 53 | 8 | 1775 | U |
| 53 | 8 | 1780 | G |
| 53 | 8 | 1781 | A |
| 53 | 8 | 1783 | C |
| 53 | 8 | 1785 | U |
| 53 | 8 | 1791 | A |

All (20) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 4 | L0 | 199 | A |
| 4 | L0 | 314 | U |
| 4 | L0 | 522 | C |
| 53 | 8 | -3 | U |
| 53 | 8 | 0 | U |
| 53 | 8 | 22 | A |
| 53 | 8 | 199 | G |
| 53 | 8 | 240 | U |
| 53 | 8 | 283 | U |
| 53 | 8 | 322 | G |
| 53 | 8 | 372 | G |
| 53 | 8 | 876 | G |
| 53 | 8 | 880 | C |
| 53 | 8 | 919 | A |
| 53 | 8 | 997 | G |
| 53 | 8 | 1057 | U |
| 53 | 8 | 1094 | G |
| 53 | 8 | 1573 | A |
| 53 | 8 | 1638 | G |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | 8 | 1790 | 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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 46 | SS | 2 |
| 22 | LN | 2 |
| 47 | ST | 2 |
| 24 | LP | 2 |
| 19 | LK | 2 |
| 38 | SI | 1 |
| 17 | LH | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | SS | 408:UNK | C | 828:ASN | N | 85.72 |
| 1 | SI | 417:UNK | C | 548:ASN | N | 63.03 |
| 1 | LN | 730:UNK | C | 731:HIS | N | 39.41 |
| 1 | ST | 316:UNK | C | 382:UNK | N | 38.49 |
| 1 | LH | 831:UNK | C | 846:ASN | N | 26.10 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | LN | 716:UNK | C | 717:UNK | N | 21.45 |
| 1 | LP | 416:UNK | C | 418:UNK | N | 15.60 |
| 1 | ST | 252:UNK | C | 264:UNK | N | 14.89 |
| 1 | LP | 369:UNK | C | 379:UNK | N | 11.71 |
| 1 | LK | 426:UNK | C | 428:ASP | N | 11.33 |
| 1 | SS | 363:UNK | C | 369:UNK | N | 10.71 |
| 1 | LK | 402:UNK | C | 404:UNK | N | 4.30 |

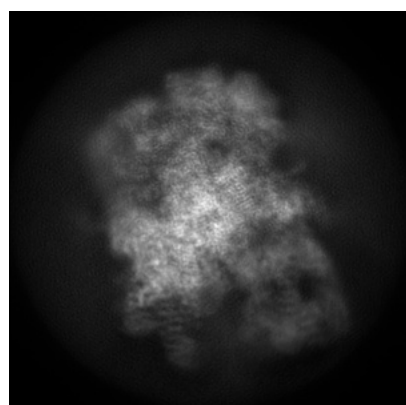
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25441. These allow visual inspection of the internal detail of the map and identification of artifacts.

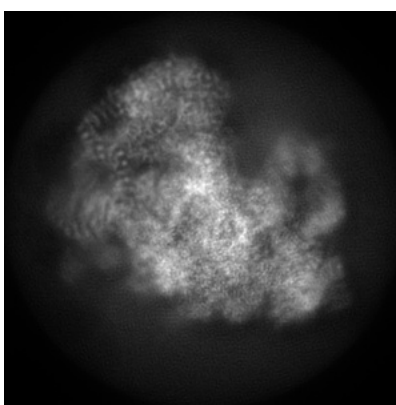
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

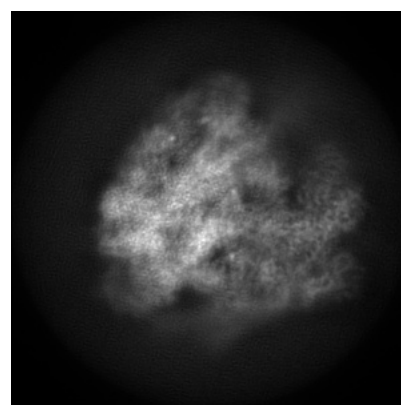
6.1.1 Primary map



X



Y

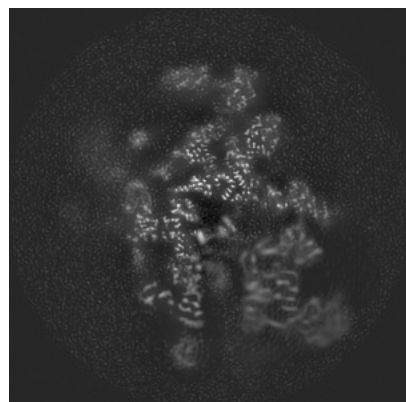


Z

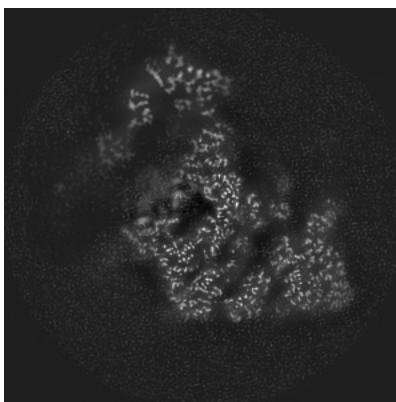
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

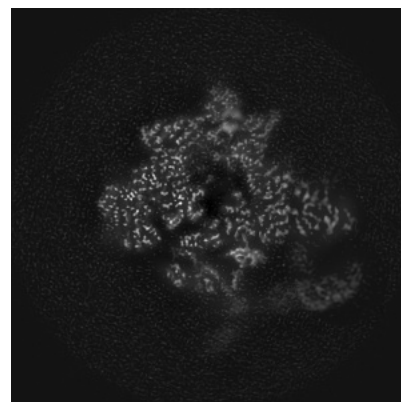
6.2.1 Primary map



X Index: 216



Y Index: 216

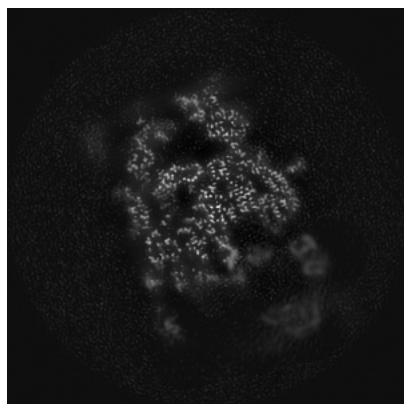


Z Index: 216

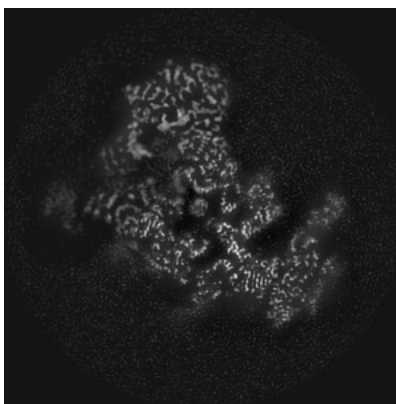
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

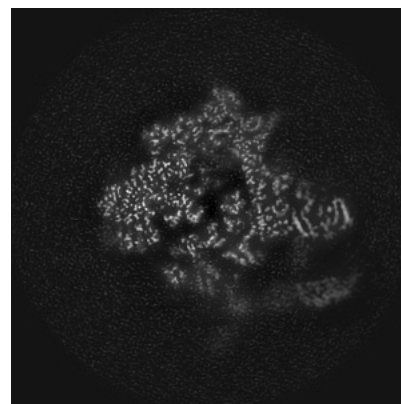
6.3.1 Primary map



X Index: 182



Y Index: 199



Z Index: 219

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

6.4 Orthogonal surface views [i](#)

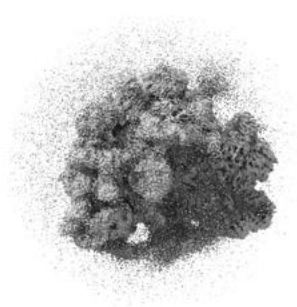
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

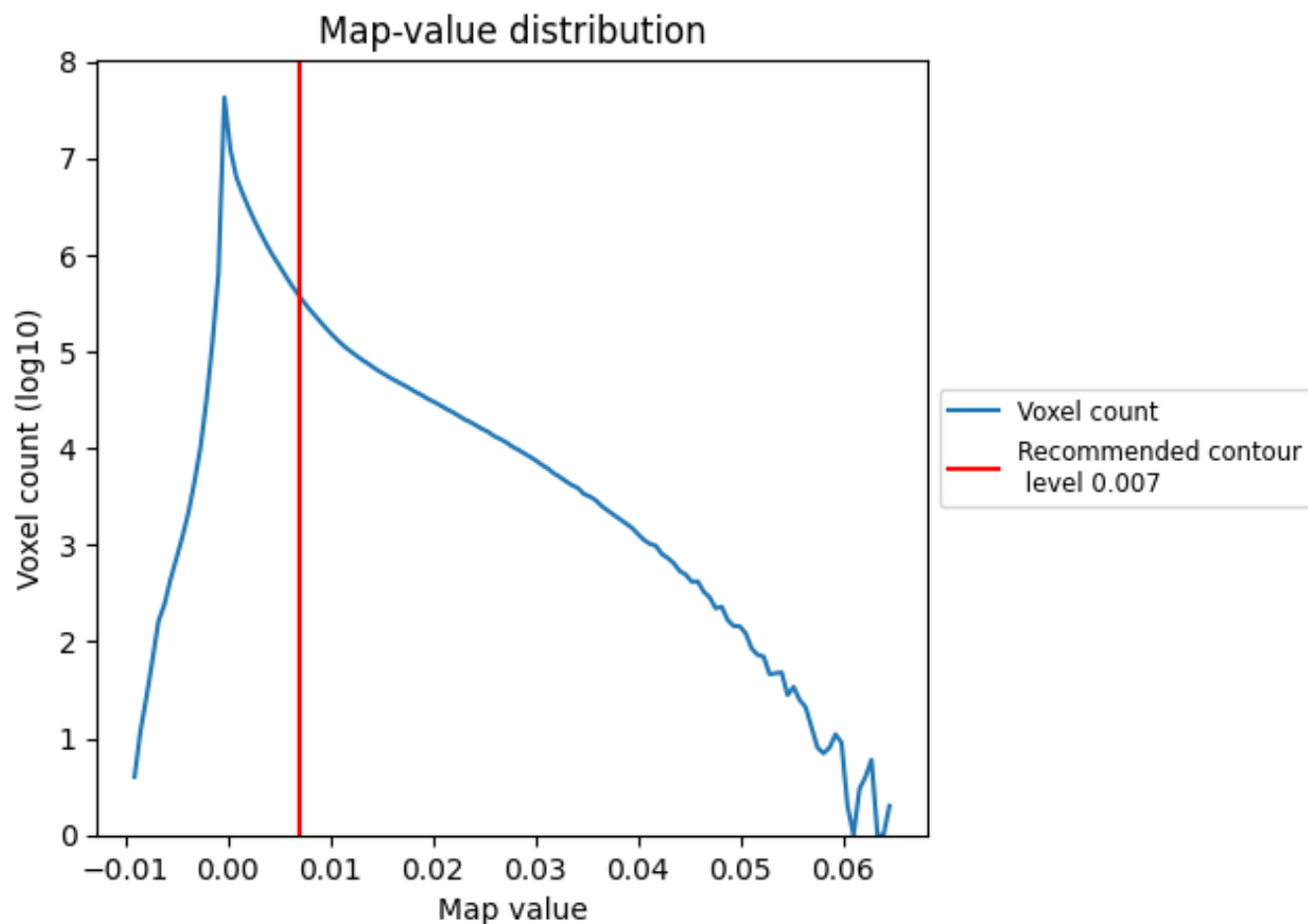
6.5 Mask visualisation

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

7 Map analysis [i](#)

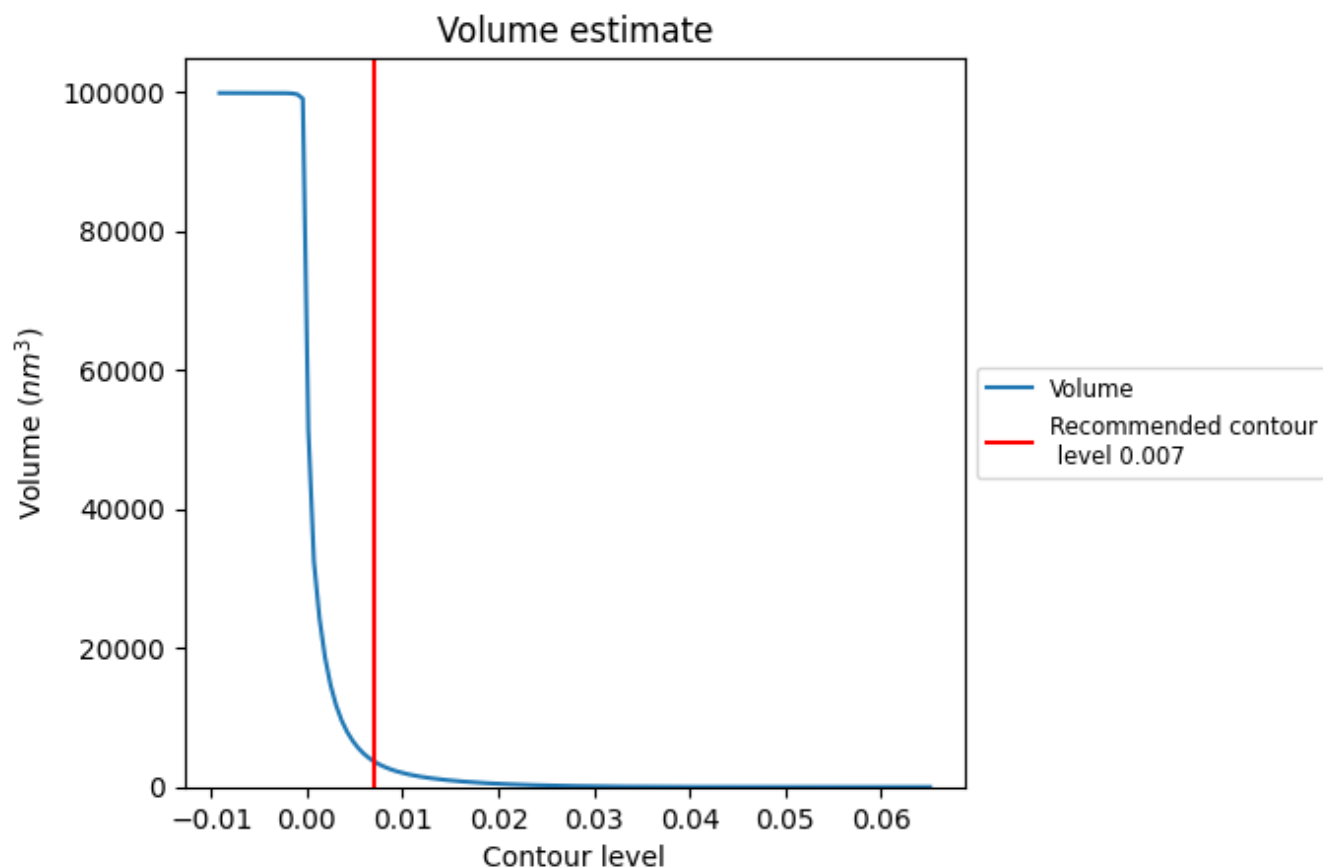
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

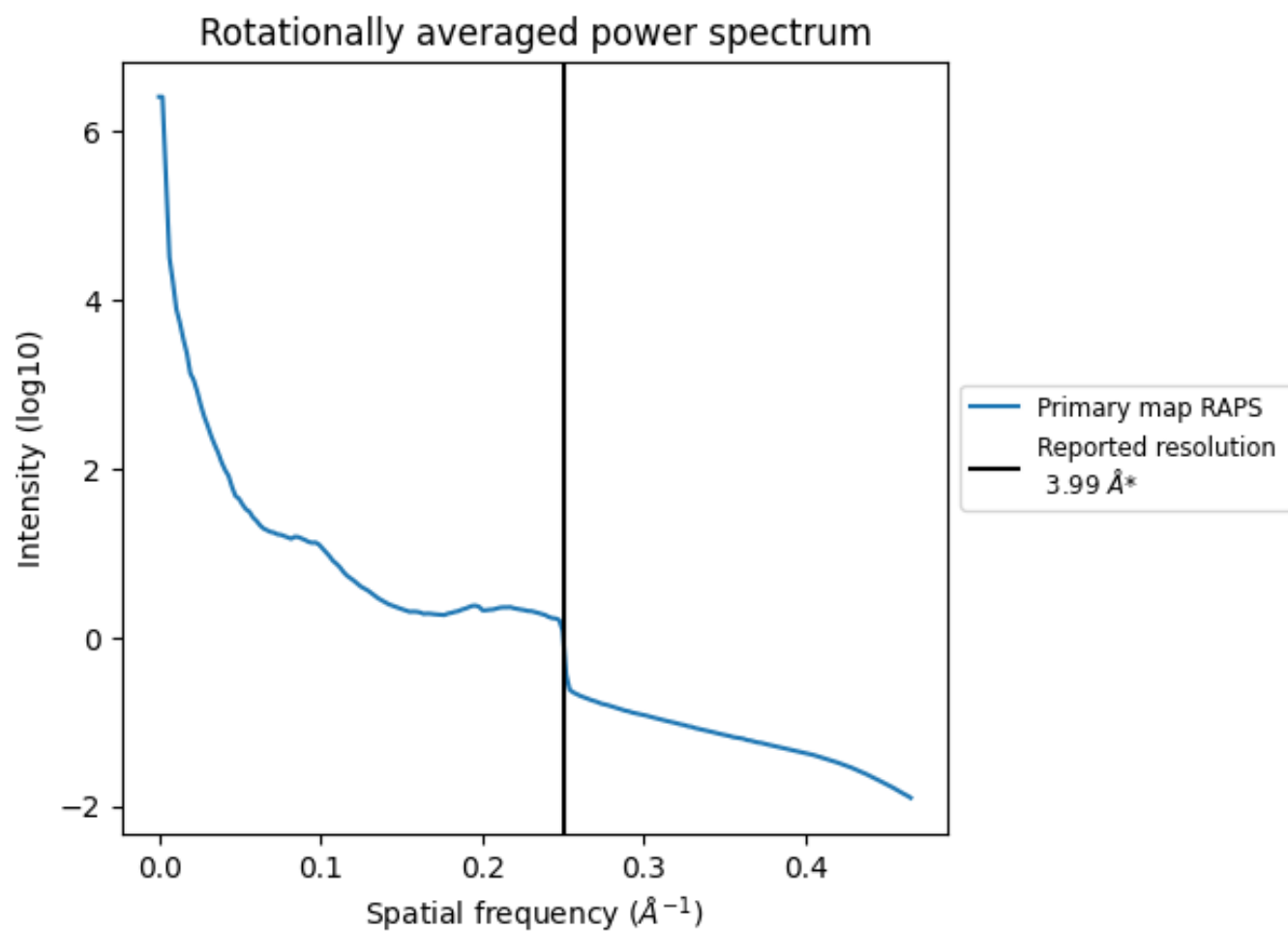
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3693 nm³; this corresponds to an approximate mass of 3336 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

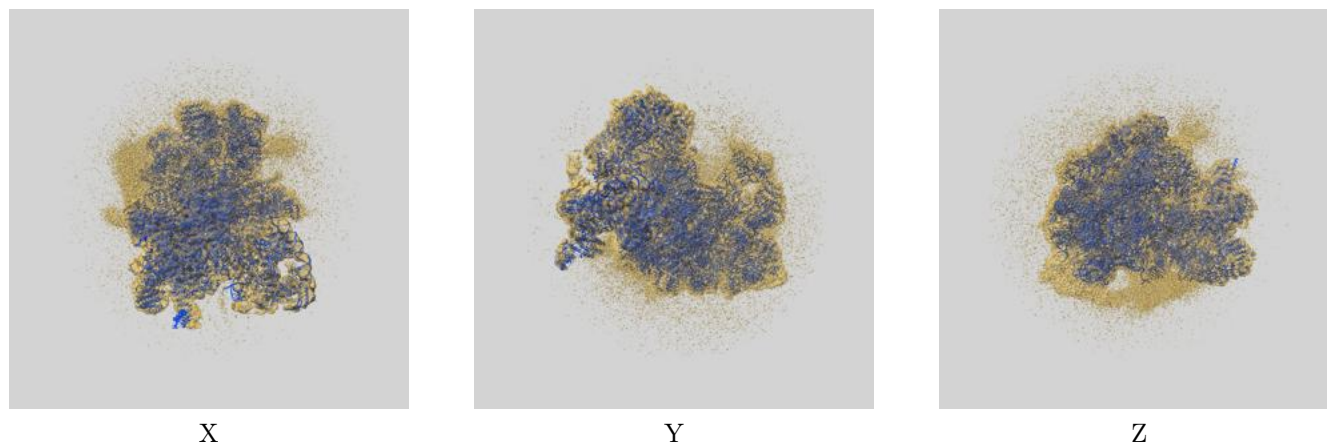
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

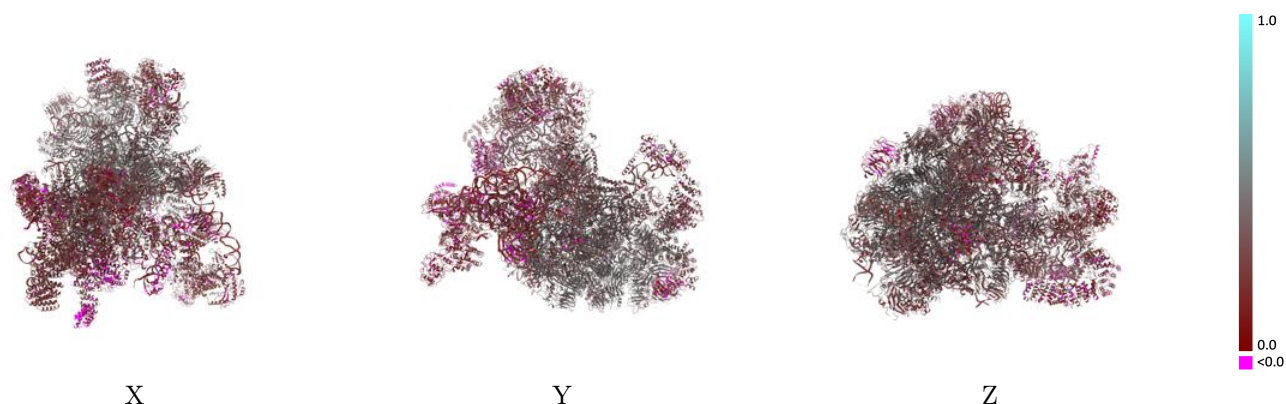
This section contains information regarding the fit between EMDB map EMD-25441 and PDB model 7SUK. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



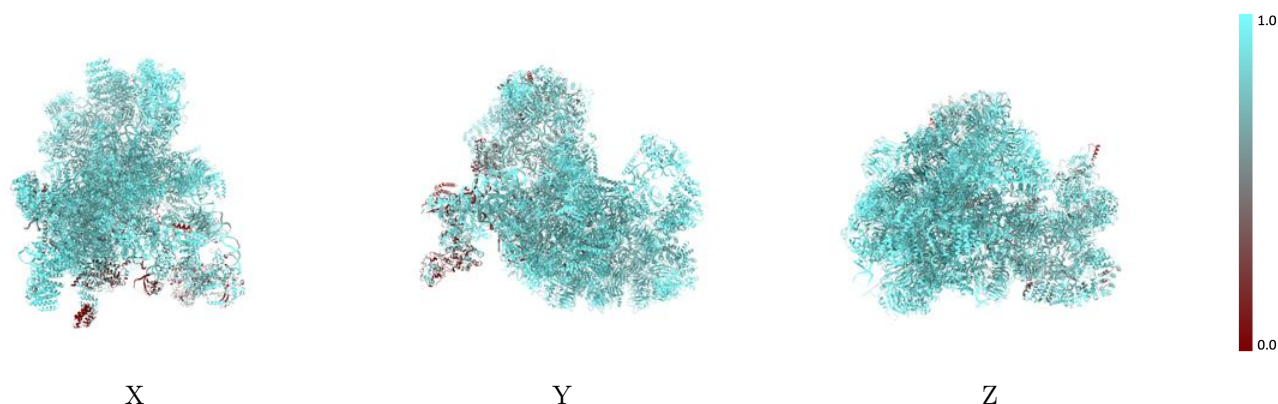
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



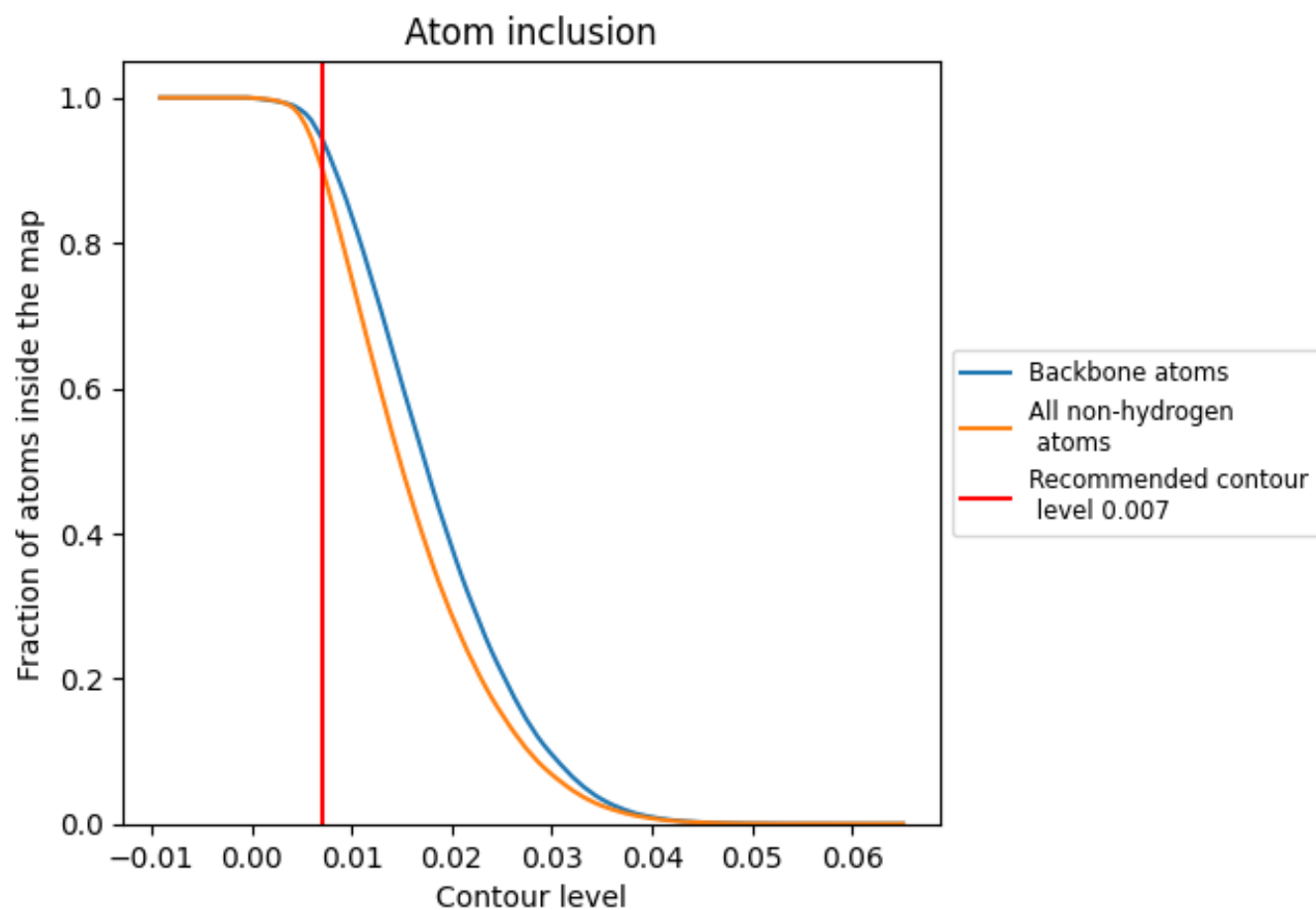
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.007) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9044 |  0.3140 |
| 5 |  0.5198 |  0.1000 |
| 6 |  0.6050 |  0.1570 |
| 8 |  0.9086 |  0.2630 |
| L0 |  0.9894 |  0.3530 |
| L2 |  0.9883 |  0.3600 |
| L3 |  0.8400 |  0.3230 |
| L4 |  0.8354 |  0.2260 |
| L5 |  0.9448 |  0.4070 |
| L6 |  0.7426 |  0.1750 |
| L7 |  0.7719 |  0.2040 |
| L8 |  0.8670 |  0.2410 |
| L9 |  0.9357 |  0.3690 |
| LC |  0.9570 |  0.4350 |
| LD |  0.8707 |  0.2350 |
| LE |  0.8462 |  0.2520 |
| LF |  0.9023 |  0.2620 |
| LG |  0.9811 |  0.4260 |
| LH |  0.9480 |  0.3750 |
| LI |  0.9288 |  0.2260 |
| LJ |  0.9540 |  0.3970 |
| LK |  0.9808 |  0.3210 |
| LL |  0.9531 |  0.3990 |
| LM |  0.9458 |  0.3870 |
| LN |  0.9490 |  0.3700 |
| LO |  0.9515 |  0.4190 |
| LP |  0.9714 |  0.3330 |
| LQ |  0.9528 |  0.3300 |
| LR |  0.8188 |  0.1640 |
| LS |  0.9552 |  0.4190 |
| LT |  0.9602 |  0.4180 |
| LU |  0.9370 |  0.3700 |
| LV |  0.8430 |  0.2340 |
| LW |  0.9490 |  0.4130 |
| LX |  0.8469 |  0.2280 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| LY |  0.8623 |  0.2620 |
| LZ |  0.9475 |  0.4160 |
| NA |  0.9012 |  0.3710 |
| NB |  0.9336 |  0.3810 |
| ND |  0.9271 |  0.3450 |
| NE |  0.7283 |  0.2910 |
| NF |  0.4853 |  0.0300 |
| NG |  0.9006 |  0.2330 |
| NH |  0.6270 |  0.1930 |
| NI |  0.3472 |  0.1710 |
| NJ |  0.9323 |  0.2520 |
| NK |  0.9505 |  0.2180 |
| SA |  0.9442 |  0.3620 |
| SB |  0.9438 |  0.3520 |
| SC |  0.9428 |  0.4130 |
| SD |  0.9385 |  0.3550 |
| SE |  0.9237 |  0.3920 |
| SF |  0.9502 |  0.3550 |
| SG |  0.9529 |  0.3100 |
| SH |  0.9470 |  0.3710 |
| SI |  0.9332 |  0.3620 |
| SJ |  0.9480 |  0.3210 |
| SK |  0.9610 |  0.3840 |
| SL |  0.9546 |  0.4140 |
| SM |  0.9257 |  0.4050 |
| SN |  0.9588 |  0.3740 |
| SO |  0.9888 |  0.3240 |
| SP |  0.8625 |  0.2240 |
| SQ |  0.8954 |  0.3950 |
| SR |  0.9206 |  0.3730 |
| SS |  0.9318 |  0.3350 |
| ST |  0.9441 |  0.3160 |
| SU |  0.9440 |  0.2940 |
| SV |  0.9074 |  0.3540 |
| SY |  0.9421 |  0.3970 |
| SZ |  0.9606 |  0.2440 |