



## Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 01:39 PM JST

PDB ID : 9XAG / pdb\_00009xag  
EMDB ID : EMD-66686  
Title : Cryo-EM structure of the 90S pre-ribosome (Enp1-Rrp12 Mut) from *Chaetomium thermophilum*, state B1  
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.  
Deposited on : 2025-10-22  
Resolution : 2.80 Å (reported)  
Based on initial model : 6RXU

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

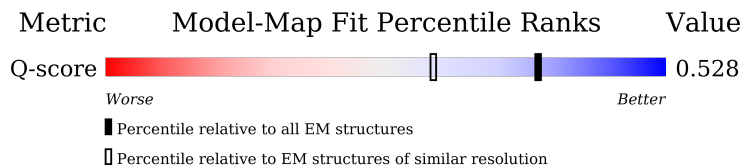
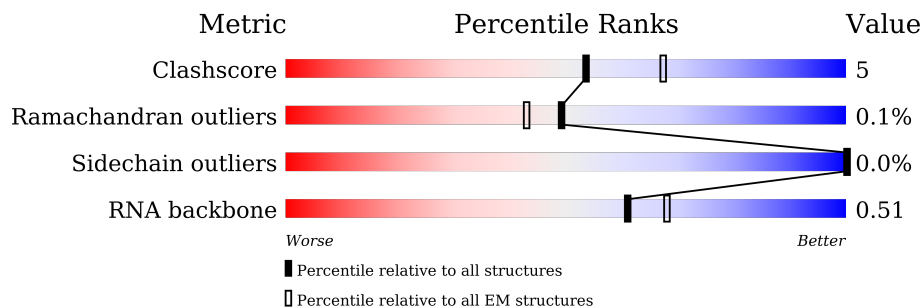
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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



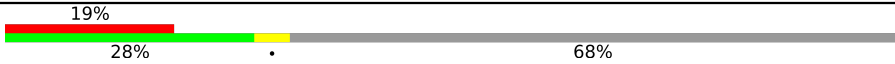
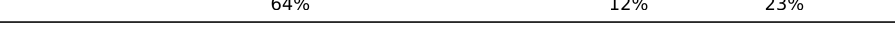
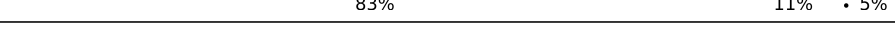
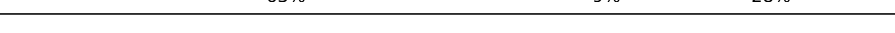
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11806 ( 2.30 - 3.30 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | UA    | 904    |                  |
| 2   | UB    | 907    |                  |

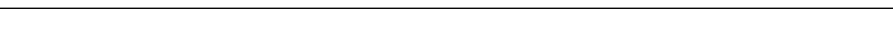
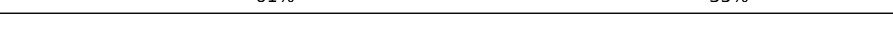
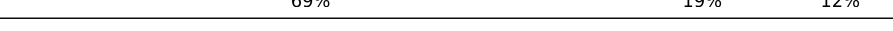
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | UC    | 648    |    |
| 4   | UD    | 884    |    |
| 5   | UF    | 414    |    |
| 6   | UG    | 558    |    |
| 7   | UJ    | 1802   |    |
| 8   | UK    | 270    |    |
| 9   | UL    | 962    |    |
| 10  | UM    | 912    |    |
| 11  | UN    | 716    |    |
| 12  | UO    | 557    |    |
| 13  | UQ    | 960    |    |
| 14  | UR    | 618    |   |
| 15  | UU    | 1049   |  |
| 16  | UX    | 193    |  |
| 17  | UZ    | 391    |  |
| 18  | CA    | 313    |  |
| 18  | CB    | 313    |  |
| 19  | CC    | 523    |  |
| 20  | CD    | 582    |  |
| 21  | CE    | 127    |  |
| 21  | CF    | 127    |  |
| 22  | CG    | 630    |  |
| 23  | CH    | 411    |  |
| 24  | CI    | 1163   |  |
| 25  | CJ    | 183    |  |

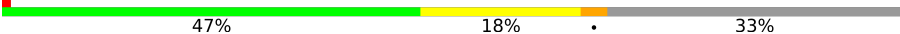
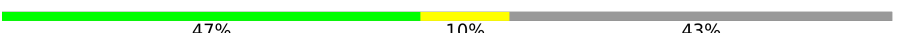
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 26  | CK    | 297    |    |
| 27  | CL    | 785    |    |
| 28  | CM    | 446    |    |
| 29  | CN    | 252    |    |
| 29  | CO    | 252    |    |
| 30  | CP    | 322    |    |
| 31  | CQ    | 259    |    |
| 32  | CR    | 1073   |    |
| 32  | CS    | 1073   |    |
| 33  | CT    | 203    |    |
| 34  | Ca    | 255    |    |
| 35  | Cb    | 264    |    |
| 36  | Cc    | 212    |  |
| 37  | Cd    | 239    |  |
| 38  | Ce    | 203    |  |
| 39  | Cf    | 202    |  |
| 40  | Cg    | 190    |  |
| 41  | Ch    | 151    |  |
| 42  | Ci    | 150    |  |
| 43  | Cj    | 143    |  |
| 44  | Ck    | 161    |  |
| 45  | Cm    | 130    |  |
| 46  | Cn    | 145    |  |
| 47  | Co    | 136    |  |
| 48  | Cp    | 68     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 49  | CU    | 311    |    |
| 50  | C1    | 2348   |    |
| 51  | C2    | 274    |    |
| 52  | CW    | 668    |    |
| 53  | UT    | 2612   |    |
| 54  | UH    | 930    |    |
| 55  | UE    | 410    |    |
| 55  | UI    | 410    |    |
| 56  | US    | 549    |    |
| 57  | Cl    | 156    |    |
| 58  | CX    | 480    |    |
| 59  | CY    | 381    |    |
| 60  | CZ    | 609    |  |
| 61  | UP    | 364    |  |

## 2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 227662 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Periodic tryptophan protein 2-like protein.

| Mol | Chain | Residues | Atoms |      |      |      |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---|---------|-------|
| 1   | UA    | 839      | Total | C    | N    | O    | P | S       |       |
|     |       |          | 6411  | 4118 | 1136 | 1132 | 1 | 24      |       |
|     |       |          |       |      |      |      |   | 0       | 0     |

- Molecule 2 is a protein called Nucleolar complex protein 14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | UB    | 566      | Total | C    | N   | O   | S  |         |       |
|     |       |          | 4506  | 2845 | 858 | 790 | 13 |         |       |
|     |       |          |       |      |     |     |    | 0       | 0     |

- Molecule 3 is a protein called Sas10 C-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | UC    | 205      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1633  | 1034 | 293 | 300 | 6 |         |       |
|     |       |          |       |      |     |     |   | 0       | 0     |

- Molecule 4 is a protein called UTP4.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | UD    | 777      | Total | C    | N    | O    | S  |         |       |
|     |       |          | 6108  | 3872 | 1099 | 1113 | 24 |         |       |
|     |       |          |       |      |      |      |    | 0       | 0     |

- Molecule 5 is a protein called U3 snoRNP protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | UF    | 331      | Total | C    | N   | O   | S  |         |       |
|     |       |          | 2599  | 1678 | 504 | 403 | 14 |         |       |
|     |       |          |       |      |     |     |    | 0       | 0     |

- Molecule 6 is a protein called U three protein 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | UG    | 479      | Total | C    | N   | O   | S  |         |       |
|     |       |          | 3765  | 2391 | 700 | 662 | 12 |         |       |
|     |       |          |       |      |     |     |    | 0       | 0     |

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 10.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 7   | UJ    | 1637     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 12592 | 8061 | 2154 | 2326 | 51 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | UK    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1066 | 351 | 273 | 5 |         |       |

- Molecule 9 is a protein called Small-subunit processome Utp12 domain-containing protein.

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

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 10  | UM    | 843      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6545  | 4139 | 1151 | 1241 | 14 |         |       |

- Molecule 11 is a protein called UTP14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | UN    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1401  | 892 | 263 | 239 | 7 |         |       |

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | UO    | 503      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3811  | 2417 | 698 | 683 | 13 |         |       |

- Molecule 13 is a protein called UTP17.

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

- Molecule 14 is a protein called UTP18.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | UR    | 447      | Total | C    | N   | O   | P | S       |       |
|     |       |          | 3495  | 2209 | 656 | 619 | 1 | 10      |       |
|     |       |          |       |      |     |     |   | 0       | 0     |

- Molecule 15 is a protein called Putative U3 snoRNP protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 15  | UU    | 908      | Total | C    | N    | O    | S  |         |       |
|     |       |          | 6778  | 4361 | 1243 | 1148 | 26 |         |       |
|     |       |          |       |      |      |      |    | 0       | 0     |

- Molecule 16 is a protein called UTP24.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | UX    | 190      | Total | C   | N   | O   | S  |         |       |
|     |       |          | 1480  | 938 | 286 | 246 | 10 |         |       |
|     |       |          |       |     |     |     |    | 0       | 0     |

- Molecule 17 is a protein called Ribosome biogenesis protein C8F11.04.

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

- Molecule 18 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

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

- Molecule 19 is a protein called Nucleolar protein 56.

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

- Molecule 20 is a protein called Nucleolar protein 58.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | CD    | 446      | Total | C    | N   | O   | S  |         |       |
|     |       |          | 3355  | 2150 | 594 | 600 | 11 |         |       |
|     |       |          |       |      |     |     |    | 0       | 0     |

- Molecule 21 is a protein called H/ACA ribonucleoprotein complex subunit 2.

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

- Molecule 22 is a protein called Ribosomal RNA-processing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | CG    | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3245  | 2065 | 587 | 580 | 13 |         |       |

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

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

- Molecule 24 is a protein called Bms1-type G domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 24  | CI    | 841      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6666  | 4277 | 1246 | 1113 | 30 |         |       |

- Molecule 25 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

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

- Molecule 26 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | CL    | 320      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2466  | 1550 | 460 | 450 | 6 |         |       |

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

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

- Molecule 29 is a protein called Nucleolar essential protein 1.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | CP    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1893  | 1209 | 340 | 335 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | CQ    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1413  | 898 | 257 | 251 | 7 |         |       |

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | CR    | 846      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6677  | 4278 | 1137 | 1233 | 29 |         |       |
| 32  | CS    | 836      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6591  | 4217 | 1118 | 1228 | 28 |         |       |

- Molecule 33 is a protein called Fcf2 pre-rRNA processing C-terminal domain-containing protein.

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

- Molecule 34 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | Ca    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1821  | 1160 | 341 | 315 | 5 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | Cb    | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1851  | 1179 | 340 | 325 | 7 |         |       |

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Cc    | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1464  | 926 | 278 | 253 | 7 |         |       |

- Molecule 37 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | Cd    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1819  | 1138 | 363 | 313 | 5 |         |       |

- Molecule 38 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 38  | Ce    | 159      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1279  | 810 | 237 | 232 |  |         |       |

- Molecule 39 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Cf    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1398  | 872 | 283 | 242 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Cg    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1248  | 804 | 258 | 184 | 2 |         |       |

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 41  | Ch    | 66       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 546   | 355 | 101 | 90 |         |       |

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | Ci    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 506 | 156 | 141 | 5 |         |       |

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Cj    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 943   | 613 | 177 | 151 | 2 |         |       |

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Ck    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1082  | 695 | 210 | 172 | 5 |         |       |

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Cm    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 632 | 184 | 164 | 5 |         |       |

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | Cn    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 702   | 456 | 134 | 110 | 2 |         |       |

- Molecule 47 is a protein called Small ribosomal subunit protein eS24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Co    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 474 | 139 | 126 | 2 |         |       |

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | Cp    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 458   | 286 | 97 | 74 | 1 |         |       |

- Molecule 49 is a protein called Faf1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | CU    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1337  | 822 | 265 | 244 | 6 |         |       |

- Molecule 50 is a RNA chain called 35s rna.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 50  | C1    | 1574     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33584 | 14984 | 6018 | 11008 | 1574 |         |       |

- Molecule 51 is a RNA chain called u3 rna.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 51  | C2    | 229      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 4869  | 2172 | 851 | 1617 | 229 |         |       |

- Molecule 52 is a protein called Ribosome biogenesis protein ENP2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | CW    | 383      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2932  | 1862 | 531 | 525 | 14 |         |       |

- Molecule 53 is a protein called utp20.

| Mol | Chain | Residues | Atoms |       |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|-------|
| 53  | UT    | 2027     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 15998 | 10300 | 2811 | 2819 | 68 |         |       |

- Molecule 54 is a protein called utp8.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 54  | UH    | 799      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6198  | 3903 | 1105 | 1171 | 19 |         |       |

- Molecule 55 is a protein called Small-subunit processome Utp12 domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | UE    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1362  | 851 | 251 | 254 | 6 |         |       |
| 55  | UI    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 622 | 187 | 181 | 6 |         |       |

- Molecule 56 is a protein called CCAAT-binding factor domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | US    | 451      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3672  | 2389 | 608 | 660 | 15 |         |       |

- Molecule 57 is a protein called Putative ribosomal protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | Cl    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 400 | 115 | 117 | 1 |         |       |

- Molecule 58 is a protein called Bystin-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | CX    | 267      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2130  | 1384 | 374 | 362 | 10 |         |       |

- Molecule 59 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59  | CY    | 264      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2095  | 1296 | 388 | 406 | 5 |         |       |

- Molecule 60 is a protein called Protein BFR2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | CZ    | 283      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2270  | 1398 | 426 | 439 | 7 |         |       |

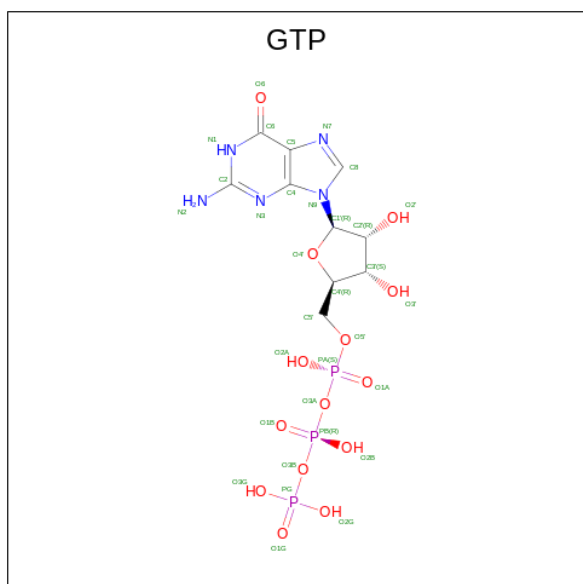
- Molecule 61 is a protein called utp16.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 61  | UP    | 54       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 422   | 264 | 88 | 70 |         |       |

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 62  | UX    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

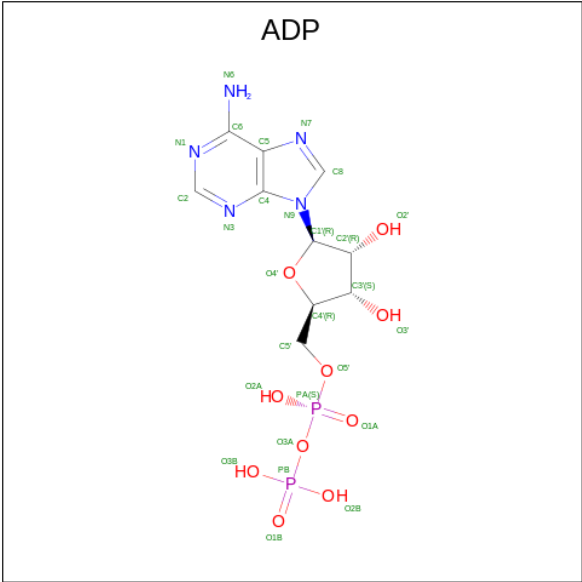


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 63  | CI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 64  | CI    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

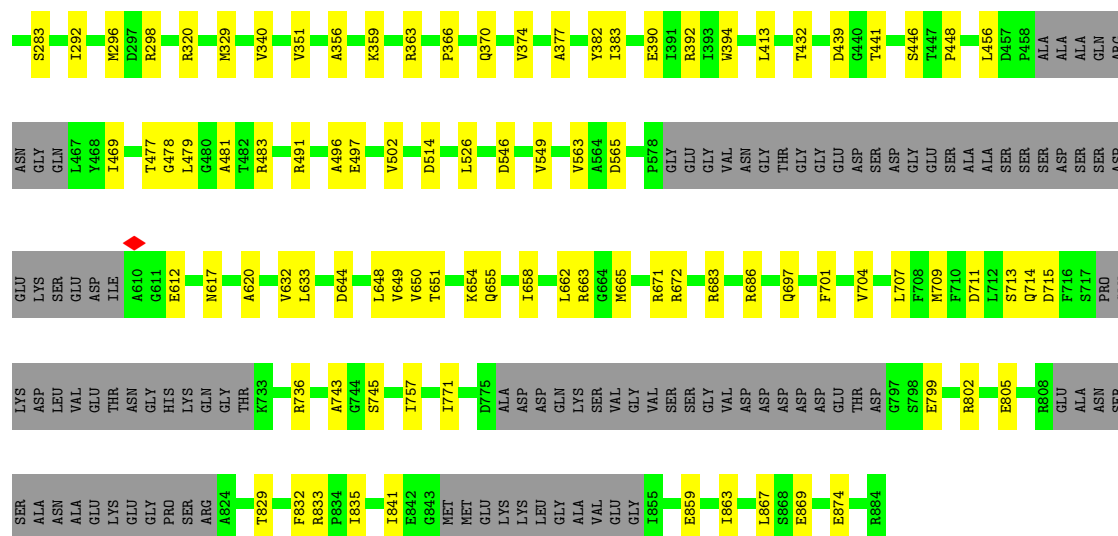
- Molecule 65 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 65  | CS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

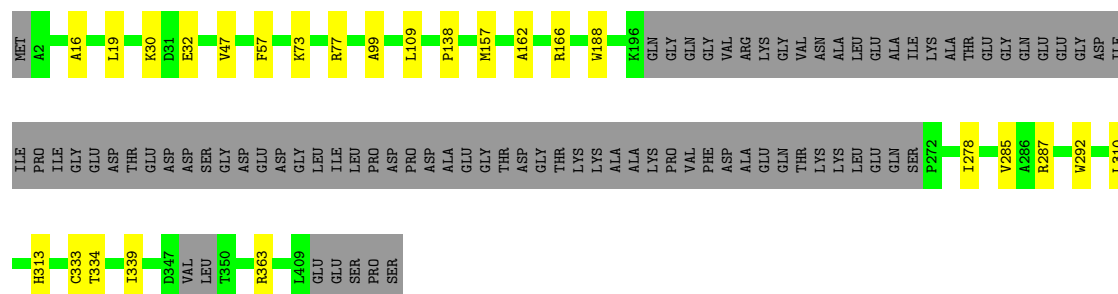






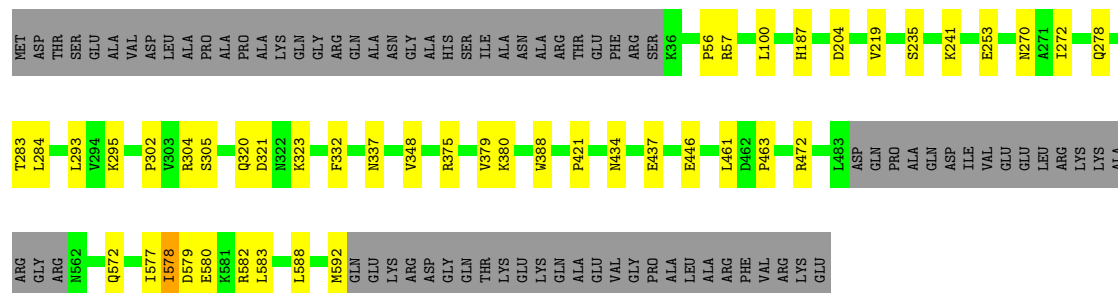
• Molecule 5: U3 snoRNP protein

Chain UF: 74% 6% 20%



• Molecule 6: U three protein 7

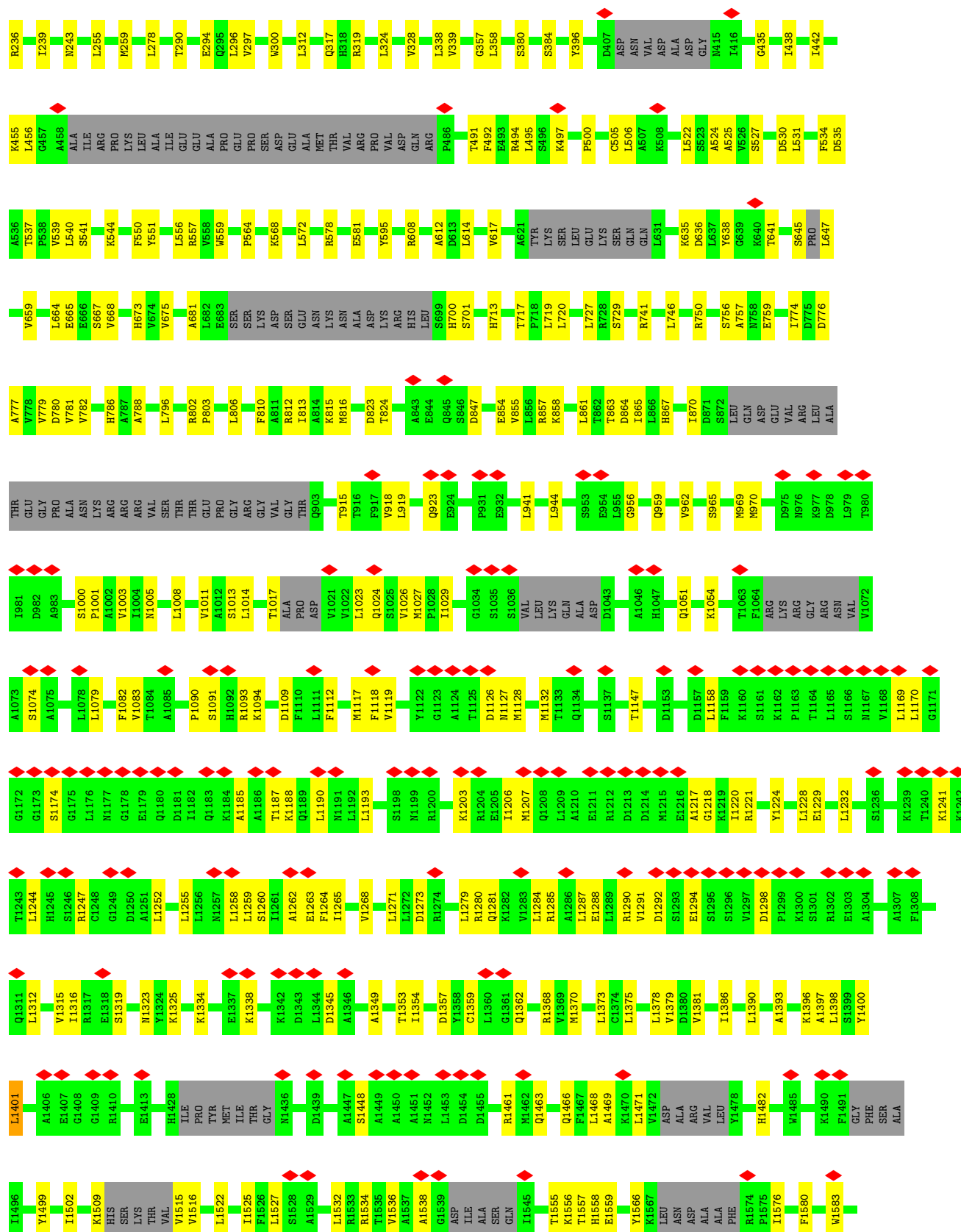
Chain UG: 78% 8% 14%

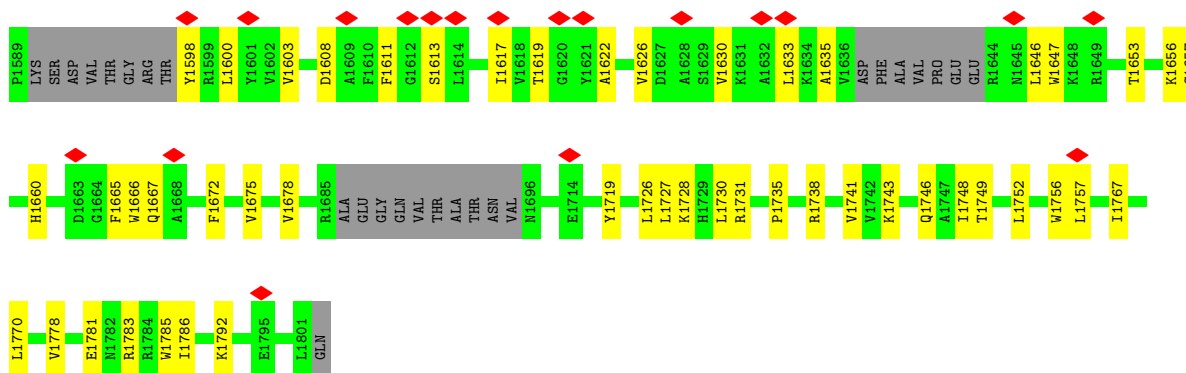


• Molecule 7: U3 small nucleolar RNA-associated protein 10

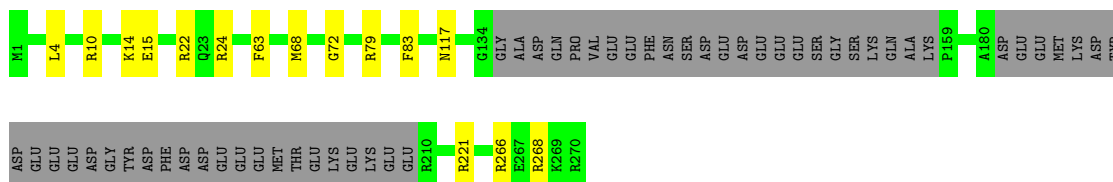
Chain UJ: 10% 71% 20% 9%



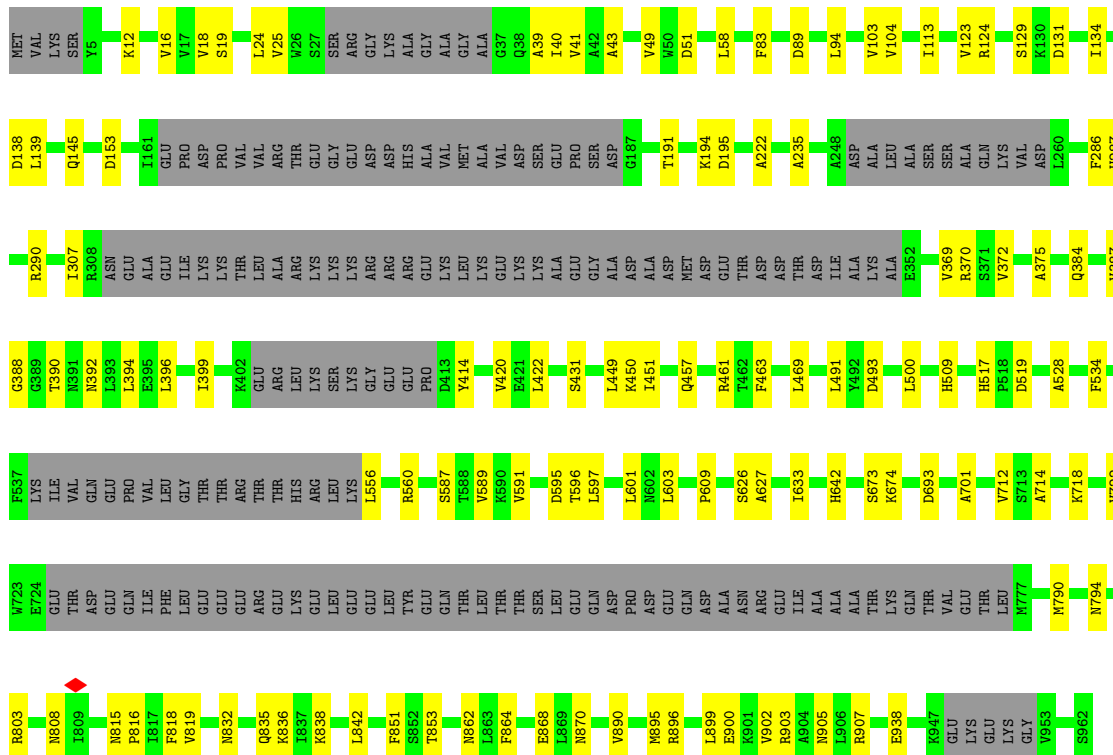




- Molecule 8: U3 small nucleolar RNA-associated protein 11

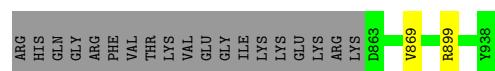


- Molecule 9: Small-subunit processome Utp12 domain-containing protein

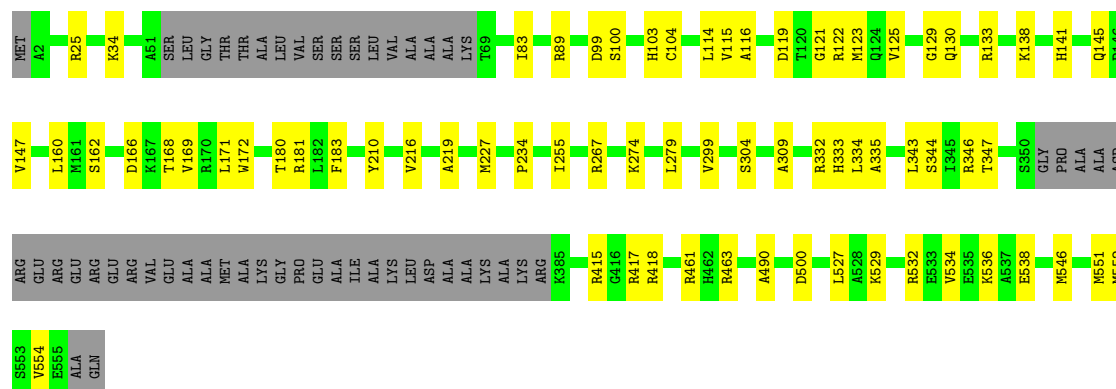
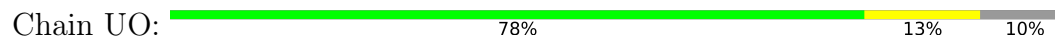


- Molecule 10: U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein

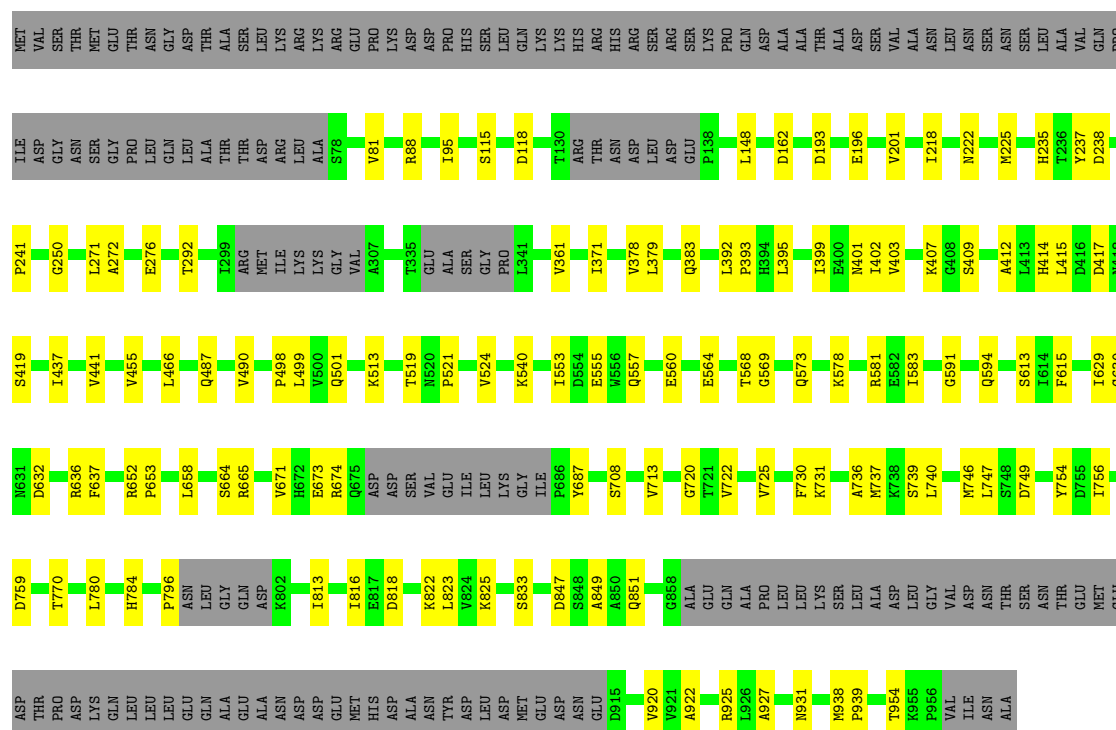




- Molecule 12: U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein

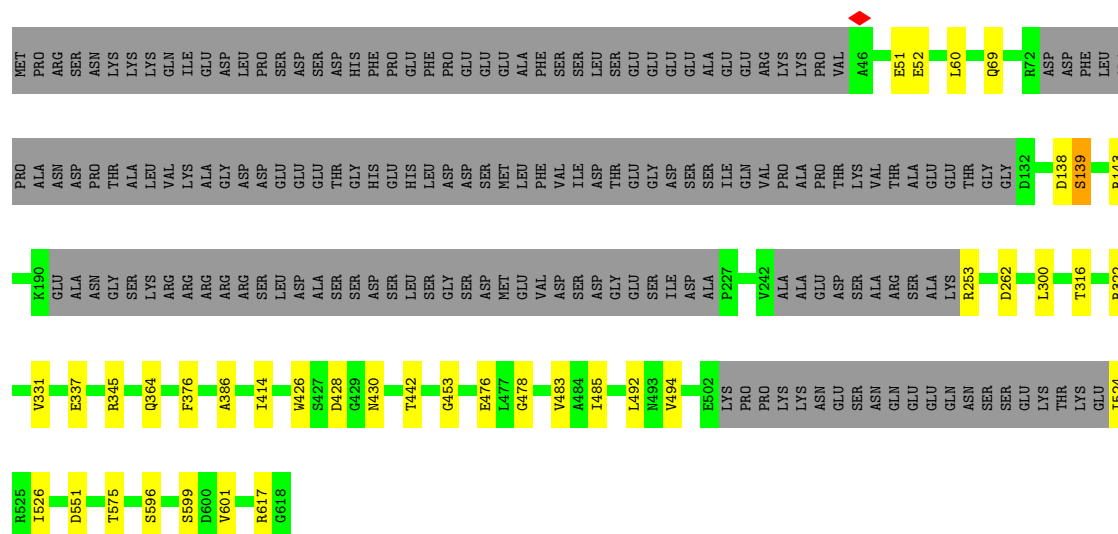


- Molecule 13: UTP17



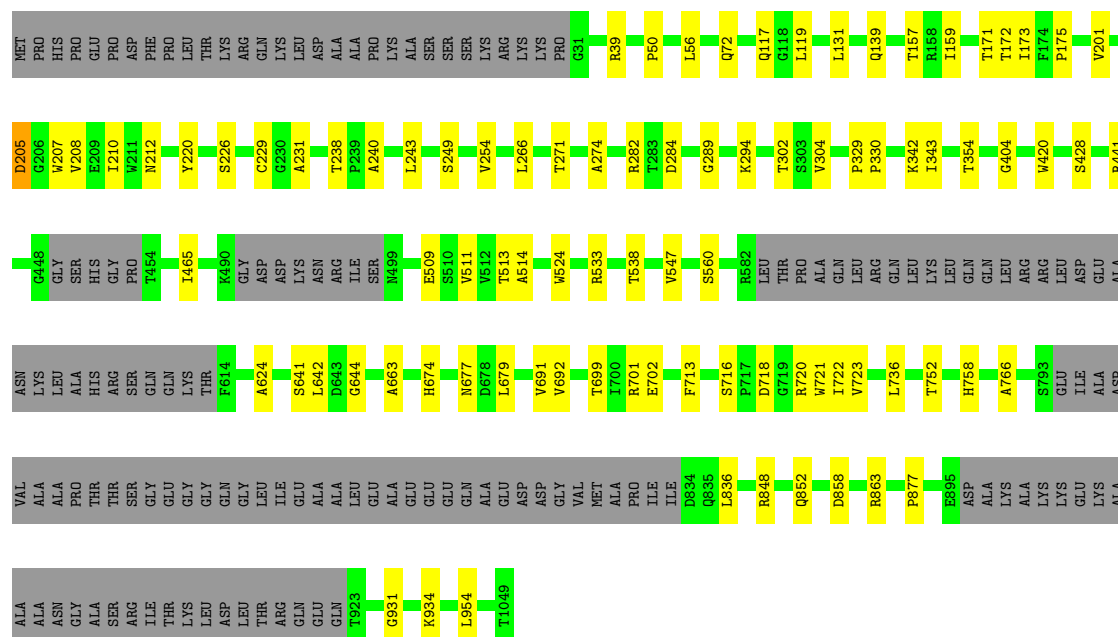
- Molecule 14: UTP18





• Molecule 15: Putative U3 snoRNP protein

Chain UU: 78% 8% 13%



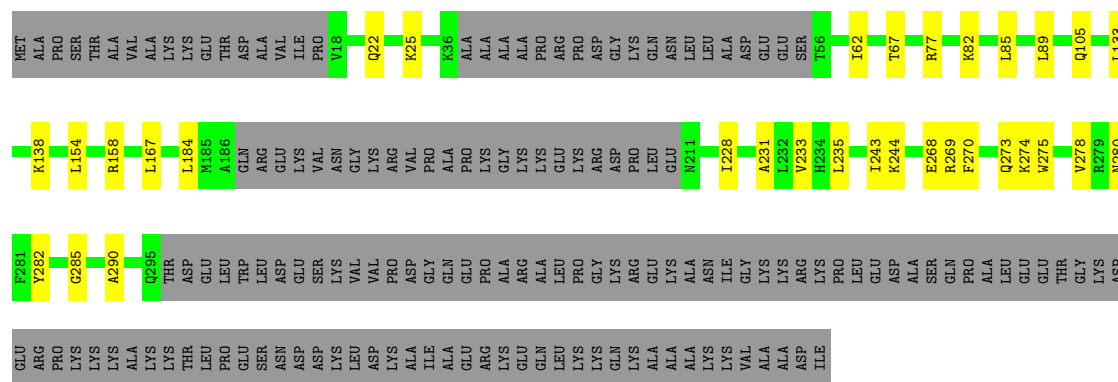
• Molecule 16: UTP24

Chain UX: 88% 10% 2%



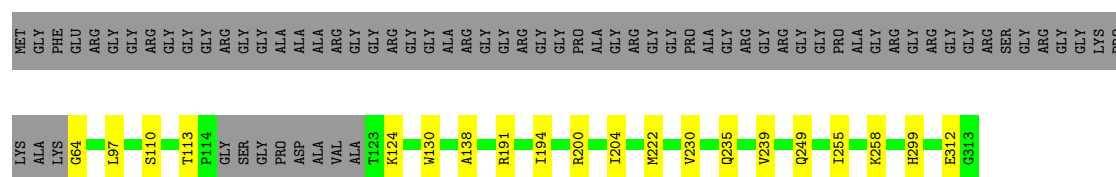
• Molecule 17: Ribosome biogenesis protein C8F11.04

Chain UZ: 52% 8% 40%



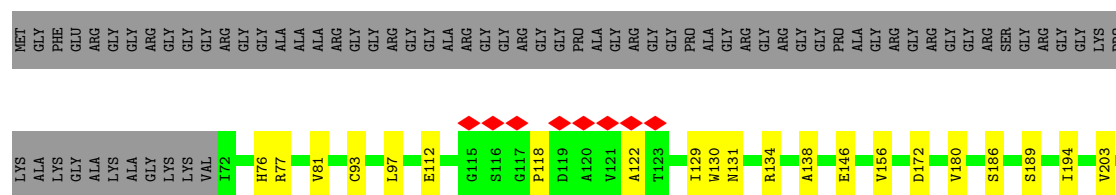
• Molecule 18: rRNA 2'-O-methyltransferase fibrillar

Chain CA: 71% 6% 23%



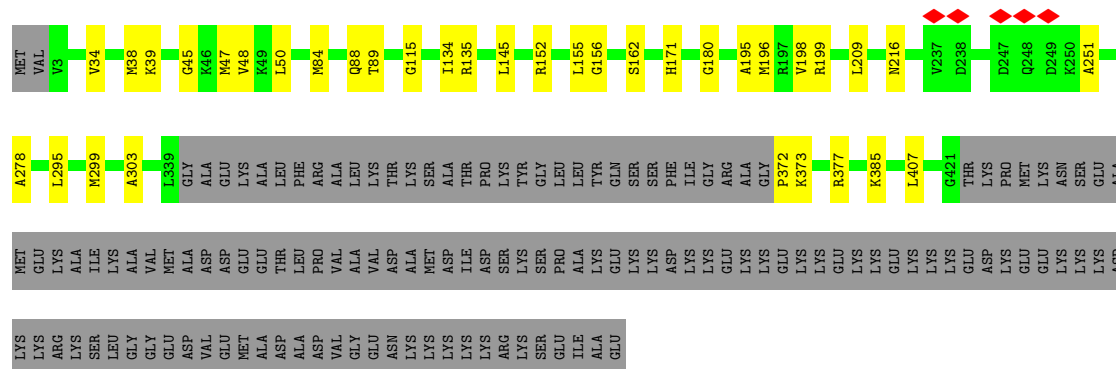
• Molecule 18: rRNA 2'-O-methyltransferase fibrillar

Chain CB: 65% 10% 24%



• Molecule 19: Nucleolar protein 56

Chain CC: 67% 7% 26%



Chain CD: 

| CD Type | Percentage | Amino Acid                                                                                                                                                                                                                                                                                                                                                 |
|---------|------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 64%     | 64%        | M1, P2, L3, F4, G12, L15, K17, A18, L24, L33, L36, I39, I40, K41, K44, A49, K50, F51, V69, L73, L77, N78, E79, L80, K85, V86, I99, L102, L118, I122, R123, L126, M133, E134, L154, S157, P158, M164                                                                                                                                                        |
| 12%     | 12%        | E178, V181, V210, L212, A213, L214, G215, A220, E227, I228, I233, K238, A239, A240, S244, M245, D253, Y254, I257, A261, V262, Q263, V264, R281, P287, I293, V297, H304, Q320, I321, L322, L328, Y341, G342, I343, Y345, I361                                                                                                                               |
| 23%     | 23%        | A391, N403, N404, L405, R406, M422, R438, G446, LEU, ALA, THR, THR, THR, MET, SER, LYS, SER, LEU, LEU, SER, LYS, LYS, PHE, THR, LYS, SER, SER, LYS, LEU, GLU, GLU, GLY, ILE, GLY, ILE, GLU, VAL, PRO, ILE, LYS, PRO, VAL, GLY, MET, LYS, ASP, ALA, SER, VAL, GLY, LYS, LYS, ASP, GLY, GLU, ASP, ALA, LYS, ALA, LYS, GLU, THR, PRO, VAL, LYS, SER, LYS, SER |

Chain CE: 

Chain CF:  80% 14% 6%

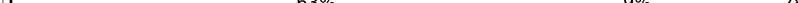
| Amino Acid | Chain CF (%) |
|------------|--------------|
| MET        | 0            |
| SER        | 0            |
| ASN        | 0            |
| ASN        | 0            |
| ASN        | 0            |
| GLU        | 0            |
| SER        | 0            |
| A7         | 80           |
| L21        | 14           |
| Q27        | 14           |
| Y31        | 14           |
| R32        | 14           |
| Q33        | 14           |
| L34        | 14           |
| K35        | 14           |
| E40        | 14           |
| E40        | 14           |
| V63        | 14           |
| H67        | 14           |
| P78        | 14           |
| Y79        | 14           |
| V101       | 14           |
| M106       | 14           |
| L111       | 14           |
| L118       | 14           |
| R119       | 14           |
| D120       | 14           |
| K121       | 14           |
| L124       | 14           |
| L125       | 14           |
| A126       | 14           |
| MET        | 6            |

[illegible]

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

Chain CH:  83% 11% 5%

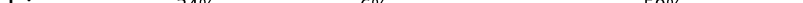
- Molecule 24: Bms1-type G domain-containing protein

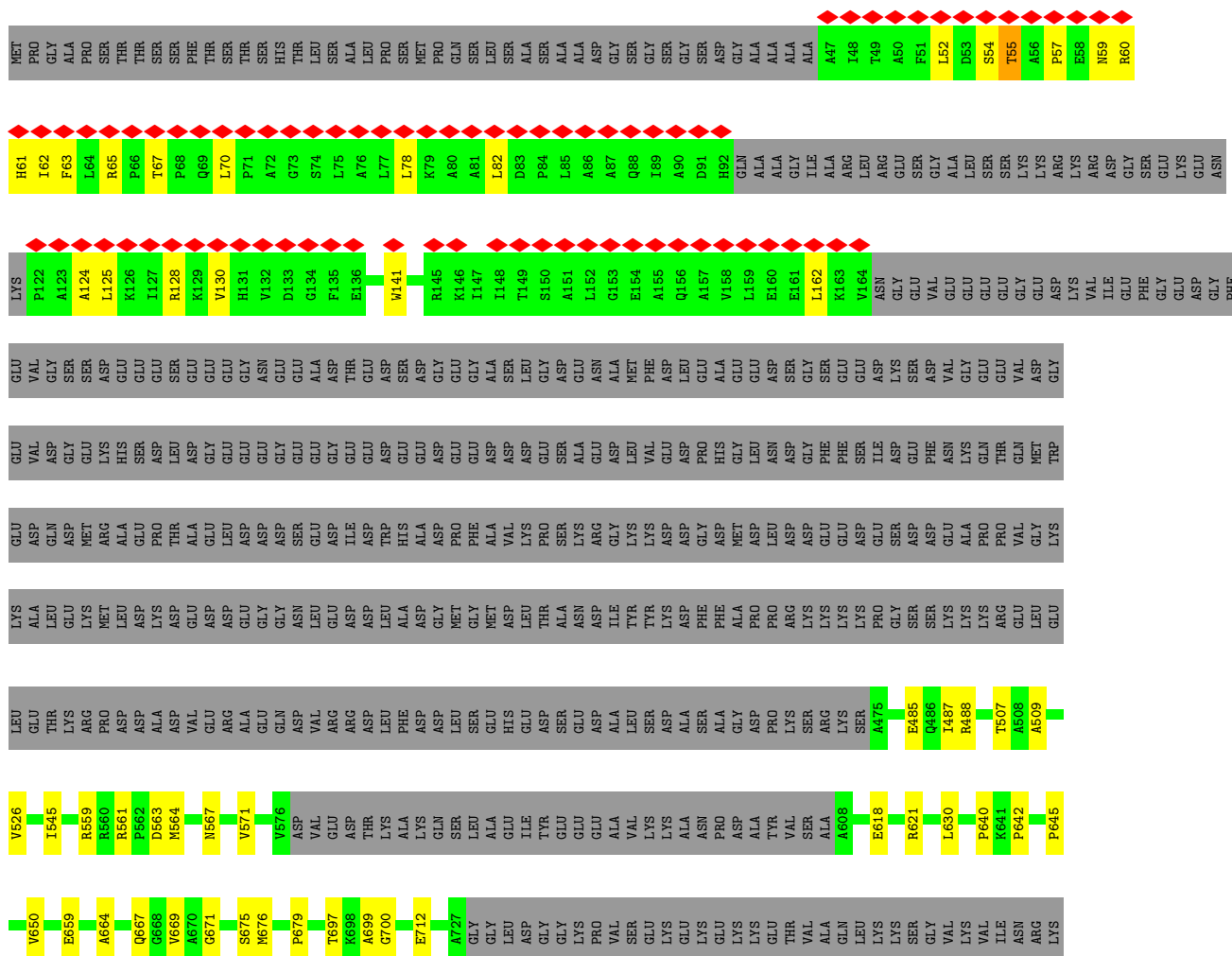
Chain CI: 

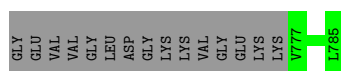
- Molecule 25: U3 small nucleolar ribonucleoprotein protein IMP3

|     |    |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |     |     |     |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|
| MET | V2 | I33 | M37 | I38 | Y44 | R49 | L50 | R72 | E75 | S89 | T102 | V103 | S104 | R108 | V113 | V114 | M115 | M120 | I170 | F180 | GLU | LEU | LEU |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|

- |      |      |
|------|------|
| R1   | V243 |
| R9   | T269 |
| K40  | M270 |
| P41  | V280 |
| R53  | Q286 |
| I73  | T288 |
| D74  | F297 |
| D75  |      |
| E76  |      |
| D85  |      |
| V88  |      |
| L89  |      |
| S93  |      |
| R94  |      |
| L100 |      |
| K105 |      |
| R108 |      |
| A114 |      |
| T115 |      |
| L116 |      |
| L117 |      |
| T123 |      |
| D126 |      |
| A131 |      |
| Q132 |      |
| R135 |      |
| I139 |      |
| T140 |      |
| E144 |      |
| T153 |      |
| H159 |      |
| G160 |      |
| S165 |      |
| R215 |      |
| N220 |      |
| T229 |      |

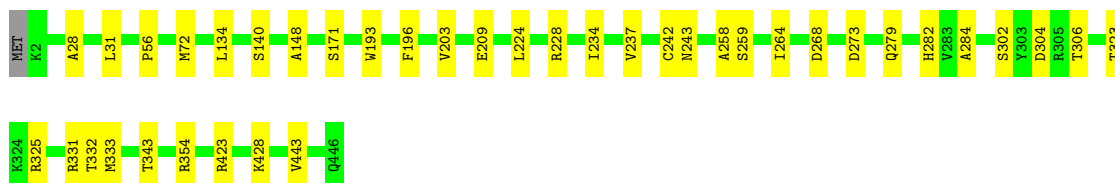
- Chain CL: 





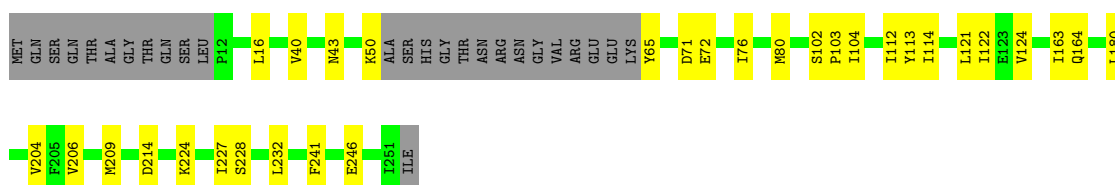
- Molecule 28: DDB1- and CUL4-associated factor 13

Chain CM: 91% 9%



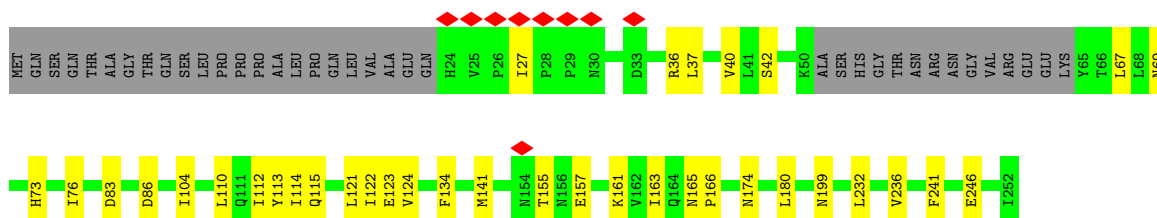
- Molecule 29: Nucleolar essential protein 1

Chain CN: 77% 12% 10%



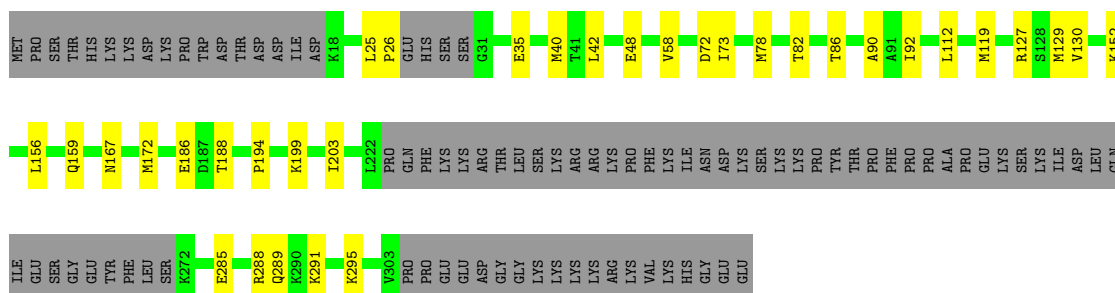
- Molecule 29: Nucleolar essential protein 1

Chain CO: 71% 14% 15%



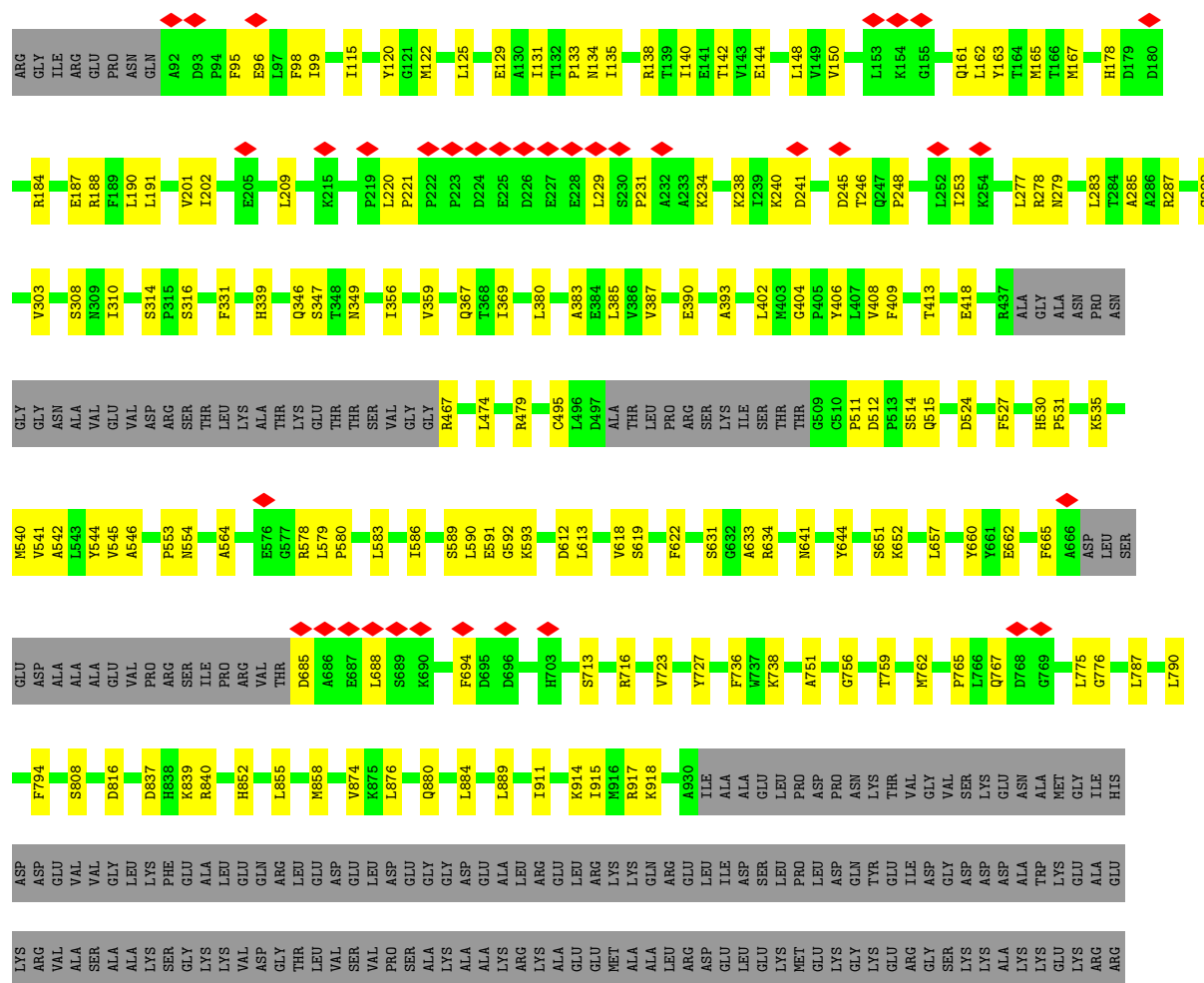
- Molecule 30: KRR1 small subunit processome component

Chain CP: 62% 11% 28%



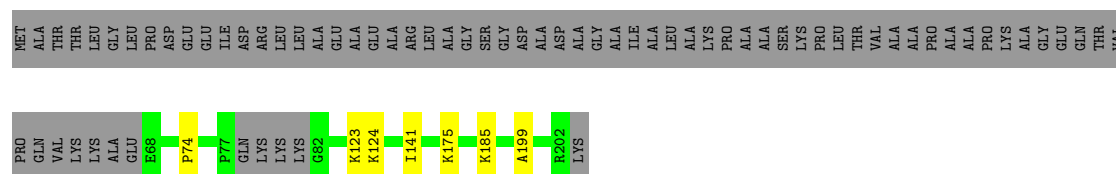
- Molecule 31: Pre-rRNA-processing protein PNO1





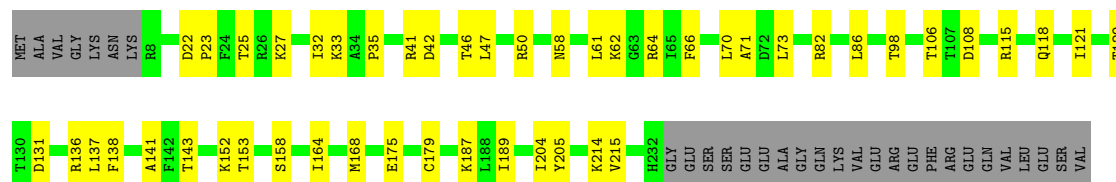
- Molecule 33: Fcf2 pre-rRNA processing C-terminal domain-containing protein

Chain CT: 61% 35%



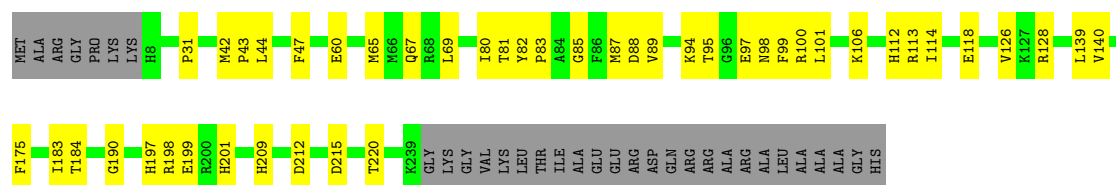
- Molecule 34: Small ribosomal subunit protein eS1

Chain Ca: 69% 19% 12%



- Molecule 35: 40S ribosomal protein S4

Chain Cb: 



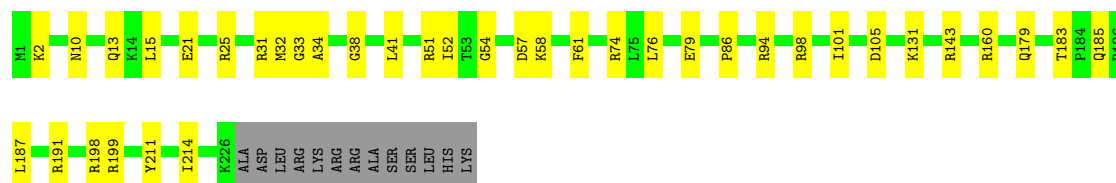
- Molecule 36: 40S ribosomal protein s5-like protein

Chain Cc: 



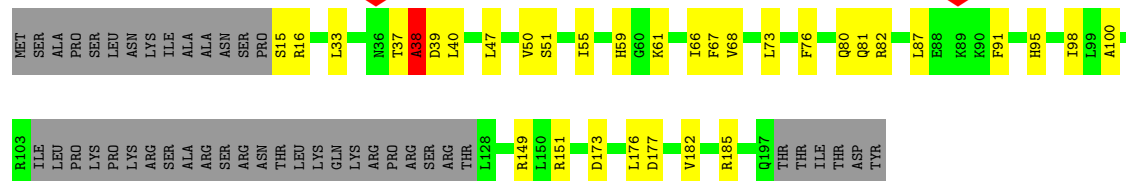
- Molecule 37: 40S ribosomal protein S6

Chain Cd: 



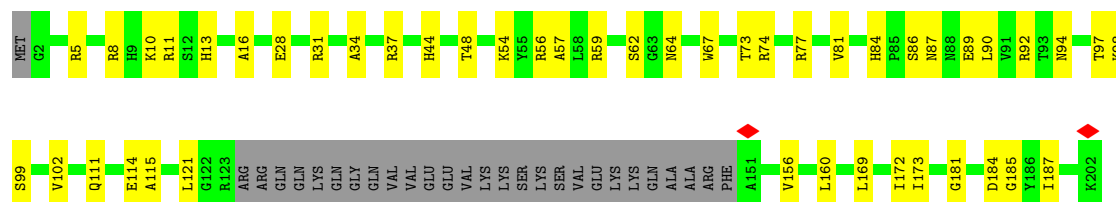
- Molecule 38: 40S ribosomal protein S7

Chain Ce: 



- Molecule 39: 40S ribosomal protein S8

Chain Cf: 



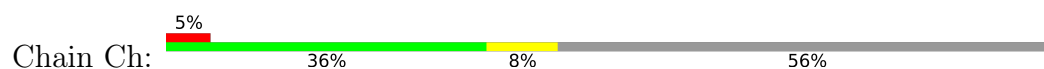
- Molecule 40: 40S ribosomal protein s9-like protein

Chain Cg: 





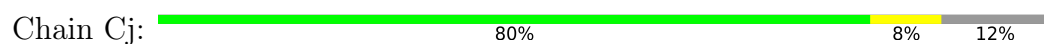
- Molecule 41: 40S ribosomal protein S13-like protein



- Molecule 42: 40S ribosomal protein S14-like protein



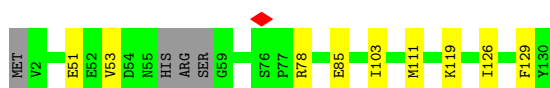
- Molecule 43: 40S ribosomal protein S16-like protein



- Molecule 44: 40S ribosomal protein S11-like protein

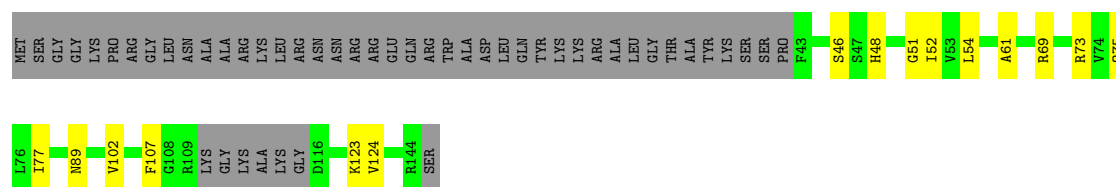


- Molecule 45: 40S ribosomal protein S22-like protein



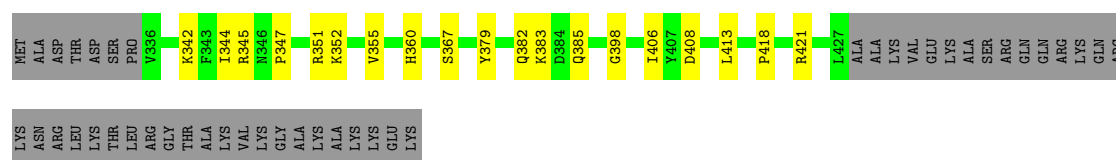
- Molecule 46: 40S ribosomal protein s23-like protein

Chain Cn:  56% 10% 34%



- Molecule 47: Small ribosomal subunit protein eS24

Chain Co:  54% 14% 32%



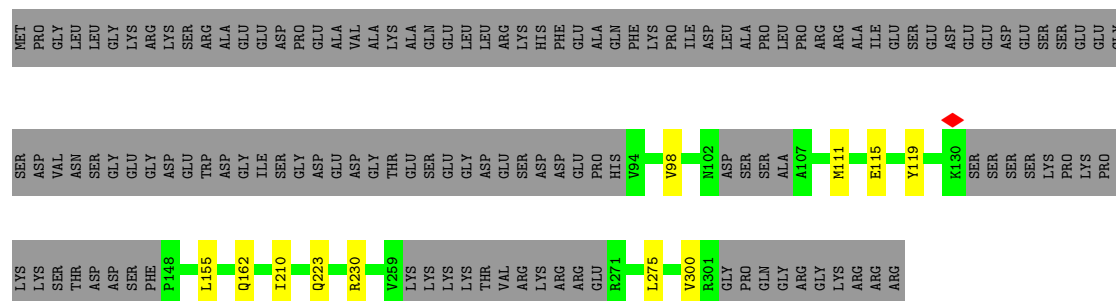
- Molecule 48: 40S ribosomal protein S28-like protein

Chain Cp:  84% 6% 10%



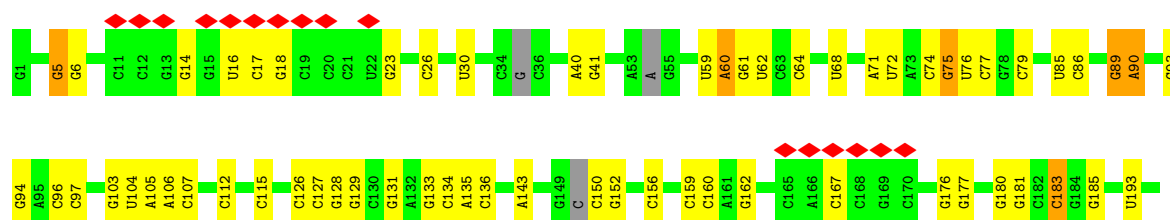
- Molecule 49: Faf1

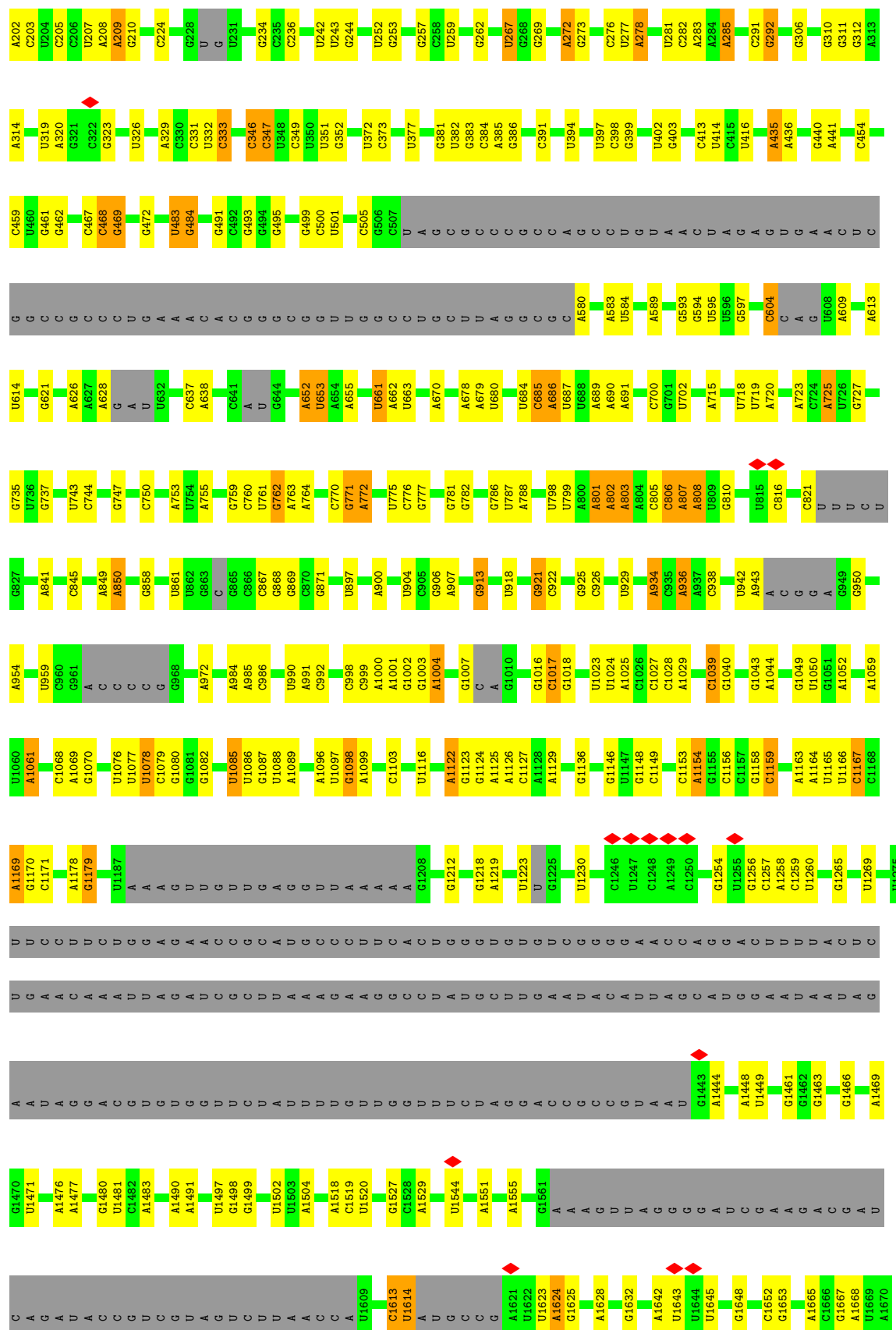
Chain CU:  53% 0% 43%



- Molecule 50: 35s rna

Chain C1:  47% 18% 33%

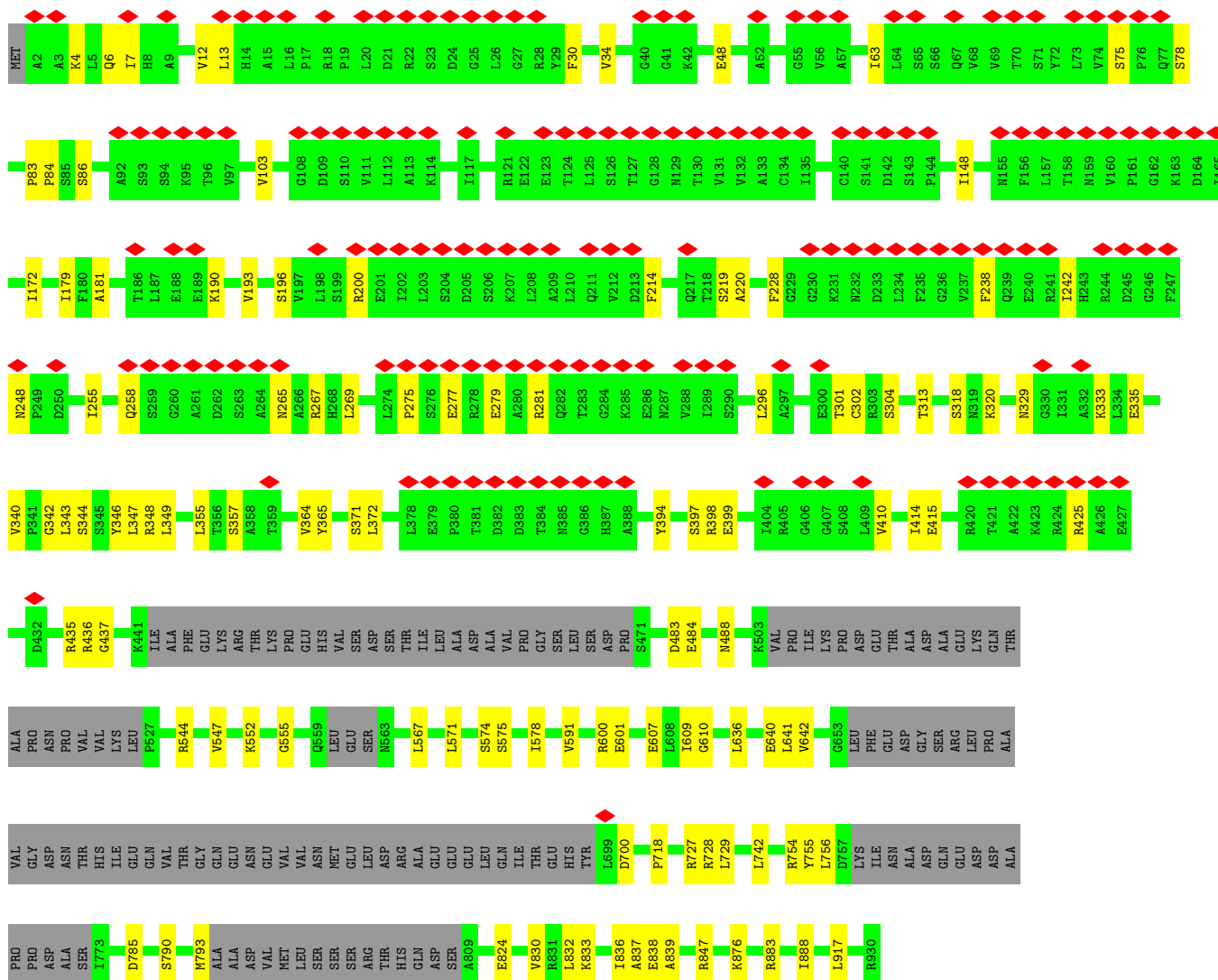




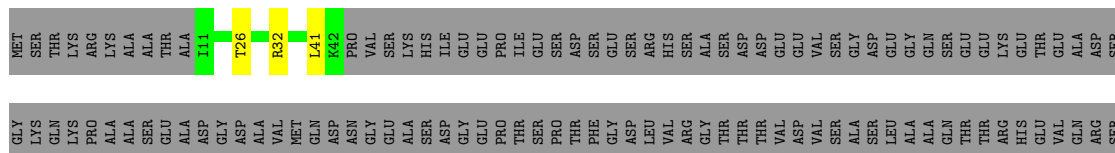
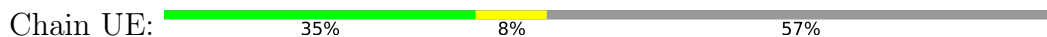


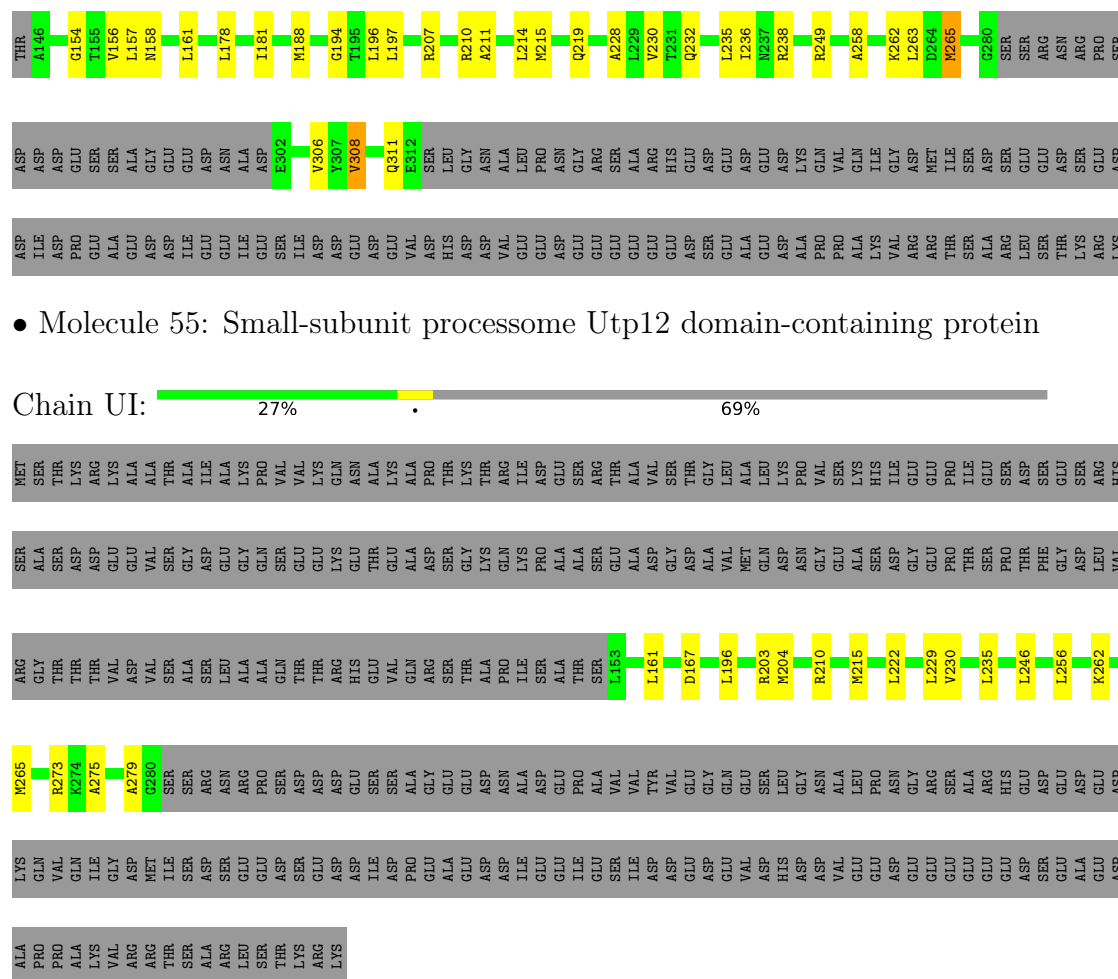




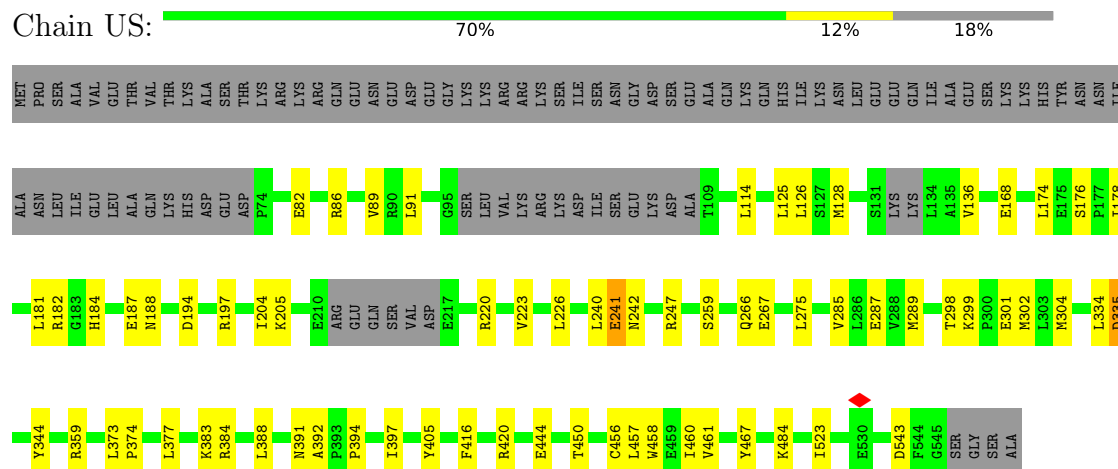


- Molecule 55: Small-subunit processome Utp12 domain-containing protein



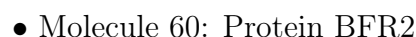


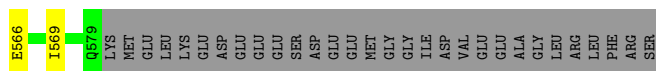
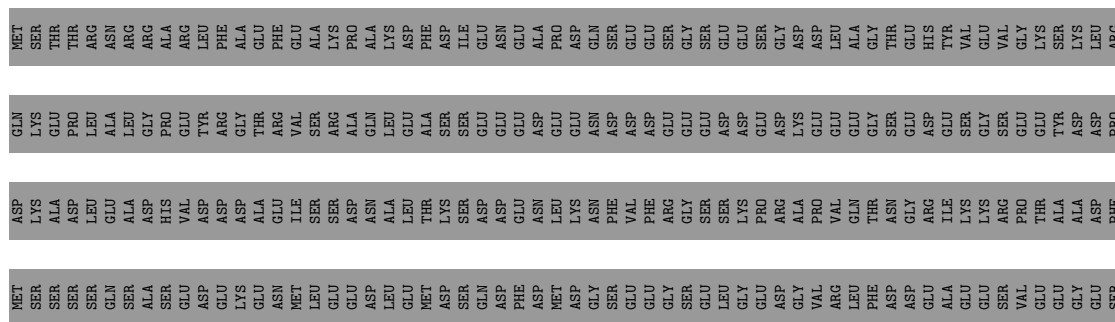
- Molecule 56: CCAAT-binding factor domain-containing protein



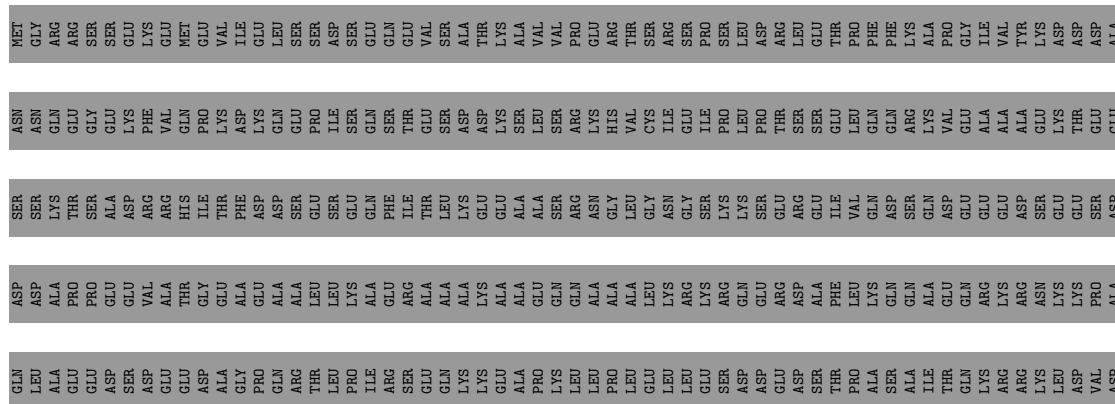
- Molecule 57: Putative ribosomal protein

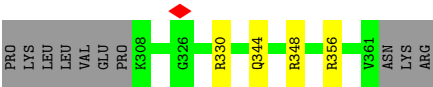






Chain UP:  14% : 85%





## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 356806                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE; Relion                    | Depositor |
| Microscope                           | TFS KRIOS                       | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 44                              | Depositor |
| Minimum defocus (nm)                 | 1000                            | Depositor |
| Maximum defocus (nm)                 | 2500                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)   | Depositor |
| Maximum map value                    | 0.637                           | Depositor |
| Minimum map value                    | -0.257                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.011                           | Depositor |
| Recommended contour level            | 0.02                            | Depositor |
| Map size ( $\text{\AA}$ )            | 501.59998, 501.59998, 501.59998 | wwPDB     |
| Map dimensions                       | 480, 480, 480                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.045, 1.045, 1.045             | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SEP, ZN, MG, OMC, A2M, GTP

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | UA    | 0.31         | 0/6555      | 0.61        | 1/8909 (0.0%)  |
| 2   | UB    | 0.22         | 0/4592      | 0.50        | 0/6178         |
| 3   | UC    | 0.23         | 0/1661      | 0.51        | 1/2228 (0.0%)  |
| 4   | UD    | 0.22         | 0/6250      | 0.47        | 0/8465         |
| 5   | UF    | 0.26         | 0/2665      | 0.51        | 0/3606         |
| 6   | UG    | 0.31         | 0/3838      | 0.60        | 0/5181         |
| 7   | UJ    | 0.27         | 0/12800     | 0.67        | 4/17357 (0.0%) |
| 8   | UK    | 0.27         | 0/1709      | 0.47        | 0/2261         |
| 9   | UL    | 0.23         | 0/6299      | 0.53        | 2/8531 (0.0%)  |
| 10  | UM    | 0.19         | 0/6680      | 0.48        | 1/9090 (0.0%)  |
| 11  | UN    | 0.27         | 0/1425      | 0.53        | 0/1913         |
| 12  | UO    | 0.26         | 0/3895      | 0.53        | 0/5302         |
| 13  | UQ    | 0.23         | 0/6136      | 0.50        | 0/8348         |
| 14  | UR    | 0.28         | 0/3557      | 0.54        | 0/4805         |
| 15  | UU    | 0.29         | 0/6947      | 0.61        | 4/9452 (0.0%)  |
| 16  | UX    | 0.30         | 0/1503      | 0.59        | 0/2022         |
| 17  | UZ    | 0.22         | 0/1857      | 0.56        | 0/2526         |
| 18  | CA    | 0.30         | 0/1814      | 0.59        | 0/2456         |
| 18  | CB    | 0.21         | 0/1853      | 0.50        | 0/2511         |
| 19  | CC    | 0.26         | 0/2911      | 0.51        | 0/3937         |
| 20  | CD    | 0.24         | 0/3412      | 0.54        | 1/4617 (0.0%)  |
| 21  | CE    | 0.28         | 0/891       | 0.54        | 0/1214         |
| 21  | CF    | 0.25         | 0/876       | 0.53        | 2/1195 (0.2%)  |
| 22  | CG    | 0.21         | 0/3307      | 0.52        | 0/4462         |
| 23  | CH    | 0.25         | 0/2939      | 0.52        | 3/3988 (0.1%)  |
| 24  | CI    | 0.25         | 0/6813      | 0.53        | 3/9182 (0.0%)  |
| 25  | CJ    | 0.34         | 0/1462      | 0.59        | 0/1967         |
| 26  | CK    | 0.32         | 0/2376      | 0.59        | 0/3214         |
| 27  | CL    | 0.26         | 0/2504      | 0.53        | 0/3377         |
| 28  | CM    | 0.29         | 0/3573      | 0.58        | 0/4829         |
| 29  | CN    | 0.26         | 0/1797      | 0.50        | 0/2443         |
| 29  | CO    | 0.20         | 0/1714      | 0.48        | 0/2325         |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5          |
| 30  | CP    | 0.26         | 0/1923   | 0.58        | 1/2577 (0.0%)    |
| 31  | CQ    | 0.22         | 0/1436   | 0.53        | 0/1932           |
| 32  | CR    | 0.21         | 0/6809   | 0.53        | 2/9215 (0.0%)    |
| 32  | CS    | 0.19         | 0/6722   | 0.53        | 2/9099 (0.0%)    |
| 33  | CT    | 0.24         | 0/1053   | 0.48        | 0/1413           |
| 34  | Ca    | 0.23         | 0/1850   | 0.49        | 0/2486           |
| 35  | Cb    | 0.20         | 0/1890   | 0.54        | 0/2548           |
| 36  | Cc    | 0.27         | 0/1485   | 0.53        | 0/2008           |
| 37  | Cd    | 0.20         | 0/1850   | 0.45        | 0/2474           |
| 38  | Ce    | 0.28         | 0/1298   | 0.76        | 4/1750 (0.2%)    |
| 39  | Cf    | 0.19         | 0/1429   | 0.49        | 0/1915           |
| 40  | Cg    | 0.28         | 0/1265   | 0.53        | 0/1694           |
| 41  | Ch    | 0.18         | 0/557    | 0.42        | 0/749            |
| 42  | Ci    | 0.21         | 0/819    | 0.49        | 0/1107           |
| 43  | Cj    | 0.30         | 0/958    | 0.58        | 0/1293           |
| 44  | Ck    | 0.14         | 0/1107   | 0.38        | 0/1486           |
| 45  | Cm    | 0.23         | 0/1001   | 0.50        | 0/1345           |
| 46  | Cn    | 0.28         | 0/712    | 0.50        | 0/954            |
| 47  | Co    | 0.23         | 0/754    | 0.72        | 2/1011 (0.2%)    |
| 48  | Cp    | 0.26         | 0/461    | 0.52        | 0/620            |
| 49  | CU    | 0.22         | 0/1350   | 0.47        | 0/1810           |
| 50  | C1    | 0.21         | 0/37474  | 0.31        | 0/58363          |
| 51  | C2    | 0.23         | 0/5434   | 0.32        | 0/8459           |
| 52  | CW    | 0.18         | 0/3004   | 0.50        | 0/4085           |
| 53  | UT    | 0.25         | 0/16312  | 0.64        | 11/22073 (0.0%)  |
| 54  | UH    | 0.18         | 0/6301   | 0.47        | 0/8526           |
| 55  | UE    | 0.25         | 0/1374   | 0.57        | 1/1852 (0.1%)    |
| 55  | UI    | 0.22         | 0/1005   | 0.54        | 0/1352           |
| 56  | US    | 0.25         | 0/3765   | 0.59        | 3/5100 (0.1%)    |
| 57  | Cl    | 0.23         | 0/638    | 0.59        | 0/857            |
| 58  | CX    | 0.24         | 0/2180   | 0.67        | 2/2956 (0.1%)    |
| 59  | CY    | 0.21         | 0/2111   | 0.50        | 0/2816           |
| 60  | CZ    | 0.21         | 0/2298   | 0.57        | 2/3080 (0.1%)    |
| 61  | UP    | 0.20         | 0/428    | 0.49        | 0/570            |
| All | All   | 0.24         | 0/235664 | 0.51        | 52/327466 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | UA    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | UG    | 0                   | 2                   |
| 15  | UU    | 0                   | 1                   |
| 16  | UX    | 0                   | 1                   |
| 17  | UZ    | 0                   | 1                   |
| 20  | CD    | 0                   | 1                   |
| 22  | CG    | 0                   | 1                   |
| 26  | CK    | 0                   | 1                   |
| 27  | CL    | 0                   | 1                   |
| 28  | CM    | 0                   | 1                   |
| 29  | CO    | 0                   | 1                   |
| 31  | CQ    | 0                   | 1                   |
| 32  | CR    | 0                   | 1                   |
| 38  | Ce    | 0                   | 1                   |
| 53  | UT    | 0                   | 3                   |
| 55  | UE    | 0                   | 1                   |
| 57  | CI    | 0                   | 1                   |
| 58  | CX    | 0                   | 1                   |
| All | All   | 0                   | 21                  |

There are no bond length outliers.

All (52) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 24  | CI    | 753  | ASN  | CA-C-N   | 8.11  | 137.03      | 121.54   |
| 24  | CI    | 753  | ASN  | C-N-CA   | 8.11  | 137.03      | 121.54   |
| 38  | Ce    | 38   | ALA  | CA-C-N   | 6.58  | 133.55      | 121.70   |
| 38  | Ce    | 38   | ALA  | C-N-CA   | 6.58  | 133.55      | 121.70   |
| 7   | UJ    | 1401 | LEU  | CA-CB-CG | 6.21  | 138.03      | 116.30   |
| 7   | UJ    | 1617 | ILE  | N-CA-C   | -6.14 | 106.52      | 112.29   |
| 23  | CH    | 120  | LEU  | CA-C-N   | 6.08  | 127.70      | 120.09   |
| 23  | CH    | 120  | LEU  | C-N-CA   | 6.08  | 127.70      | 120.09   |
| 56  | US    | 335  | ASP  | CA-C-N   | 6.06  | 139.61      | 122.21   |
| 56  | US    | 335  | ASP  | C-N-CA   | 6.06  | 139.61      | 122.21   |
| 21  | CF    | 67   | HIS  | CA-C-N   | 6.06  | 124.06      | 120.24   |
| 21  | CF    | 67   | HIS  | C-N-CA   | 6.06  | 124.06      | 120.24   |
| 53  | UT    | 1802 | ILE  | CA-C-N   | -5.89 | 112.65      | 120.96   |
| 53  | UT    | 1802 | ILE  | C-N-CA   | -5.89 | 112.65      | 120.96   |
| 20  | CD    | 233  | ILE  | N-CA-C   | -5.88 | 104.59      | 111.00   |
| 58  | CX    | 268  | MET  | CA-C-N   | -5.79 | 117.30      | 122.97   |
| 58  | CX    | 268  | MET  | C-N-CA   | -5.79 | 117.30      | 122.97   |
| 24  | CI    | 183  | LYS  | CA-CB-CG | 5.58  | 125.27      | 114.10   |
| 3   | UC    | 609  | GLU  | N-CA-CB  | 5.58  | 118.41      | 110.16   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23  | CH    | 90   | ASN  | N-CA-C   | -5.52 | 107.80      | 114.75   |
| 9   | UL    | 853  | THR  | CA-C-N   | 5.48  | 123.69      | 120.24   |
| 9   | UL    | 853  | THR  | C-N-CA   | 5.48  | 123.69      | 120.24   |
| 53  | UT    | 553  | GLU  | N-CA-CB  | 5.46  | 118.74      | 110.28   |
| 60  | CZ    | 565  | GLU  | CA-C-N   | 5.46  | 131.96      | 121.54   |
| 60  | CZ    | 565  | GLU  | C-N-CA   | 5.46  | 131.96      | 121.54   |
| 53  | UT    | 612  | ARG  | CA-C-N   | 5.41  | 130.26      | 121.83   |
| 53  | UT    | 612  | ARG  | C-N-CA   | 5.41  | 130.26      | 121.83   |
| 53  | UT    | 1917 | GLU  | N-CA-CB  | 5.39  | 118.63      | 110.28   |
| 53  | UT    | 479  | LEU  | CA-CB-CG | 5.36  | 135.06      | 116.30   |
| 56  | US    | 82   | GLU  | N-CA-CB  | 5.35  | 118.55      | 110.30   |
| 30  | CP    | 289  | GLN  | N-CA-CB  | 5.28  | 118.43      | 110.30   |
| 15  | UU    | 171  | THR  | CA-C-N   | 5.24  | 128.67      | 121.33   |
| 15  | UU    | 171  | THR  | C-N-CA   | 5.24  | 128.67      | 121.33   |
| 15  | UU    | 641  | SER  | CA-C-N   | 5.24  | 129.07      | 120.63   |
| 15  | UU    | 641  | SER  | C-N-CA   | 5.24  | 129.07      | 120.63   |
| 32  | CR    | 157  | THR  | CA-C-N   | 5.24  | 131.55      | 121.54   |
| 32  | CR    | 157  | THR  | C-N-CA   | 5.24  | 131.55      | 121.54   |
| 47  | Co    | 379  | TYR  | CA-C-N   | 5.17  | 131.41      | 121.54   |
| 47  | Co    | 379  | TYR  | C-N-CA   | 5.17  | 131.41      | 121.54   |
| 55  | UE    | 308  | VAL  | N-CA-C   | -5.17 | 107.67      | 112.43   |
| 32  | CS    | 619  | SER  | CA-C-N   | -5.16 | 110.65      | 121.64   |
| 32  | CS    | 619  | SER  | C-N-CA   | -5.16 | 110.65      | 121.64   |
| 53  | UT    | 2193 | GLU  | N-CA-CB  | 5.16  | 118.24      | 110.30   |
| 1   | UA    | 254  | ASN  | N-CA-C   | 5.15  | 116.97      | 111.36   |
| 53  | UT    | 830  | GLU  | N-CA-CB  | 5.12  | 117.73      | 110.16   |
| 7   | UJ    | 1557 | THR  | CA-C-N   | -5.11 | 112.56      | 122.06   |
| 7   | UJ    | 1557 | THR  | C-N-CA   | -5.11 | 112.56      | 122.06   |
| 38  | Ce    | 81   | GLN  | CA-C-N   | 5.08  | 131.25      | 121.54   |
| 38  | Ce    | 81   | GLN  | C-N-CA   | 5.08  | 131.25      | 121.54   |
| 10  | UM    | 580  | GLY  | N-CA-C   | 5.05  | 118.65      | 110.87   |
| 53  | UT    | 677  | LEU  | CA-C-N   | 5.00  | 132.21      | 123.91   |
| 53  | UT    | 677  | LEU  | C-N-CA   | 5.00  | 132.21      | 123.91   |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 20  | CD    | 157 | SER  | Peptide |
| 22  | CG    | 178 | VAL  | Peptide |
| 26  | CK    | 93  | SER  | Peptide |
| 27  | CL    | 55  | THR  | Peptide |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 28  | CM    | 140  | SER  | Peptide   |
| 29  | CO    | 165  | ASN  | Peptide   |
| 31  | CQ    | 83   | ARG  | Peptide   |
| 32  | CR    | 729  | LEU  | Peptide   |
| 58  | CX    | 373  | LYS  | Peptide   |
| 38  | Ce    | 38   | ALA  | Peptide   |
| 57  | Cl    | 25   | LYS  | Peptide   |
| 1   | UA    | 645  | ALA  | Mainchain |
| 55  | UE    | 265  | MET  | Peptide   |
| 6   | UG    | 388  | TRP  | Peptide   |
| 6   | UG    | 578  | ILE  | Peptide   |
| 53  | UT    | 1516 | LEU  | Peptide   |
| 53  | UT    | 1566 | GLU  | Peptide   |
| 53  | UT    | 2233 | ARG  | Sidechain |
| 15  | UU    | 205  | ASP  | Peptide   |
| 16  | UX    | -2   | ARG  | Sidechain |
| 17  | UZ    | 273  | GLN  | 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   | UA    | 6411  | 0        | 6306     | 55      | 0            |
| 2   | UB    | 4506  | 0        | 4633     | 43      | 0            |
| 3   | UC    | 1633  | 0        | 1696     | 19      | 0            |
| 4   | UD    | 6108  | 0        | 6108     | 74      | 0            |
| 5   | UF    | 2599  | 0        | 2650     | 17      | 0            |
| 6   | UG    | 3765  | 0        | 3800     | 26      | 0            |
| 7   | UJ    | 12592 | 0        | 12889    | 213     | 0            |
| 8   | UK    | 1695  | 0        | 1828     | 14      | 0            |
| 9   | UL    | 6175  | 0        | 6188     | 70      | 0            |
| 10  | UM    | 6545  | 0        | 6547     | 78      | 0            |
| 11  | UN    | 1401  | 0        | 1455     | 9       | 0            |
| 12  | UO    | 3811  | 0        | 3861     | 53      | 0            |
| 13  | UQ    | 6008  | 0        | 6033     | 77      | 0            |
| 14  | UR    | 3495  | 0        | 3506     | 30      | 0            |
| 15  | UU    | 6778  | 0        | 6782     | 56      | 0            |
| 16  | UX    | 1480  | 0        | 1554     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | UZ    | 1815  | 0        | 1896     | 17      | 0            |
| 18  | CA    | 1778  | 0        | 1830     | 14      | 0            |
| 18  | CB    | 1816  | 0        | 1847     | 20      | 0            |
| 19  | CC    | 2866  | 0        | 2960     | 27      | 0            |
| 20  | CD    | 3355  | 0        | 3483     | 44      | 0            |
| 21  | CE    | 879   | 0        | 918      | 10      | 0            |
| 21  | CF    | 864   | 0        | 900      | 9       | 0            |
| 22  | CG    | 3245  | 0        | 3262     | 43      | 0            |
| 23  | CH    | 2888  | 0        | 2979     | 34      | 0            |
| 24  | CI    | 6666  | 0        | 6825     | 69      | 0            |
| 25  | CJ    | 1434  | 0        | 1482     | 12      | 0            |
| 26  | CK    | 2329  | 0        | 2373     | 30      | 0            |
| 27  | CL    | 2466  | 0        | 2532     | 40      | 0            |
| 28  | CM    | 3501  | 0        | 3498     | 22      | 0            |
| 29  | CN    | 1762  | 0        | 1807     | 20      | 0            |
| 29  | CO    | 1683  | 0        | 1726     | 19      | 0            |
| 30  | CP    | 1893  | 0        | 1993     | 22      | 0            |
| 31  | CQ    | 1413  | 0        | 1479     | 14      | 0            |
| 32  | CR    | 6677  | 0        | 6809     | 91      | 0            |
| 32  | CS    | 6591  | 0        | 6674     | 118     | 0            |
| 33  | CT    | 1035  | 0        | 1063     | 7       | 0            |
| 34  | Ca    | 1821  | 0        | 1936     | 33      | 0            |
| 35  | Cb    | 1851  | 0        | 1905     | 32      | 0            |
| 36  | Cc    | 1464  | 0        | 1504     | 12      | 0            |
| 37  | Cd    | 1819  | 0        | 1920     | 28      | 0            |
| 38  | Ce    | 1279  | 0        | 1322     | 21      | 0            |
| 39  | Cf    | 1398  | 0        | 1401     | 33      | 0            |
| 40  | Cg    | 1248  | 0        | 1365     | 6       | 0            |
| 41  | Ch    | 546   | 0        | 580      | 7       | 0            |
| 42  | Ci    | 808   | 0        | 831      | 12      | 0            |
| 43  | Cj    | 943   | 0        | 1002     | 7       | 0            |
| 44  | Ck    | 1082  | 0        | 1138     | 10      | 0            |
| 45  | Cm    | 985   | 0        | 1021     | 6       | 0            |
| 46  | Cn    | 702   | 0        | 750      | 9       | 0            |
| 47  | Co    | 741   | 0        | 785      | 12      | 0            |
| 48  | Cp    | 458   | 0        | 489      | 3       | 0            |
| 49  | CU    | 1337  | 0        | 1376     | 9       | 0            |
| 50  | C1    | 33584 | 0        | 17007    | 173     | 0            |
| 51  | C2    | 4869  | 0        | 2465     | 24      | 0            |
| 52  | CW    | 2932  | 0        | 2866     | 48      | 0            |
| 53  | UT    | 15998 | 0        | 16397    | 280     | 0            |
| 54  | UH    | 6198  | 0        | 6272     | 78      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55  | UE    | 1362   | 0        | 1440     | 30      | 0            |
| 55  | UI    | 996    | 0        | 1054     | 17      | 0            |
| 56  | US    | 3672   | 0        | 3679     | 38      | 0            |
| 57  | CI    | 633    | 0        | 676      | 10      | 0            |
| 58  | CX    | 2130   | 0        | 2219     | 36      | 0            |
| 59  | CY    | 2095   | 0        | 2185     | 38      | 0            |
| 60  | CZ    | 2270   | 0        | 2273     | 40      | 0            |
| 61  | UP    | 422    | 0        | 457      | 4       | 0            |
| 62  | UX    | 1      | 0        | 0        | 0       | 0            |
| 63  | CI    | 32     | 0        | 12       | 0       | 0            |
| 64  | CI    | 1      | 0        | 0        | 0       | 0            |
| 65  | CS    | 27     | 0        | 11       | 2       | 0            |
| All | All   | 227662 | 0        | 212510   | 2265    | 0            |

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

All (2265) 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) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:UD:441:THR:HA    | 4:UD:456:LEU:O      | 1.31                     | 1.24              |
| 12:UO:333:HIS:HA   | 12:UO:346:ARG:O     | 1.49                     | 1.11              |
| 54:UH:555:GLY:O    | 54:UH:567:LEU:HA    | 1.55                     | 1.06              |
| 15:UU:159:ILE:O    | 15:UU:172:THR:HA    | 1.61                     | 1.00              |
| 14:UR:485:ILE:O    | 14:UR:492:LEU:HA    | 1.66                     | 0.95              |
| 38:Ce:76:PHE:O     | 38:Ce:80:GLN:HB2    | 1.65                     | 0.95              |
| 12:UO:335:ALA:HA   | 12:UO:344:SER:O     | 1.67                     | 0.95              |
| 22:CG:176:VAL:HA   | 22:CG:184:TYR:O     | 1.70                     | 0.91              |
| 47:Co:360:HIS:O    | 47:Co:398:GLY:HA2   | 1.72                     | 0.90              |
| 29:CO:121:LEU:HB3  | 29:CO:163:ILE:O     | 1.73                     | 0.86              |
| 14:UR:483:VAL:O    | 14:UR:494:VAL:HA    | 1.76                     | 0.85              |
| 37:Cd:34:ALA:O     | 37:Cd:51:ARG:HA     | 1.78                     | 0.84              |
| 53:UT:1143:ARG:O   | 53:UT:1147:ASN:HB2  | 1.83                     | 0.78              |
| 53:UT:1759:SER:HB2 | 53:UT:1800:VAL:HG21 | 1.66                     | 0.77              |
| 23:CH:269:GLN:N    | 23:CH:269:GLN:HE21  | 1.83                     | 0.76              |
| 29:CN:121:LEU:HB3  | 29:CN:163:ILE:O     | 1.86                     | 0.75              |
| 2:UB:43:GLN:N      | 2:UB:43:GLN:HE21    | 1.85                     | 0.75              |
| 32:CS:188:ARG:NH1  | 32:CS:527:PHE:O     | 2.20                     | 0.75              |
| 15:UU:238:THR:HG22 | 15:UU:240:ALA:H     | 1.52                     | 0.74              |
| 22:CG:221:LYS:N    | 51:C2:180:U:HO2'    | 1.85                     | 0.74              |
| 32:CR:851:TYR:HA   | 32:CR:854:VAL:HG12  | 1.70                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:Cb:98:ASN:HB2   | 35:Cb:114:ILE:O    | 1.89                     | 0.73              |
| 50:C1:661:U:H3     | 53:UT:801:CYS:HG   | 1.35                     | 0.73              |
| 1:UA:706:PHE:O     | 15:UU:677:ASN:ND2  | 2.22                     | 0.72              |
| 7:UJ:1600:LEU:HD23 | 7:UJ:1646:LEU:HB3  | 1.69                     | 0.72              |
| 16:UX:1:ALA:HB1    | 25:CJ:37:MET:HE1   | 1.71                     | 0.72              |
| 5:UF:157:MET:HE3   | 5:UF:188:TRP:HB2   | 1.71                     | 0.72              |
| 12:UO:274:LYS:HE2  | 56:US:335:ASP:HB3  | 1.71                     | 0.72              |
| 1:UA:316:ALA:O     | 1:UA:320:GLY:O     | 2.09                     | 0.71              |
| 12:UO:181:ARG:NH1  | 12:UO:219:ALA:O    | 2.23                     | 0.71              |
| 20:CD:133:MET:HE3  | 20:CD:134:GLU:H    | 1.54                     | 0.71              |
| 32:CS:855:LEU:HA   | 32:CS:858:MET:HG2  | 1.72                     | 0.71              |
| 26:CK:53:ARG:HD3   | 49:CU:210:ILE:HG21 | 1.70                     | 0.71              |
| 50:C1:60:A:H62     | 54:UH:876:LYS:HA   | 1.55                     | 0.71              |
| 1:UA:364:ILE:HG12  | 1:UA:399:THR:HG21  | 1.73                     | 0.71              |
| 32:CS:738:LYS:HE2  | 32:CS:808:SER:HB3  | 1.73                     | 0.70              |
| 59:CY:106:LYS:HG2  | 60:CZ:433:ASN:HB2  | 1.71                     | 0.70              |
| 12:UO:104:CYS:O    | 12:UO:116:ALA:HA   | 1.91                     | 0.70              |
| 53:UT:453:ILE:O    | 53:UT:457:TRP:HB3  | 1.91                     | 0.70              |
| 60:CZ:301:SER:OG   | 60:CZ:305:ARG:NH1  | 2.25                     | 0.70              |
| 8:UK:268:ARG:HE    | 21:CE:95:SER:HB3   | 1.56                     | 0.70              |
| 54:UH:267:ARG:HH12 | 54:UH:302:CYS:HB2  | 1.55                     | 0.70              |
| 21:CF:33:GLN:HG3   | 21:CF:106:ASN:HD22 | 1.56                     | 0.70              |
| 52:CW:40:GLU:O     | 52:CW:44:ASN:HB2   | 1.92                     | 0.70              |
| 42:CI:29:VAL:HG12  | 42:CI:93:HIS:HB2   | 1.74                     | 0.69              |
| 59:CY:318:ALA:HA   | 59:CY:321:ILE:HD12 | 1.74                     | 0.69              |
| 39:Cf:87:ASN:HB2   | 39:Cf:90:LEU:HG    | 1.74                     | 0.69              |
| 15:UU:863:ARG:NH2  | 27:CL:664:ALA:O    | 2.25                     | 0.69              |
| 54:UH:832:LEU:HD11 | 55:UI:215:MET:HG2  | 1.73                     | 0.69              |
| 56:US:285:VAL:O    | 56:US:289:MET:HB2  | 1.93                     | 0.69              |
| 7:UJ:1023:LEU:HA   | 7:UJ:1026:VAL:HG12 | 1.74                     | 0.69              |
| 7:UJ:505:CYS:SG    | 7:UJ:557:ARG:NH2   | 2.66                     | 0.68              |
| 30:CP:119:MET:HE3  | 30:CP:172:MET:HG2  | 1.75                     | 0.68              |
| 54:UH:267:ARG:HB2  | 54:UH:296:LEU:O    | 1.93                     | 0.68              |
| 57:Cl:80:LYS:HD3   | 57:Cl:81:ILE:H     | 1.58                     | 0.68              |
| 7:UJ:1023:LEU:HD22 | 7:UJ:1074:SER:HB3  | 1.76                     | 0.68              |
| 58:CX:267:GLU:HA   | 58:CX:271:LEU:HD23 | 1.76                     | 0.68              |
| 24:CI:920:LEU:HD12 | 24:CI:989:LEU:HD23 | 1.74                     | 0.68              |
| 50:C1:1122:A:H5'   | 50:C1:1127:C:H41   | 1.59                     | 0.68              |
| 9:UL:19:SER:OG     | 9:UL:43:ALA:O      | 2.12                     | 0.68              |
| 18:CB:156:VAL:HG12 | 18:CB:225:VAL:HB   | 1.75                     | 0.68              |
| 15:UU:718:ASP:HB3  | 15:UU:720:ARG:HG3  | 1.75                     | 0.67              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 32:CR:23:LYS:O      | 32:CR:146:GLY:N     | 2.27                     | 0.67              |
| 38:Ce:51:SER:HB3    | 38:Ce:67:PHE:HB2    | 1.75                     | 0.67              |
| 39:Cf:67:TRP:HB2    | 39:Cf:187:ILE:HD12  | 1.76                     | 0.67              |
| 27:CL:52:LEU:O      | 27:CL:55:THR:C      | 2.37                     | 0.67              |
| 9:UL:890:VAL:HA     | 10:UM:891:MET:HG2   | 1.74                     | 0.67              |
| 26:CK:132:GLN:O     | 26:CK:135:ARG:NH1   | 2.24                     | 0.67              |
| 56:US:194:ASP:OD1   | 56:US:197:ARG:NH2   | 2.26                     | 0.67              |
| 26:CK:117:LEU:HD11  | 43:Cj:126:PRO:HG2   | 1.77                     | 0.67              |
| 32:CS:511:PRO:HG2   | 32:CS:583:LEU:HD21  | 1.77                     | 0.67              |
| 53:UT:1512:LEU:O    | 53:UT:1516:LEU:HB2  | 1.94                     | 0.67              |
| 4:UD:479:LEU:HA     | 61:UP:330:ARG:HH12  | 1.59                     | 0.67              |
| 13:UQ:401:ASN:HB2   | 13:UQ:414:HIS:HB3   | 1.76                     | 0.67              |
| 60:CZ:494:PHE:HA    | 60:CZ:497:LEU:HG    | 1.74                     | 0.67              |
| 31:CQ:111:LEU:HD21  | 31:CQ:136:LEU:HA    | 1.76                     | 0.67              |
| 35:Cb:67:GLN:HG3    | 35:Cb:69:LEU:HD13   | 1.76                     | 0.66              |
| 58:CX:422:ARG:HH12  | 58:CX:453:LEU:HD22  | 1.60                     | 0.66              |
| 29:CO:112:ILE:HB    | 29:CO:124:VAL:HB    | 1.78                     | 0.66              |
| 39:Cf:16:ALA:HB2    | 50:C1:938:C:H5"     | 1.78                     | 0.66              |
| 50:C1:2168:U:H3     | 50:C1:2194:A:H2     | 1.43                     | 0.66              |
| 32:CR:291:LYS:HD3   | 32:CR:411:ALA:HB1   | 1.78                     | 0.66              |
| 59:CY:52:LEU:HD21   | 60:CZ:328:ARG:HD2   | 1.78                     | 0.66              |
| 13:UQ:581:ARG:HH12  | 13:UQ:613:SER:HB3   | 1.61                     | 0.66              |
| 53:UT:1211:VAL:HG11 | 53:UT:1263:ILE:HG22 | 1.78                     | 0.66              |
| 32:CS:187:GLU:OE1   | 32:CS:188:ARG:NH1   | 2.29                     | 0.66              |
| 9:UL:589:VAL:HB     | 9:UL:603:LEU:HB2    | 1.78                     | 0.65              |
| 26:CK:108:ARG:HG3   | 26:CK:116:ARG:HB2   | 1.78                     | 0.65              |
| 7:UJ:812:ARG:HD2    | 7:UJ:815:LYS:HE3    | 1.78                     | 0.65              |
| 7:UJ:1783:ARG:NH1   | 53:UT:49:HIS:O      | 2.29                     | 0.65              |
| 15:UU:238:THR:HB    | 15:UU:243:LEU:O     | 1.96                     | 0.65              |
| 6:UG:270:ASN:ND2    | 6:UG:461:LEU:O      | 2.30                     | 0.65              |
| 9:UL:835:GLN:HE21   | 9:UL:870:ASN:HD22   | 1.45                     | 0.65              |
| 15:UU:226:SER:HG    | 15:UU:229:CYS:HG    | 1.43                     | 0.65              |
| 50:C1:950:G:H1      | 50:C1:959:U:H3      | 1.42                     | 0.65              |
| 18:CA:130:TRP:HE3   | 18:CA:138:ALA:HB2   | 1.61                     | 0.65              |
| 32:CS:592:GLY:HA3   | 32:CS:631:SER:HA    | 1.78                     | 0.65              |
| 39:Cf:99:SER:N      | 39:Cf:173:ILE:O     | 2.28                     | 0.65              |
| 53:UT:1490:ILE:HA   | 53:UT:1505:ILE:HD11 | 1.79                     | 0.65              |
| 1:UA:445:ILE:HA     | 1:UA:470:PRO:HB3    | 1.78                     | 0.65              |
| 12:UO:554:VAL:HA    | 55:UE:230:VAL:HG13  | 1.78                     | 0.65              |
| 20:CD:361:ILE:HG13  | 20:CD:405:LEU:HD13  | 1.79                     | 0.65              |
| 59:CY:43:VAL:HB     | 60:CZ:418:ARG:HH12  | 1.61                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:UQ:466:LEU:HB3   | 13:UQ:833:SER:HB2   | 1.77                     | 0.64              |
| 32:CR:790:LEU:HA    | 32:CR:794:PHE:HB2   | 1.78                     | 0.64              |
| 1:UA:408:ALA:HB3    | 1:UA:418:ARG:HB2    | 1.80                     | 0.64              |
| 24:CI:282:GLN:HE22  | 24:CI:767:GLN:HE22  | 1.43                     | 0.64              |
| 1:UA:448:PHE:HB2    | 26:CK:135:ARG:HH21  | 1.62                     | 0.64              |
| 4:UD:19:VAL:HG12    | 4:UD:46:ILE:HG12    | 1.78                     | 0.64              |
| 53:UT:1633:TRP:HB3  | 53:UT:1636:ARG:HD3  | 1.79                     | 0.64              |
| 22:CG:110:LYS:NZ    | 59:CY:324:LEU:O     | 2.29                     | 0.64              |
| 13:UQ:652:ARG:HD3   | 13:UQ:653:PRO:HD2   | 1.80                     | 0.64              |
| 37:CD:79:GLU:HG2    | 37:CD:86:PRO:HG3    | 1.78                     | 0.64              |
| 32:CR:248:PRO:HB3   | 32:CR:334:LEU:HD11  | 1.80                     | 0.64              |
| 53:UT:176:SER:HB2   | 53:UT:217:LYS:HG3   | 1.77                     | 0.64              |
| 58:CX:422:ARG:HH22  | 58:CX:453:LEU:HD13  | 1.62                     | 0.64              |
| 61:UP:344:GLN:OE1   | 61:UP:348:ARG:NH1   | 2.31                     | 0.64              |
| 7:UJ:1727:LEU:HA    | 7:UJ:1730:LEU:HG    | 1.79                     | 0.64              |
| 20:CD:122:ILE:O     | 20:CD:126:LEU:HB2   | 1.98                     | 0.64              |
| 32:CR:593:LYS:HG2   | 32:CR:631:SER:HB3   | 1.80                     | 0.64              |
| 29:CO:123:GLU:HB3   | 29:CO:161:LYS:HB2   | 1.78                     | 0.64              |
| 34:Ca:136:ARG:NH2   | 50:C1:1469:A:OP1    | 2.31                     | 0.64              |
| 32:CR:814:MET:HE1   | 32:CR:821:PRO:HD3   | 1.79                     | 0.63              |
| 48:Cp:13:VAL:O      | 48:Cp:52:ASN:N      | 2.31                     | 0.63              |
| 53:UT:442:ARG:HE    | 53:UT:480:PRO:HD3   | 1.63                     | 0.63              |
| 54:UH:371:SER:HA    | 54:UH:437:GLY:HA2   | 1.80                     | 0.63              |
| 26:CK:286:GLN:HE21  | 27:CL:526:VAL:HG12  | 1.63                     | 0.63              |
| 56:US:178:ILE:HG22  | 56:US:181:LEU:H     | 1.62                     | 0.63              |
| 60:CZ:456:GLN:O     | 60:CZ:460:SER:HB2   | 1.98                     | 0.63              |
| 9:UL:712:VAL:HG12   | 9:UL:722:VAL:HG22   | 1.80                     | 0.63              |
| 59:CY:17:SER:O      | 60:CZ:330:ARG:NH1   | 2.32                     | 0.63              |
| 24:CI:536:PRO:HB2   | 24:CI:537:TRP:HD1   | 1.62                     | 0.63              |
| 32:CR:283:LEU:HD11  | 32:CR:474:LEU:HG    | 1.79                     | 0.63              |
| 50:C1:68:U:H3       | 54:UH:883:ARG:HH21  | 1.47                     | 0.63              |
| 58:CX:371:LEU:HD21  | 58:CX:417:PHE:HB2   | 1.80                     | 0.63              |
| 7:UJ:1657:CYS:HA    | 7:UJ:1660:HIS:CE1   | 2.34                     | 0.63              |
| 9:UL:451:ILE:HB     | 9:UL:461:ARG:HB2    | 1.81                     | 0.63              |
| 15:UU:858:ASP:OD1   | 31:CQ:254:ARG:NH2   | 2.32                     | 0.62              |
| 50:C1:954:A:N3      | 59:CY:320:ARG:NH1   | 2.46                     | 0.62              |
| 53:UT:777:PRO:HA    | 53:UT:844:ARG:HH21  | 1.63                     | 0.62              |
| 53:UT:1649:ARG:HH22 | 53:UT:1764:ILE:HG23 | 1.65                     | 0.62              |
| 4:UD:651:THR:O      | 4:UD:654:LYS:N      | 2.32                     | 0.62              |
| 21:CE:63:SER:HA     | 21:CE:66:LEU:HB2    | 1.81                     | 0.62              |
| 53:UT:2065:ARG:O    | 53:UT:2105:ARG:NH2  | 2.32                     | 0.62              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:UJ:1770:LEU:HD21  | 7:UJ:1778:VAL:HG22 | 1.81                     | 0.62              |
| 28:CM:268:ASP:OD2   | 50:C1:580:A:N6     | 2.32                     | 0.62              |
| 32:CS:162:LEU:HA    | 32:CS:165:MET:HG3  | 1.81                     | 0.62              |
| 54:UH:833:LYS:HB3   | 55:UI:246:LEU:HB3  | 1.81                     | 0.62              |
| 2:UB:6:LEU:HB2      | 26:CK:243:VAL:HG21 | 1.80                     | 0.62              |
| 24:CI:519:TRP:O     | 24:CI:526:ARG:NH2  | 2.32                     | 0.62              |
| 34:Ca:143:THR:HG23  | 34:Ca:205:TYR:HE2  | 1.65                     | 0.62              |
| 53:UT:1157:ARG:HH12 | 53:UT:1198:PRO:HB2 | 1.64                     | 0.62              |
| 56:US:86:ARG:HA     | 56:US:89:VAL:HG12  | 1.80                     | 0.62              |
| 32:CS:512:ASP:HB3   | 32:CS:515:GLN:HE21 | 1.63                     | 0.62              |
| 7:UJ:1316:ILE:O     | 7:UJ:1325:LYS:NZ   | 2.31                     | 0.62              |
| 7:UJ:1499:TYR:HA    | 7:UJ:1502:ILE:HG22 | 1.80                     | 0.62              |
| 32:CR:834:THR:HG23  | 32:CR:837:ASP:H    | 1.65                     | 0.62              |
| 35:Cb:87:MET:N      | 35:Cb:101:LEU:O    | 2.32                     | 0.62              |
| 50:C1:929:U:O4      | 60:CZ:537:ARG:NH1  | 2.33                     | 0.62              |
| 53:UT:282:MET:O     | 53:UT:334:GLN:NE2  | 2.32                     | 0.62              |
| 32:CS:874:VAL:HG12  | 32:CS:918:LYS:HZ2  | 1.64                     | 0.62              |
| 39:Cf:111:GLN:NE2   | 53:UT:1082:GLU:O   | 2.32                     | 0.62              |
| 10:UM:277:LEU:HD21  | 10:UM:280:VAL:HG13 | 1.82                     | 0.62              |
| 29:CN:112:ILE:HB    | 29:CN:124:VAL:HB   | 1.81                     | 0.62              |
| 32:CS:402:LEU:O     | 32:CS:406:TYR:OH   | 2.18                     | 0.62              |
| 56:US:174:LEU:HD13  | 56:US:223:VAL:HG12 | 1.82                     | 0.62              |
| 10:UM:271:MET:HE2   | 10:UM:273:ARG:HH22 | 1.65                     | 0.62              |
| 26:CK:9:ARG:HH22    | 26:CK:270:MET:HE3  | 1.65                     | 0.62              |
| 53:UT:437:ASN:HB3   | 53:UT:440:ARG:HH21 | 1.64                     | 0.62              |
| 32:CR:243:LEU:HD21  | 32:CR:249:ILE:HG23 | 1.81                     | 0.61              |
| 42:Ci:44:THR:HG22   | 42:Ci:51:THR:HA    | 1.81                     | 0.61              |
| 50:C1:115:C:OP2     | 55:UE:207:ARG:NH1  | 2.33                     | 0.61              |
| 58:CX:390:LEU:HD11  | 58:CX:432:ALA:HB1  | 1.81                     | 0.61              |
| 7:UJ:1229:GLU:HG2   | 7:UJ:1279:LEU:HD21 | 1.81                     | 0.61              |
| 9:UL:94:LEU:HB2     | 9:UL:104:VAL:HG12  | 1.82                     | 0.61              |
| 8:UK:68:MET:HG3     | 51:C2:58:A:H4'     | 1.80                     | 0.61              |
| 5:UF:77:ARG:NH1     | 14:UR:52:GLU:OE2   | 2.33                     | 0.61              |
| 7:UJ:1203:LYS:HG3   | 7:UJ:1207:MET:HE1  | 1.83                     | 0.61              |
| 10:UM:335:LEU:HD11  | 10:UM:343:LEU:HB3  | 1.81                     | 0.61              |
| 21:CF:106:ASN:HD21  | 21:CF:111:LEU:HD23 | 1.66                     | 0.61              |
| 24:CI:819:ARG:NH1   | 24:CI:823:HIS:O    | 2.33                     | 0.61              |
| 28:CM:332:THR:HG22  | 28:CM:343:THR:HG22 | 1.82                     | 0.61              |
| 35:Cb:126:VAL:HG13  | 35:Cb:139:LEU:HD11 | 1.81                     | 0.61              |
| 55:UE:161:LEU:HD21  | 55:UE:196:LEU:HB2  | 1.83                     | 0.61              |
| 4:UD:33:LYS:HG3     | 4:UD:36:LEU:HD12   | 1.82                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:UL:534:PHE:HB2   | 9:UL:560:ARG:HB2   | 1.81                     | 0.61              |
| 30:CP:127:ARG:NH1  | 30:CP:130:VAL:O    | 2.33                     | 0.61              |
| 50:C1:462:G:N7     | 59:CY:374:ARG:NH1  | 2.48                     | 0.61              |
| 53:UT:149:VAL:HA   | 53:UT:193:LEU:HD11 | 1.82                     | 0.61              |
| 9:UL:509:HIS:HB3   | 9:UL:528:ALA:HB3   | 1.83                     | 0.61              |
| 12:UO:415:ARG:NH2  | 50:C1:131:G:N7     | 2.49                     | 0.61              |
| 20:CD:17:LYS:HB2   | 20:CD:44:LYS:HB2   | 1.83                     | 0.61              |
| 35:Cb:69:LEU:HD21  | 35:Cb:94:LYS:HD3   | 1.82                     | 0.61              |
| 53:UT:324:ARG:NH1  | 53:UT:328:ASP:OD2  | 2.32                     | 0.61              |
| 53:UT:1609:LEU:HB3 | 53:UT:1647:ALA:HB1 | 1.83                     | 0.61              |
| 24:CI:622:THR:HG23 | 24:CI:623:ARG:HG2  | 1.81                     | 0.61              |
| 54:UH:313:THR:OG1  | 54:UH:348:ARG:NH1  | 2.34                     | 0.61              |
| 10:UM:258:LEU:O    | 10:UM:268:GLY:HA3  | 2.01                     | 0.60              |
| 15:UU:159:ILE:HB   | 15:UU:173:ILE:HB   | 1.83                     | 0.60              |
| 4:UD:799:GLU:HA    | 4:UD:802:ARG:HG2   | 1.83                     | 0.60              |
| 5:UF:166:ARG:NH2   | 11:UN:358:GLN:O    | 2.34                     | 0.60              |
| 12:UO:333:HIS:CA   | 12:UO:346:ARG:O    | 2.40                     | 0.60              |
| 24:CI:944:ILE:HD13 | 24:CI:973:PHE:HB3  | 1.83                     | 0.60              |
| 24:CI:1085:ARG:NE  | 50:C1:391:C:OP1    | 2.34                     | 0.60              |
| 56:US:388:LEU:O    | 56:US:392:ALA:HB2  | 2.01                     | 0.60              |
| 7:UJ:150:THR:HG22  | 33:CT:74:PRO:HD3   | 1.82                     | 0.60              |
| 13:UQ:540:LYS:HB2  | 13:UQ:553:ILE:HB   | 1.82                     | 0.60              |
| 16:UX:54:PRO:HB3   | 16:UX:85:ALA:HB1   | 1.83                     | 0.60              |
| 18:CB:76:HIS:HB3   | 18:CB:81:VAL:HG23  | 1.83                     | 0.60              |
| 18:CB:112:GLU:HB2  | 18:CB:122:ALA:HA   | 1.82                     | 0.60              |
| 32:CR:822:THR:OG1  | 32:CR:869:ARG:NH2  | 2.35                     | 0.60              |
| 53:UT:111:ILE:O    | 53:UT:114:HIS:ND1  | 2.34                     | 0.60              |
| 13:UQ:437:ILE:O    | 13:UQ:501:GLN:NE2  | 2.35                     | 0.60              |
| 19:CC:198:VAL:HG21 | 19:CC:278:ALA:HB2  | 1.84                     | 0.60              |
| 20:CD:69:VAL:HG11  | 20:CD:102:LEU:HD11 | 1.83                     | 0.60              |
| 53:UT:462:ASN:HA   | 53:UT:465:LEU:HB2  | 1.84                     | 0.60              |
| 5:UF:285:VAL:HG11  | 11:UN:369:LEU:HB2  | 1.83                     | 0.60              |
| 24:CI:1096:LYS:HE3 | 33:CT:175:LYS:HD2  | 1.83                     | 0.60              |
| 7:UJ:317:GLN:HG2   | 13:UQ:954:THR:HG21 | 1.84                     | 0.60              |
| 7:UJ:810:PHE:HA    | 7:UJ:813:ILE:HG12  | 1.82                     | 0.60              |
| 7:UJ:1288:GLU:HG3  | 7:UJ:1334:LYS:HE2  | 1.83                     | 0.60              |
| 21:CE:21:LEU:HD23  | 21:CE:118:LEU:HD13 | 1.84                     | 0.60              |
| 27:CL:54:SER:O     | 27:CL:59:ASN:ND2   | 2.32                     | 0.60              |
| 32:CS:406:TYR:O    | 32:CS:467:ARG:NH2  | 2.35                     | 0.60              |
| 37:Cd:131:LYS:NZ   | 50:C1:750:C:OP1    | 2.34                     | 0.60              |
| 39:Cf:89:GLU:HA    | 39:Cf:92:ARG:HG2   | 1.83                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:UJ:1284:LEU:HA    | 7:UJ:1287:LEU:HD12 | 1.84                     | 0.60              |
| 20:CD:403:ASN:OD1   | 20:CD:406:ARG:NH2  | 2.35                     | 0.60              |
| 24:CI:843:GLN:HB3   | 24:CI:1002:ASN:HB3 | 1.84                     | 0.60              |
| 51:C2:137:U:H3      | 51:C2:150:G:H1     | 1.50                     | 0.60              |
| 53:UT:107:LEU:HD21  | 53:UT:126:VAL:HG22 | 1.84                     | 0.60              |
| 4:UD:446:SER:HB2    | 4:UD:481:ALA:HB3   | 1.84                     | 0.60              |
| 19:CC:155:LEU:HG    | 20:CD:245:MET:HE1  | 1.84                     | 0.60              |
| 23:CH:152:THR:O     | 23:CH:156:ALA:HB3  | 2.02                     | 0.60              |
| 23:CH:217:ARG:NH2   | 49:CU:119:TYR:OH   | 2.35                     | 0.60              |
| 32:CR:837:ASP:HA    | 32:CR:840:ARG:HD3  | 1.84                     | 0.59              |
| 37:Cd:33:GLY:N      | 37:Cd:52:ILE:O     | 2.35                     | 0.59              |
| 50:C1:761:U:O2      | 50:C1:762:G:N2     | 2.35                     | 0.59              |
| 53:UT:539:LYS:HG2   | 53:UT:587:ARG:HD3  | 1.84                     | 0.59              |
| 53:UT:1154:VAL:HG23 | 53:UT:1157:ARG:HE  | 1.67                     | 0.59              |
| 38:Ce:73:LEU:HD11   | 38:Ce:100:ALA:HB2  | 1.84                     | 0.59              |
| 19:CC:196:MET:SD    | 19:CC:199:ARG:NH2  | 2.76                     | 0.59              |
| 36:Cc:176:THR:OG1   | 36:Cc:179:GLU:OE1  | 2.16                     | 0.59              |
| 53:UT:2153:TRP:NE1  | 53:UT:2193:GLU:OE2 | 2.35                     | 0.59              |
| 7:UJ:1118:PHE:HB3   | 7:UJ:1128:MET:HE2  | 1.83                     | 0.59              |
| 14:UR:253:ARG:HH22  | 14:UR:599:SER:HB2  | 1.68                     | 0.59              |
| 22:CG:575:GLY:N     | 22:CG:606:VAL:O    | 2.35                     | 0.59              |
| 27:CL:712:GLU:OE2   | 50:C1:2222:C:N4    | 2.35                     | 0.59              |
| 9:UL:862:ASN:OD1    | 9:UL:905:ASN:ND2   | 2.36                     | 0.59              |
| 10:UM:400:ILE:HB    | 10:UM:427:ALA:HB3  | 1.83                     | 0.59              |
| 12:UO:417:ARG:NH2   | 50:C1:129:G:O6     | 2.35                     | 0.59              |
| 15:UU:511:VAL:HB    | 15:UU:524:TRP:HB2  | 1.83                     | 0.59              |
| 27:CL:571:VAL:HG21  | 27:CL:645:PRO:HB3  | 1.83                     | 0.59              |
| 52:CW:292:ASN:HB2   | 52:CW:308:ALA:HB3  | 1.84                     | 0.59              |
| 12:UO:417:ARG:HH12  | 50:C1:79:C:H41     | 1.50                     | 0.59              |
| 38:Ce:185:ARG:NH2   | 50:C1:1269:U:OP1   | 2.31                     | 0.59              |
| 52:CW:277:ARG:HH11  | 59:CY:123:ARG:HH21 | 1.50                     | 0.59              |
| 7:UJ:578:ARG:NH1    | 7:UJ:581:GLU:OE1   | 2.36                     | 0.59              |
| 7:UJ:1555:THR:HA    | 7:UJ:1558:HIS:CE1  | 2.38                     | 0.59              |
| 31:CQ:111:LEU:HD23  | 31:CQ:124:LEU:HD12 | 1.84                     | 0.59              |
| 32:CS:134:ASN:OD1   | 32:CS:554:ASN:ND2  | 2.36                     | 0.59              |
| 53:UT:130:ALA:O     | 53:UT:133:LEU:C    | 2.46                     | 0.59              |
| 54:UH:793:MET:SD    | 55:UI:273:ARG:NH1  | 2.75                     | 0.59              |
| 6:UG:283:THR:HG22   | 6:UG:295:LYS:HG2   | 1.85                     | 0.59              |
| 13:UQ:196:GLU:HB3   | 13:UQ:201:VAL:HG22 | 1.83                     | 0.59              |
| 23:CH:131:ARG:NH1   | 23:CH:193:GLU:OE2  | 2.35                     | 0.59              |
| 53:UT:753:MET:HA    | 53:UT:756:VAL:HG12 | 1.83                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:UT:1252:LYS:NZ   | 53:UT:1295:MET:SD   | 2.76                     | 0.59              |
| 58:CX:422:ARG:NH1   | 58:CX:452:GLU:OE1   | 2.32                     | 0.59              |
| 10:UM:344:VAL:HG12  | 10:UM:368:ARG:HG2   | 1.84                     | 0.59              |
| 15:UU:722:ILE:HG12  | 15:UU:736:LEU:HD11  | 1.85                     | 0.59              |
| 32:CR:143:VAL:HG21  | 32:CR:149:VAL:HG22  | 1.84                     | 0.59              |
| 6:UG:241:LYS:HG2    | 6:UG:253:GLU:HG2    | 1.84                     | 0.59              |
| 10:UM:324:SER:HB3   | 10:UM:337:ALA:HB3   | 1.85                     | 0.59              |
| 32:CS:540:MET:O     | 32:CS:544:TYR:HB2   | 2.02                     | 0.59              |
| 37:CD:199:ARG:NH1   | 50:C1:869:G:OP1     | 2.36                     | 0.59              |
| 7:UJ:1534:ARG:HB2   | 7:UJ:1598:TYR:HB3   | 1.84                     | 0.58              |
| 13:UQ:674:ARG:NH2   | 13:UQ:708:SER:O     | 2.36                     | 0.58              |
| 15:UU:289:GLY:HA3   | 15:UU:294:LYS:HD3   | 1.85                     | 0.58              |
| 26:CK:100:LEU:HB2   | 26:CK:144:GLU:HG2   | 1.84                     | 0.58              |
| 29:CN:214:ASP:O     | 29:CN:224:LYS:NZ    | 2.36                     | 0.58              |
| 19:CC:299:MET:HE3   | 19:CC:303:ALA:HB3   | 1.84                     | 0.58              |
| 32:CR:210:PRO:O     | 32:CR:212:SER:N     | 2.36                     | 0.58              |
| 32:CS:283:LEU:HD11  | 32:CS:474:LEU:HG    | 1.84                     | 0.58              |
| 38:Ce:55:ILE:HD11   | 38:Ce:182:VAL:HG22  | 1.84                     | 0.58              |
| 53:UT:208:ALA:O     | 53:UT:212:SER:HB2   | 2.03                     | 0.58              |
| 29:CO:69:ASN:HD22   | 29:CO:134:PHE:HE2   | 1.51                     | 0.58              |
| 32:CR:252:LEU:HB3   | 32:CR:265:LEU:HD21  | 1.86                     | 0.58              |
| 32:CS:24:ARG:NH1    | 32:CS:140:ILE:O     | 2.36                     | 0.58              |
| 50:C1:805:C:H5"     | 53:UT:1318:ARG:HH21 | 1.66                     | 0.58              |
| 53:UT:1471:ALA:O    | 53:UT:1475:GLN:N    | 2.34                     | 0.58              |
| 54:UH:269:LEU:HD23  | 54:UH:296:LEU:HD13  | 1.85                     | 0.58              |
| 54:UH:333:LYS:NZ    | 54:UH:335:GLU:OE2   | 2.36                     | 0.58              |
| 7:UJ:1466:GLN:HA    | 7:UJ:1469:ALA:HB3   | 1.86                     | 0.58              |
| 13:UQ:756:ILE:O     | 54:UH:435:ARG:NH2   | 2.33                     | 0.58              |
| 24:CI:169:ILE:HG23  | 24:CI:206:LEU:HD13  | 1.85                     | 0.58              |
| 32:CS:38:ILE:HG21   | 32:CS:150:VAL:HG11  | 1.85                     | 0.58              |
| 53:UT:64:ARG:NH1    | 53:UT:87:ASN:OD1    | 2.37                     | 0.58              |
| 53:UT:1024:ILE:HD11 | 53:UT:1075:MET:HE3  | 1.85                     | 0.58              |
| 2:UB:672:ARG:NH2    | 2:UB:684:GLU:OE1    | 2.36                     | 0.58              |
| 10:UM:557:LYS:HG3   | 10:UM:558:LEU:HG    | 1.86                     | 0.58              |
| 53:UT:2202:LEU:HA   | 53:UT:2205:VAL:HG22 | 1.85                     | 0.58              |
| 7:UJ:1767:ILE:HG21  | 7:UJ:1786:ILE:HD13  | 1.85                     | 0.58              |
| 24:CI:807:GLU:O     | 24:CI:840:ARG:NH2   | 2.37                     | 0.58              |
| 28:CM:209:GLU:OE2   | 28:CM:228:ARG:NH2   | 2.36                     | 0.58              |
| 37:CD:13:GLN:NE2    | 50:C1:735:G:N3      | 2.51                     | 0.58              |
| 38:Ce:151:ARG:NH1   | 45:Cm:51:GLU:OE1    | 2.36                     | 0.58              |
| 53:UT:2159:PHE:O    | 53:UT:2163:ASN:ND2  | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:UD:549:VAL:HG21  | 4:UD:563:VAL:HB    | 1.85                     | 0.58              |
| 8:UK:14:LYS:NZ     | 50:C1:1167:C:O2    | 2.37                     | 0.58              |
| 21:CE:94:VAL:HG12  | 21:CE:96:ARG:H     | 1.68                     | 0.58              |
| 32:CS:129:GLU:HA   | 32:CS:167:MET:HG3  | 1.84                     | 0.58              |
| 32:CS:787:LEU:HG   | 32:CS:889:LEU:HD21 | 1.85                     | 0.58              |
| 32:CS:641:ASN:HB3  | 32:CS:644:TYR:HB2  | 1.85                     | 0.58              |
| 35:Cb:95:THR:HG22  | 47:Co:347:PRO:HG2  | 1.86                     | 0.58              |
| 38:Ce:47:LEU:HD22  | 38:Ce:76:PHE:HZ    | 1.69                     | 0.58              |
| 59:CY:98:LYS:HB3   | 60:CZ:441:LEU:HD22 | 1.86                     | 0.58              |
| 4:UD:841:ILE:HG13  | 4:UD:859:GLU:HB3   | 1.84                     | 0.58              |
| 53:UT:1874:GLN:NE2 | 53:UT:1921:GLU:OE1 | 2.37                     | 0.58              |
| 1:UA:126:SER:OG    | 1:UA:131:ASN:OD1   | 2.22                     | 0.57              |
| 3:UC:230:ASP:OD1   | 27:CL:60:ARG:NH2   | 2.36                     | 0.57              |
| 4:UD:456:LEU:HG    | 4:UD:469:ILE:HG12  | 1.86                     | 0.57              |
| 9:UL:372:VAL:HG12  | 9:UL:387:VAL:HG22  | 1.85                     | 0.57              |
| 52:CW:227:GLU:HG3  | 52:CW:239:VAL:HG22 | 1.86                     | 0.57              |
| 55:UE:210:ARG:HB3  | 55:UE:214:LEU:HD13 | 1.86                     | 0.57              |
| 59:CY:106:LYS:O    | 60:CZ:433:ASN:ND2  | 2.32                     | 0.57              |
| 4:UD:869:GLU:O     | 61:UP:356:ARG:NH1  | 2.37                     | 0.57              |
| 7:UJ:776:ASP:HA    | 7:UJ:779:VAL:HG12  | 1.86                     | 0.57              |
| 13:UQ:818:ASP:OD2  | 13:UQ:822:LYS:NZ   | 2.37                     | 0.57              |
| 15:UU:441:ARG:NE   | 51:C2:68:A:OP1     | 2.37                     | 0.57              |
| 28:CM:171:SER:HB3  | 28:CM:203:VAL:HB   | 1.86                     | 0.57              |
| 38:Ce:15:SER:OG    | 38:Ce:16:ARG:N     | 2.37                     | 0.57              |
| 50:C1:1070:G:H1    | 50:C1:1085:U:H3    | 1.52                     | 0.57              |
| 52:CW:119:ARG:NH2  | 60:CZ:540:LYS:O    | 2.37                     | 0.57              |
| 52:CW:183:GLN:O    | 52:CW:236:ARG:NH2  | 2.37                     | 0.57              |
| 53:UT:233:GLU:HA   | 53:UT:236:LYS:HG2  | 1.85                     | 0.57              |
| 56:US:176:SER:O    | 56:US:182:ARG:NH2  | 2.36                     | 0.57              |
| 6:UG:304:ARG:NH1   | 6:UG:320:GLN:OE1   | 2.38                     | 0.57              |
| 7:UJ:1292:ASP:O    | 7:UJ:1338:LYS:NZ   | 2.38                     | 0.57              |
| 32:CR:659:ASP:HB2  | 32:CR:664:LYS:HD2  | 1.86                     | 0.57              |
| 39:Cf:84:HIS:NE2   | 39:Cf:97:THR:OG1   | 2.36                     | 0.57              |
| 52:CW:210:ALA:O    | 52:CW:215:GLY:CA   | 2.52                     | 0.57              |
| 53:UT:621:LEU:HB3  | 53:UT:673:ILE:HG13 | 1.86                     | 0.57              |
| 56:US:266:GLN:NE2  | 56:US:298:THR:OG1  | 2.37                     | 0.57              |
| 7:UJ:855:VAL:HA    | 7:UJ:858:LYS:HG2   | 1.87                     | 0.57              |
| 7:UJ:1091:SER:HA   | 7:UJ:1094:LYS:HD2  | 1.87                     | 0.57              |
| 7:UJ:1359:CYS:H    | 7:UJ:1396:LYS:HE3  | 1.70                     | 0.57              |
| 12:UO:169:VAL:HG13 | 12:UO:183:PHE:HB2  | 1.86                     | 0.57              |
| 13:UQ:555:GLU:HG3  | 13:UQ:583:ILE:HG12 | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:UU:343:ILE:HG22 | 15:UU:354:THR:HG22 | 1.85                     | 0.57              |
| 15:UU:863:ARG:NH1  | 27:CL:659:GLU:OE1  | 2.36                     | 0.57              |
| 34:Ca:64:ARG:HG2   | 42:Ca:49:ARG:HD3   | 1.87                     | 0.57              |
| 52:CW:347:THR:HB   | 52:CW:355:HIS:HB2  | 1.84                     | 0.57              |
| 7:UJ:1190:LEU:HD23 | 7:UJ:1193:LEU:HD21 | 1.86                     | 0.57              |
| 23:CH:7:GLU:HA     | 23:CH:32:HIS:HB2   | 1.87                     | 0.57              |
| 28:CM:323:THR:HG22 | 28:CM:325:ARG:H    | 1.69                     | 0.57              |
| 53:UT:1472:THR:HA  | 53:UT:1475:GLN:HB2 | 1.87                     | 0.57              |
| 1:UA:21:LEU:HB2    | 1:UA:30:PHE:HB2    | 1.86                     | 0.57              |
| 32:CS:633:ALA:O    | 32:CS:723:VAL:HA   | 2.04                     | 0.57              |
| 34:Ca:32:ILE:HD11  | 34:Ca:46:THR:HG23  | 1.86                     | 0.57              |
| 35:Cb:85:GLY:N     | 35:Cb:88:ASP:OD2   | 2.29                     | 0.57              |
| 53:UT:442:ARG:HH21 | 53:UT:480:PRO:HG3  | 1.70                     | 0.57              |
| 32:CR:280:THR:HA   | 32:CR:408:VAL:O    | 2.05                     | 0.57              |
| 35:Cb:197:HIS:HB3  | 35:Cb:209:HIS:HB2  | 1.87                     | 0.57              |
| 37:Cd:76:LEU:O     | 52:CW:49:GLN:NE2   | 2.35                     | 0.57              |
| 7:UJ:535:ASP:OD1   | 7:UJ:551:TYR:OH    | 2.23                     | 0.57              |
| 7:UJ:1635:ALA:O    | 7:UJ:1647:TRP:NE1  | 2.37                     | 0.57              |
| 10:UM:484:ALA:HB1  | 10:UM:550:LEU:HB2  | 1.87                     | 0.57              |
| 13:UQ:920:VAL:HG21 | 14:UR:575:THR:HG21 | 1.86                     | 0.57              |
| 14:UR:428:ASP:OD2  | 14:UR:430:ASN:ND2  | 2.38                     | 0.57              |
| 19:CC:385:LYS:HD3  | 19:CC:407:LEU:HD22 | 1.87                     | 0.57              |
| 32:CR:858:MET:HA   | 32:CR:861:ILE:HG12 | 1.85                     | 0.57              |
| 53:UT:1028:ASP:O   | 53:UT:1032:MET:N   | 2.38                     | 0.57              |
| 2:UB:531:ILE:HD11  | 2:UB:567:VAL:HG23  | 1.87                     | 0.57              |
| 12:UO:267:ARG:NH1  | 12:UO:304:SER:O    | 2.38                     | 0.57              |
| 17:UZ:133:LEU:HD11 | 17:UZ:167:LEU:HD21 | 1.87                     | 0.57              |
| 27:CL:485:GLU:OE1  | 27:CL:488:ARG:NH2  | 2.38                     | 0.57              |
| 32:CS:131:ILE:HA   | 32:CS:135:ILE:HD11 | 1.85                     | 0.57              |
| 50:C1:782:G:OP1    | 53:UT:1134:ARG:NH2 | 2.38                     | 0.57              |
| 53:UT:612:ARG:NH2  | 53:UT:836:ILE:O    | 2.38                     | 0.57              |
| 54:UH:349:LEU:HD21 | 54:UH:355:LEU:HD12 | 1.87                     | 0.57              |
| 9:UL:129:SER:OG    | 9:UL:131:ASP:OD2   | 2.23                     | 0.56              |
| 19:CC:377:ARG:NH2  | 51:C2:197:C:OP2    | 2.38                     | 0.56              |
| 46:Cn:107:PHE:HD2  | 46:Cn:123:LYS:HB3  | 1.70                     | 0.56              |
| 6:UG:100:LEU:HD13  | 6:UG:421:PRO:HG2   | 1.86                     | 0.56              |
| 20:CD:341:TYR:HB3  | 20:CD:345:TYR:HB2  | 1.87                     | 0.56              |
| 53:UT:208:ALA:O    | 53:UT:212:SER:CB   | 2.53                     | 0.56              |
| 1:UA:23:SER:HB3    | 1:UA:28:HIS:HB2    | 1.87                     | 0.56              |
| 1:UA:170:SER:OG    | 1:UA:172:ASP:OD1   | 2.22                     | 0.56              |
| 7:UJ:861:LEU:HD12  | 7:UJ:865:ILE:HG21  | 1.88                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 20:CD:297:VAL:HG13  | 20:CD:343:ILE:HG22  | 1.87                     | 0.56              |
| 29:CN:180:LEU:HD21  | 29:CN:206:VAL:HG13  | 1.87                     | 0.56              |
| 52:CW:60:VAL:HG23   | 52:CW:348:ALA:HB2   | 1.88                     | 0.56              |
| 54:UH:836:ILE:HD13  | 55:UI:222:LEU:HD11  | 1.86                     | 0.56              |
| 56:US:205:LYS:HD2   | 56:US:267:GLU:HB3   | 1.86                     | 0.56              |
| 59:CY:109:PHE:HD1   | 60:CZ:433:ASN:HD21  | 1.53                     | 0.56              |
| 4:UD:4:HIS:NE2      | 4:UD:859:GLU:OE2    | 2.39                     | 0.56              |
| 7:UJ:1291:VAL:HG23  | 7:UJ:1334:LYS:HZ1   | 1.71                     | 0.56              |
| 9:UL:138:ASP:HB2    | 9:UL:145:GLN:HG3    | 1.88                     | 0.56              |
| 9:UL:864:PHE:O      | 9:UL:868:GLU:HA     | 2.06                     | 0.56              |
| 15:UU:159:ILE:O     | 15:UU:172:THR:CA    | 2.45                     | 0.56              |
| 22:CG:172:THR:HG23  | 22:CG:583:GLY:HA3   | 1.87                     | 0.56              |
| 39:Cf:98:LYS:HB3    | 50:C1:913:G:H5''    | 1.86                     | 0.56              |
| 60:CZ:280:ASP:OD2   | 60:CZ:284:LYS:NZ    | 2.39                     | 0.56              |
| 1:UA:558:ARG:HB2    | 1:UA:566:ALA:HB2    | 1.86                     | 0.56              |
| 18:CB:217:ARG:O     | 20:CD:123:ARG:NH1   | 2.39                     | 0.56              |
| 30:CP:35:GLU:OE2    | 42:CI:127:ARG:NH1   | 2.38                     | 0.56              |
| 32:CR:62:LYS:HG2    | 32:CR:63:GLU:HG2    | 1.86                     | 0.56              |
| 53:UT:740:VAL:O     | 53:UT:746:TRP:NE1   | 2.29                     | 0.56              |
| 54:UH:607:GLU:OE1   | 54:UH:728:ARG:NH1   | 2.38                     | 0.56              |
| 2:UB:497:VAL:HA     | 2:UB:500:LEU:HD23   | 1.88                     | 0.56              |
| 7:UJ:541:SER:HB3    | 7:UJ:544:LYS:HB2    | 1.86                     | 0.56              |
| 7:UJ:1672:PHE:HA    | 7:UJ:1675:VAL:HG22  | 1.88                     | 0.56              |
| 24:CI:1033:SER:OG   | 50:C1:1159:C:N3     | 2.35                     | 0.56              |
| 32:CR:623:GLN:OE1   | 32:CS:839:LYS:NZ    | 2.38                     | 0.56              |
| 53:UT:1389:SER:OG   | 53:UT:1393:ARG:NH1  | 2.38                     | 0.56              |
| 53:UT:1755:ARG:HG2  | 53:UT:1793:THR:HG22 | 1.86                     | 0.56              |
| 54:UH:790:SER:HA    | 54:UH:793:MET:HE2   | 1.88                     | 0.56              |
| 2:UB:553:SER:HA     | 2:UB:556:VAL:HG12   | 1.86                     | 0.56              |
| 7:UJ:324:LEU:HD13   | 7:UJ:357:GLY:HA3    | 1.88                     | 0.56              |
| 39:Cf:11:ARG:O      | 44:Ck:138:LYS:NZ    | 2.38                     | 0.56              |
| 49:CU:155:LEU:O     | 49:CU:162:GLN:NE2   | 2.35                     | 0.56              |
| 53:UT:109:GLU:OE2   | 53:UT:113:ARG:NH2   | 2.35                     | 0.56              |
| 53:UT:578:THR:O     | 53:UT:582:PHE:HB2   | 2.05                     | 0.56              |
| 53:UT:587:ARG:NH1   | 53:UT:588:MET:SD    | 2.79                     | 0.56              |
| 7:UJ:915:THR:HA     | 7:UJ:918:VAL:HG12   | 1.88                     | 0.56              |
| 9:UL:803:ARG:NH2    | 9:UL:808:ASN:OD1    | 2.38                     | 0.56              |
| 13:UQ:499:LEU:HD22  | 13:UQ:513:LYS:HE2   | 1.87                     | 0.56              |
| 32:CS:285:ALA:HB2   | 32:CS:474:LEU:HB2   | 1.87                     | 0.56              |
| 8:UK:221:ARG:NH1    | 50:C1:377:U:OP1     | 2.39                     | 0.56              |
| 24:CI:1116:ARG:HH11 | 50:C1:1078:U:HI'    | 1.71                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 32:CS:837:ASP:OD1   | 32:CS:840:ARG:NH2   | 2.39                     | 0.56              |
| 53:UT:306:ILE:HG23  | 53:UT:345:MET:HE3   | 1.88                     | 0.56              |
| 55:UE:156:VAL:HG21  | 56:US:301:GLU:HB2   | 1.88                     | 0.56              |
| 57:CI:24:GLY:HA2    | 57:CI:58:ALA:HB3    | 1.88                     | 0.56              |
| 2:UB:88:PRO:HB3     | 50:C1:1762:G:H5''   | 1.88                     | 0.56              |
| 4:UD:374:VAL:HG11   | 4:UD:863:ILE:HD13   | 1.88                     | 0.56              |
| 9:UL:449:LEU:HB3    | 9:UL:463:PHE:HB2    | 1.88                     | 0.56              |
| 10:UM:200:TRP:HZ3   | 10:UM:210:PHE:HB2   | 1.70                     | 0.56              |
| 32:CS:246:THR:HG22  | 32:CS:248:PRO:HD2   | 1.88                     | 0.56              |
| 35:Cb:212:ASP:O     | 35:Cb:215:ASP:N     | 2.39                     | 0.56              |
| 50:C1:926:C:H5''    | 52:CW:194:GLY:HA3   | 1.88                     | 0.56              |
| 53:UT:414:GLN:NE2   | 53:UT:418:THR:OG1   | 2.36                     | 0.56              |
| 53:UT:1433:PRO:O    | 53:UT:1437:ASN:ND2  | 2.39                     | 0.56              |
| 53:UT:1900:LEU:HD23 | 53:UT:1969:ILE:HD13 | 1.88                     | 0.56              |
| 7:UJ:919:LEU:O      | 7:UJ:923:GLN:NE2    | 2.38                     | 0.55              |
| 7:UJ:1522:LEU:HA    | 7:UJ:1525:ILE:HG12  | 1.88                     | 0.55              |
| 9:UL:153:ASP:HB3    | 9:UL:194:LYS:HB3    | 1.88                     | 0.55              |
| 24:CI:325:ARG:NH1   | 50:C1:637:C:OP2     | 2.39                     | 0.55              |
| 32:CR:310:ILE:HD12  | 32:CR:385:LEU:HD23  | 1.86                     | 0.55              |
| 45:Cm:85:GLU:HA     | 49:CU:300:VAL:HG21  | 1.88                     | 0.55              |
| 58:CX:278:ILE:HD11  | 58:CX:320:GLU:HG2   | 1.87                     | 0.55              |
| 9:UL:899:LEU:HA     | 9:UL:902:VAL:HG12   | 1.88                     | 0.55              |
| 39:Cf:73:THR:O      | 39:Cf:74:ARG:NH1    | 2.37                     | 0.55              |
| 53:UT:1092:ASP:O    | 53:UT:1096:ASN:ND2  | 2.34                     | 0.55              |
| 53:UT:1375:LEU:HD22 | 53:UT:1395:LEU:HD21 | 1.86                     | 0.55              |
| 12:UO:122:ARG:HB2   | 12:UO:141:HIS:HD2   | 1.71                     | 0.55              |
| 26:CK:40:LYS:NZ     | 26:CK:41:PRO:O      | 2.39                     | 0.55              |
| 50:C1:807:A:O2'     | 53:UT:1495:ARG:NH2  | 2.39                     | 0.55              |
| 53:UT:1013:ARG:O    | 53:UT:1017:HIS:HB3  | 2.05                     | 0.55              |
| 6:UG:332:PHE:HB3    | 11:UN:869:VAL:HG11  | 1.87                     | 0.55              |
| 22:CG:110:LYS:HZ2   | 59:CY:328:LYS:HD3   | 1.71                     | 0.55              |
| 22:CG:195:TRP:HD1   | 22:CG:226:ARG:HA    | 1.72                     | 0.55              |
| 24:CI:63:PRO:HG2    | 24:CI:66:PRO:HA     | 1.87                     | 0.55              |
| 29:CN:76:ILE:HG22   | 29:CN:80:MET:HE2    | 1.88                     | 0.55              |
| 53:UT:419:LYS:HG3   | 53:UT:421:PRO:HD2   | 1.87                     | 0.55              |
| 54:UH:84:PRO:HB3    | 54:UH:103:VAL:HG12  | 1.88                     | 0.55              |
| 15:UU:205:ASP:O     | 15:UU:207:TRP:N     | 2.39                     | 0.55              |
| 18:CB:131:ASN:HD22  | 18:CB:134:ARG:HD3   | 1.72                     | 0.55              |
| 23:CH:213:GLY:O     | 24:CI:623:ARG:NH1   | 2.35                     | 0.55              |
| 32:CS:13:THR:O      | 32:CS:17:ASN:ND2    | 2.39                     | 0.55              |
| 32:CS:618:VAL:O     | 32:CS:622:PHE:HB2   | 2.05                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:Ce:66:ILE:HD11  | 38:Ce:98:ILE:HG12   | 1.89                     | 0.55              |
| 53:UT:1552:LEU:HB3 | 53:UT:1556:ARG:HH12 | 1.71                     | 0.55              |
| 1:UA:393:LYS:HG3   | 1:UA:395:SER:H      | 1.71                     | 0.55              |
| 24:CI:881:ASN:N    | 24:CI:905:VAL:O     | 2.39                     | 0.55              |
| 31:CQ:119:GLU:OE2  | 31:CQ:121:ARG:NH2   | 2.39                     | 0.55              |
| 53:UT:454:VAL:HG12 | 53:UT:491:PRO:HG3   | 1.88                     | 0.55              |
| 53:UT:692:GLN:HA   | 53:UT:695:GLU:HG3   | 1.89                     | 0.55              |
| 53:UT:2068:ILE:O   | 53:UT:2105:ARG:NH1  | 2.40                     | 0.55              |
| 56:US:91:LEU:HD21  | 56:US:114:LEU:HD23  | 1.88                     | 0.55              |
| 4:UD:672:ARG:NH1   | 4:UD:715:ASP:OD1    | 2.40                     | 0.55              |
| 7:UJ:608:ARG:NH1   | 7:UJ:668:VAL:O      | 2.40                     | 0.55              |
| 9:UL:94:LEU:HD11   | 9:UL:139:LEU:HD22   | 1.89                     | 0.55              |
| 10:UM:647:LYS:HD2  | 10:UM:699:LEU:H     | 1.71                     | 0.55              |
| 10:UM:889:ARG:NH2  | 10:UM:890:GLU:OE2   | 2.38                     | 0.55              |
| 12:UO:552:MET:O    | 54:UH:727:ARG:NH2   | 2.39                     | 0.55              |
| 26:CK:288:THR:HG23 | 50:C1:1146:G:C5     | 2.41                     | 0.55              |
| 27:CL:697:THR:O    | 27:CL:700:GLY:N     | 2.37                     | 0.55              |
| 53:UT:1908:SER:HB2 | 53:UT:1980:LEU:HD21 | 1.88                     | 0.55              |
| 1:UA:115:LEU:HD12  | 1:UA:118:LYS:HE3    | 1.88                     | 0.55              |
| 13:UQ:383:GLN:NE2  | 14:UR:364:GLN:O     | 2.40                     | 0.55              |
| 18:CB:180:VAL:HB   | 18:CB:203:VAL:HG12  | 1.89                     | 0.55              |
| 23:CH:235:MET:HB3  | 23:CH:279:LEU:HD22  | 1.87                     | 0.55              |
| 25:CJ:108:ARG:HA   | 25:CJ:113:VAL:HG11  | 1.89                     | 0.55              |
| 34:Ca:35:PRO:O     | 34:Ca:41:ARG:NH1    | 2.40                     | 0.55              |
| 50:C1:2120:C:H1'   | 50:C1:2155:G:H22    | 1.72                     | 0.55              |
| 53:UT:424:LYS:NZ   | 53:UT:461:ASN:OD1   | 2.35                     | 0.55              |
| 55:UE:154:GLY:O    | 55:UE:158:ASN:ND2   | 2.34                     | 0.55              |
| 23:CH:110:ILE:HG12 | 23:CH:192:VAL:HG11  | 1.88                     | 0.55              |
| 58:CX:239:PRO:O    | 58:CX:273:ARG:NH2   | 2.40                     | 0.55              |
| 7:UJ:757:ALA:HA    | 7:UJ:802:ARG:HH12   | 1.72                     | 0.55              |
| 7:UJ:1468:LEU:HA   | 7:UJ:1471:LEU:HG    | 1.89                     | 0.55              |
| 15:UU:254:VAL:HG12 | 15:UU:266:LEU:HD13  | 1.88                     | 0.55              |
| 20:CD:341:TYR:HD2  | 51:C2:90:C:H5'      | 1.71                     | 0.55              |
| 26:CK:89:LEU:HD11  | 26:CK:117:LEU:HB2   | 1.88                     | 0.55              |
| 34:Ca:214:LYS:NZ   | 50:C1:1471:U:OP1    | 2.38                     | 0.55              |
| 53:UT:63:LEU:N     | 53:UT:132:ASP:OD2   | 2.40                     | 0.55              |
| 7:UJ:645:SER:O     | 7:UJ:647:LEU:N      | 2.40                     | 0.54              |
| 7:UJ:1726:LEU:HD12 | 7:UJ:1741:VAL:HG23  | 1.88                     | 0.54              |
| 8:UK:15:GLU:OE2    | 24:CI:1040:ARG:NH2  | 2.40                     | 0.54              |
| 12:UO:546:MET:HG2  | 55:UI:265:MET:HB2   | 1.88                     | 0.54              |
| 20:CD:77:LEU:HD11  | 20:CD:99:ILE:HD11   | 1.89                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 34:Ca:129:THR:HG23  | 34:Ca:131:ASP:H     | 1.72                     | 0.54              |
| 53:UT:1047:ARG:NH2  | 53:UT:1092:ASP:O    | 2.40                     | 0.54              |
| 53:UT:1367:ASN:HA   | 53:UT:1370:THR:HG22 | 1.90                     | 0.54              |
| 54:UH:484:GLU:OE2   | 54:UH:488:ASN:ND2   | 2.40                     | 0.54              |
| 32:CS:404:GLY:O     | 32:CS:467:ARG:NH1   | 2.40                     | 0.54              |
| 53:UT:585:TYR:O     | 53:UT:589:CYS:HB2   | 2.07                     | 0.54              |
| 7:UJ:1187:THR:O     | 7:UJ:1247:ARG:NH2   | 2.40                     | 0.54              |
| 17:UZ:22:GLN:HA     | 17:UZ:25:LYS:HG2    | 1.89                     | 0.54              |
| 29:CO:114:ILE:HB    | 29:CO:122:ILE:HB    | 1.88                     | 0.54              |
| 32:CS:184:ARG:NH1   | 32:CS:524:ASP:OD1   | 2.40                     | 0.54              |
| 34:Ca:137:LEU:HD22  | 34:Ca:215:VAL:HG22  | 1.88                     | 0.54              |
| 53:UT:1652:VAL:HG12 | 53:UT:1656:LYS:HE3  | 1.88                     | 0.54              |
| 4:UD:51:GLY:HA2     | 4:UD:77:VAL:HG23    | 1.89                     | 0.54              |
| 13:UQ:88:ARG:HD3    | 13:UQ:441:VAL:HG21  | 1.88                     | 0.54              |
| 34:Ca:115:ARG:NH2   | 34:Ca:118:GLN:OE1   | 2.41                     | 0.54              |
| 41:Ch:130:LYS:NZ    | 41:Ch:139:TRP:O     | 2.40                     | 0.54              |
| 7:UJ:813:ILE:HA     | 7:UJ:816:MET:HG2    | 1.88                     | 0.54              |
| 24:CI:86:LYS:HG3    | 24:CI:100:PRO:HG3   | 1.90                     | 0.54              |
| 24:CI:379:LEU:HD22  | 32:CR:211:ILE:HD13  | 1.88                     | 0.54              |
| 32:CS:310:ILE:HD12  | 32:CS:385:LEU:HD23  | 1.90                     | 0.54              |
| 35:Cb:60:GLU:OE1    | 47:Co:351:ARG:NH2   | 2.33                     | 0.54              |
| 10:UM:777:VAL:HG21  | 10:UM:794:VAL:HG21  | 1.90                     | 0.54              |
| 12:UO:100:SER:HB3   | 12:UO:119:ASP:HB2   | 1.88                     | 0.54              |
| 12:UO:334:LEU:HB3   | 12:UO:346:ARG:HB3   | 1.88                     | 0.54              |
| 13:UQ:713:VAL:HG22  | 13:UQ:725:VAL:HG22  | 1.89                     | 0.54              |
| 23:CH:80:GLY:O      | 24:CI:809:ARG:NH2   | 2.40                     | 0.54              |
| 25:CJ:49:ARG:NH1    | 50:C1:292:G:OP2     | 2.41                     | 0.54              |
| 32:CS:287:ARG:NH1   | 32:CS:418:GLU:OE1   | 2.41                     | 0.54              |
| 53:UT:313:SER:O     | 53:UT:353:ARG:NH1   | 2.40                     | 0.54              |
| 53:UT:426:TYR:OH    | 53:UT:448:GLU:OE1   | 2.24                     | 0.54              |
| 24:CI:754:LYS:HA    | 24:CI:757:TYR:HB2   | 1.90                     | 0.54              |
| 47:Co:345:ARG:NE    | 53:UT:73:LEU:O      | 2.39                     | 0.54              |
| 58:CX:325:SER:HB2   | 58:CX:369:VAL:HG11  | 1.88                     | 0.54              |
| 10:UM:865:VAL:HG12  | 27:CL:679:PRO:HG3   | 1.89                     | 0.54              |
| 32:CR:749:GLN:NE2   | 32:CS:852:HIS:O     | 2.40                     | 0.54              |
| 35:Cb:100:ARG:HB2   | 35:Cb:114:ILE:HG13  | 1.89                     | 0.54              |
| 50:C1:314:A:H61     | 50:C1:326:U:H3      | 1.54                     | 0.54              |
| 50:C1:372:U:H3      | 50:C1:394:U:H3      | 1.54                     | 0.54              |
| 53:UT:1412:LEU:O    | 53:UT:1416:ASN:ND2  | 2.41                     | 0.54              |
| 56:US:126:LEU:HD21  | 56:US:168:GLU:HB3   | 1.90                     | 0.54              |
| 1:UA:381:HIS:CE1    | 1:UA:407:ARG:HG3    | 2.43                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:UQ:115:SER:OG   | 13:UQ:118:ASP:OD1   | 2.25                     | 0.54              |
| 13:UQ:770:THR:HG22 | 13:UQ:796:PRO:HB3   | 1.90                     | 0.54              |
| 15:UU:302:THR:HG22 | 15:UU:304:VAL:H     | 1.73                     | 0.54              |
| 23:CH:139:THR:HB   | 23:CH:179:SER:H     | 1.71                     | 0.54              |
| 32:CS:28:VAL:HB    | 32:CS:201:VAL:HG12  | 1.89                     | 0.54              |
| 35:Cb:87:MET:HA    | 35:Cb:101:LEU:O     | 2.08                     | 0.54              |
| 37:Cd:143:ARG:NH1  | 50:C1:727:G:OP1     | 2.41                     | 0.54              |
| 53:UT:1368:ARG:HA  | 53:UT:1371:LEU:HD12 | 1.90                     | 0.54              |
| 17:UZ:82:LYS:O     | 17:UZ:269:ARG:NH2   | 2.41                     | 0.54              |
| 18:CB:130:TRP:CD1  | 18:CB:138:ALA:HB3   | 2.43                     | 0.54              |
| 20:CD:240:ALA:O    | 20:CD:244:SER:HB2   | 2.08                     | 0.54              |
| 21:CF:21:LEU:HD23  | 21:CF:118:LEU:HD13  | 1.90                     | 0.54              |
| 7:UJ:1224:TYR:HE2  | 7:UJ:1264:PHE:HA    | 1.72                     | 0.53              |
| 23:CH:269:GLN:N    | 23:CH:269:GLN:NE2   | 2.55                     | 0.53              |
| 30:CP:199:LYS:HE3  | 30:CP:203:ILE:HD11  | 1.90                     | 0.53              |
| 32:CR:344:ILE:HA   | 32:CR:359:VAL:HG12  | 1.89                     | 0.53              |
| 34:Ca:33:LYS:NZ    | 34:Ca:42:ASP:OD2    | 2.41                     | 0.53              |
| 50:C1:652:A:N6     | 50:C1:670:A:OP2     | 2.39                     | 0.53              |
| 53:UT:1313:LEU:O   | 53:UT:1325:LYS:NZ   | 2.41                     | 0.53              |
| 56:US:304:MET:HG2  | 56:US:334:LEU:HD23  | 1.90                     | 0.53              |
| 7:UJ:713:HIS:O     | 7:UJ:717:THR:OG1    | 2.19                     | 0.53              |
| 20:CD:320:GLN:OE1  | 51:C2:262:C:N4      | 2.37                     | 0.53              |
| 23:CH:151:ASP:OD1  | 23:CH:154:ARG:NH2   | 2.41                     | 0.53              |
| 23:CH:251:HIS:HB3  | 49:CU:111:MET:HG2   | 1.89                     | 0.53              |
| 32:CR:24:ARG:NH1   | 32:CR:140:ILE:O     | 2.41                     | 0.53              |
| 32:CS:129:GLU:HB3  | 32:CS:165:MET:HE1   | 1.90                     | 0.53              |
| 39:Cf:31:ARG:HH12  | 39:Cf:48:THR:HG22   | 1.72                     | 0.53              |
| 53:UT:263:MET:HE1  | 53:UT:305:VAL:HB    | 1.89                     | 0.53              |
| 56:US:383:LYS:NZ   | 56:US:456:CYS:O     | 2.41                     | 0.53              |
| 59:CY:291:ARG:HG2  | 59:CY:294:ARG:HH21  | 1.73                     | 0.53              |
| 6:UG:580:GLU:HA    | 6:UG:583:LEU:HB2    | 1.90                     | 0.53              |
| 9:UL:587:SER:HA    | 9:UL:609:PRO:HA     | 1.89                     | 0.53              |
| 29:CN:228:SER:HB3  | 29:CN:232:LEU:HD11  | 1.90                     | 0.53              |
| 30:CP:129:MET:HE1  | 30:CP:186:GLU:HG2   | 1.90                     | 0.53              |
| 39:Cf:8:ARG:NH2    | 39:Cf:28:GLU:OE2    | 2.37                     | 0.53              |
| 53:UT:39:SER:OG    | 53:UT:209:GLU:OE1   | 2.26                     | 0.53              |
| 2:UB:670:PRO:HG3   | 2:UB:691:ILE:HB     | 1.90                     | 0.53              |
| 7:UJ:854:GLU:OE1   | 7:UJ:857:ARG:NH2    | 2.41                     | 0.53              |
| 15:UU:50:PRO:HB2   | 15:UU:342:LYS:HD2   | 1.90                     | 0.53              |
| 24:CI:56:VAL:HG22  | 46:Cn:52:ILE:HG12   | 1.91                     | 0.53              |
| 24:CI:346:ILE:HG12 | 24:CI:351:ILE:HG12  | 1.91                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 26:CK:73:ILE:HG13   | 26:CK:75:ASP:HB2    | 1.91                     | 0.53              |
| 27:CL:561:ARG:NH2   | 27:CL:567:ASN:O     | 2.42                     | 0.53              |
| 38:Ce:50:VAL:HG21   | 38:Ce:68:VAL:HG12   | 1.89                     | 0.53              |
| 50:C1:806:C:OP2     | 53:UT:1318:ARG:NH2  | 2.42                     | 0.53              |
| 52:CW:170:ARG:HG3   | 52:CW:179:LEU:HB2   | 1.90                     | 0.53              |
| 53:UT:402:PRO:O     | 53:UT:406:LEU:HB2   | 2.08                     | 0.53              |
| 53:UT:2083:LYS:HA   | 53:UT:2086:LEU:HD12 | 1.91                     | 0.53              |
| 54:UH:483:ASP:OD1   | 54:UH:552:LYS:NZ    | 2.41                     | 0.53              |
| 10:UM:345:LEU:HD12  | 10:UM:367:ARG:HB3   | 1.89                     | 0.53              |
| 15:UU:752:THR:N     | 15:UU:766:ALA:O     | 2.39                     | 0.53              |
| 32:CS:32:ASP:O      | 32:CS:35:LYS:NZ     | 2.37                     | 0.53              |
| 2:UB:479:PHE:HB2    | 2:UB:507:ILE:HD13   | 1.90                     | 0.53              |
| 7:UJ:746:LEU:HD12   | 7:UJ:750:ARG:HE     | 1.74                     | 0.53              |
| 7:UJ:782:VAL:O      | 7:UJ:812:ARG:NH2    | 2.41                     | 0.53              |
| 7:UJ:803:PRO:HA     | 7:UJ:806:LEU:HB2    | 1.91                     | 0.53              |
| 22:CG:593:TYR:OH    | 51:C2:189:G:O2'     | 2.24                     | 0.53              |
| 27:CL:507:THR:HG22  | 27:CL:509:ALA:H     | 1.74                     | 0.53              |
| 42:CI:33:PHE:HB3    | 42:CI:40:PHE:HB2    | 1.91                     | 0.53              |
| 45:Cm:103:ILE:HD11  | 45:Cm:129:PHE:HE1   | 1.73                     | 0.53              |
| 52:CW:183:GLN:O     | 52:CW:229:TYR:OH    | 2.27                     | 0.53              |
| 53:UT:1601:THR:HG22 | 53:UT:1640:LEU:HD12 | 1.90                     | 0.53              |
| 53:UT:1859:LYS:O    | 53:UT:1903:ASN:ND2  | 2.42                     | 0.53              |
| 53:UT:1964:ARG:HB3  | 53:UT:2004:VAL:HG12 | 1.91                     | 0.53              |
| 54:UH:642:VAL:HG23  | 54:UH:729:LEU:HD22  | 1.90                     | 0.53              |
| 14:UR:322:ARG:HH21  | 50:C1:133:G:H22     | 1.54                     | 0.53              |
| 25:CJ:72:ARG:NH1    | 25:CJ:75:GLU:OE2    | 2.42                     | 0.53              |
| 32:CR:8:ASP:OD2     | 32:CR:10:ARG:NH2    | 2.41                     | 0.53              |
| 32:CS:279:ASN:H     | 32:CS:467:ARG:HH21  | 1.55                     | 0.53              |
| 37:CD:198:ARG:NH2   | 50:C1:868:G:OP1     | 2.40                     | 0.53              |
| 40:Cg:38:ARG:HH22   | 50:C1:1179:G:H5'    | 1.73                     | 0.53              |
| 1:UA:534:LEU:HB2    | 1:UA:548:VAL:HG22   | 1.91                     | 0.53              |
| 5:UF:73:LYS:HE3     | 14:UR:51:GLU:HG3    | 1.91                     | 0.53              |
| 7:UJ:1746:GLN:NE2   | 7:UJ:1781:GLU:O     | 2.42                     | 0.53              |
| 9:UL:701:ALA:HB3    | 9:UL:714:ALA:HB3    | 1.91                     | 0.53              |
| 18:CA:222:MET:HG2   | 19:CC:135:ARG:HG2   | 1.91                     | 0.53              |
| 19:CC:89:THR:HG23   | 19:CC:115:GLY:HA3   | 1.91                     | 0.53              |
| 28:CM:224:LEU:HB2   | 28:CM:234:ILE:HG22  | 1.91                     | 0.53              |
| 32:CS:292:SER:OG    | 65:CS:1101:ADP:O1A  | 2.26                     | 0.53              |
| 34:Ca:82:ARG:NH2    | 34:Ca:189:ILE:O     | 2.41                     | 0.53              |
| 54:UH:148:ILE:HG22  | 54:UH:172:ILE:HG12  | 1.91                     | 0.53              |
| 4:UD:115:ASP:HB2    | 4:UD:122:LYS:HB2    | 1.91                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:UD:617:ASN:HB3    | 4:UD:620:ALA:HB2    | 1.90                     | 0.53              |
| 10:UM:18:GLN:HG3    | 10:UM:53:ARG:HH21   | 1.72                     | 0.53              |
| 12:UO:418:ARG:NH2   | 50:C1:76:U:OP1      | 2.41                     | 0.53              |
| 15:UU:119:LEU:HD22  | 15:UU:131:LEU:HD22  | 1.90                     | 0.53              |
| 19:CC:152:ARG:NH1   | 20:CD:245:MET:SD    | 2.82                     | 0.53              |
| 22:CG:176:VAL:CA    | 22:CG:184:TYR:O     | 2.50                     | 0.53              |
| 24:CI:349:ASP:OD1   | 32:CR:16:ARG:NH1    | 2.42                     | 0.53              |
| 49:CU:223:GLN:O     | 49:CU:230:ARG:NH2   | 2.42                     | 0.53              |
| 53:UT:2079:LEU:HD22 | 53:UT:2115:THR:HG21 | 1.91                     | 0.53              |
| 5:UF:339:ILE:HG22   | 5:UF:363:ARG:HB3    | 1.91                     | 0.53              |
| 12:UO:125:VAL:HB    | 12:UO:138:LYS:HB3   | 1.90                     | 0.53              |
| 20:CD:69:VAL:HG13   | 20:CD:73:LEU:HD23   | 1.92                     | 0.53              |
| 20:CD:227:GLU:HG2   | 20:CD:228:ILE:HG13  | 1.91                     | 0.53              |
| 27:CL:59:ASN:OD1    | 27:CL:61:HIS:NE2    | 2.42                     | 0.53              |
| 32:CS:163:TYR:HE1   | 32:CS:190:LEU:HD12  | 1.74                     | 0.53              |
| 32:CS:542:ALA:O     | 32:CS:546:ALA:HB2   | 2.09                     | 0.53              |
| 53:UT:43:LEU:HD11   | 53:UT:170:PHE:HA    | 1.91                     | 0.53              |
| 53:UT:182:ASP:O     | 53:UT:184:ARG:NH1   | 2.42                     | 0.53              |
| 53:UT:335:GLN:HA    | 53:UT:367:MET:HE1   | 1.91                     | 0.53              |
| 53:UT:2104:ASP:OD1  | 53:UT:2141:GLN:NE2  | 2.42                     | 0.53              |
| 35:Cb:100:ARG:NH2   | 35:Cb:118:GLU:O     | 2.40                     | 0.52              |
| 54:UH:555:GLY:O     | 54:UH:567:LEU:CA    | 2.43                     | 0.52              |
| 54:UH:785:ASP:OD2   | 55:UI:262:LYS:NZ    | 2.42                     | 0.52              |
| 7:UJ:1090:PRO:O     | 7:UJ:1094:LYS:N     | 2.40                     | 0.52              |
| 9:UL:896:ARG:NE     | 10:UM:892:ASP:OD1   | 2.41                     | 0.52              |
| 23:CH:375:TRP:O     | 24:CI:763:HIS:NE2   | 2.43                     | 0.52              |
| 32:CS:776:GLY:HA3   | 32:CS:816:ASP:HB2   | 1.91                     | 0.52              |
| 60:CZ:415:MET:HA    | 60:CZ:418:ARG:HB3   | 1.90                     | 0.52              |
| 13:UQ:564:GLU:OE2   | 13:UQ:573:GLN:NE2   | 2.43                     | 0.52              |
| 20:CD:15:LEU:HD11   | 20:CD:80:LEU:HD11   | 1.90                     | 0.52              |
| 28:CM:72:MET:HE3    | 28:CM:333:MET:HG2   | 1.91                     | 0.52              |
| 53:UT:130:ALA:O     | 53:UT:133:LEU:O     | 2.26                     | 0.52              |
| 54:UH:214:PHE:HB3   | 54:UH:255:ILE:HB    | 1.91                     | 0.52              |
| 4:UD:491:ARG:NH2    | 4:UD:612:GLU:OE2    | 2.43                     | 0.52              |
| 23:CH:368:LYS:HZ1   | 23:CH:374:SER:HB2   | 1.74                     | 0.52              |
| 32:CR:263:LYS:HD3   | 32:CR:266:LEU:HD21  | 1.92                     | 0.52              |
| 43:Cj:11:GLY:HA2    | 43:Cj:83:GLN:HE21   | 1.74                     | 0.52              |
| 52:CW:210:ALA:O     | 52:CW:215:GLY:HA2   | 2.09                     | 0.52              |
| 53:UT:1036:LEU:HD12 | 53:UT:1079:VAL:HG11 | 1.92                     | 0.52              |
| 53:UT:1161:VAL:HG21 | 53:UT:1202:VAL:HG11 | 1.90                     | 0.52              |
| 54:UH:830:VAL:HA    | 54:UH:833:LYS:HG2   | 1.91                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:UH:847:ARG:NH1   | 55:UI:230:VAL:O     | 2.43                     | 0.52              |
| 2:UB:43:GLN:N       | 2:UB:43:GLN:NE2     | 2.56                     | 0.52              |
| 4:UD:377:ALA:HB3    | 4:UD:382:TYR:HB2    | 1.91                     | 0.52              |
| 7:UJ:1378:LEU:HA    | 7:UJ:1381:VAL:HG22  | 1.92                     | 0.52              |
| 9:UL:16:VAL:HA      | 9:UL:392:ASN:HD21   | 1.74                     | 0.52              |
| 26:CK:100:LEU:HD13  | 26:CK:144:GLU:HB3   | 1.92                     | 0.52              |
| 32:CR:771:ASP:N     | 32:CR:771:ASP:OD1   | 2.43                     | 0.52              |
| 32:CS:727:TYR:CE1   | 32:CS:762:MET:HG2   | 2.45                     | 0.52              |
| 47:Co:352:LYS:HB2   | 47:Co:406:ILE:HG23  | 1.91                     | 0.52              |
| 1:UA:268:ASN:HB3    | 1:UA:285:PRO:HD3    | 1.91                     | 0.52              |
| 4:UD:390:GLU:OE2    | 4:UD:392:ARG:NE     | 2.40                     | 0.52              |
| 7:UJ:525:ALA:HA     | 7:UJ:531:LEU:HD21   | 1.91                     | 0.52              |
| 10:UM:520:GLN:OE1   | 10:UM:522:ARG:NH2   | 2.39                     | 0.52              |
| 13:UQ:636:ARG:NH1   | 55:UE:41:LEU:O      | 2.42                     | 0.52              |
| 18:CB:186:SER:OG    | 18:CB:189:SER:OG    | 2.28                     | 0.52              |
| 20:CD:287:PRO:HB2   | 20:CD:391:ALA:HB2   | 1.92                     | 0.52              |
| 22:CG:416:GLY:HA2   | 22:CG:466:ILE:HG13  | 1.91                     | 0.52              |
| 28:CM:273:ASP:OD2   | 28:CM:273:ASP:N     | 2.43                     | 0.52              |
| 32:CS:662:GLU:OE2   | 32:CS:767:GLN:NE2   | 2.41                     | 0.52              |
| 53:UT:1201:ASN:HD22 | 53:UT:1250:LEU:HD12 | 1.75                     | 0.52              |
| 56:US:444:GLU:HB3   | 56:US:450:THR:HG22  | 1.90                     | 0.52              |
| 3:UC:639:LYS:HG3    | 33:CT:123:LYS:HD3   | 1.92                     | 0.52              |
| 6:UG:270:ASN:HB3    | 6:UG:272:ILE:HG12   | 1.90                     | 0.52              |
| 23:CH:9:LEU:HB3     | 23:CH:31:ILE:HG22   | 1.92                     | 0.52              |
| 43:Cj:97:VAL:HG12   | 43:Cj:98:ASP:H      | 1.75                     | 0.52              |
| 54:UH:219:SER:HB2   | 54:UH:248:ASN:HD21  | 1.74                     | 0.52              |
| 59:CY:64:ARG:HH12   | 60:CZ:399:ALA:HA    | 1.73                     | 0.52              |
| 12:UO:25:ARG:NH1    | 50:C1:85:U:OP2      | 2.43                     | 0.52              |
| 18:CA:230:VAL:O     | 18:CA:235:GLN:NE2   | 2.42                     | 0.52              |
| 20:CD:438:ARG:HB3   | 50:C1:272:A:H5''    | 1.92                     | 0.52              |
| 24:CI:1130:ARG:HH22 | 50:C1:604:C:H5''    | 1.73                     | 0.52              |
| 26:CK:131:ALA:HB2   | 26:CK:139:ILE:HD11  | 1.90                     | 0.52              |
| 32:CR:745:VAL:HB    | 32:CR:761:VAL:HG13  | 1.91                     | 0.52              |
| 35:Cb:44:LEU:HB3    | 35:Cb:65:MET:HE1    | 1.91                     | 0.52              |
| 40:Cg:146:VAL:HG11  | 40:Cg:154:ILE:HD11  | 1.92                     | 0.52              |
| 53:UT:1065:PRO:HD2  | 53:UT:1068:LYS:HD2  | 1.90                     | 0.52              |
| 53:UT:1479:ILE:HD11 | 53:UT:1519:TRP:CD1  | 2.45                     | 0.52              |
| 55:UE:157:LEU:HD23  | 55:UE:188:MET:HG3   | 1.92                     | 0.52              |
| 56:US:405:TYR:OH    | 56:US:484:LYS:O     | 2.27                     | 0.52              |
| 10:UM:62:GLU:HG3    | 10:UM:82:SER:HB3    | 1.92                     | 0.52              |
| 12:UO:216:VAL:HB    | 12:UO:227:MET:HB2   | 1.92                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 14:UR:322:ARG:NH2  | 50:C1:76:U:OP2      | 2.36                     | 0.52              |
| 53:UT:433:LEU:HD11 | 53:UT:440:ARG:HH12  | 1.75                     | 0.52              |
| 53:UT:1567:PHE:HB3 | 53:UT:1572:ILE:HD11 | 1.91                     | 0.52              |
| 54:UH:34:VAL:HG22  | 54:UH:86:SER:HB3    | 1.92                     | 0.52              |
| 2:UB:730:THR:HG23  | 2:UB:780:LEU:HD22   | 1.91                     | 0.52              |
| 4:UD:683:ARG:O     | 4:UD:736:ARG:NH1    | 2.42                     | 0.52              |
| 10:UM:48:LEU:HB3   | 10:UM:367:ARG:HH22  | 1.75                     | 0.52              |
| 24:CI:68:PRO:HB3   | 24:CI:113:ARG:HG3   | 1.92                     | 0.52              |
| 50:C1:906:G:H4'    | 50:C1:907:A:H5'     | 1.92                     | 0.52              |
| 2:UB:701:GLN:NE2   | 56:US:543:ASP:OD1   | 2.36                     | 0.51              |
| 6:UG:284:LEU:O     | 6:UG:293:LEU:N      | 2.42                     | 0.51              |
| 10:UM:12:GLU:OE1   | 10:UM:721:ARG:NH2   | 2.42                     | 0.51              |
| 13:UQ:403:VAL:HB   | 13:UQ:412:ALA:HB3   | 1.92                     | 0.51              |
| 16:UX:62:THR:HG23  | 16:UX:99:LEU:HG     | 1.92                     | 0.51              |
| 32:CR:108:TYR:HB2  | 32:CR:111:GLU:HG3   | 1.92                     | 0.51              |
| 37:CD:74:ARG:NH2   | 50:C1:1004:A2M:OP2  | 2.43                     | 0.51              |
| 53:UT:858:ALA:HB1  | 53:UT:865:LEU:HD22  | 1.91                     | 0.51              |
| 53:UT:1305:MET:HA  | 53:UT:1308:ILE:HG12 | 1.92                     | 0.51              |
| 1:UA:507:LEU:HD21  | 1:UA:542:ALA:HB1    | 1.92                     | 0.51              |
| 7:UJ:1224:TYR:HE1  | 7:UJ:1255:LEU:HD12  | 1.73                     | 0.51              |
| 9:UL:900:GLU:OE2   | 9:UL:903:ARG:NH2    | 2.43                     | 0.51              |
| 12:UO:171:LEU:O    | 12:UO:180:THR:N     | 2.43                     | 0.51              |
| 29:CN:114:ILE:HB   | 29:CN:122:ILE:HB    | 1.92                     | 0.51              |
| 37:CD:98:ARG:NH2   | 37:CD:101:ILE:O     | 2.42                     | 0.51              |
| 52:CW:210:ALA:O    | 52:CW:215:GLY:N     | 2.43                     | 0.51              |
| 53:UT:1601:THR:HB  | 53:UT:1643:LYS:HD2  | 1.92                     | 0.51              |
| 58:CX:275:ARG:NH2  | 58:CX:315:THR:OG1   | 2.43                     | 0.51              |
| 59:CY:43:VAL:HG11  | 60:CZ:421:VAL:HG11  | 1.92                     | 0.51              |
| 7:UJ:1185:ALA:HA   | 7:UJ:1188:LYS:HE3   | 1.93                     | 0.51              |
| 9:UL:375:ALA:HB3   | 9:UL:384:GLN:HB2    | 1.91                     | 0.51              |
| 10:UM:452:SER:OG   | 10:UM:453:LYS:N     | 2.43                     | 0.51              |
| 18:CB:239:VAL:HG21 | 18:CB:255:ILE:HD12  | 1.92                     | 0.51              |
| 32:CS:713:SER:O    | 32:CS:716:ARG:NH2   | 2.43                     | 0.51              |
| 47:Co:342:LYS:HB2  | 47:Co:355:VAL:HG12  | 1.92                     | 0.51              |
| 48:Cp:23:ARG:NH2   | 50:C1:1746:C:OP1    | 2.43                     | 0.51              |
| 53:UT:135:VAL:HG12 | 53:UT:177:ARG:HH22  | 1.74                     | 0.51              |
| 58:CX:255:VAL:HG11 | 58:CX:295:ALA:HA    | 1.92                     | 0.51              |
| 4:UD:711:ASP:OD2   | 4:UD:714:GLN:NE2    | 2.42                     | 0.51              |
| 6:UG:187:HIS:NE2   | 6:UG:446:GLU:OE1    | 2.33                     | 0.51              |
| 7:UJ:500:PRO:HB3   | 7:UJ:539:VAL:HA     | 1.91                     | 0.51              |
| 12:UO:461:ARG:NH1  | 12:UO:500:ASP:OD2   | 2.41                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:UQ:665:ARG:HD3   | 13:UQ:720:GLY:HA3   | 1.92                     | 0.51              |
| 15:UU:139:GLN:NE2   | 15:UU:157:THR:OG1   | 2.32                     | 0.51              |
| 15:UU:274:ALA:HB1   | 15:UU:302:THR:HG21  | 1.93                     | 0.51              |
| 17:UZ:89:LEU:HD11   | 17:UZ:244:LYS:HE3   | 1.91                     | 0.51              |
| 53:UT:1310:THR:HG21 | 53:UT:1351:VAL:HG12 | 1.92                     | 0.51              |
| 53:UT:1864:THR:HG23 | 53:UT:1865:ARG:HG2  | 1.92                     | 0.51              |
| 12:UO:115:VAL:HG11  | 12:UO:160:LEU:HD11  | 1.92                     | 0.51              |
| 32:CR:374:PRO:HB2   | 32:CR:398:LEU:HD13  | 1.93                     | 0.51              |
| 37:Cd:38:GLY:HA2    | 37:Cd:41:LEU:HD13   | 1.92                     | 0.51              |
| 54:UH:397:SER:OG    | 54:UH:398:ARG:NH1   | 2.42                     | 0.51              |
| 54:UH:397:SER:O     | 54:UH:425:ARG:NH1   | 2.43                     | 0.51              |
| 7:UJ:1312:LEU:HA    | 7:UJ:1315:VAL:HG12  | 1.92                     | 0.51              |
| 12:UO:166:ASP:OD1   | 12:UO:168:THR:OG1   | 2.29                     | 0.51              |
| 14:UR:138:ASP:OD2   | 15:UU:212:ASN:ND2   | 2.43                     | 0.51              |
| 32:CS:613:LEU:H     | 32:CS:634:ARG:HH22  | 1.57                     | 0.51              |
| 50:C1:467:C:H4'     | 50:C1:468:C:H5'     | 1.93                     | 0.51              |
| 54:UH:13:LEU:HD11   | 54:UH:63:ILE:HG23   | 1.91                     | 0.51              |
| 4:UD:651:THR:OG1    | 4:UD:655:GLN:OE1    | 2.28                     | 0.51              |
| 7:UJ:1728:LYS:O     | 7:UJ:1731:ARG:NH1   | 2.42                     | 0.51              |
| 20:CD:210:VAL:O     | 20:CD:214:LEU:HB3   | 2.11                     | 0.51              |
| 22:CG:307:SER:OG    | 22:CG:308:LYS:N     | 2.43                     | 0.51              |
| 24:CI:183:LYS:NZ    | 50:C1:1050:U:OP2    | 2.41                     | 0.51              |
| 38:Ce:173:ASP:HA    | 38:Ce:176:LEU:HG    | 1.93                     | 0.51              |
| 46:Cn:61:ALA:HB3    | 46:Cn:69:ARG:HG2    | 1.91                     | 0.51              |
| 6:UG:472:ARG:NH1    | 50:C1:333:C:OP1     | 2.43                     | 0.51              |
| 7:UJ:7:GLN:HG2      | 20:CD:422:ASN:HB2   | 1.93                     | 0.51              |
| 7:UJ:756:SER:N      | 7:UJ:759:GLU:OE2    | 2.42                     | 0.51              |
| 9:UL:394:LEU:HB2    | 9:UL:420:VAL:HB     | 1.93                     | 0.51              |
| 10:UM:47:GLU:OE1    | 10:UM:50:THR:N      | 2.35                     | 0.51              |
| 27:CL:618:GLU:OE2   | 27:CL:621:ARG:NH2   | 2.43                     | 0.51              |
| 32:CS:303:VAL:HG11  | 32:CS:331:PHE:HE1   | 1.76                     | 0.51              |
| 32:CS:347:SER:OG    | 32:CS:349:ASN:OD1   | 2.28                     | 0.51              |
| 56:US:344:TYR:O     | 56:US:384:ARG:NH1   | 2.44                     | 0.51              |
| 57:Cl:70:VAL:HA     | 57:Cl:73:ILE:HG22   | 1.93                     | 0.51              |
| 58:CX:383:ASP:OD2   | 58:CX:459:ARG:NH2   | 2.42                     | 0.51              |
| 6:UG:278:GLN:HA     | 6:UG:302:PRO:HB3    | 1.93                     | 0.51              |
| 9:UL:718:LYS:NZ     | 50:C1:2238:A:OP1    | 2.38                     | 0.51              |
| 14:UR:253:ARG:NH2   | 14:UR:551:ASP:OD2   | 2.43                     | 0.51              |
| 32:CR:311:PHE:HB2   | 32:CR:386:VAL:HG12  | 1.93                     | 0.51              |
| 39:Cf:156:VAL:HB    | 39:Cf:160:LEU:HD23  | 1.93                     | 0.51              |
| 53:UT:1572:ILE:HG23 | 53:UT:1607:LEU:HD12 | 1.92                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 58:CX:275:ARG:O    | 58:CX:279:HIS:HB2   | 2.11                     | 0.51              |
| 60:CZ:331:LEU:HD21 | 60:CZ:366:LEU:HD21  | 1.93                     | 0.51              |
| 7:UJ:1354:ILE:HD12 | 7:UJ:1375:LEU:HD22  | 1.92                     | 0.51              |
| 20:CD:178:GLU:HA   | 20:CD:181:VAL:HG12  | 1.93                     | 0.51              |
| 24:CI:113:ARG:NH2  | 24:CI:304:ASP:OD2   | 2.44                     | 0.51              |
| 29:CN:104:ILE:N    | 29:CN:246:GLU:OE2   | 2.44                     | 0.51              |
| 32:CR:88:GLU:HB2   | 32:CR:91:GLN:HB2    | 1.92                     | 0.51              |
| 35:Cb:97:GLU:HA    | 35:Cb:113:ARG:HH12  | 1.76                     | 0.51              |
| 52:CW:296:LEU:HD13 | 52:CW:362:LEU:HD11  | 1.92                     | 0.51              |
| 53:UT:1505:ILE:HA  | 53:UT:1508:VAL:HG22 | 1.92                     | 0.51              |
| 10:UM:864:LYS:NZ   | 10:UM:868:GLU:OE2   | 2.44                     | 0.50              |
| 14:UR:139:SEP:O2P  | 14:UR:143:ARG:NH2   | 2.40                     | 0.50              |
| 14:UR:322:ARG:HE   | 50:C1:133:G:H1      | 1.59                     | 0.50              |
| 32:CR:622:PHE:O    | 32:CS:839:LYS:NZ    | 2.40                     | 0.50              |
| 32:CS:120:TYR:HB2  | 32:CS:142:THR:HB    | 1.94                     | 0.50              |
| 32:CS:589:SER:HB3  | 32:CS:634:ARG:HG2   | 1.94                     | 0.50              |
| 32:CS:613:LEU:N    | 32:CS:634:ARG:HH22  | 2.08                     | 0.50              |
| 34:Ca:204:ILE:O    | 50:C1:1648:G:O2'    | 2.29                     | 0.50              |
| 50:C1:808:A:H61    | 50:C1:821:C:H2'     | 1.75                     | 0.50              |
| 52:CW:170:ARG:HH12 | 52:CW:234:LYS:HG2   | 1.76                     | 0.50              |
| 53:UT:1580:PHE:HB2 | 53:UT:1604:ILE:HD11 | 1.92                     | 0.50              |
| 2:UB:14:ARG:NH1    | 50:C1:1733:G:OP1    | 2.44                     | 0.50              |
| 4:UD:477:THR:OG1   | 4:UD:478:GLY:N      | 2.42                     | 0.50              |
| 5:UF:278:ILE:HG23  | 11:UN:373:ILE:HD12  | 1.93                     | 0.50              |
| 10:UM:638:PHE:HE1  | 10:UM:683:GLY:HA2   | 1.76                     | 0.50              |
| 35:Cb:80:ILE:HG23  | 35:Cb:81:THR:HG23   | 1.93                     | 0.50              |
| 53:UT:364:LEU:HD22 | 53:UT:397:VAL:HG11  | 1.92                     | 0.50              |
| 7:UJ:1749:THR:HG21 | 7:UJ:1785:TRP:HE1   | 1.76                     | 0.50              |
| 9:UL:517:HIS:ND1   | 9:UL:519:ASP:OD1    | 2.44                     | 0.50              |
| 10:UM:623:THR:HG22 | 10:UM:639:GLU:HG3   | 1.93                     | 0.50              |
| 28:CM:193:TRP:HB3  | 28:CM:196:PHE:HB2   | 1.93                     | 0.50              |
| 32:CS:278:ARG:HG2  | 32:CS:467:ARG:HA    | 1.93                     | 0.50              |
| 39:Cf:172:ILE:O    | 39:Cf:185:GLY:HA3   | 2.11                     | 0.50              |
| 60:CZ:566:GLU:HA   | 60:CZ:569:ILE:HG12  | 1.92                     | 0.50              |
| 6:UG:578:ILE:HB    | 30:CP:72:ASP:HA     | 1.92                     | 0.50              |
| 10:UM:259:TRP:HA   | 10:UM:268:GLY:HA3   | 1.93                     | 0.50              |
| 18:CA:239:VAL:HG21 | 18:CA:255:ILE:HD12  | 1.93                     | 0.50              |
| 22:CG:124:ASP:HB3  | 22:CG:127:GLU:HG2   | 1.94                     | 0.50              |
| 34:Ca:66:PHE:HE1   | 42:CI:47:SER:HB3    | 1.76                     | 0.50              |
| 34:Ca:164:ILE:HD11 | 34:Ca:205:TYR:HB3   | 1.93                     | 0.50              |
| 53:UT:232:ILE:HA   | 53:UT:235:VAL:HG22  | 1.92                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:UT:490:LEU:HD21 | 53:UT:494:TRP:HB2  | 1.94                     | 0.50              |
| 4:UD:366:PRO:HB3   | 4:UD:704:VAL:HG21  | 1.92                     | 0.50              |
| 6:UG:588:LEU:HG    | 6:UG:592:MET:HE2   | 1.94                     | 0.50              |
| 18:CA:110:SER:HB3  | 33:CT:141:ILE:HD11 | 1.93                     | 0.50              |
| 31:CQ:116:ASN:ND2  | 31:CQ:119:GLU:OE2  | 2.43                     | 0.50              |
| 32:CR:592:GLY:HA3  | 32:CR:631:SER:HA   | 1.94                     | 0.50              |
| 32:CS:380:LEU:O    | 32:CS:383:ALA:HB3  | 2.12                     | 0.50              |
| 37:Cd:183:THR:HG22 | 37:Cd:185:GLN:H    | 1.75                     | 0.50              |
| 39:Cf:34:ALA:HB2   | 39:Cf:56:ARG:HD2   | 1.93                     | 0.50              |
| 54:UH:347:LEU:HD21 | 54:UH:394:TYR:HB2  | 1.93                     | 0.50              |
| 58:CX:199:VAL:HA   | 58:CX:236:LEU:HD21 | 1.93                     | 0.50              |
| 13:UQ:713:VAL:HG13 | 13:UQ:722:VAL:HG13 | 1.93                     | 0.50              |
| 14:UR:253:ARG:HG2  | 14:UR:617:ARG:HA   | 1.93                     | 0.50              |
| 17:UZ:105:GLN:NE2  | 50:C1:2062:A:OP1   | 2.44                     | 0.50              |
| 28:CM:242:CYS:HA   | 28:CM:259:SER:HA   | 1.93                     | 0.50              |
| 30:CP:285:GLU:O    | 30:CP:288:ARG:HD3  | 2.12                     | 0.50              |
| 32:CR:425:SER:O    | 32:CR:429:ILE:HB   | 2.11                     | 0.50              |
| 50:C1:934:A:H5''   | 50:C1:936:A:H5'    | 1.94                     | 0.50              |
| 54:UH:6:GLN:HB2    | 54:UH:415:GLU:HB3  | 1.92                     | 0.50              |
| 55:UE:194:GLY:HA3  | 55:UE:235:LEU:HD11 | 1.93                     | 0.50              |
| 7:UJ:717:THR:HG22  | 7:UJ:719:LEU:H     | 1.75                     | 0.50              |
| 22:CG:177:ALA:HB3  | 22:CG:184:TYR:HB2  | 1.94                     | 0.50              |
| 24:CI:358:GLY:HA2  | 32:CR:3:VAL:HG21   | 1.94                     | 0.50              |
| 34:Ca:129:THR:OG1  | 34:Ca:179:CYS:O    | 2.30                     | 0.50              |
| 44:Ck:78:GLY:HA3   | 44:Ck:91:ILE:HD12  | 1.93                     | 0.50              |
| 49:CU:111:MET:HB3  | 49:CU:115:GLU:HB2  | 1.94                     | 0.50              |
| 53:UT:283:ARG:HA   | 53:UT:334:GLN:HE22 | 1.76                     | 0.50              |
| 54:UH:571:LEU:HB3  | 54:UH:574:SER:HB2  | 1.93                     | 0.50              |
| 58:CX:270:ILE:HA   | 58:CX:273:ARG:HB3  | 1.94                     | 0.50              |
| 1:UA:392:LYS:HE2   | 1:UA:435:PRO:HB2   | 1.94                     | 0.50              |
| 1:UA:565:THR:HG23  | 51:C2:61:G:H5'     | 1.92                     | 0.50              |
| 7:UJ:1290:ARG:HE   | 7:UJ:1294:GLU:HG3  | 1.77                     | 0.50              |
| 7:UJ:1370:MET:HA   | 7:UJ:1373:LEU:HD23 | 1.93                     | 0.50              |
| 24:CI:273:TYR:OH   | 24:CI:304:ASP:OD1  | 2.27                     | 0.50              |
| 32:CR:112:THR:HA   | 32:CR:115:ILE:HG12 | 1.93                     | 0.50              |
| 32:CS:495:CYS:HB3  | 32:CS:541:VAL:HG11 | 1.94                     | 0.50              |
| 7:UJ:1051:GLN:HA   | 7:UJ:1054:LYS:HG2  | 1.94                     | 0.50              |
| 10:UM:53:ARG:NH1   | 10:UM:56:GLU:OE2   | 2.44                     | 0.50              |
| 32:CS:240:LYS:HD3  | 32:CS:253:ILE:HG22 | 1.93                     | 0.50              |
| 46:Cn:102:VAL:HG13 | 46:Cn:124:VAL:HG13 | 1.94                     | 0.50              |
| 53:UT:184:ARG:HH22 | 53:UT:231:PHE:HD1  | 1.60                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:UT:299:SER:OG   | 53:UT:340:ARG:NH1   | 2.44                     | 0.50              |
| 53:UT:1577:ILE:O   | 53:UT:1581:GLU:HB2  | 2.12                     | 0.50              |
| 3:UC:279:ILE:HD13  | 27:CL:141:TRP:HE1   | 1.76                     | 0.49              |
| 4:UD:439:ASP:OD1   | 4:UD:439:ASP:N      | 2.41                     | 0.49              |
| 7:UJ:1398:LEU:HA   | 7:UJ:1401:LEU:HD23  | 1.94                     | 0.49              |
| 7:UJ:1600:LEU:HA   | 7:UJ:1603:VAL:HG22  | 1.92                     | 0.49              |
| 24:CI:617:ASP:OD1  | 24:CI:620:ARG:NH2   | 2.32                     | 0.49              |
| 53:UT:1274:GLN:HG3 | 53:UT:1276:ASP:H    | 1.76                     | 0.49              |
| 59:CY:92:LEU:HD23  | 59:CY:95:TYR:HD2    | 1.76                     | 0.49              |
| 4:UD:65:GLN:HB3    | 4:UD:370:GLN:HB2    | 1.94                     | 0.49              |
| 7:UJ:727:LEU:HD11  | 7:UJ:781:VAL:HG12   | 1.93                     | 0.49              |
| 8:UK:63:PHE:HB2    | 25:CJ:170:ILE:HD11  | 1.94                     | 0.49              |
| 24:CI:70:LEU:HD12  | 24:CI:115:THR:HG23  | 1.94                     | 0.49              |
| 32:CR:155:GLY:O    | 32:CR:159:LEU:HB2   | 2.11                     | 0.49              |
| 32:CR:641:ASN:HD21 | 32:CR:643:ASP:HB2   | 1.77                     | 0.49              |
| 39:Cf:81:VAL:HG12  | 39:Cf:102:VAL:HG12  | 1.93                     | 0.49              |
| 53:UT:1552:LEU:HB3 | 53:UT:1556:ARG:NH1  | 2.27                     | 0.49              |
| 56:US:187:GLU:OE2  | 56:US:188:ASN:ND2   | 2.45                     | 0.49              |
| 59:CY:32:GLU:O     | 60:CZ:316:LYS:NZ    | 2.44                     | 0.49              |
| 7:UJ:636:ASP:OD1   | 7:UJ:636:ASP:N      | 2.42                     | 0.49              |
| 13:UQ:847:ASP:OD1  | 13:UQ:847:ASP:N     | 2.43                     | 0.49              |
| 20:CD:36:LEU:HA    | 20:CD:39:ILE:HG22   | 1.93                     | 0.49              |
| 34:Ca:25:THR:O     | 34:Ca:50:ARG:NH2    | 2.45                     | 0.49              |
| 35:Cb:87:MET:CA    | 35:Cb:101:LEU:O     | 2.61                     | 0.49              |
| 50:C1:461:G:N7     | 59:CY:377:ARG:NH2   | 2.60                     | 0.49              |
| 52:CW:298:THR:HB   | 52:CW:302:GLU:HB2   | 1.93                     | 0.49              |
| 1:UA:11:LEU:HB2    | 1:UA:695:LEU:HB2    | 1.94                     | 0.49              |
| 7:UJ:786:HIS:HE1   | 7:UJ:788:ALA:HB3    | 1.75                     | 0.49              |
| 12:UO:551:MET:HE1  | 55:UE:236:ILE:HG13  | 1.94                     | 0.49              |
| 13:UQ:736:ALA:HB3  | 13:UQ:747:LEU:HB3   | 1.94                     | 0.49              |
| 27:CL:667:GLN:HB3  | 27:CL:671:GLY:HA3   | 1.94                     | 0.49              |
| 55:UI:275:ALA:O    | 55:UI:279:ALA:HB3   | 2.13                     | 0.49              |
| 2:UB:659:ASN:OD1   | 56:US:391:ASN:ND2   | 2.44                     | 0.49              |
| 2:UB:661:LEU:HD13  | 2:UB:733:LEU:HD22   | 1.95                     | 0.49              |
| 7:UJ:1273:ASP:O    | 7:UJ:1280:ARG:NH2   | 2.45                     | 0.49              |
| 10:UM:70:THR:HB    | 10:UM:123:SER:HB2   | 1.95                     | 0.49              |
| 16:UX:108:VAL:HA   | 16:UX:111:MET:HE3   | 1.93                     | 0.49              |
| 32:CS:660:TYR:HD1  | 32:CS:665:PHE:HB2   | 1.78                     | 0.49              |
| 53:UT:1328:ILE:HA  | 53:UT:1331:ILE:HG22 | 1.95                     | 0.49              |
| 59:CY:47:LEU:HD21  | 60:CZ:418:ARG:HD3   | 1.94                     | 0.49              |
| 59:CY:317:GLY:O    | 59:CY:320:ARG:HG2   | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:UB:652:ARG:HD3   | 56:US:467:TYR:HA   | 1.95                     | 0.49              |
| 4:UD:481:ALA:HA    | 4:UD:497:GLU:HA    | 1.93                     | 0.49              |
| 4:UD:686:ARG:NH2   | 4:UD:745:SER:OG    | 2.44                     | 0.49              |
| 11:UN:282:LEU:HD11 | 53:UT:2158:LYS:HG2 | 1.94                     | 0.49              |
| 13:UQ:455:VAL:HA   | 54:UH:888:ILE:HD11 | 1.94                     | 0.49              |
| 13:UQ:521:PRO:HG3  | 55:UE:26:THR:HG21  | 1.93                     | 0.49              |
| 22:CG:314:VAL:HG13 | 22:CG:323:VAL:HG23 | 1.94                     | 0.49              |
| 30:CP:291:LYS:HB3  | 30:CP:295:LYS:HZ3  | 1.78                     | 0.49              |
| 34:Ca:71:ALA:HB3   | 42:CI:127:ARG:HH21 | 1.77                     | 0.49              |
| 39:Cf:114:GLU:OE2  | 39:Cf:121:LEU:N    | 2.45                     | 0.49              |
| 52:CW:284:GLN:HE22 | 52:CW:309:ASP:HB2  | 1.77                     | 0.49              |
| 56:US:394:PRO:HA   | 56:US:397:ILE:HD12 | 1.95                     | 0.49              |
| 2:UB:608:HIS:HB3   | 2:UB:611:CYS:HB2   | 1.94                     | 0.49              |
| 3:UC:209:VAL:HB    | 27:CL:65:ARG:HB2   | 1.94                     | 0.49              |
| 4:UD:6:CYS:HB2     | 4:UD:863:ILE:HG13  | 1.93                     | 0.49              |
| 7:UJ:1259:LEU:HD11 | 7:UJ:1262:ALA:HB3  | 1.94                     | 0.49              |
| 9:UL:693:ASP:OD1   | 9:UL:693:ASP:N     | 2.46                     | 0.49              |
| 24:CI:867:MET:HB2  | 50:C1:1156:C:C4    | 2.48                     | 0.49              |
| 32:CR:282:THR:OG1  | 32:CR:471:GLU:OE1  | 2.31                     | 0.49              |
| 32:CR:913:MET:HA   | 32:CR:916:MET:HE2  | 1.94                     | 0.49              |
| 32:CS:178:HIS:HE1  | 32:CS:590:LEU:HD23 | 1.78                     | 0.49              |
| 32:CS:586:ILE:HG21 | 32:CS:657:LEU:HD22 | 1.94                     | 0.49              |
| 54:UH:4:LYS:NZ     | 54:UH:601:GLU:O    | 2.46                     | 0.49              |
| 7:UJ:297:VAL:HG11  | 7:UJ:328:VAL:HG23  | 1.94                     | 0.49              |
| 9:UL:399:ILE:HD13  | 9:UL:414:TYR:HB3   | 1.95                     | 0.49              |
| 9:UL:431:SER:OG    | 9:UL:469:LEU:O     | 2.29                     | 0.49              |
| 13:UQ:927:ALA:O    | 13:UQ:931:ASN:HB2  | 2.13                     | 0.49              |
| 17:UZ:138:LYS:NZ   | 50:C1:2108:A:OP1   | 2.35                     | 0.49              |
| 18:CB:93:CYS:HB3   | 18:CB:129:ILE:HD13 | 1.94                     | 0.49              |
| 22:CG:486:CYS:SG   | 22:CG:488:ARG:NE   | 2.78                     | 0.49              |
| 29:CO:42:SER:HA    | 29:CO:115:GLN:HB3  | 1.95                     | 0.49              |
| 30:CP:188:THR:HG23 | 30:CP:194:PRO:HD3  | 1.95                     | 0.49              |
| 32:CR:188:ARG:NH1  | 32:CR:493:LEU:O    | 2.36                     | 0.49              |
| 32:CS:917:ARG:NH2  | 52:CW:380:GLU:O    | 2.46                     | 0.49              |
| 41:Ch:147:SER:HA   | 41:Ch:150:VAL:HG22 | 1.94                     | 0.49              |
| 53:UT:275:PRO:HD3  | 53:UT:321:VAL:HG22 | 1.94                     | 0.49              |
| 53:UT:279:SER:OG   | 53:UT:324:ARG:NH1  | 2.46                     | 0.49              |
| 54:UH:277:GLU:OE2  | 54:UH:281:ARG:NH2  | 2.43                     | 0.49              |
| 2:UB:713:LEU:HD13  | 2:UB:717:GLU:HG3   | 1.94                     | 0.49              |
| 4:UD:483:ARG:HB2   | 4:UD:496:ALA:HB3   | 1.94                     | 0.49              |
| 4:UD:644:ASP:HA    | 4:UD:662:LEU:HD12  | 1.95                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:UQ:218:ILE:HD12  | 13:UQ:235:HIS:HB3   | 1.94                     | 0.49              |
| 53:UT:387:TRP:CH2   | 53:UT:428:PRO:HB2   | 2.48                     | 0.49              |
| 53:UT:416:ALA:O     | 53:UT:419:LYS:NZ    | 2.36                     | 0.49              |
| 53:UT:969:PHE:HZ    | 53:UT:1023:ILE:HD11 | 1.76                     | 0.49              |
| 53:UT:1313:LEU:HD22 | 53:UT:1358:LEU:HD21 | 1.95                     | 0.49              |
| 53:UT:1347:LEU:HA   | 53:UT:1350:LYS:HG2  | 1.95                     | 0.49              |
| 58:CX:277:ASP:OD1   | 58:CX:278:ILE:N     | 2.45                     | 0.49              |
| 60:CZ:301:SER:HG    | 60:CZ:305:ARG:HH12  | 1.58                     | 0.49              |
| 1:UA:713:MET:HE3    | 15:UU:702:GLU:HB2   | 1.95                     | 0.49              |
| 7:UJ:170:TYR:O      | 7:UJ:173:SER:O      | 2.30                     | 0.49              |
| 10:UM:540:ARG:NH2   | 10:UM:575:LYS:O     | 2.46                     | 0.49              |
| 17:UZ:282:TYR:HB3   | 17:UZ:290:ALA:HB1   | 1.94                     | 0.49              |
| 53:UT:264:LYS:HG2   | 53:UT:312:HIS:ND1   | 2.28                     | 0.49              |
| 53:UT:1037:ASP:O    | 53:UT:1044:ARG:NH1  | 2.43                     | 0.49              |
| 54:UH:220:ALA:HB1   | 54:UH:242:ILE:HD13  | 1.94                     | 0.49              |
| 55:UE:232:GLN:HG3   | 55:UE:235:LEU:HD23  | 1.94                     | 0.49              |
| 2:UB:574:ARG:HG2    | 2:UB:593:ILE:HD13   | 1.95                     | 0.48              |
| 4:UD:633:LEU:HD12   | 4:UD:649:VAL:HG22   | 1.95                     | 0.48              |
| 7:UJ:1241:LYS:HB2   | 7:UJ:1244:LEU:HB2   | 1.95                     | 0.48              |
| 10:UM:389:MET:O     | 10:UM:400:ILE:HA    | 2.13                     | 0.48              |
| 15:UU:404:GLY:HA3   | 15:UU:758:HIS:HB2   | 1.95                     | 0.48              |
| 17:UZ:235:LEU:HD11  | 17:UZ:270:PHE:HB3   | 1.95                     | 0.48              |
| 18:CA:113:THR:HG21  | 18:CA:124:LYS:HE3   | 1.94                     | 0.48              |
| 20:CD:293:ILE:HD12  | 20:CD:297:VAL:HG12  | 1.95                     | 0.48              |
| 37:Cd:58:LYS:HE2    | 37:Cd:105:ASP:HA    | 1.95                     | 0.48              |
| 45:Cm:78:ARG:HD3    | 45:Cm:126:ILE:HG22  | 1.95                     | 0.48              |
| 53:UT:830:GLU:O     | 53:UT:834:LYS:HB2   | 2.12                     | 0.48              |
| 21:CF:35:LYS:HB3    | 21:CF:40:GLU:HG2    | 1.95                     | 0.48              |
| 26:CK:76:GLU:HG2    | 26:CK:160:GLY:HA2   | 1.95                     | 0.48              |
| 27:CL:67:THR:HB     | 27:CL:70:LEU:HD12   | 1.95                     | 0.48              |
| 32:CR:281:VAL:HG22  | 32:CR:409:PHE:CD2   | 2.48                     | 0.48              |
| 32:CS:651:SER:HA    | 32:CS:736:PHE:HE1   | 1.77                     | 0.48              |
| 53:UT:1919:ILE:HD13 | 53:UT:1992:VAL:HG11 | 1.94                     | 0.48              |
| 57:Cl:12:ASN:HA     | 57:Cl:25:LYS:HB2    | 1.95                     | 0.48              |
| 7:UJ:741:ARG:NH2    | 7:UJ:780:ASP:O      | 2.45                     | 0.48              |
| 9:UL:12:LYS:HD3     | 9:UL:457:GLN:HG2    | 1.96                     | 0.48              |
| 13:UQ:487:GLN:HA    | 13:UQ:490:VAL:HG22  | 1.94                     | 0.48              |
| 22:CG:593:TYR:HH    | 51:C2:189:G:HO2'    | 1.52                     | 0.48              |
| 32:CR:586:ILE:HG21  | 32:CR:657:LEU:HD22  | 1.95                     | 0.48              |
| 32:CS:96:GLU:HA     | 32:CS:99:ILE:HG12   | 1.94                     | 0.48              |
| 53:UT:2164:LEU:HD23 | 53:UT:2175:VAL:HG13 | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:CX:307:LEU:HA   | 58:CX:310:LEU:HD12 | 1.96                     | 0.48              |
| 60:CZ:367:TRP:HZ3  | 60:CZ:374:ARG:HH12 | 1.60                     | 0.48              |
| 1:UA:425:ARG:HD3   | 27:CL:642:PRO:HA   | 1.95                     | 0.48              |
| 2:UB:615:MET:HA    | 2:UB:618:ILE:HG22  | 1.94                     | 0.48              |
| 2:UB:618:ILE:HG13  | 2:UB:639:LEU:HD13  | 1.96                     | 0.48              |
| 7:UJ:1315:VAL:O    | 7:UJ:1319:SER:OG   | 2.25                     | 0.48              |
| 14:UR:253:ARG:NH1  | 14:UR:599:SER:O    | 2.45                     | 0.48              |
| 14:UR:476:GLU:HB2  | 14:UR:524:ILE:HD11 | 1.95                     | 0.48              |
| 53:UT:300:ASP:OD1  | 53:UT:340:ARG:NH2  | 2.36                     | 0.48              |
| 4:UD:757:ILE:HB    | 4:UD:771:ILE:O     | 2.14                     | 0.48              |
| 7:UJ:338:LEU:HD21  | 7:UJ:358:LEU:HD21  | 1.96                     | 0.48              |
| 7:UJ:1008:LEU:HA   | 7:UJ:1011:VAL:HG22 | 1.95                     | 0.48              |
| 15:UU:677:ASN:HB3  | 15:UU:679:LEU:HG   | 1.95                     | 0.48              |
| 24:CI:523:MET:HA   | 24:CI:526:ARG:HE   | 1.78                     | 0.48              |
| 32:CR:271:ALA:O    | 32:CR:279:ASN:ND2  | 2.46                     | 0.48              |
| 32:CS:188:ARG:HH21 | 32:CS:191:LEU:HG   | 1.79                     | 0.48              |
| 38:Ce:50:VAL:HG23  | 38:Ce:51:SER:H     | 1.78                     | 0.48              |
| 53:UT:1608:THR:HA  | 53:UT:1611:LEU:HG  | 1.96                     | 0.48              |
| 54:UH:700:ASP:OD1  | 54:UH:700:ASP:N    | 2.47                     | 0.48              |
| 4:UD:158:THR:O     | 4:UD:161:GLY:N     | 2.47                     | 0.48              |
| 4:UD:632:VAL:O     | 4:UD:649:VAL:HA    | 2.13                     | 0.48              |
| 7:UJ:296:LEU:HD22  | 7:UJ:312:LEU:HG    | 1.95                     | 0.48              |
| 7:UJ:1228:LEU:HD23 | 7:UJ:1271:LEU:HD12 | 1.96                     | 0.48              |
| 10:UM:45:LEU:HB2   | 10:UM:55:ALA:HB3   | 1.95                     | 0.48              |
| 15:UU:420:TRP:HA   | 15:UU:428:SER:HB2  | 1.96                     | 0.48              |
| 27:CL:82:LEU:HD13  | 27:CL:130:VAL:HG21 | 1.95                     | 0.48              |
| 32:CS:229:LEU:O    | 32:CS:234:LYS:NZ   | 2.46                     | 0.48              |
| 34:Ca:141:ALA:HB2  | 34:Ca:168:MET:HE1  | 1.96                     | 0.48              |
| 53:UT:559:LEU:HD11 | 53:UT:578:THR:HA   | 1.96                     | 0.48              |
| 56:US:287:GLU:HG3  | 56:US:359:ARG:HH12 | 1.79                     | 0.48              |
| 58:CX:424:ASP:O    | 58:CX:459:ARG:NH1  | 2.46                     | 0.48              |
| 60:CZ:411:GLU:HA   | 60:CZ:414:VAL:HG22 | 1.96                     | 0.48              |
| 1:UA:751:GLN:HG2   | 15:UU:836:LEU:HD21 | 1.94                     | 0.48              |
| 4:UD:356:ALA:HB1   | 4:UD:359:LYS:HB3   | 1.95                     | 0.48              |
| 13:UQ:747:LEU:HD13 | 13:UQ:780:LEU:HB2  | 1.95                     | 0.48              |
| 23:CH:22:VAL:HG13  | 23:CH:120:LEU:HD13 | 1.94                     | 0.48              |
| 24:CI:308:THR:H    | 24:CI:311:MET:HE2  | 1.79                     | 0.48              |
| 29:CN:164:GLN:HB3  | 50:C1:2158:G:H5''  | 1.95                     | 0.48              |
| 32:CR:395:PRO:HG2  | 32:CR:398:LEU:HD12 | 1.95                     | 0.48              |
| 32:CR:723:VAL:HG23 | 32:CR:766:LEU:HD11 | 1.95                     | 0.48              |
| 32:CR:905:GLY:HA2  | 32:CR:908:VAL:HB   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:Ca:158:SER:OG   | 50:C1:1461:G:OP1    | 2.30                     | 0.48              |
| 35:Cb:199:GLU:OE1  | 35:Cb:201:HIS:ND1   | 2.43                     | 0.48              |
| 39:Cf:10:LYS:NZ    | 50:C1:921:G:O3'     | 2.47                     | 0.48              |
| 7:UJ:780:ASP:HA    | 7:UJ:812:ARG:HE     | 1.79                     | 0.48              |
| 10:UM:619:SER:OG   | 10:UM:620:GLY:N     | 2.47                     | 0.48              |
| 17:UZ:275:TRP:HA   | 17:UZ:278:VAL:HG12  | 1.94                     | 0.48              |
| 20:CD:24:LEU:HD21  | 20:CD:118:LEU:HD22  | 1.95                     | 0.48              |
| 22:CG:95:THR:HB    | 22:CG:98:GLU:HG2    | 1.95                     | 0.48              |
| 26:CK:85:ASP:OD2   | 27:CL:559:ARG:NH2   | 2.46                     | 0.48              |
| 32:CR:284:THR:HB   | 32:CR:414:ILE:HG13  | 1.96                     | 0.48              |
| 32:CS:285:ALA:O    | 32:CS:413:THR:HA    | 2.14                     | 0.48              |
| 32:CS:387:VAL:HG22 | 32:CS:409:PHE:HB2   | 1.95                     | 0.48              |
| 38:Ce:38:ALA:HA    | 38:Ce:39:ASP:HB2    | 1.96                     | 0.48              |
| 50:C1:103:G:O2'    | 50:C1:106:A:N6      | 2.46                     | 0.48              |
| 50:C1:781:G:H2'    | 50:C1:782:G:H8      | 1.77                     | 0.48              |
| 53:UT:1055:ARG:HE  | 53:UT:1058:VAL:HG21 | 1.78                     | 0.48              |
| 53:UT:1504:GLU:HA  | 53:UT:1507:ARG:HG2  | 1.95                     | 0.48              |
| 56:US:416:PHE:O    | 56:US:420:ARG:HB2   | 2.12                     | 0.48              |
| 55:UI:161:LEU:HD21 | 55:UI:196:LEU:HD12  | 1.96                     | 0.48              |
| 1:UA:323:LEU:HD12  | 1:UA:335:LYS:HG3    | 1.96                     | 0.48              |
| 7:UJ:1218:GLY:O    | 7:UJ:1221:ARG:NH1   | 2.47                     | 0.48              |
| 10:UM:563:SER:OG   | 10:UM:564:GLN:N     | 2.47                     | 0.48              |
| 13:UQ:671:VAL:HG22 | 54:UH:718:PRO:HD3   | 1.96                     | 0.48              |
| 20:CD:33:LEU:HD22  | 20:CD:39:ILE:HD12   | 1.96                     | 0.48              |
| 24:CI:544:ARG:O    | 24:CI:548:ASP:HB2   | 2.13                     | 0.48              |
| 29:CO:83:ASP:HB3   | 29:CO:86:ASP:HB2    | 1.96                     | 0.48              |
| 32:CS:59:ALA:HB3   | 32:CS:125:LEU:HD13  | 1.96                     | 0.48              |
| 38:Ce:76:PHE:O     | 38:Ce:80:GLN:CB     | 2.51                     | 0.48              |
| 50:C1:626:A:OP2    | 59:CY:291:ARG:NH2   | 2.47                     | 0.48              |
| 53:UT:259:PHE:O    | 53:UT:263:MET:HG2   | 2.13                     | 0.48              |
| 58:CX:371:LEU:HD11 | 58:CX:417:PHE:HD1   | 1.78                     | 0.48              |
| 1:UA:832:ARG:HH21  | 27:CL:669:VAL:HG13  | 1.78                     | 0.48              |
| 7:UJ:1112:PHE:HA   | 7:UJ:1147:THR:HG23  | 1.96                     | 0.48              |
| 7:UJ:1534:ARG:HA   | 7:UJ:1538:ALA:HB3   | 1.94                     | 0.48              |
| 26:CK:229:THR:HG21 | 27:CL:545:ILE:HD11  | 1.96                     | 0.48              |
| 32:CS:876:LEU:HD12 | 32:CS:880:GLN:HB3   | 1.96                     | 0.48              |
| 32:CS:911:ILE:HA   | 32:CS:914:LYS:HD2   | 1.96                     | 0.48              |
| 36:Cc:35:TYR:CD1   | 36:Cc:54:PRO:HB3    | 2.49                     | 0.48              |
| 39:Cf:57:ALA:HB2   | 39:Cf:181:GLY:HA2   | 1.95                     | 0.48              |
| 50:C1:176:G:H2'    | 50:C1:177:G:H8      | 1.79                     | 0.48              |
| 53:UT:575:ASN:OD1  | 53:UT:576:PHE:N     | 2.47                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:UT:1625:SER:O   | 53:UT:1629:SER:HB3  | 2.14                     | 0.48              |
| 56:US:220:ARG:HD2  | 56:US:275:LEU:HD13  | 1.95                     | 0.48              |
| 1:UA:195:ARG:HH22  | 50:C1:285:A:H5''    | 1.79                     | 0.47              |
| 1:UA:716:THR:HG22  | 1:UA:718:ALA:H      | 1.79                     | 0.47              |
| 4:UD:802:ARG:HA    | 4:UD:805:GLU:HG3    | 1.96                     | 0.47              |
| 7:UJ:970:MET:HE3   | 7:UJ:1013:SER:HB2   | 1.96                     | 0.47              |
| 9:UL:815:ASN:HB3   | 9:UL:818:PHE:HD2    | 1.78                     | 0.47              |
| 10:UM:132:ASP:HB2  | 10:UM:152:PRO:HB3   | 1.95                     | 0.47              |
| 15:UU:514:ALA:HB2  | 15:UU:547:VAL:HG13  | 1.96                     | 0.47              |
| 35:Cb:89:VAL:HA    | 35:Cb:99:PHE:O      | 2.14                     | 0.47              |
| 38:Ce:40:LEU:HD22  | 38:Ce:82:ARG:HH21   | 1.79                     | 0.47              |
| 50:C1:858:G:OP2    | 53:UT:198:LYS:NZ    | 2.47                     | 0.47              |
| 51:C2:160:U:H2'    | 51:C2:161:G:H8      | 1.79                     | 0.47              |
| 1:UA:195:ARG:NH2   | 50:C1:285:A:H5''    | 2.29                     | 0.47              |
| 7:UJ:380:SER:O     | 7:UJ:384:SER:HB3    | 2.14                     | 0.47              |
| 7:UJ:491:THR:HA    | 7:UJ:494:ARG:HG2    | 1.96                     | 0.47              |
| 13:UQ:754:TYR:OH   | 13:UQ:759:ASP:OD1   | 2.26                     | 0.47              |
| 14:UR:322:ARG:NH2  | 50:C1:133:G:H22     | 2.12                     | 0.47              |
| 22:CG:401:VAL:HG23 | 22:CG:411:THR:HG22  | 1.95                     | 0.47              |
| 29:CN:40:VAL:HG22  | 29:CN:113:TYR:HB2   | 1.96                     | 0.47              |
| 39:Cf:81:VAL:HG22  | 39:Cf:94:ASN:HA     | 1.96                     | 0.47              |
| 44:Ck:11:ARG:NH2   | 50:C1:926:C:O2'     | 2.48                     | 0.47              |
| 50:C1:661:U:N3     | 53:UT:801:CYS:SG    | 2.76                     | 0.47              |
| 53:UT:1852:ASP:OD1 | 53:UT:1852:ASP:N    | 2.44                     | 0.47              |
| 54:UH:372:LEU:HD23 | 54:UH:600:ARG:HH12  | 1.79                     | 0.47              |
| 1:UA:364:ILE:HD11  | 1:UA:381:HIS:HD2    | 1.79                     | 0.47              |
| 7:UJ:1730:LEU:HB3  | 7:UJ:1741:VAL:HG21  | 1.96                     | 0.47              |
| 9:UL:25:VAL:HB     | 9:UL:40:ILE:HB      | 1.96                     | 0.47              |
| 21:CF:34:LEU:HD11  | 21:CF:101:VAL:HB    | 1.96                     | 0.47              |
| 21:CF:121:LYS:HG2  | 21:CF:124:ARG:HH21  | 1.78                     | 0.47              |
| 32:CS:20:GLN:HG2   | 32:CS:220:LEU:HD11  | 1.96                     | 0.47              |
| 53:UT:1982:THR:OG1 | 53:UT:1985:ASN:OD1  | 2.33                     | 0.47              |
| 7:UJ:556:LEU:HD11  | 7:UJ:595:TYR:HB3    | 1.96                     | 0.47              |
| 50:C1:1613:C:H4'   | 50:C1:1614:U:H5'    | 1.97                     | 0.47              |
| 53:UT:1447:GLU:H   | 53:UT:1451:LEU:HD21 | 1.79                     | 0.47              |
| 55:UE:211:ALA:HB1  | 55:UE:215:MET:HE2   | 1.97                     | 0.47              |
| 2:UB:599:THR:HG21  | 56:US:523:ILE:HG23  | 1.97                     | 0.47              |
| 2:UB:710:LYS:HB2   | 2:UB:713:LEU:HD23   | 1.96                     | 0.47              |
| 4:UD:549:VAL:HA    | 4:UD:565:ASP:HA     | 1.96                     | 0.47              |
| 7:UJ:864:ASP:OD1   | 7:UJ:864:ASP:N      | 2.48                     | 0.47              |
| 9:UL:222:ALA:HB3   | 9:UL:235:ALA:HB3    | 1.97                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:UL:384:GLN:HB3    | 9:UL:396:LEU:HD11   | 1.95                     | 0.47              |
| 13:UQ:637:PHE:O     | 13:UQ:664:SER:N     | 2.47                     | 0.47              |
| 23:CH:405:ASN:C     | 23:CH:405:ASN:HD22  | 2.19                     | 0.47              |
| 24:CI:954:THR:O     | 24:CI:957:GLY:N     | 2.34                     | 0.47              |
| 29:CN:71:ASP:OD1    | 29:CN:72:GLU:N      | 2.48                     | 0.47              |
| 30:CP:291:LYS:HB3   | 30:CP:295:LYS:NZ    | 2.29                     | 0.47              |
| 37:Cd:57:ASP:OD1    | 37:Cd:61:PHE:N      | 2.46                     | 0.47              |
| 37:Cd:179:GLN:HG2   | 50:C1:753:A:H5'     | 1.97                     | 0.47              |
| 53:UT:490:LEU:HD12  | 53:UT:541:THR:HG21  | 1.95                     | 0.47              |
| 53:UT:2218:ALA:O    | 53:UT:2222:ILE:HD12 | 2.14                     | 0.47              |
| 54:UH:575:SER:HA    | 54:UH:578:ILE:HG22  | 1.94                     | 0.47              |
| 7:UJ:1119:VAL:HG12  | 7:UJ:1188:LYS:HZ2   | 1.79                     | 0.47              |
| 8:UK:266:ARG:HH12   | 50:C1:205:C:N4      | 2.13                     | 0.47              |
| 10:UM:511:ILE:HG13  | 10:UM:550:LEU:HD21  | 1.97                     | 0.47              |
| 12:UO:417:ARG:HH22  | 50:C1:79:C:H42      | 1.62                     | 0.47              |
| 30:CP:127:ARG:HB2   | 30:CP:167:ASN:HB3   | 1.97                     | 0.47              |
| 32:CR:281:VAL:HG12  | 32:CR:470:LYS:HB2   | 1.97                     | 0.47              |
| 54:UH:344:SER:OG    | 54:UH:357:SER:O     | 2.32                     | 0.47              |
| 3:UC:642:LEU:HD21   | 50:C1:1082:G:H5''   | 1.97                     | 0.47              |
| 4:UD:363:ARG:NH2    | 4:UD:686:ARG:O      | 2.47                     | 0.47              |
| 7:UJ:59:LEU:HD11    | 7:UJ:114:ALA:HA     | 1.96                     | 0.47              |
| 7:UJ:1024:GLN:HA    | 7:UJ:1027:MET:HE1   | 1.96                     | 0.47              |
| 8:UK:10:ARG:NH2     | 50:C1:1136:G:N7     | 2.63                     | 0.47              |
| 10:UM:514:SER:OG    | 10:UM:515:GLN:N     | 2.47                     | 0.47              |
| 13:UQ:849:ALA:O     | 13:UQ:851:GLN:N     | 2.48                     | 0.47              |
| 13:UQ:922:ALA:HB3   | 13:UQ:925:ARG:HG2   | 1.97                     | 0.47              |
| 23:CH:219:ARG:HA    | 23:CH:251:HIS:O     | 2.14                     | 0.47              |
| 27:CL:650:VAL:HG23  | 27:CL:676:MET:HE2   | 1.95                     | 0.47              |
| 32:CR:361:ILE:HB    | 32:CR:367:GLN:HB2   | 1.95                     | 0.47              |
| 32:CR:776:GLY:HA3   | 32:CR:816:ASP:HB2   | 1.96                     | 0.47              |
| 32:CR:916:MET:HA    | 32:CR:919:VAL:HG22  | 1.97                     | 0.47              |
| 32:CS:134:ASN:HB3   | 32:CS:138:ARG:HH21  | 1.80                     | 0.47              |
| 32:CS:135:ILE:HA    | 32:CS:138:ARG:HG2   | 1.96                     | 0.47              |
| 37:Cd:2:LYS:HD3     | 37:Cd:15:LEU:HD21   | 1.96                     | 0.47              |
| 47:Co:352:LYS:NZ    | 47:Co:408:ASP:OD1   | 2.45                     | 0.47              |
| 50:C1:678:A:H5''    | 50:C1:679:A:H5''    | 1.97                     | 0.47              |
| 50:C1:782:G:OP2     | 53:UT:1131:ARG:NH1  | 2.47                     | 0.47              |
| 53:UT:1746:LYS:O    | 53:UT:1751:ARG:NH1  | 2.48                     | 0.47              |
| 53:UT:1877:LEU:HD12 | 53:UT:1958:HIS:HB2  | 1.95                     | 0.47              |
| 54:UH:258:GLN:O     | 54:UH:265:ASN:HA    | 2.15                     | 0.47              |
| 60:CZ:539:SER:OG    | 60:CZ:542:ARG:NH2   | 2.48                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:UD:874:GLU:HG2   | 61:UP:356:ARG:HH21 | 1.79                     | 0.47              |
| 7:UJ:1281:GLN:NE2  | 7:UJ:1323:ASN:OD1  | 2.47                     | 0.47              |
| 14:UR:596:SER:HB2  | 14:UR:601:VAL:HB   | 1.97                     | 0.47              |
| 22:CG:195:TRP:CD1  | 22:CG:226:ARG:HA   | 2.49                     | 0.47              |
| 24:CI:1130:ARG:O   | 24:CI:1134:GLN:HG2 | 2.14                     | 0.47              |
| 26:CK:94:ARG:NH2   | 50:C1:2189:C:OP2   | 2.38                     | 0.47              |
| 32:CR:38:ILE:HD11  | 32:CR:152:LEU:HD21 | 1.96                     | 0.47              |
| 53:UT:5:THR:HB     | 53:UT:10:LEU:HD21  | 1.96                     | 0.47              |
| 4:UD:833:ARG:NH1   | 50:C1:62:U:O2'     | 2.48                     | 0.47              |
| 9:UL:51:ASP:HB2    | 9:UL:58:LEU:HD11   | 1.96                     | 0.47              |
| 9:UL:907:ARG:HA    | 9:UL:907:ARG:HD3   | 1.77                     | 0.47              |
| 10:UM:458:ARG:HG2  | 10:UM:474:VAL:HG22 | 1.96                     | 0.47              |
| 13:UQ:615:PHE:N    | 13:UQ:629:ILE:O    | 2.46                     | 0.47              |
| 15:UU:691:VAL:HB   | 15:UU:701:ARG:HB2  | 1.97                     | 0.47              |
| 16:UX:72:LYS:NZ    | 49:CU:275:LEU:O    | 2.46                     | 0.47              |
| 24:CI:72:VAL:HG11  | 24:CI:129:MET:HB3  | 1.96                     | 0.47              |
| 24:CI:826:ILE:HD12 | 24:CI:862:TYR:HB3  | 1.96                     | 0.47              |
| 26:CK:140:ILE:HA   | 26:CK:153:THR:O    | 2.15                     | 0.47              |
| 41:Ch:124:ARG:NH1  | 50:C1:1212:G:OP1   | 2.44                     | 0.47              |
| 53:UT:240:GLU:HA   | 53:UT:243:VAL:HG13 | 1.96                     | 0.47              |
| 54:UH:320:LYS:HD3  | 54:UH:342:GLY:H    | 1.80                     | 0.47              |
| 54:UH:610:GLY:HA2  | 54:UH:640:GLU:HG3  | 1.96                     | 0.47              |
| 7:UJ:1158:LEU:HD21 | 7:UJ:1170:LEU:HD21 | 1.97                     | 0.47              |
| 7:UJ:1469:ALA:HB1  | 7:UJ:1509:LYS:HG3  | 1.96                     | 0.47              |
| 13:UQ:271:LEU:HD23 | 13:UQ:276:GLU:HG3  | 1.97                     | 0.47              |
| 24:CI:246:ILE:HB   | 24:CI:798:ILE:HB   | 1.95                     | 0.47              |
| 24:CI:945:ALA:HA   | 24:CI:948:GLU:HG3  | 1.97                     | 0.47              |
| 25:CJ:33:ILE:HA    | 25:CJ:38:ILE:HD12  | 1.97                     | 0.47              |
| 52:CW:156:VAL:HA   | 52:CW:203:ALA:HA   | 1.96                     | 0.47              |
| 52:CW:221:THR:OG1  | 52:CW:225:THR:OG1  | 2.32                     | 0.47              |
| 52:CW:310:LYS:HA   | 52:CW:333:LEU:HB2  | 1.96                     | 0.47              |
| 15:UU:210:ILE:HD12 | 15:UU:220:TYR:HB3  | 1.97                     | 0.46              |
| 15:UU:848:ARG:HG2  | 15:UU:852:GLN:OE1  | 2.15                     | 0.46              |
| 32:CR:618:VAL:O    | 32:CR:622:PHE:HB2  | 2.15                     | 0.46              |
| 39:Cf:44:HIS:HB3   | 39:Cf:56:ARG:HB2   | 1.97                     | 0.46              |
| 42:CI:49:ARG:HG2   | 50:C1:1504:A:H1'   | 1.98                     | 0.46              |
| 52:CW:136:PRO:HG2  | 60:CZ:544:LEU:HD12 | 1.97                     | 0.46              |
| 57:CI:53:ASP:HB3   | 57:CI:56:LYS:HG3   | 1.97                     | 0.46              |
| 4:UD:697:GLN:HG3   | 4:UD:713:SER:HB3   | 1.95                     | 0.46              |
| 7:UJ:1448:SER:O    | 7:UJ:1461:ARG:NH2  | 2.47                     | 0.46              |
| 10:UM:251:SER:OG   | 10:UM:252:ARG:N    | 2.47                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:UO:463:ARG:NH1  | 13:UQ:524:VAL:O     | 2.39                     | 0.46              |
| 17:UZ:154:LEU:HD11 | 17:UZ:228:ILE:HG13  | 1.97                     | 0.46              |
| 32:CR:880:GLN:HE21 | 32:CR:911:ILE:HD11  | 1.80                     | 0.46              |
| 32:CS:277:LEU:HB3  | 32:CS:406:TYR:HA    | 1.97                     | 0.46              |
| 32:CS:579:LEU:HD12 | 32:CS:580:PRO:HD2   | 1.98                     | 0.46              |
| 37:Cd:160:ARG:NE   | 50:C1:653:U:O2      | 2.44                     | 0.46              |
| 53:UT:372:GLY:HA2  | 53:UT:421:PRO:HG2   | 1.98                     | 0.46              |
| 53:UT:1210:ILE:O   | 53:UT:1213:THR:OG1  | 2.28                     | 0.46              |
| 53:UT:1757:THR:O   | 53:UT:1761:ILE:HG12 | 2.14                     | 0.46              |
| 58:CX:274:VAL:O    | 58:CX:278:ILE:HG12  | 2.15                     | 0.46              |
| 55:UI:167:ASP:N    | 55:UI:167:ASP:OD1   | 2.46                     | 0.46              |
| 6:UG:579:ASP:O     | 6:UG:582:ARG:N      | 2.48                     | 0.46              |
| 12:UO:527:LEU:HB2  | 55:UE:263:LEU:HB3   | 1.98                     | 0.46              |
| 13:UQ:193:ASP:OD2  | 13:UQ:250:GLY:N     | 2.48                     | 0.46              |
| 15:UU:509:GLU:OE2  | 15:UU:533:ARG:HG2   | 2.14                     | 0.46              |
| 15:UU:644:GLY:HA3  | 15:UU:663:ALA:HA    | 1.96                     | 0.46              |
| 18:CA:194:ILE:HD11 | 19:CC:162:SER:HB3   | 1.97                     | 0.46              |
| 19:CC:199:ARG:NH1  | 19:CC:216:ASN:OD1   | 2.48                     | 0.46              |
| 22:CG:420:LEU:O    | 22:CG:429:LEU:N     | 2.48                     | 0.46              |
| 46:Cn:54:LEU:HD11  | 46:Cn:75:GLN:HB2    | 1.96                     | 0.46              |
| 53:UT:1516:LEU:O   | 53:UT:1518:GLN:N    | 2.48                     | 0.46              |
| 3:UC:632:GLN:HG2   | 18:CA:64:GLY:HA3    | 1.97                     | 0.46              |
| 4:UD:671:ARG:NE    | 7:UJ:665:GLU:OE2    | 2.47                     | 0.46              |
| 7:UJ:1117:MET:HE3  | 7:UJ:1169:LEU:HD13  | 1.98                     | 0.46              |
| 10:UM:692:HIS:CG   | 10:UM:696:LEU:HD21  | 2.50                     | 0.46              |
| 23:CH:328:MET:HE2  | 23:CH:330:ALA:HB3   | 1.97                     | 0.46              |
| 32:CS:408:VAL:HG23 | 32:CS:467:ARG:HH22  | 1.81                     | 0.46              |
| 37:Cd:2:LYS:HB3    | 37:Cd:15:LEU:HD11   | 1.97                     | 0.46              |
| 45:Cm:111:MET:HE1  | 45:Cm:119:LYS:HD2   | 1.97                     | 0.46              |
| 53:UT:554:VAL:HA   | 53:UT:557:LYS:HE2   | 1.98                     | 0.46              |
| 53:UT:868:HIS:HB3  | 53:UT:895:TRP:HZ2   | 1.81                     | 0.46              |
| 7:UJ:1281:GLN:HB3  | 7:UJ:1285:ARG:HH21  | 1.80                     | 0.46              |
| 9:UL:633:ILE:O     | 9:UL:642:HIS:N      | 2.49                     | 0.46              |
| 13:UQ:272:ALA:N    | 13:UQ:276:GLU:OE2   | 2.49                     | 0.46              |
| 18:CB:130:TRP:NE1  | 18:CB:138:ALA:HB3   | 2.30                     | 0.46              |
| 20:CD:3:LEU:HB3    | 20:CD:18:ALA:HB3    | 1.98                     | 0.46              |
| 32:CS:346:GLN:HE22 | 32:CS:356:ILE:HG13  | 1.80                     | 0.46              |
| 53:UT:287:LYS:HD3  | 53:UT:290:LEU:HD12  | 1.97                     | 0.46              |
| 2:UB:576:GLN:NE2   | 2:UB:580:GLU:OE1    | 2.43                     | 0.46              |
| 4:UD:54:GLU:OE1    | 4:UD:65:GLN:NE2     | 2.49                     | 0.46              |
| 5:UF:99:ALA:HB1    | 5:UF:109:LEU:HD21   | 1.96                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:UJ:1170:LEU:HA    | 7:UJ:1174:SER:HB2   | 1.97                     | 0.46              |
| 13:UQ:379:LEU:HB3   | 13:UQ:392:LEU:HB3   | 1.98                     | 0.46              |
| 24:CI:835:PHE:O     | 24:CI:841:ARG:HA    | 2.16                     | 0.46              |
| 32:CR:559:MET:HE3   | 32:CR:559:MET:HB2   | 1.87                     | 0.46              |
| 40:Cg:103:LEU:HD23  | 40:Cg:106:ARG:HD2   | 1.98                     | 0.46              |
| 52:CW:254:ARG:HH12  | 52:CW:297:THR:HB    | 1.80                     | 0.46              |
| 52:CW:342:SER:OG    | 52:CW:343:GLY:N     | 2.47                     | 0.46              |
| 58:CX:342:ILE:HG21  | 58:CX:377:LEU:HD21  | 1.98                     | 0.46              |
| 2:UB:65:ARG:HH21    | 50:C1:2047:G:H5''   | 1.81                     | 0.46              |
| 4:UD:663:ARG:HG3    | 4:UD:665:MET:HG2    | 1.98                     | 0.46              |
| 5:UF:162:ALA:HB2    | 11:UN:359:PRO:HA    | 1.98                     | 0.46              |
| 6:UG:305:SER:HB3    | 6:UG:348:VAL:HG12   | 1.98                     | 0.46              |
| 10:UM:273:ARG:HD3   | 10:UM:299:ARG:HH21  | 1.81                     | 0.46              |
| 18:CA:258:LYS:HG3   | 18:CA:299:HIS:CE1   | 2.51                     | 0.46              |
| 25:CJ:180:PHE:CD2   | 43:Cj:87:LYS:HD2    | 2.51                     | 0.46              |
| 29:CO:174:ASN:ND2   | 29:CO:199:ASN:O     | 2.49                     | 0.46              |
| 35:Cb:42:MET:HE1    | 35:Cb:47:PHE:HD1    | 1.81                     | 0.46              |
| 53:UT:1874:GLN:HA   | 53:UT:1877:LEU:HD23 | 1.97                     | 0.46              |
| 54:UH:636:LEU:HB3   | 54:UH:641:LEU:HG    | 1.97                     | 0.46              |
| 56:US:241:GLU:HA    | 56:US:247:ARG:HH22  | 1.79                     | 0.46              |
| 58:CX:193:GLU:HB3   | 58:CX:194:ILE:H     | 1.62                     | 0.46              |
| 59:CY:43:VAL:HB     | 60:CZ:418:ARG:NH1   | 2.29                     | 0.46              |
| 60:CZ:374:ARG:O     | 60:CZ:378:MET:HG2   | 2.16                     | 0.46              |
| 9:UL:491:LEU:HD21   | 9:UL:556:LEU:HD22   | 1.97                     | 0.46              |
| 12:UO:115:VAL:HG21  | 12:UO:160:LEU:HD21  | 1.96                     | 0.46              |
| 27:CL:125:LEU:HD13  | 27:CL:128:ARG:HH21  | 1.81                     | 0.46              |
| 32:CS:29:VAL:HG23   | 32:CS:202:ILE:HG23  | 1.98                     | 0.46              |
| 32:CS:591:GLU:HG2   | 32:CS:612:ASP:HA    | 1.98                     | 0.46              |
| 50:C1:718:U:H2'     | 53:UT:1004:ILE:HD11 | 1.97                     | 0.46              |
| 53:UT:1877:LEU:HD21 | 53:UT:1962:MET:HE3  | 1.98                     | 0.46              |
| 59:CY:41:LEU:HB2    | 60:CZ:317:GLN:HG2   | 1.98                     | 0.46              |
| 3:UC:639:LYS:NZ     | 33:CT:124:LYS:O     | 2.48                     | 0.46              |
| 4:UD:502:VAL:HG13   | 4:UD:526:LEU:HB2    | 1.97                     | 0.46              |
| 7:UJ:667:SER:HA     | 7:UJ:673:HIS:HB3    | 1.98                     | 0.46              |
| 24:CI:518:ARG:NH2   | 32:CS:339:HIS:O     | 2.38                     | 0.46              |
| 32:CS:564:ALA:HB1   | 32:CS:590:LEU:HB3   | 1.97                     | 0.46              |
| 50:C1:1480:G:H1     | 50:C1:1502:U:H3     | 1.63                     | 0.46              |
| 53:UT:43:LEU:HD12   | 53:UT:173:LYS:HD2   | 1.96                     | 0.46              |
| 53:UT:428:PRO:HA    | 53:UT:431:SER:HB3   | 1.98                     | 0.46              |
| 53:UT:1040:LEU:HD23 | 53:UT:1072:LEU:HD11 | 1.97                     | 0.46              |
| 59:CY:94:LEU:HD21   | 60:CZ:463:LEU:HD13  | 1.98                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:UB:747:ILE:HD12   | 2:UB:795:ARG:HH21   | 1.81                     | 0.46              |
| 7:UJ:229:ILE:HD11   | 7:UJ:278:LEU:HD23   | 1.98                     | 0.46              |
| 10:UM:651:LEU:HB2   | 10:UM:665:GLN:HG3   | 1.98                     | 0.46              |
| 26:CK:123:ILE:HG13  | 26:CK:126:ASP:H     | 1.81                     | 0.46              |
| 32:CS:540:MET:O     | 32:CS:544:TYR:CB    | 2.64                     | 0.46              |
| 34:Ca:27:LYS:HB3    | 34:Ca:47:LEU:HD22   | 1.98                     | 0.46              |
| 37:Cd:33:GLY:CA     | 37:Cd:52:ILE:O      | 2.64                     | 0.46              |
| 37:Cd:191:ARG:NH1   | 50:C1:867:C:OP2     | 2.49                     | 0.46              |
| 40:Cg:139:VAL:HG13  | 59:CY:257:GLY:HA3   | 1.98                     | 0.46              |
| 50:C1:156:C:H42     | 50:C1:180:G:H1      | 1.63                     | 0.46              |
| 50:C1:725:A:H2      | 50:C1:850:A:H4'     | 1.80                     | 0.46              |
| 53:UT:1901:LEU:HD21 | 53:UT:1972:ALA:HB1  | 1.96                     | 0.46              |
| 53:UT:2238:LEU:HA   | 53:UT:2241:LEU:HG   | 1.97                     | 0.46              |
| 2:UB:769:LEU:HD12   | 2:UB:773:LEU:HD23   | 1.98                     | 0.45              |
| 10:UM:482:VAL:HA    | 10:UM:514:SER:HA    | 1.98                     | 0.45              |
| 25:CJ:115:MET:HB2   | 25:CJ:120:MET:HB2   | 1.97                     | 0.45              |
| 29:CN:227:ILE:HG21  | 29:CN:241:PHE:HE1   | 1.81                     | 0.45              |
| 32:CR:912:PHE:O     | 32:CR:916:MET:HG2   | 2.16                     | 0.45              |
| 52:CW:243:GLN:HG3   | 52:CW:247:ILE:HD11  | 1.99                     | 0.45              |
| 53:UT:1075:MET:O    | 53:UT:1079:VAL:HG23 | 2.16                     | 0.45              |
| 5:UF:287:ARG:HA     | 5:UF:292:TRP:CD2    | 2.51                     | 0.45              |
| 9:UL:24:LEU:HD22    | 9:UL:41:VAL:HG12    | 1.99                     | 0.45              |
| 9:UL:493:ASP:HB2    | 9:UL:500:LEU:HD21   | 1.97                     | 0.45              |
| 10:UM:774:PHE:HA    | 10:UM:777:VAL:HG12  | 1.98                     | 0.45              |
| 12:UO:103:HIS:NE2   | 12:UO:119:ASP:OD1   | 2.35                     | 0.45              |
| 12:UO:145:GLN:HE21  | 29:CN:16:LEU:HD21   | 1.80                     | 0.45              |
| 13:UQ:740:LEU:HD12  | 13:UQ:816:ILE:HD13  | 1.96                     | 0.45              |
| 19:CC:50:LEU:HD21   | 19:CC:145:LEU:HD12  | 1.98                     | 0.45              |
| 23:CH:292:TYR:OH    | 24:CI:623:ARG:NH2   | 2.49                     | 0.45              |
| 26:CK:40:LYS:HD2    | 26:CK:41:PRO:HD2    | 1.99                     | 0.45              |
| 30:CP:82:THR:HB     | 30:CP:86:THR:HG21   | 1.98                     | 0.45              |
| 32:CR:246:THR:O     | 32:CR:250:GLY:N     | 2.47                     | 0.45              |
| 32:CS:727:TYR:HE1   | 32:CS:762:MET:HG2   | 1.81                     | 0.45              |
| 34:Ca:58:ASN:O      | 34:Ca:62:LYS:HG2    | 2.16                     | 0.45              |
| 35:Cb:97:GLU:OE1    | 35:Cb:113:ARG:NH1   | 2.49                     | 0.45              |
| 50:C1:311:G:H21     | 50:C1:329:A:H62     | 1.65                     | 0.45              |
| 54:UH:756:LEU:HG    | 55:UI:203:ARG:HH22  | 1.81                     | 0.45              |
| 55:UE:235:LEU:HD13  | 55:UE:238:ARG:HB2   | 1.98                     | 0.45              |
| 3:UC:213:MET:O      | 3:UC:218:ARG:NH2    | 2.46                     | 0.45              |
| 4:UD:158:THR:HB     | 4:UD:162:ASN:HB2    | 1.97                     | 0.45              |
| 7:UJ:1026:VAL:HA    | 7:UJ:1029:ILE:HD12  | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:UJ:1357:ASP:O    | 7:UJ:1368:ARG:NH2  | 2.50                     | 0.45              |
| 9:UL:591:VAL:HB    | 9:UL:601:LEU:HB2   | 1.98                     | 0.45              |
| 13:UQ:498:PRO:HG2  | 13:UQ:499:LEU:HD12 | 1.98                     | 0.45              |
| 13:UQ:557:GLN:HB3  | 13:UQ:581:ARG:HG2  | 1.98                     | 0.45              |
| 13:UQ:615:PHE:H    | 13:UQ:630:GLY:HA2  | 1.82                     | 0.45              |
| 20:CD:212:LEU:HD21 | 20:CD:262:VAL:HG23 | 1.98                     | 0.45              |
| 50:C1:801:A:H4'    | 50:C1:802:A:H3'    | 1.97                     | 0.45              |
| 53:UT:256:MET:HE1  | 53:UT:305:VAL:HA   | 1.98                     | 0.45              |
| 53:UT:1242:GLU:HA  | 53:UT:1245:SER:OG  | 2.17                     | 0.45              |
| 55:UI:275:ALA:O    | 55:UI:279:ALA:CB   | 2.64                     | 0.45              |
| 4:UD:648:LEU:HD13  | 4:UD:658:ILE:HG12  | 1.98                     | 0.45              |
| 21:CF:53:VAL:O     | 21:CF:79:TYR:HA    | 2.16                     | 0.45              |
| 52:CW:165:TYR:HB3  | 52:CW:183:GLN:HE21 | 1.82                     | 0.45              |
| 53:UT:538:LEU:HD21 | 53:UT:551:ILE:HD13 | 1.98                     | 0.45              |
| 53:UT:1749:GLU:HG3 | 53:UT:1753:MET:HE3 | 1.97                     | 0.45              |
| 54:UH:365:TYR:CZ   | 54:UH:372:LEU:HD13 | 2.52                     | 0.45              |
| 58:CX:428:ASP:OD1  | 58:CX:429:GLN:N    | 2.49                     | 0.45              |
| 2:UB:723:ILE:HG23  | 2:UB:773:LEU:HD22  | 1.97                     | 0.45              |
| 4:UD:351:VAL:HG12  | 4:UD:743:ALA:HB2   | 1.99                     | 0.45              |
| 7:UJ:1014:LEU:O    | 7:UJ:1017:THR:OG1  | 2.24                     | 0.45              |
| 7:UJ:1109:ASP:OD1  | 7:UJ:1109:ASP:N    | 2.48                     | 0.45              |
| 7:UJ:1743:LYS:NZ   | 7:UJ:1781:GLU:OE1  | 2.36                     | 0.45              |
| 9:UL:134:ILE:HD13  | 9:UL:191:THR:HG21  | 1.99                     | 0.45              |
| 12:UO:332:ARG:O    | 12:UO:347:THR:HA   | 2.16                     | 0.45              |
| 12:UO:532:ARG:HG3  | 12:UO:536:LYS:HE3  | 1.99                     | 0.45              |
| 13:UQ:95:ILE:HG21  | 13:UQ:148:LEU:HG   | 1.98                     | 0.45              |
| 22:CG:136:ARG:HG3  | 47:Co:344:ILE:HD12 | 1.98                     | 0.45              |
| 24:CI:156:ILE:HG13 | 24:CI:899:ILE:HD11 | 1.98                     | 0.45              |
| 24:CI:753:ASN:O    | 24:CI:754:LYS:HG2  | 2.17                     | 0.45              |
| 37:Cd:10:ASN:HD21  | 53:UT:708:ALA:HB2  | 1.82                     | 0.45              |
| 43:Cj:7:VAL:HG12   | 43:Cj:95:LYS:HD3   | 1.98                     | 0.45              |
| 53:UT:560:LYS:HE3  | 53:UT:602:LEU:HD21 | 1.99                     | 0.45              |
| 1:UA:706:PHE:HB2   | 15:UU:720:ARG:HG2  | 1.99                     | 0.45              |
| 2:UB:579:GLU:OE1   | 2:UB:620:ARG:NH1   | 2.49                     | 0.45              |
| 10:UM:132:ASP:OD1  | 10:UM:133:GLY:N    | 2.49                     | 0.45              |
| 10:UM:256:MET:HE2  | 10:UM:291:SER:HB2  | 1.98                     | 0.45              |
| 12:UO:299:VAL:HB   | 12:UO:309:ALA:HB3  | 1.99                     | 0.45              |
| 13:UQ:560:GLU:HB3  | 13:UQ:573:GLN:HB3  | 1.98                     | 0.45              |
| 13:UQ:813:ILE:HB   | 13:UQ:823:LEU:HB3  | 1.98                     | 0.45              |
| 32:CR:844:TYR:CE2  | 32:CR:916:MET:HE1  | 2.51                     | 0.45              |
| 32:CS:727:TYR:O    | 32:CS:759:THR:HA   | 2.17                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:Ca:106:THR:OG1  | 34:Ca:108:ASP:OD2   | 2.27                     | 0.45              |
| 35:Cb:183:ILE:O    | 35:Cb:190:GLY:N     | 2.50                     | 0.45              |
| 51:C2:164:U:O2     | 51:C2:166:G:N2      | 2.50                     | 0.45              |
| 58:CX:220:PRO:HA   | 58:CX:223:VAL:HG22  | 1.98                     | 0.45              |
| 59:CY:119:ASP:OD1  | 60:CZ:315:ARG:NH2   | 2.49                     | 0.45              |
| 3:UC:239:LEU:HB3   | 3:UC:266:LEU:HD11   | 1.99                     | 0.45              |
| 9:UL:24:LEU:HD11   | 9:UL:388:GLY:N      | 2.32                     | 0.45              |
| 9:UL:422:LEU:O     | 9:UL:450:LYS:NZ     | 2.29                     | 0.45              |
| 12:UO:129:GLY:HA3  | 12:UO:133:ARG:HH11  | 1.82                     | 0.45              |
| 13:UQ:568:THR:HG21 | 55:UE:258:ALA:HB1   | 1.98                     | 0.45              |
| 14:UR:331:VAL:HB   | 14:UR:337:GLU:HB2   | 1.99                     | 0.45              |
| 17:UZ:268:GLU:HA   | 17:UZ:274:LYS:HD2   | 1.99                     | 0.45              |
| 22:CG:123:PHE:O    | 35:Cb:106:LYS:NZ    | 2.50                     | 0.45              |
| 23:CH:151:ASP:OD2  | 23:CH:178:ARG:NH2   | 2.45                     | 0.45              |
| 35:Cb:183:ILE:HG12 | 35:Cb:220:THR:HG21  | 1.98                     | 0.45              |
| 2:UB:817:ASP:N     | 2:UB:817:ASP:OD1    | 2.50                     | 0.45              |
| 7:UJ:506:LEU:HD23  | 7:UJ:557:ARG:HH11   | 1.81                     | 0.45              |
| 7:UJ:1126:ASP:OD1  | 7:UJ:1127:ASN:N     | 2.48                     | 0.45              |
| 7:UJ:1262:ALA:O    | 7:UJ:1265:ILE:N     | 2.49                     | 0.45              |
| 14:UR:322:ARG:HH21 | 50:C1:133:G:N2      | 2.15                     | 0.45              |
| 18:CB:265:THR:HG21 | 21:CE:124:ARG:HH11  | 1.81                     | 0.45              |
| 22:CG:356:TYR:HB3  | 22:CG:365:LEU:HB2   | 1.99                     | 0.45              |
| 24:CI:786:ALA:O    | 24:CI:790:LYS:HG3   | 2.16                     | 0.45              |
| 24:CI:829:THR:HG23 | 24:CI:847:ILE:HA    | 1.99                     | 0.45              |
| 27:CL:52:LEU:O     | 27:CL:57:PRO:HD2    | 2.17                     | 0.45              |
| 28:CM:72:MET:HE2   | 28:CM:331:ARG:HB3   | 1.97                     | 0.45              |
| 32:CS:593:LYS:HG2  | 32:CS:631:SER:HB3   | 1.99                     | 0.45              |
| 39:Cf:64:ASN:O     | 39:Cf:184:ASP:HA    | 2.17                     | 0.45              |
| 43:Cj:86:ALA:HB1   | 43:Cj:109:LEU:HD13  | 1.98                     | 0.45              |
| 50:C1:1039:C:H3'   | 50:C1:1040:G:H8     | 1.82                     | 0.45              |
| 51:C2:134:C:O2'    | 51:C2:181:A:N6      | 2.49                     | 0.45              |
| 53:UT:122:LEU:O    | 53:UT:126:VAL:HG23  | 2.17                     | 0.45              |
| 53:UT:236:LYS:HE2  | 53:UT:236:LYS:HB2   | 1.82                     | 0.45              |
| 53:UT:586:LEU:O    | 53:UT:590:LYS:HG2   | 2.16                     | 0.45              |
| 53:UT:1479:ILE:HA  | 53:UT:1482:VAL:HG12 | 1.98                     | 0.45              |
| 54:UH:179:ILE:HB   | 54:UH:193:VAL:HB    | 1.99                     | 0.45              |
| 57:Cl:45:LEU:HD21  | 57:Cl:80:LYS:HD2    | 1.99                     | 0.45              |
| 7:UJ:559:TRP:CD1   | 7:UJ:572:LEU:HD22   | 2.52                     | 0.45              |
| 7:UJ:664:LEU:O     | 7:UJ:667:SER:OG     | 2.34                     | 0.45              |
| 7:UJ:1252:LEU:HA   | 7:UJ:1255:LEU:HD23  | 1.98                     | 0.45              |
| 9:UL:286:PHE:HE1   | 9:UL:307:ILE:HD11   | 1.82                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:UM:14:ALA:HB2    | 10:UM:721:ARG:HB2   | 1.99                     | 0.45              |
| 10:UM:207:ILE:HB    | 10:UM:220:VAL:HB    | 1.98                     | 0.45              |
| 13:UQ:238:ASP:OD1   | 13:UQ:238:ASP:N     | 2.49                     | 0.45              |
| 13:UQ:591:GLY:O     | 13:UQ:594:GLN:N     | 2.50                     | 0.45              |
| 18:CB:118:PRO:HA    | 51:C2:243:G:H5''    | 1.99                     | 0.45              |
| 20:CD:4:PHE:HD2     | 20:CD:86:VAL:HG13   | 1.81                     | 0.45              |
| 27:CL:564:MET:HE3   | 27:CL:564:MET:HB3   | 1.87                     | 0.45              |
| 29:CN:50:LYS:HD3    | 29:CN:65:TYR:CZ     | 2.51                     | 0.45              |
| 34:Ca:152:LYS:HG3   | 34:Ca:153:THR:HG23  | 1.99                     | 0.45              |
| 35:Cb:114:ILE:HD12  | 35:Cb:118:GLU:HG2   | 1.98                     | 0.45              |
| 36:Cc:129:PRO:HA    | 36:Cc:201:LYS:HE3   | 1.99                     | 0.45              |
| 50:C1:1016:G:H5''   | 50:C1:1017:C:H5''   | 1.97                     | 0.45              |
| 50:C1:1623:U:H5''   | 50:C1:1624:A:H2'    | 1.99                     | 0.45              |
| 50:C1:2182:C:H2'    | 50:C1:2183:A:C8     | 2.52                     | 0.45              |
| 53:UT:1274:GLN:HB3  | 53:UT:1277:ILE:HD11 | 1.99                     | 0.45              |
| 53:UT:1552:LEU:HD21 | 53:UT:1596:LEU:HA   | 1.97                     | 0.45              |
| 54:UH:7:ILE:HD11    | 54:UH:364:VAL:HG23  | 1.98                     | 0.45              |
| 1:UA:149:GLN:NE2    | 50:C1:267:U:OP2     | 2.39                     | 0.45              |
| 6:UG:204:ASP:CG     | 16:UX:13:ARG:HH12   | 2.25                     | 0.45              |
| 7:UJ:67:VAL:HG23    | 7:UJ:68:PRO:HD3     | 1.99                     | 0.45              |
| 7:UJ:614:LEU:HA     | 7:UJ:617:VAL:HG12   | 1.99                     | 0.45              |
| 9:UL:89:ASP:OD1     | 9:UL:89:ASP:N       | 2.50                     | 0.45              |
| 10:UM:479:LEU:N     | 10:UM:516:ASP:OD2   | 2.48                     | 0.45              |
| 10:UM:546:ASP:OD1   | 10:UM:546:ASP:N     | 2.50                     | 0.45              |
| 13:UQ:632:ASP:OD2   | 13:UQ:636:ARG:NH2   | 2.50                     | 0.45              |
| 15:UU:716:SER:HB3   | 15:UU:721:TRP:HB2   | 1.99                     | 0.45              |
| 18:CA:249:GLN:HG2   | 19:CC:39:LYS:HE2    | 1.97                     | 0.45              |
| 26:CK:9:ARG:HD3     | 26:CK:159:HIS:HB2   | 1.98                     | 0.45              |
| 41:Ch:129:TYR:HA    | 41:Ch:132:VAL:HG12  | 1.98                     | 0.45              |
| 50:C1:381:G:H21     | 50:C1:385:A:H62     | 1.64                     | 0.45              |
| 50:C1:686:A:H2'     | 50:C1:687:U:H4'     | 1.99                     | 0.45              |
| 50:C1:759:G:H22     | 50:C1:850:A:H5'     | 1.82                     | 0.45              |
| 50:C1:799:U:O2'     | 53:UT:1279:ARG:NH1  | 2.40                     | 0.45              |
| 1:UA:316:ALA:O      | 1:UA:320:GLY:C      | 2.59                     | 0.44              |
| 2:UB:550:GLU:O      | 2:UB:554:ARG:HG2    | 2.17                     | 0.44              |
| 7:UJ:1735:PRO:HA    | 7:UJ:1738:ARG:HB2   | 1.98                     | 0.44              |
| 8:UK:79:ARG:HB2     | 8:UK:83:PHE:HB2     | 1.99                     | 0.44              |
| 10:UM:696:LEU:HA    | 10:UM:712:GLY:HA3   | 1.99                     | 0.44              |
| 13:UQ:569:GLY:HA2   | 54:UH:837:ALA:HB1   | 1.98                     | 0.44              |
| 19:CC:195:ALA:HB1   | 19:CC:216:ASN:HB3   | 1.98                     | 0.44              |
| 28:CM:56:PRO:HA     | 28:CM:354:ARG:HG2   | 1.99                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:CO:40:VAL:HG22   | 29:CO:113:TYR:HB2   | 1.98                     | 0.44              |
| 32:CS:161:GLN:HG2   | 32:CS:688:LEU:HD22  | 1.99                     | 0.44              |
| 53:UT:245:THR:OG1   | 53:UT:247:GLN:OE1   | 2.32                     | 0.44              |
| 53:UT:343:GLY:HA3   | 53:UT:393:ASN:ND2   | 2.32                     | 0.44              |
| 53:UT:472:ARG:HH12  | 53:UT:473:MET:HE2   | 1.81                     | 0.44              |
| 53:UT:1805:PHE:O    | 53:UT:1809:SER:OG   | 2.34                     | 0.44              |
| 54:UH:238:PHE:HE1   | 54:UH:275:PRO:HB3   | 1.82                     | 0.44              |
| 1:UA:82:THR:HG22    | 1:UA:89:VAL:HA      | 1.99                     | 0.44              |
| 3:UC:255:ALA:HA     | 3:UC:260:VAL:HG11   | 1.99                     | 0.44              |
| 4:UD:165:LEU:HD13   | 4:UD:179:LEU:HD11   | 1.99                     | 0.44              |
| 6:UG:270:ASN:ND2    | 6:UG:463:PRO:HD3    | 2.32                     | 0.44              |
| 7:UJ:1482:HIS:ND1   | 7:UJ:1522:LEU:HB3   | 2.32                     | 0.44              |
| 9:UL:595:ASP:OD1    | 9:UL:596:THR:N      | 2.50                     | 0.44              |
| 10:UM:604:GLY:HA2   | 10:UM:636:ARG:HH21  | 1.81                     | 0.44              |
| 13:UQ:737:MET:HG3   | 13:UQ:746:MET:HG2   | 2.00                     | 0.44              |
| 15:UU:231:ALA:O     | 15:UU:249:SER:N     | 2.43                     | 0.44              |
| 19:CC:38:MET:SD     | 19:CC:47:MET:HE1    | 2.57                     | 0.44              |
| 31:CQ:84:LYS:HD2    | 31:CQ:121:ARG:NH1   | 2.31                     | 0.44              |
| 32:CR:268:PHE:CZ    | 32:CR:298:ALA:HB1   | 2.51                     | 0.44              |
| 32:CS:144:GLU:HA    | 32:CS:479:ARG:HB3   | 1.99                     | 0.44              |
| 32:CS:220:LEU:HD12  | 32:CS:221:PRO:HD2   | 1.99                     | 0.44              |
| 36:Cc:35:TYR:HA     | 36:Cc:38:ILE:HD12   | 1.99                     | 0.44              |
| 36:Cc:179:GLU:O     | 36:Cc:183:GLU:HG3   | 2.17                     | 0.44              |
| 39:Cf:84:HIS:HE2    | 39:Cf:97:THR:HG1    | 1.64                     | 0.44              |
| 53:UT:690:MET:HE1   | 53:UT:733:PHE:CG    | 2.51                     | 0.44              |
| 53:UT:797:THR:HG23  | 53:UT:799:PHE:H     | 1.82                     | 0.44              |
| 53:UT:901:LYS:HE2   | 53:UT:937:LEU:HB2   | 1.99                     | 0.44              |
| 53:UT:1168:ARG:HA   | 53:UT:1168:ARG:HD3  | 1.82                     | 0.44              |
| 53:UT:1621:ARG:HH21 | 53:UT:1689:ASN:HD22 | 1.65                     | 0.44              |
| 60:CZ:536:ARG:HD2   | 60:CZ:536:ARG:HA    | 1.79                     | 0.44              |
| 1:UA:787:MET:HG3    | 1:UA:826:MET:HE3    | 1.99                     | 0.44              |
| 4:UD:296:MET:C      | 4:UD:298:ARG:H      | 2.26                     | 0.44              |
| 8:UK:72:GLY:O       | 8:UK:79:ARG:NH2     | 2.42                     | 0.44              |
| 10:UM:126:LEU:O     | 10:UM:137:ILE:HA    | 2.18                     | 0.44              |
| 10:UM:636:ARG:HE    | 10:UM:636:ARG:HB2   | 1.69                     | 0.44              |
| 10:UM:804:GLU:HG3   | 10:UM:847:VAL:HG13  | 1.99                     | 0.44              |
| 28:CM:304:ASP:O     | 28:CM:306:THR:N     | 2.47                     | 0.44              |
| 32:CS:245:ASP:OD1   | 32:CS:245:ASP:N     | 2.50                     | 0.44              |
| 35:Cb:31:PRO:HG3    | 35:Cb:43:PRO:HG3    | 1.99                     | 0.44              |
| 50:C1:181:G:O2'     | 50:C1:183:C:N4      | 2.50                     | 0.44              |
| 51:C2:135:U:H4'     | 51:C2:136:C:H4'     | 2.00                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:UT:1432:MET:HA   | 53:UT:1435:VAL:HG12 | 2.00                     | 0.44              |
| 53:UT:1720:LEU:HD13 | 53:UT:1732:LEU:HD22 | 1.99                     | 0.44              |
| 56:US:204:ILE:HD11  | 56:US:226:LEU:HD23  | 1.99                     | 0.44              |
| 4:UD:50:ASN:ND2     | 4:UD:52:ASP:OD2     | 2.51                     | 0.44              |
| 8:UK:117:ASN:HB3    | 51:C2:260:G:H4'     | 2.00                     | 0.44              |
| 10:UM:290:TYR:HB2   | 10:UM:298:LEU:HD11  | 1.99                     | 0.44              |
| 10:UM:589:VAL:HG22  | 10:UM:619:SER:HB2   | 2.00                     | 0.44              |
| 13:UQ:673:GLU:OE2   | 13:UQ:687:TYR:OH    | 2.32                     | 0.44              |
| 21:CF:78:PRO:HG2    | 21:CF:119:ARG:HG3   | 1.99                     | 0.44              |
| 24:CI:968:LYS:HA    | 24:CI:968:LYS:HD2   | 1.82                     | 0.44              |
| 25:CJ:89:SER:OG     | 50:C1:352:G:N7      | 2.49                     | 0.44              |
| 26:CK:215:ARG:NH1   | 26:CK:220:ASN:OD1   | 2.44                     | 0.44              |
| 32:CS:593:LYS:HE3   | 32:CS:631:SER:HB3   | 2.00                     | 0.44              |
| 52:CW:264:SER:HA    | 52:CW:289:PRO:HA    | 1.99                     | 0.44              |
| 53:UT:680:THR:HB    | 53:UT:725:TRP:CE2   | 2.53                     | 0.44              |
| 53:UT:901:LYS:HD3   | 53:UT:937:LEU:HD13  | 2.00                     | 0.44              |
| 54:UH:372:LEU:N     | 54:UH:436:ARG:O     | 2.49                     | 0.44              |
| 1:UA:288:ASN:HB3    | 15:UU:877:PRO:HG3   | 1.98                     | 0.44              |
| 1:UA:773:LEU:HD23   | 1:UA:797:LEU:HD21   | 1.99                     | 0.44              |
| 7:UJ:1783:ARG:HA    | 7:UJ:1786:ILE:HG22  | 2.00                     | 0.44              |
| 9:UL:370:ARG:HB2    | 9:UL:390:THR:HG22   | 2.00                     | 0.44              |
| 14:UR:376:PHE:HA    | 14:UR:386:ALA:O     | 2.18                     | 0.44              |
| 18:CB:97:LEU:HD13   | 18:CB:172:ASP:HA    | 1.99                     | 0.44              |
| 20:CD:41:LYS:O      | 20:CD:44:LYS:NZ     | 2.51                     | 0.44              |
| 30:CP:156:LEU:O     | 30:CP:159:GLN:NE2   | 2.48                     | 0.44              |
| 39:Cf:5:ARG:NH2     | 50:C1:918:U:O4      | 2.44                     | 0.44              |
| 39:Cf:48:THR:HG21   | 39:Cf:54:LYS:HG3    | 1.99                     | 0.44              |
| 50:C1:331:C:N4      | 50:C1:332:U:O4      | 2.50                     | 0.44              |
| 51:C2:177:G:H4'     | 51:C2:178:U:H5      | 1.83                     | 0.44              |
| 59:CY:100:THR:O     | 59:CY:104:GLU:N     | 2.46                     | 0.44              |
| 1:UA:558:ARG:HA     | 1:UA:558:ARG:HD2    | 1.86                     | 0.44              |
| 2:UB:747:ILE:HA     | 2:UB:788:LEU:HD22   | 1.99                     | 0.44              |
| 3:UC:582:GLN:O      | 3:UC:585:LYS:O      | 2.35                     | 0.44              |
| 4:UD:650:VAL:HA     | 4:UD:655:GLN:O      | 2.18                     | 0.44              |
| 10:UM:497:GLU:HA    | 10:UM:500:LYS:HB2   | 2.00                     | 0.44              |
| 17:UZ:233:VAL:HG22  | 17:UZ:243:ILE:HD13  | 1.99                     | 0.44              |
| 18:CB:77:ARG:HH22   | 18:CB:146:GLU:HA    | 1.82                     | 0.44              |
| 31:CQ:116:ASN:HD22  | 31:CQ:121:ARG:HH21  | 1.66                     | 0.44              |
| 32:CR:829:LEU:O     | 32:CR:832:LEU:C     | 2.61                     | 0.44              |
| 50:C1:787:U:H2'     | 50:C1:788:A:H8      | 1.83                     | 0.44              |
| 50:C1:2175:A:H2'    | 50:C1:2176:A:C8     | 2.52                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:UT:1482:VAL:HG23 | 53:UT:1486:ILE:HD13 | 1.99                     | 0.44              |
| 53:UT:1579:LEU:HA   | 53:UT:1582:HIS:CE1  | 2.52                     | 0.44              |
| 2:UB:820:ASP:OD1    | 2:UB:820:ASP:N      | 2.51                     | 0.44              |
| 4:UD:292:ILE:HD13   | 4:UD:340:VAL:HG21   | 2.00                     | 0.44              |
| 5:UF:47:VAL:HG13    | 5:UF:57:PHE:CE2     | 2.53                     | 0.44              |
| 7:UJ:492:PHE:HA     | 7:UJ:495:LEU:HG     | 1.99                     | 0.44              |
| 7:UJ:1397:ALA:HA    | 7:UJ:1400:TYR:CE1   | 2.53                     | 0.44              |
| 7:UJ:1665:PHE:HD2   | 7:UJ:1667:GLN:HB2   | 1.82                     | 0.44              |
| 9:UL:25:VAL:HG11    | 9:UL:83:PHE:HE2     | 1.82                     | 0.44              |
| 9:UL:838:LYS:O      | 9:UL:842:LEU:N      | 2.50                     | 0.44              |
| 10:UM:397:ASP:OD1   | 10:UM:397:ASP:N     | 2.50                     | 0.44              |
| 16:UX:135:VAL:HG13  | 16:UX:160:ILE:HD11  | 1.99                     | 0.44              |
| 20:CD:85:LYS:HA     | 20:CD:85:LYS:HD3    | 1.81                     | 0.44              |
| 22:CG:343:ARG:HD3   | 22:CG:358:LYS:HA    | 1.98                     | 0.44              |
| 22:CG:471:THR:HG22  | 22:CG:478:ILE:HG12  | 1.99                     | 0.44              |
| 26:CK:269:THR:HG22  | 26:CK:280:VAL:HG22  | 1.99                     | 0.44              |
| 29:CO:155:THR:HG23  | 29:CO:157:GLU:H     | 1.82                     | 0.44              |
| 50:C1:1230:U:H5'    | 53:UT:1894:LEU:HD21 | 2.00                     | 0.44              |
| 53:UT:290:LEU:HD21  | 53:UT:334:GLN:HB3   | 1.98                     | 0.44              |
| 53:UT:927:LEU:HD21  | 53:UT:994:VAL:HG22  | 2.00                     | 0.44              |
| 53:UT:2161:VAL:HA   | 53:UT:2164:LEU:HD12 | 1.99                     | 0.44              |
| 56:US:299:LYS:HB2   | 56:US:302:MET:HE2   | 2.00                     | 0.44              |
| 3:UC:305:MET:N      | 3:UC:305:MET:SD     | 2.91                     | 0.44              |
| 7:UJ:339:VAL:HG21   | 7:UJ:380:SER:HB3    | 1.99                     | 0.44              |
| 7:UJ:1217:ALA:HA    | 7:UJ:1220:ILE:HB    | 2.00                     | 0.44              |
| 7:UJ:1232:LEU:HD21  | 7:UJ:1252:LEU:HD13  | 1.99                     | 0.44              |
| 7:UJ:1630:VAL:HG23  | 7:UJ:1678:VAL:HG21  | 2.00                     | 0.44              |
| 8:UK:4:LEU:HB3      | 46:Cn:89:ASN:HD22   | 1.82                     | 0.44              |
| 9:UL:626:SER:OG     | 9:UL:627:ALA:N      | 2.51                     | 0.44              |
| 10:UM:567:THR:HG22  | 10:UM:583:ARG:HG3   | 1.99                     | 0.44              |
| 12:UO:490:ALA:O     | 55:UE:249:ARG:NH2   | 2.51                     | 0.44              |
| 23:CH:240:ARG:O     | 23:CH:244:ASN:ND2   | 2.51                     | 0.44              |
| 24:CI:302:LEU:HD11  | 24:CI:778:ARG:HB2   | 2.00                     | 0.44              |
| 29:CN:227:ILE:HG21  | 29:CN:241:PHE:CE1   | 2.53                     | 0.44              |
| 32:CS:541:VAL:O     | 32:CS:545:VAL:HG12  | 2.18                     | 0.44              |
| 37:Cd:32:MET:HE3    | 37:Cd:54:GLY:HA2    | 1.99                     | 0.44              |
| 39:Cf:48:THR:HG21   | 39:Cf:54:LYS:HE2    | 2.00                     | 0.44              |
| 50:C1:483:U:H4'     | 50:C1:484:G:H5''    | 2.00                     | 0.44              |
| 52:CW:297:THR:HA    | 52:CW:302:GLU:O     | 2.18                     | 0.44              |
| 53:UT:1302:ILE:HG23 | 53:UT:1335:PHE:HE2  | 1.83                     | 0.44              |
| 57:Cl:25:LYS:HD2    | 57:Cl:25:LYS:O      | 2.18                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 58:CX:373:LYS:NZ   | 58:CX:375:TYR:OH    | 2.40                     | 0.44              |
| 60:CZ:493:ASP:OD1  | 60:CZ:493:ASP:N     | 2.51                     | 0.44              |
| 9:UL:18:VAL:HG23   | 9:UL:41:VAL:HB      | 1.99                     | 0.44              |
| 22:CG:127:GLU:HA   | 22:CG:130:ARG:HG3   | 2.00                     | 0.44              |
| 24:CI:739:TYR:CZ   | 24:CI:743:LYS:HD2   | 2.53                     | 0.44              |
| 27:CL:59:ASN:HB3   | 27:CL:62:ILE:HG22   | 2.00                     | 0.44              |
| 38:Ce:149:ARG:HG3  | 45:Cm:53:VAL:HG22   | 1.99                     | 0.44              |
| 44:Ck:115:HIS:HB3  | 44:Ck:143:ASN:ND2   | 2.32                     | 0.44              |
| 50:C1:208:A:O2'    | 50:C1:209:A:O4'     | 2.32                     | 0.44              |
| 50:C1:747:G:OP2    | 50:C1:747:G:N2      | 2.38                     | 0.44              |
| 54:UH:824:GLU:OE2  | 55:UI:210:ARG:NH1   | 2.51                     | 0.44              |
| 58:CX:242:TRP:HB2  | 58:CX:273:ARG:HH22  | 1.83                     | 0.44              |
| 60:CZ:326:ASN:O    | 60:CZ:330:ARG:HG2   | 2.18                     | 0.44              |
| 10:UM:815:ASP:O    | 10:UM:818:THR:OG1   | 2.30                     | 0.43              |
| 12:UO:417:ARG:HH12 | 50:C1:79:C:N4       | 2.16                     | 0.43              |
| 15:UU:713:PHE:HA   | 15:UU:723:VAL:O     | 2.18                     | 0.43              |
| 16:UX:138:VAL:HG12 | 16:UX:144:TYR:HB2   | 2.00                     | 0.43              |
| 22:CG:341:GLN:NE2  | 22:CG:406:ASP:OD2   | 2.51                     | 0.43              |
| 23:CH:153:PHE:O    | 23:CH:157:VAL:HG22  | 2.18                     | 0.43              |
| 32:CR:504:LYS:O    | 32:CR:508:THR:OG1   | 2.31                     | 0.43              |
| 32:CS:209:LEU:HD11 | 32:CS:694:PHE:HA    | 2.00                     | 0.43              |
| 34:Ca:22:ASP:O     | 34:Ca:25:THR:OG1    | 2.32                     | 0.43              |
| 42:Ci:65:ARG:HB3   | 50:C1:1490:A:H5'    | 2.00                     | 0.43              |
| 47:Co:385:GLN:HA   | 47:Co:413:LEU:HD13  | 1.99                     | 0.43              |
| 58:CX:290:ASN:HA   | 58:CX:293:LYS:HD3   | 1.99                     | 0.43              |
| 4:UD:249:ILE:HB    | 4:UD:261:TRP:HB2    | 1.99                     | 0.43              |
| 12:UO:145:GLN:HE21 | 29:CN:16:LEU:HD11   | 1.81                     | 0.43              |
| 16:UX:56:TYR:HB2   | 16:UX:87:VAL:HG12   | 2.00                     | 0.43              |
| 28:CM:423:ARG:HA   | 28:CM:428:LYS:HB2   | 2.01                     | 0.43              |
| 32:CR:385:LEU:HD11 | 32:CR:409:PHE:CD1   | 2.53                     | 0.43              |
| 32:CS:133:PRO:HB2  | 32:CS:553:PRO:HB2   | 1.99                     | 0.43              |
| 36:Cc:173:ASN:OD1  | 36:Cc:174:VAL:N     | 2.51                     | 0.43              |
| 39:Cf:13:HIS:HB3   | 44:Ck:139:THR:HG21  | 2.00                     | 0.43              |
| 39:Cf:37:ARG:HB2   | 39:Cf:59:ARG:HG3    | 1.99                     | 0.43              |
| 53:UT:255:ILE:HA   | 53:UT:258:MET:HG3   | 2.00                     | 0.43              |
| 53:UT:1161:VAL:O   | 53:UT:1165:ILE:HG12 | 2.18                     | 0.43              |
| 54:UH:275:PRO:HB2  | 54:UH:279:GLU:HB2   | 1.99                     | 0.43              |
| 54:UH:591:VAL:HG21 | 54:UH:609:ILE:HG21  | 2.00                     | 0.43              |
| 4:UD:832:PHE:HB2   | 4:UD:835:ILE:HD11   | 2.00                     | 0.43              |
| 7:UJ:941:LEU:HD12  | 7:UJ:944:LEU:HD11   | 2.00                     | 0.43              |
| 9:UL:851:PHE:CZ    | 9:UL:895:MET:HE1    | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:UM:522:ARG:HD3  | 10:UM:522:ARG:HA   | 1.82                     | 0.43              |
| 13:UQ:417:ASP:OD1  | 13:UQ:419:SER:OG   | 2.35                     | 0.43              |
| 13:UQ:658:LEU:HD21 | 55:UE:32:ARG:HB3   | 2.00                     | 0.43              |
| 18:CA:204:ILE:HG13 | 19:CC:155:LEU:HD12 | 1.99                     | 0.43              |
| 23:CH:281:LEU:HB3  | 23:CH:317:LEU:HD22 | 2.00                     | 0.43              |
| 32:CR:620:GLN:O    | 32:CR:623:GLN:NE2  | 2.51                     | 0.43              |
| 39:Cf:86:SER:O     | 50:C1:925:G:O2'    | 2.27                     | 0.43              |
| 50:C1:278:A:OP2    | 50:C1:278:A:H8     | 2.01                     | 0.43              |
| 50:C1:990:U:H2'    | 50:C1:991:A:C8     | 2.53                     | 0.43              |
| 53:UT:2192:GLN:HG2 | 53:UT:2233:ARG:CZ  | 2.48                     | 0.43              |
| 55:UE:178:LEU:HA   | 55:UE:181:ILE:HD12 | 1.99                     | 0.43              |
| 4:UD:432:THR:HG23  | 4:UD:448:PRO:HD3   | 1.99                     | 0.43              |
| 7:UJ:959:GLN:HA    | 7:UJ:962:VAL:HG22  | 2.01                     | 0.43              |
| 7:UJ:965:SER:O     | 7:UJ:969:MET:HG2   | 2.19                     | 0.43              |
| 7:UJ:1090:PRO:HD2  | 7:UJ:1093:ARG:HD2  | 2.00                     | 0.43              |
| 8:UK:22:ARG:NH2    | 24:CI:984:SER:O    | 2.51                     | 0.43              |
| 13:UQ:407:LYS:O    | 13:UQ:409:SER:N    | 2.44                     | 0.43              |
| 22:CG:339:LEU:HD23 | 22:CG:339:LEU:HA   | 1.88                     | 0.43              |
| 37:Cd:187:LEU:HD12 | 50:C1:725:A:H62    | 1.83                     | 0.43              |
| 39:Cf:169:LEU:HD13 | 39:Cf:187:ILE:HD13 | 1.99                     | 0.43              |
| 42:CI:81:ALA:HB2   | 42:CI:118:LEU:HD23 | 2.01                     | 0.43              |
| 52:CW:204:VAL:HG13 | 52:CW:221:THR:HG22 | 1.99                     | 0.43              |
| 52:CW:247:ILE:HG12 | 52:CW:263:THR:HG22 | 2.00                     | 0.43              |
| 53:UT:1062:GLU:HA  | 53:UT:1063:PRO:HD3 | 1.90                     | 0.43              |
| 54:UH:824:GLU:OE1  | 55:UI:210:ARG:NH2  | 2.52                     | 0.43              |
| 60:CZ:497:LEU:HA   | 60:CZ:500:LYS:HG3  | 2.00                     | 0.43              |
| 3:UC:642:LEU:HD23  | 3:UC:644:LYS:HE3   | 2.00                     | 0.43              |
| 4:UD:47:GLY:HA3    | 4:UD:77:VAL:HG11   | 2.00                     | 0.43              |
| 4:UD:256:GLY:HA2   | 4:UD:279:VAL:HG23  | 2.00                     | 0.43              |
| 7:UJ:294:GLU:HA    | 7:UJ:297:VAL:HG22  | 2.00                     | 0.43              |
| 7:UJ:297:VAL:HG12  | 7:UJ:300:TRP:CZ3   | 2.53                     | 0.43              |
| 10:UM:874:ILE:HD13 | 10:UM:877:LEU:HD12 | 2.01                     | 0.43              |
| 11:UN:305:ARG:NH2  | 38:Ce:177:ASP:OD1  | 2.46                     | 0.43              |
| 13:UQ:730:PHE:CZ   | 13:UQ:746:MET:HE3  | 2.53                     | 0.43              |
| 22:CG:483:TRP:HB3  | 22:CG:559:ILE:HG12 | 2.01                     | 0.43              |
| 22:CG:504:ILE:HB   | 22:CG:507:VAL:HG22 | 1.99                     | 0.43              |
| 29:CN:204:VAL:HG11 | 29:CN:241:PHE:CD2  | 2.53                     | 0.43              |
| 29:CO:73:HIS:HB3   | 29:CO:76:ILE:HG12  | 2.00                     | 0.43              |
| 32:CR:753:ASP:OD1  | 32:CR:754:LEU:N    | 2.52                     | 0.43              |
| 37:Cd:94:ARG:NE    | 50:C1:991:A:OP1    | 2.51                     | 0.43              |
| 47:Co:418:PRO:HD2  | 47:Co:421:ARG:HD2  | 2.01                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 52:CW:270:ILE:HB    | 52:CW:280:LEU:HB2   | 2.01                     | 0.43              |
| 52:CW:271:PHE:HE1   | 52:CW:278:PRO:HB3   | 1.82                     | 0.43              |
| 53:UT:613:SER:HA    | 53:UT:614:PRO:HD3   | 1.93                     | 0.43              |
| 53:UT:1272:HIS:HA   | 53:UT:1311:TRP:HZ3  | 1.82                     | 0.43              |
| 53:UT:1778:ARG:HH11 | 53:UT:1816:ILE:HG13 | 1.84                     | 0.43              |
| 53:UT:2189:GLU:O    | 53:UT:2192:GLN:HB2  | 2.18                     | 0.43              |
| 55:UE:228:ALA:O     | 55:UE:232:GLN:HG2   | 2.18                     | 0.43              |
| 60:CZ:325:LEU:HD23  | 60:CZ:502:LEU:HD12  | 2.00                     | 0.43              |
| 3:UC:602:VAL:HG21   | 50:C1:1061:A:H5'    | 2.00                     | 0.43              |
| 4:UD:104:SER:HB3    | 4:UD:114:TRP:HE1    | 1.84                     | 0.43              |
| 4:UD:632:VAL:HB     | 4:UD:650:VAL:HB     | 2.01                     | 0.43              |
| 6:UG:375:ARG:HH21   | 6:UG:379:VAL:H      | 1.65                     | 0.43              |
| 7:UJ:255:LEU:O      | 7:UJ:259:MET:HG3    | 2.18                     | 0.43              |
| 7:UJ:1128:MET:HE3   | 7:UJ:1132:MET:HE3   | 2.00                     | 0.43              |
| 7:UJ:1566:TYR:HE2   | 7:UJ:1613:SER:HA    | 1.83                     | 0.43              |
| 13:UQ:399:ILE:HA    | 13:UQ:415:LEU:HD23  | 2.01                     | 0.43              |
| 18:CB:250:GLY:CA    | 18:CB:306:TYR:O     | 2.66                     | 0.43              |
| 32:CS:29:VAL:HA     | 32:CS:202:ILE:O     | 2.19                     | 0.43              |
| 32:CS:514:SER:HB2   | 59:CY:116:ARG:HH12  | 1.83                     | 0.43              |
| 34:Ca:175:GLU:O     | 34:Ca:187:LYS:NZ    | 2.45                     | 0.43              |
| 38:Ce:33:LEU:HA     | 38:Ce:37:THR:HG21   | 1.99                     | 0.43              |
| 44:Ck:43:VAL:HG21   | 44:Ck:145:LEU:HD11  | 1.98                     | 0.43              |
| 51:C2:160:U:H2'     | 51:C2:161:G:C8      | 2.54                     | 0.43              |
| 53:UT:306:ILE:HD13  | 53:UT:341:VAL:HG13  | 2.01                     | 0.43              |
| 53:UT:929:LEU:HD12  | 53:UT:929:LEU:HA    | 1.81                     | 0.43              |
| 3:UC:321:LEU:HD11   | 27:CL:162:LEU:HD11  | 1.99                     | 0.43              |
| 9:UL:832:ASN:O      | 9:UL:836:LYS:HG2    | 2.18                     | 0.43              |
| 10:UM:311:LYS:HZ1   | 10:UM:362:LEU:HD13  | 1.84                     | 0.43              |
| 13:UQ:731:LYS:HB3   | 13:UQ:749:ASP:HB2   | 1.99                     | 0.43              |
| 15:UU:117:GLN:NE2   | 15:UU:139:GLN:O     | 2.46                     | 0.43              |
| 15:UU:271:THR:HB    | 15:UU:274:ALA:HB3   | 2.00                     | 0.43              |
| 25:CJ:102:THR:HG22  | 25:CJ:104:SER:H     | 1.83                     | 0.43              |
| 32:CR:255:LEU:O     | 32:CR:257:ARG:NH1   | 2.52                     | 0.43              |
| 32:CS:359:VAL:HB    | 32:CS:369:ILE:HB    | 2.00                     | 0.43              |
| 32:CS:685:ASP:OD1   | 32:CS:685:ASP:N     | 2.51                     | 0.43              |
| 41:Ch:108:ASP:OD1   | 50:C1:1463:G:O2'    | 2.27                     | 0.43              |
| 44:Ck:137:SER:O     | 44:Ck:141:ARG:NH1   | 2.50                     | 0.43              |
| 47:Co:382:GLN:HE21  | 47:Co:383:LYS:H     | 1.67                     | 0.43              |
| 50:C1:5:G:H1        | 50:C1:30:U:H3       | 1.66                     | 0.43              |
| 50:C1:1097:U:H2'    | 50:C1:1098:G:C8     | 2.53                     | 0.43              |
| 53:UT:713:LEU:HA    | 53:UT:716:VAL:HG22  | 1.99                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:UT:1235:ILE:HD12 | 53:UT:1295:MET:HG3  | 2.01                     | 0.43              |
| 53:UT:1342:GLN:HG2  | 53:UT:1381:ARG:NH2  | 2.34                     | 0.43              |
| 54:UH:544:ARG:HA    | 54:UH:547:VAL:HG22  | 2.01                     | 0.43              |
| 54:UH:839:ALA:HB2   | 55:UE:265:MET:HE1   | 1.99                     | 0.43              |
| 7:UJ:1619:THR:HB    | 7:UJ:1666:TRP:HZ3   | 1.83                     | 0.43              |
| 7:UJ:1748:ILE:O     | 7:UJ:1752:LEU:HB2   | 2.18                     | 0.43              |
| 9:UL:123:VAL:HG13   | 9:UL:124:ARG:HG3    | 2.01                     | 0.43              |
| 10:UM:137:ILE:HD12  | 10:UM:147:HIS:HB2   | 2.01                     | 0.43              |
| 10:UM:819:ASN:ND2   | 27:CL:699:ALA:O     | 2.36                     | 0.43              |
| 13:UQ:162:ASP:OD1   | 13:UQ:162:ASP:N     | 2.49                     | 0.43              |
| 26:CK:9:ARG:HA      | 26:CK:9:ARG:HD2     | 1.86                     | 0.43              |
| 27:CL:124:ALA:HB1   | 27:CL:125:LEU:HD23  | 2.01                     | 0.43              |
| 28:CM:243:ASN:N     | 28:CM:258:ALA:O     | 2.43                     | 0.43              |
| 29:CO:67:LEU:HD11   | 29:CO:141:MET:HB2   | 2.01                     | 0.43              |
| 32:CR:824:LEU:HD22  | 32:CR:864:LEU:HD21  | 2.01                     | 0.43              |
| 46:Cn:51:GLY:HA2    | 46:Cn:77:ILE:HG13   | 2.01                     | 0.43              |
| 53:UT:587:ARG:HG3   | 53:UT:588:MET:SD    | 2.58                     | 0.43              |
| 53:UT:2191:THR:HA   | 53:UT:2194:VAL:HG22 | 2.01                     | 0.43              |
| 54:UH:181:ALA:O     | 54:UH:190:LYS:N     | 2.51                     | 0.43              |
| 54:UH:399:GLU:HB3   | 54:UH:414:ILE:HG13  | 2.00                     | 0.43              |
| 1:UA:183:GLU:HB2    | 1:UA:186:PHE:HB3    | 1.99                     | 0.43              |
| 1:UA:204:SER:OG     | 1:UA:206:ASP:O      | 2.34                     | 0.43              |
| 1:UA:730:TYR:HB3    | 1:UA:753:ILE:HG12   | 2.01                     | 0.43              |
| 4:UD:129:HIS:HB2    | 4:UD:158:THR:HG21   | 2.01                     | 0.43              |
| 7:UJ:142:TYR:O      | 7:UJ:145:ILE:HG12   | 2.19                     | 0.43              |
| 7:UJ:494:ARG:HA     | 7:UJ:497:LYS:HG2    | 2.00                     | 0.43              |
| 7:UJ:522:LEU:HD11   | 7:UJ:564:PRO:HD2    | 2.00                     | 0.43              |
| 7:UJ:700:HIS:HA     | 7:UJ:701:SER:HA     | 1.73                     | 0.43              |
| 13:UQ:938:MET:HG3   | 13:UQ:939:PRO:HD2   | 2.01                     | 0.43              |
| 17:UZ:77:ARG:HD2    | 50:C1:373:C:H4'     | 2.00                     | 0.43              |
| 24:CI:1076:MET:HA   | 24:CI:1079:ARG:HG2  | 2.01                     | 0.43              |
| 25:CJ:44:TYR:CD1    | 25:CJ:103:VAL:HG11  | 2.54                     | 0.43              |
| 31:CQ:84:LYS:HD2    | 31:CQ:121:ARG:HH11  | 1.84                     | 0.43              |
| 32:CR:837:ASP:HB3   | 32:CR:857:LEU:HD11  | 1.99                     | 0.43              |
| 32:CS:884:LEU:HD13  | 32:CS:915:ILE:HG21  | 1.99                     | 0.43              |
| 50:C1:252:U:H2'     | 50:C1:253:G:C8      | 2.54                     | 0.43              |
| 50:C1:1652:C:H2'    | 50:C1:1653:G:C8     | 2.54                     | 0.43              |
| 50:C1:2158:G:H2'    | 50:C1:2159:A:C8     | 2.54                     | 0.43              |
| 53:UT:278:PHE:HB3   | 53:UT:324:ARG:HH22  | 1.83                     | 0.43              |
| 53:UT:717:TYR:CD1   | 53:UT:756:VAL:HG23  | 2.54                     | 0.43              |
| 53:UT:2005:LYS:NZ   | 53:UT:2035:GLU:OE1  | 2.52                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:UH:75:SER:HB3    | 54:UH:78:SER:HB3    | 2.01                     | 0.43              |
| 58:CX:406:LEU:HA    | 58:CX:407:PRO:HD3   | 1.88                     | 0.43              |
| 7:UJ:541:SER:O      | 7:UJ:544:LYS:N      | 2.51                     | 0.43              |
| 7:UJ:1224:TYR:CE2   | 7:UJ:1259:LEU:HD23  | 2.54                     | 0.43              |
| 10:UM:628:ASN:HB2   | 10:UM:635:ILE:HD11  | 2.00                     | 0.43              |
| 12:UO:162:SER:HB3   | 12:UO:172:TRP:HE1   | 1.84                     | 0.43              |
| 15:UU:56:LEU:HD23   | 50:C1:262:G:C8      | 2.54                     | 0.43              |
| 17:UZ:158:ARG:NH2   | 17:UZ:184:LEU:O     | 2.51                     | 0.43              |
| 22:CG:221:LYS:N     | 51:C2:180:U:O2'     | 2.50                     | 0.43              |
| 23:CH:236:ILE:HD12  | 23:CH:252:ILE:HB    | 2.01                     | 0.43              |
| 24:CI:113:ARG:HD3   | 24:CI:308:THR:HG23  | 2.00                     | 0.43              |
| 27:CL:675:SER:O     | 27:CL:675:SER:OG    | 2.36                     | 0.43              |
| 32:CS:911:ILE:O     | 32:CS:915:ILE:HG12  | 2.19                     | 0.43              |
| 53:UT:2010:LYS:O    | 53:UT:2013:THR:OG1  | 2.31                     | 0.43              |
| 53:UT:2075:LEU:HD11 | 53:UT:2107:LEU:HD13 | 2.00                     | 0.43              |
| 7:UJ:635:LYS:HD3    | 7:UJ:641:THR:HA     | 2.01                     | 0.42              |
| 7:UJ:847:ASP:N      | 7:UJ:847:ASP:OD1    | 2.51                     | 0.42              |
| 7:UJ:1608:ASP:HA    | 7:UJ:1611:PHE:CD2   | 2.54                     | 0.42              |
| 14:UR:262:ASP:CB    | 14:UR:617:ARG:O     | 2.67                     | 0.42              |
| 14:UR:300:LEU:HB2   | 14:UR:316:THR:HG22  | 2.00                     | 0.42              |
| 22:CG:352:ARG:HH11  | 22:CG:396:GLY:HA2   | 1.84                     | 0.42              |
| 32:CR:557:GLN:NE2   | 32:CR:561:ASP:OD2   | 2.51                     | 0.42              |
| 37:Cd:21:GLU:O      | 37:Cd:25:ARG:HG3    | 2.19                     | 0.42              |
| 53:UT:1504:GLU:HG3  | 53:UT:1507:ARG:HH11 | 1.84                     | 0.42              |
| 54:UH:34:VAL:HB     | 54:UH:48:GLU:HB2    | 2.01                     | 0.42              |
| 56:US:458:TRP:HA    | 56:US:461:VAL:HG22  | 2.00                     | 0.42              |
| 59:CY:252:ASN:HB2   | 59:CY:261:LYS:HB2   | 2.00                     | 0.42              |
| 1:UA:346:LEU:HA     | 1:UA:356:VAL:O      | 2.19                     | 0.42              |
| 7:UJ:194:SER:OG     | 7:UJ:198:ARG:NH2    | 2.48                     | 0.42              |
| 7:UJ:1117:MET:SD    | 7:UJ:1169:LEU:HD22  | 2.59                     | 0.42              |
| 7:UJ:1600:LEU:HB3   | 7:UJ:1646:LEU:HD22  | 1.99                     | 0.42              |
| 20:CD:304:HIS:CD2   | 20:CD:322:LEU:HD22  | 2.54                     | 0.42              |
| 22:CG:418:LEU:HD12  | 22:CG:418:LEU:HA    | 1.90                     | 0.42              |
| 29:CO:37:LEU:HD23   | 29:CO:110:LEU:HD12  | 2.02                     | 0.42              |
| 31:CQ:109:CYS:HB3   | 31:CQ:111:LEU:HD13  | 2.00                     | 0.42              |
| 32:CR:282:THR:HA    | 32:CR:410:MET:HB2   | 2.00                     | 0.42              |
| 32:CR:744:PRO:HA    | 32:CR:762:MET:HG2   | 2.00                     | 0.42              |
| 37:Cd:31:ARG:NH1    | 52:CW:42:LEU:O      | 2.47                     | 0.42              |
| 50:C1:770:C:H42     | 50:C1:781:G:H1      | 1.65                     | 0.42              |
| 50:C1:771:G:O2'     | 50:C1:772:A:O5'     | 2.33                     | 0.42              |
| 50:C1:781:G:H2'     | 50:C1:782:G:C8      | 2.54                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:UT:913:PRO:HG3  | 53:UT:948:TRP:HA    | 2.00                     | 0.42              |
| 7:UJ:48:ILE:HD13   | 7:UJ:123:ARG:HE     | 1.83                     | 0.42              |
| 7:UJ:232:MET:HB3   | 7:UJ:243:ASN:HB3    | 2.01                     | 0.42              |
| 7:UJ:612:ALA:HA    | 7:UJ:664:LEU:HD11   | 2.01                     | 0.42              |
| 7:UJ:1268:VAL:HG21 | 7:UJ:1287:LEU:HD21  | 2.01                     | 0.42              |
| 7:UJ:1463:GLN:HA   | 7:UJ:1466:GLN:HE22  | 1.84                     | 0.42              |
| 12:UO:121:GLY:HA2  | 12:UO:147:VAL:HG23  | 2.01                     | 0.42              |
| 15:UU:538:THR:HB   | 15:UU:560:SER:HB3   | 2.02                     | 0.42              |
| 15:UU:624:ALA:HB3  | 15:UU:642:LEU:HD12  | 2.01                     | 0.42              |
| 19:CC:372:PRO:HB2  | 19:CC:373:LYS:H     | 1.63                     | 0.42              |
| 22:CG:119:ASP:N    | 22:CG:119:ASP:OD1   | 2.53                     | 0.42              |
| 34:Ca:70:LEU:HA    | 34:Ca:73:LEU:HB2    | 2.01                     | 0.42              |
| 39:Cf:115:ALA:HA   | 53:UT:1084:GLY:HA3  | 2.01                     | 0.42              |
| 53:UT:673:ILE:O    | 53:UT:677:LEU:HB2   | 2.20                     | 0.42              |
| 53:UT:1242:GLU:HA  | 53:UT:1245:SER:HG   | 1.83                     | 0.42              |
| 53:UT:1600:ALA:O   | 53:UT:1604:ILE:HG12 | 2.19                     | 0.42              |
| 59:CY:258:ARG:HE   | 59:CY:258:ARG:HB3   | 1.74                     | 0.42              |
| 1:UA:15:TYR:HD2    | 1:UA:320:GLY:O      | 2.01                     | 0.42              |
| 5:UF:16:ALA:HA     | 5:UF:19:LEU:HD12    | 2.02                     | 0.42              |
| 7:UJ:720:LEU:HD13  | 7:UJ:774:ILE:HG12   | 2.02                     | 0.42              |
| 7:UJ:863:THR:O     | 7:UJ:867:HIS:ND1    | 2.47                     | 0.42              |
| 18:CB:194:ILE:HD12 | 20:CD:154:LEU:HD11  | 2.00                     | 0.42              |
| 22:CG:438:LEU:HA   | 22:CG:463:PRO:HA    | 2.01                     | 0.42              |
| 24:Cl:183:LYS:HZ2  | 50:C1:1049:G:H5'    | 1.84                     | 0.42              |
| 29:CN:102:SER:HA   | 29:CO:236:VAL:HG21  | 2.01                     | 0.42              |
| 32:CR:658:VAL:O    | 32:CR:662:GLU:HG2   | 2.19                     | 0.42              |
| 32:CS:35:LYS:H     | 32:CS:35:LYS:HG2    | 1.61                     | 0.42              |
| 32:CS:95:PHE:HA    | 32:CS:98:PHE:CE1    | 2.54                     | 0.42              |
| 36:Cc:50:GLN:NE2   | 36:Cc:53:ALA:H      | 2.18                     | 0.42              |
| 50:C1:94:G:OP1     | 56:US:259:SER:OG    | 2.29                     | 0.42              |
| 52:CW:137:ARG:NE   | 52:CW:167:GLU:OE2   | 2.40                     | 0.42              |
| 53:UT:1434:LEU:O   | 53:UT:1438:LEU:HB2  | 2.19                     | 0.42              |
| 53:UT:1640:LEU:O   | 53:UT:1644:GLU:HG2  | 2.19                     | 0.42              |
| 53:UT:2142:PHE:O   | 53:UT:2146:TYR:HB2  | 2.19                     | 0.42              |
| 1:UA:505:GLU:OE2   | 36:Cc:70:ARG:NH1    | 2.36                     | 0.42              |
| 1:UA:705:GLN:HE21  | 15:UU:674:HIS:HE1   | 1.67                     | 0.42              |
| 2:UB:482:PRO:HB2   | 2:UB:529:VAL:HG11   | 2.02                     | 0.42              |
| 10:UM:145:VAL:O    | 50:C1:2359:A:O2'    | 2.32                     | 0.42              |
| 23:CH:240:ARG:NH1  | 23:CH:250:VAL:O     | 2.53                     | 0.42              |
| 24:Cl:254:HIS:ND1  | 24:Cl:256:THR:HG22  | 2.34                     | 0.42              |
| 32:CR:158:SER:HA   | 32:CR:161:GLN:HB2   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 32:CR:754:LEU:HD12 | 32:CR:755:THR:HG23  | 2.00                     | 0.42              |
| 50:C1:992:C:O2'    | 52:CW:127:MET:SD    | 2.68                     | 0.42              |
| 58:CX:338:SER:HB2  | 58:CX:370:LEU:HD11  | 2.01                     | 0.42              |
| 7:UJ:956:GLY:HA2   | 7:UJ:959:GLN:HG2    | 2.02                     | 0.42              |
| 7:UJ:1379:VAL:HG22 | 7:UJ:1386:ILE:HG12  | 2.02                     | 0.42              |
| 9:UL:673:SER:OG    | 9:UL:674:LYS:N      | 2.53                     | 0.42              |
| 12:UO:529:LYS:NZ   | 50:C1:112:C:O2'     | 2.48                     | 0.42              |
| 17:UZ:67:THR:HG22  | 17:UZ:280:ASN:HB2   | 2.02                     | 0.42              |
| 19:CC:45:GLY:HA3   | 50:C1:435:A:N1      | 2.35                     | 0.42              |
| 20:CD:253:ASP:O    | 20:CD:257:ILE:HG12  | 2.20                     | 0.42              |
| 21:CE:67:HIS:CE1   | 21:CE:68:ILE:HG13   | 2.54                     | 0.42              |
| 24:CI:87:SER:HB3   | 24:CI:219:ILE:HG13  | 2.00                     | 0.42              |
| 27:CL:63:PHE:CE1   | 27:CL:70:LEU:HD13   | 2.55                     | 0.42              |
| 32:CR:835:PRO:HA   | 32:CR:838:HIS:HB2   | 2.00                     | 0.42              |
| 32:CS:530:HIS:CE1  | 60:CZ:289:ALA:HA    | 2.55                     | 0.42              |
| 50:C1:1476:A:H2'   | 50:C1:1477:A:H8     | 1.85                     | 0.42              |
| 56:US:240:LEU:O    | 56:US:242:ASN:N     | 2.52                     | 0.42              |
| 5:UF:310:LEU:O     | 5:UF:313:HIS:ND1    | 2.45                     | 0.42              |
| 7:UJ:540:LEU:HA    | 7:UJ:550:PHE:HE2    | 1.85                     | 0.42              |
| 7:UJ:1657:CYS:HA   | 7:UJ:1660:HIS:ND1   | 2.34                     | 0.42              |
| 17:UZ:62:ILE:HG22  | 17:UZ:285:GLY:HA2   | 2.01                     | 0.42              |
| 19:CC:48:VAL:HG11  | 19:CC:134:ILE:HD11  | 2.02                     | 0.42              |
| 24:CI:1013:MET:HG3 | 27:CL:487:ILE:HG23  | 2.02                     | 0.42              |
| 29:CO:104:ILE:HB   | 29:CO:246:GLU:HG3   | 2.02                     | 0.42              |
| 31:CQ:166:ILE:HA   | 31:CQ:218:ILE:O     | 2.20                     | 0.42              |
| 50:C1:801:A:O2'    | 53:UT:1321:ASN:OD1  | 2.34                     | 0.42              |
| 50:C1:1701:U:H2'   | 50:C1:1702:G:C8     | 2.54                     | 0.42              |
| 53:UT:387:TRP:HA   | 53:UT:391:ILE:HG22  | 2.02                     | 0.42              |
| 53:UT:402:PRO:HG2  | 53:UT:405:ALA:HB3   | 2.01                     | 0.42              |
| 53:UT:1194:PRO:HA  | 53:UT:1237:LEU:HD11 | 2.01                     | 0.42              |
| 53:UT:1256:LEU:O   | 53:UT:1260:THR:OG1  | 2.31                     | 0.42              |
| 54:UH:228:PHE:HA   | 54:UH:329:ASN:HA    | 2.01                     | 0.42              |
| 55:UE:306:VAL:O    | 55:UE:311:GLN:NE2   | 2.51                     | 0.42              |
| 58:CX:217:LEU:HD11 | 58:CX:249:ALA:HB1   | 2.02                     | 0.42              |
| 1:UA:548:VAL:HG12  | 1:UA:604:MET:HB3    | 2.00                     | 0.42              |
| 1:UA:832:ARG:NH2   | 27:CL:669:VAL:HG13  | 2.34                     | 0.42              |
| 2:UB:736:ALA:HA    | 2:UB:739:THR:HG22   | 2.01                     | 0.42              |
| 4:UD:709:MET:HE2   | 54:UH:917:LEU:HD23  | 2.02                     | 0.42              |
| 7:UJ:86:MET:HE1    | 7:UJ:94:LEU:HD22    | 2.02                     | 0.42              |
| 7:UJ:540:LEU:HD12  | 7:UJ:551:TYR:HD1    | 1.85                     | 0.42              |
| 7:UJ:1206:ILE:HG21 | 7:UJ:1259:LEU:HD13  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:UL:790:MET:O     | 9:UL:794:ASN:ND2    | 2.42                     | 0.42              |
| 29:CO:27:ILE:HD12  | 29:CO:36:ARG:HH11   | 1.84                     | 0.42              |
| 32:CS:41:LEU:HA    | 32:CS:44:ILE:HG12   | 2.02                     | 0.42              |
| 35:Cb:175:PHE:O    | 35:Cb:198:ARG:NH1   | 2.49                     | 0.42              |
| 50:C1:1153:C:H2'   | 50:C1:1154:A:O4'    | 2.19                     | 0.42              |
| 53:UT:1582:HIS:O   | 53:UT:1586:ASP:HB2  | 2.20                     | 0.42              |
| 3:UC:239:LEU:HD23  | 3:UC:242:LEU:HD12   | 2.02                     | 0.42              |
| 6:UG:219:VAL:HA    | 6:UG:235:SER:HA     | 2.02                     | 0.42              |
| 7:UJ:52:CYS:HB3    | 7:UJ:120:TRP:HB2    | 2.02                     | 0.42              |
| 7:UJ:396:TYR:HE1   | 7:UJ:442:ILE:HD11   | 1.84                     | 0.42              |
| 7:UJ:506:LEU:HD13  | 7:UJ:638:TYR:CE2    | 2.54                     | 0.42              |
| 7:UJ:1719:TYR:HB3  | 7:UJ:1756:TRP:HZ3   | 1.84                     | 0.42              |
| 9:UL:40:ILE:HG13   | 9:UL:49:VAL:HG12    | 2.02                     | 0.42              |
| 9:UL:938:GLU:OE1   | 31:CQ:240:GLN:NE2   | 2.53                     | 0.42              |
| 11:UN:279:SER:O    | 11:UN:283:MET:HG2   | 2.20                     | 0.42              |
| 12:UO:335:ALA:HB1  | 12:UO:343:LEU:HD11  | 2.01                     | 0.42              |
| 16:UX:17:GLU:HA    | 16:UX:20:LYS:HD3    | 2.01                     | 0.42              |
| 24:CI:934:ILE:HD12 | 24:CI:987:VAL:HG21  | 2.02                     | 0.42              |
| 32:CR:201:VAL:HG12 | 32:CR:209:LEU:HD12  | 2.02                     | 0.42              |
| 35:Cb:184:THR:HA   | 35:Cb:190:GLY:H     | 1.85                     | 0.42              |
| 38:Ce:59:HIS:HB3   | 53:UT:2087:THR:HG22 | 2.02                     | 0.42              |
| 50:C1:89:G:O2'     | 50:C1:90:A:O5'      | 2.36                     | 0.42              |
| 51:C2:125:U:O2'    | 51:C2:126:U:O4'     | 2.36                     | 0.42              |
| 52:CW:298:THR:O    | 52:CW:301:GLU:N     | 2.53                     | 0.42              |
| 53:UT:685:ASN:O    | 53:UT:688:SER:OG    | 2.38                     | 0.42              |
| 53:UT:1783:LYS:HB2 | 53:UT:1786:GLN:HG3  | 2.01                     | 0.42              |
| 53:UT:2155:LYS:HA  | 53:UT:2158:LYS:HE2  | 2.01                     | 0.42              |
| 55:UE:308:VAL:HG23 | 55:UE:311:GLN:HE21  | 1.85                     | 0.42              |
| 56:US:373:LEU:HD22 | 56:US:377:LEU:HD22  | 2.02                     | 0.42              |
| 58:CX:391:ARG:NH2  | 58:CX:392:TYR:OH    | 2.53                     | 0.42              |
| 58:CX:445:ILE:HG22 | 58:CX:449:ILE:HD11  | 2.02                     | 0.42              |
| 2:UB:738:ASP:OD1   | 2:UB:783:HIS:NE2    | 2.41                     | 0.42              |
| 4:UD:383:ILE:HG13  | 4:UD:394:TRP:HB2    | 2.01                     | 0.42              |
| 7:UJ:455:LYS:HD3   | 7:UJ:456:LEU:HD22   | 2.02                     | 0.42              |
| 7:UJ:727:LEU:HD23  | 7:UJ:777:ALA:HB1    | 2.02                     | 0.42              |
| 7:UJ:1515:VAL:HG13 | 7:UJ:1516:VAL:HG23  | 2.02                     | 0.42              |
| 12:UO:83:ILE:HD11  | 12:UO:114:LEU:HD13  | 2.01                     | 0.42              |
| 13:UQ:81:VAL:HG21  | 13:UQ:825:LYS:HD2   | 2.00                     | 0.42              |
| 13:UQ:378:VAL:HG13 | 13:UQ:393:PRO:HA    | 2.02                     | 0.42              |
| 14:UR:426:TRP:HB3  | 14:UR:478:GLY:HA3   | 2.02                     | 0.42              |
| 18:CB:250:GLY:HA2  | 18:CB:306:TYR:O     | 2.20                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 19:CC:251:ALA:O     | 19:CC:255:ILE:HG12  | 2.20                     | 0.42              |
| 23:CH:222:ALA:HB2   | 23:CH:279:LEU:HD13  | 2.01                     | 0.42              |
| 24:CI:246:ILE:HD12  | 24:CI:270:LEU:HB3   | 2.02                     | 0.42              |
| 32:CR:544:TYR:OH    | 32:CR:587:GLN:OE1   | 2.30                     | 0.42              |
| 51:C2:246:G:H3'     | 51:C2:247:G:H5''    | 2.01                     | 0.42              |
| 53:UT:1415:PHE:HB3  | 53:UT:1454:ASN:HB3  | 2.02                     | 0.42              |
| 2:UB:473:ASN:HB3    | 2:UB:499:LYS:HE2    | 2.02                     | 0.41              |
| 2:UB:704:CYS:HA     | 2:UB:707:CYS:SG     | 2.60                     | 0.41              |
| 4:UD:514:ASP:N      | 4:UD:514:ASP:OD1    | 2.52                     | 0.41              |
| 5:UF:32:GLU:HG2     | 14:UR:60:LEU:HD13   | 2.02                     | 0.41              |
| 7:UJ:559:TRP:O      | 7:UJ:568:LYS:NZ     | 2.42                     | 0.41              |
| 7:UJ:1653:THR:HA    | 7:UJ:1656:LYS:HG2   | 2.02                     | 0.41              |
| 9:UL:287:HIS:HB3    | 9:UL:290:ARG:H      | 1.85                     | 0.41              |
| 12:UO:534:VAL:O     | 12:UO:538:GLU:HG2   | 2.20                     | 0.41              |
| 13:UQ:292:THR:HG23  | 13:UQ:361:VAL:HG12  | 2.03                     | 0.41              |
| 14:UR:414:ILE:HG22  | 14:UR:442:THR:HG21  | 2.03                     | 0.41              |
| 15:UU:282:ARG:HE    | 15:UU:284:ASP:HB3   | 1.85                     | 0.41              |
| 20:CD:321:ILE:HD12  | 20:CD:328:LEU:HD22  | 2.02                     | 0.41              |
| 22:CG:343:ARG:HA    | 22:CG:357:TRP:O     | 2.19                     | 0.41              |
| 24:CI:514:GLU:HA    | 24:CI:517:VAL:HG22  | 2.02                     | 0.41              |
| 32:CS:238:LYS:HA    | 32:CS:241:ASP:HB2   | 2.01                     | 0.41              |
| 35:Cb:99:PHE:HA     | 35:Cb:112:HIS:O     | 2.19                     | 0.41              |
| 53:UT:287:LYS:HE2   | 53:UT:287:LYS:HB2   | 1.92                     | 0.41              |
| 53:UT:578:THR:O     | 53:UT:582:PHE:CB    | 2.68                     | 0.41              |
| 53:UT:601:PRO:HA    | 53:UT:604:ARG:HG2   | 2.02                     | 0.41              |
| 53:UT:1027:LEU:HD23 | 53:UT:1027:LEU:HA   | 1.92                     | 0.41              |
| 55:UE:158:ASN:HD21  | 55:UE:188:MET:HA    | 1.85                     | 0.41              |
| 55:UE:197:LEU:HD23  | 55:UE:197:LEU:HA    | 1.93                     | 0.41              |
| 59:CY:120:ASP:OD1   | 59:CY:123:ARG:NH1   | 2.53                     | 0.41              |
| 1:UA:196:GLN:HG3    | 1:UA:216:ASP:HB3    | 2.02                     | 0.41              |
| 2:UB:685:PRO:HA     | 2:UB:686:PRO:HD3    | 1.91                     | 0.41              |
| 7:UJ:72:THR:HG22    | 14:UR:69:GLN:HB3    | 2.01                     | 0.41              |
| 7:UJ:126:ARG:NH1    | 7:UJ:129:GLU:OE1    | 2.53                     | 0.41              |
| 15:UU:931:GLY:O     | 15:UU:934:LYS:C     | 2.64                     | 0.41              |
| 30:CP:25:LEU:HD23   | 30:CP:26:PRO:HD3    | 2.02                     | 0.41              |
| 32:CR:61:LYS:HD2    | 32:CR:130:ALA:HB3   | 2.02                     | 0.41              |
| 50:C1:2086:A:H5''   | 50:C1:2087:G:C8     | 2.55                     | 0.41              |
| 53:UT:442:ARG:NH2   | 53:UT:486:GLU:OE1   | 2.53                     | 0.41              |
| 53:UT:1143:ARG:HH11 | 53:UT:1146:GLN:HE21 | 1.68                     | 0.41              |
| 54:UH:838:GLU:HB3   | 55:UE:265:MET:HE2   | 2.02                     | 0.41              |
| 58:CX:367:LEU:O     | 58:CX:371:LEU:HB2   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:UG:321:ASP:O     | 6:UG:323:LYS:N     | 2.47                     | 0.41              |
| 6:UG:337:ASN:HB3   | 6:UG:380:LYS:HD2   | 2.01                     | 0.41              |
| 7:UJ:823:ASP:OD1   | 7:UJ:824:THR:N     | 2.54                     | 0.41              |
| 9:UL:12:LYS:HB2    | 9:UL:722:VAL:HB    | 2.02                     | 0.41              |
| 9:UL:113:ILE:HD13  | 9:UL:129:SER:HB3   | 2.01                     | 0.41              |
| 12:UO:210:TYR:HB3  | 56:US:374:PRO:HB3  | 2.03                     | 0.41              |
| 13:UQ:237:TYR:CZ   | 13:UQ:241:PRO:HB3  | 2.55                     | 0.41              |
| 13:UQ:739:SER:O    | 13:UQ:784:HIS:NE2  | 2.50                     | 0.41              |
| 15:UU:954:LEU:HD22 | 31:CQ:254:ARG:HB3  | 2.02                     | 0.41              |
| 16:UX:13:ARG:H     | 16:UX:13:ARG:HG2   | 1.54                     | 0.41              |
| 18:CA:97:LEU:HD23  | 18:CA:200:ARG:HG2  | 2.01                     | 0.41              |
| 20:CD:220:ALA:O    | 20:CD:238:LYS:NZ   | 2.51                     | 0.41              |
| 22:CG:272:VAL:HG12 | 22:CG:282:LYS:HB3  | 2.02                     | 0.41              |
| 23:CH:152:THR:O    | 23:CH:156:ALA:CB   | 2.67                     | 0.41              |
| 29:CO:37:LEU:O     | 29:CO:110:LEU:HA   | 2.20                     | 0.41              |
| 32:CR:224:ASP:HB3  | 32:CR:227:GLU:HG3  | 2.02                     | 0.41              |
| 32:CR:331:PHE:HB3  | 32:CR:336:TYR:HB2  | 2.02                     | 0.41              |
| 32:CS:115:ILE:HB   | 32:CS:120:TYR:HE2  | 1.85                     | 0.41              |
| 32:CS:162:LEU:HD21 | 32:CS:190:LEU:HD11 | 2.02                     | 0.41              |
| 33:CT:185:LYS:HD3  | 50:C1:399:G:H5'    | 2.02                     | 0.41              |
| 37:Cd:211:TYR:HA   | 37:Cd:214:ILE:HG22 | 2.01                     | 0.41              |
| 44:Ck:43:VAL:HG11  | 44:Ck:145:LEU:HD12 | 2.02                     | 0.41              |
| 50:C1:1169:A:O2'   | 50:C1:1170:G:N2    | 2.48                     | 0.41              |
| 52:CW:366:PRO:HD2  | 52:CW:369:CYS:SG   | 2.60                     | 0.41              |
| 53:UT:649:GLU:HA   | 53:UT:652:ILE:HG12 | 2.02                     | 0.41              |
| 53:UT:964:LEU:HD23 | 53:UT:964:LEU:HA   | 1.87                     | 0.41              |
| 53:UT:992:ILE:HD13 | 53:UT:992:ILE:HA   | 1.96                     | 0.41              |
| 53:UT:1255:LEU:O   | 53:UT:1259:ASN:ND2 | 2.49                     | 0.41              |
| 53:UT:1359:PHE:O   | 53:UT:1368:ARG:NH2 | 2.43                     | 0.41              |
| 54:UH:30:PHE:HB3   | 54:UH:83:PRO:HA    | 2.02                     | 0.41              |
| 56:US:136:VAL:HG13 | 56:US:184:HIS:CD2  | 2.55                     | 0.41              |
| 59:CY:110:GLN:HA   | 59:CY:113:LYS:HG2  | 2.02                     | 0.41              |
| 4:UD:298:ARG:HG3   | 4:UD:320:ARG:HD2   | 2.03                     | 0.41              |
| 7:UJ:109:LEU:HD11  | 7:UJ:138:THR:HG22  | 2.01                     | 0.41              |
| 7:UJ:1083:VAL:HG22 | 7:UJ:1118:PHE:CE2  | 2.55                     | 0.41              |
| 7:UJ:1527:LEU:HD11 | 7:UJ:1583:TRP:CD1  | 2.55                     | 0.41              |
| 9:UL:816:PRO:HA    | 9:UL:819:VAL:HG22  | 2.02                     | 0.41              |
| 13:UQ:568:THR:HG22 | 55:UE:262:LYS:HE2  | 2.03                     | 0.41              |
| 14:UR:453:GLY:HA3  | 14:UR:526:ILE:HD12 | 2.01                     | 0.41              |
| 21:CE:60:GLN:OE1   | 21:CE:85:LYS:NZ    | 2.48                     | 0.41              |
| 22:CG:312:VAL:O    | 22:CG:326:LEU:N    | 2.50                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:CH:232:ASN:O    | 23:CH:236:ILE:HG12  | 2.20                     | 0.41              |
| 24:CI:382:GLU:HG2  | 24:CI:384:LYS:H     | 1.85                     | 0.41              |
| 29:CO:180:LEU:HD21 | 29:CO:241:PHE:HE2   | 1.85                     | 0.41              |
| 32:CS:161:GLN:HE21 | 32:CS:688:LEU:HB3   | 1.85                     | 0.41              |
| 32:CS:390:GLU:HB3  | 32:CS:393:ALA:HB3   | 2.01                     | 0.41              |
| 32:CS:479:ARG:NH2  | 65:CS:1101:ADP:O3'  | 2.53                     | 0.41              |
| 35:Cb:128:ARG:HB3  | 35:Cb:140:VAL:HB    | 2.02                     | 0.41              |
| 47:Co:345:ARG:HG2  | 53:UT:75:ILE:HG22   | 2.02                     | 0.41              |
| 52:CW:329:PRO:HG2  | 52:CW:333:LEU:HD11  | 2.02                     | 0.41              |
| 58:CX:446:ALA:HA   | 58:CX:449:ILE:HD12  | 2.02                     | 0.41              |
| 59:CY:270:GLU:HG3  | 59:CY:273:ARG:HH21  | 1.84                     | 0.41              |
| 1:UA:29:LEU:HD21   | 1:UA:322:LEU:HD11   | 2.03                     | 0.41              |
| 1:UA:558:ARG:NH2   | 51:C2:62:A:OP2      | 2.47                     | 0.41              |
| 4:UD:283:SER:HB2   | 4:UD:329:MET:HG3    | 2.01                     | 0.41              |
| 4:UD:413:LEU:HD23  | 4:UD:413:LEU:HA     | 1.95                     | 0.41              |
| 7:UJ:78:SER:HA     | 7:UJ:81:VAL:HG12    | 2.01                     | 0.41              |
| 9:UL:369:VAL:HG13  | 9:UL:387:VAL:HG13   | 2.03                     | 0.41              |
| 19:CC:156:GLY:HA2  | 20:CD:245:MET:HE3   | 2.01                     | 0.41              |
| 19:CC:180:GLY:HA3  | 19:CC:295:LEU:HD11  | 2.03                     | 0.41              |
| 22:CG:334:LEU:HD23 | 22:CG:334:LEU:HA    | 1.87                     | 0.41              |
| 23:CH:170:ARG:HB2  | 23:CH:198:SER:HB3   | 2.02                     | 0.41              |
| 24:CI:950:ALA:O    | 24:CI:961:GLN:HA    | 2.20                     | 0.41              |
| 28:CM:134:LEU:HB3  | 28:CM:148:ALA:HB3   | 2.01                     | 0.41              |
| 32:CS:917:ARG:HE   | 52:CW:381:SER:HA    | 1.86                     | 0.41              |
| 36:Cc:152:LEU:HD23 | 48:Cp:48:PRO:HG2    | 2.02                     | 0.41              |
| 46:Cn:54:LEU:HD12  | 46:Cn:73:ARG:HG2    | 2.02                     | 0.41              |
| 50:C1:493:G:H1     | 50:C1:505:C:H42     | 1.68                     | 0.41              |
| 53:UT:437:ASN:HD22 | 53:UT:440:ARG:HE    | 1.68                     | 0.41              |
| 53:UT:1285:ALA:O   | 53:UT:1289:VAL:HG23 | 2.21                     | 0.41              |
| 56:US:457:LEU:HD13 | 56:US:460:ILE:HG13  | 2.03                     | 0.41              |
| 3:UC:305:MET:HE3   | 3:UC:305:MET:HB3    | 1.95                     | 0.41              |
| 5:UF:138:PRO:HB3   | 19:CC:84:MET:HE1    | 2.02                     | 0.41              |
| 5:UF:333:CYS:SG    | 5:UF:334:THR:N      | 2.94                     | 0.41              |
| 7:UJ:675:VAL:HG13  | 7:UJ:729:SER:HA     | 2.02                     | 0.41              |
| 7:UJ:1000:SER:HB3  | 7:UJ:1003:VAL:HG12  | 2.01                     | 0.41              |
| 9:UL:94:LEU:O      | 9:UL:103:VAL:N      | 2.54                     | 0.41              |
| 10:UM:54:LEU:HD23  | 10:UM:99:VAL:HG23   | 2.03                     | 0.41              |
| 10:UM:788:LEU:HD22 | 10:UM:835:LYS:HD3   | 2.03                     | 0.41              |
| 13:UQ:222:ASN:OD1  | 13:UQ:225:MET:HG3   | 2.21                     | 0.41              |
| 15:UU:173:ILE:HG22 | 15:UU:175:PRO:HD3   | 2.02                     | 0.41              |
| 18:CB:213:PRO:HB2  | 18:CB:245:LEU:HD23  | 2.03                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 28:CM:237:VAL:HB    | 28:CM:443:VAL:HG12  | 2.01                     | 0.41              |
| 52:CW:71:SER:O      | 52:CW:79:PHE:HA     | 2.21                     | 0.41              |
| 52:CW:140:ARG:N     | 52:CW:154:PRO:O     | 2.45                     | 0.41              |
| 53:UT:278:PHE:HB3   | 53:UT:324:ARG:NH2   | 2.35                     | 0.41              |
| 53:UT:1173:PRO:HA   | 53:UT:1213:THR:HG22 | 2.03                     | 0.41              |
| 53:UT:1629:SER:OG   | 53:UT:1630:LYS:N    | 2.54                     | 0.41              |
| 53:UT:1710:VAL:HB   | 53:UT:1757:THR:HG21 | 2.02                     | 0.41              |
| 54:UH:340:VAL:HB    | 54:UH:343:LEU:HB2   | 2.01                     | 0.41              |
| 58:CX:369:VAL:HA    | 58:CX:372:GLU:HG3   | 2.02                     | 0.41              |
| 60:CZ:565:GLU:O     | 60:CZ:566:GLU:HG3   | 2.21                     | 0.41              |
| 4:UD:648:LEU:HD21   | 4:UD:701:PHE:HZ     | 1.86                     | 0.41              |
| 6:UG:375:ARG:NH2    | 6:UG:379:VAL:H      | 2.19                     | 0.41              |
| 6:UG:572:GLN:HE21   | 6:UG:577:ILE:HB     | 1.85                     | 0.41              |
| 9:UL:39:ALA:O       | 9:UL:49:VAL:HA      | 2.20                     | 0.41              |
| 12:UO:123:MET:HE1   | 12:UO:172:TRP:CE2   | 2.55                     | 0.41              |
| 13:UQ:371:ILE:HG22  | 13:UQ:402:ILE:HD13  | 2.02                     | 0.41              |
| 19:CC:34:VAL:O      | 19:CC:38:MET:HG2    | 2.21                     | 0.41              |
| 20:CD:1:MET:HA      | 20:CD:2:PRO:HD2     | 1.98                     | 0.41              |
| 22:CG:583:GLY:HA2   | 22:CG:599:CYS:HA    | 2.03                     | 0.41              |
| 26:CK:105:LYS:NZ    | 50:C1:1743:C:H5'    | 2.36                     | 0.41              |
| 30:CP:127:ARG:HD2   | 30:CP:127:ARG:HA    | 1.84                     | 0.41              |
| 32:CS:231:PRO:HA    | 32:CS:234:LYS:HG2   | 2.01                     | 0.41              |
| 34:Ca:61:LEU:HA     | 34:Ca:64:ARG:HD3    | 2.03                     | 0.41              |
| 50:C1:1652:C:H2'    | 50:C1:1653:G:H8     | 1.85                     | 0.41              |
| 52:CW:224:GLY:HA2   | 52:CW:247:ILE:HG13  | 2.03                     | 0.41              |
| 53:UT:46:VAL:HG23   | 53:UT:48:ARG:HD2    | 2.02                     | 0.41              |
| 53:UT:1260:THR:HG21 | 53:UT:1296:ILE:HG12 | 2.03                     | 0.41              |
| 53:UT:1427:THR:OG1  | 53:UT:1430:GLN:OE1  | 2.35                     | 0.41              |
| 55:UE:207:ARG:HD3   | 55:UE:207:ARG:HA    | 1.80                     | 0.41              |
| 58:CX:263:GLN:O     | 58:CX:267:GLU:HG2   | 2.20                     | 0.41              |
| 1:UA:3:THR:HG21     | 1:UA:607:LEU:HD13   | 2.02                     | 0.41              |
| 1:UA:486:GLY:HA3    | 1:UA:513:VAL:HG11   | 2.03                     | 0.41              |
| 3:UC:210:THR:OG1    | 3:UC:212:ASP:OD1    | 2.32                     | 0.41              |
| 6:UG:57:ARG:O       | 11:UN:899:ARG:HD3   | 2.21                     | 0.41              |
| 7:UJ:32:SER:OG      | 7:UJ:119:GLU:OE2    | 2.38                     | 0.41              |
| 7:UJ:236:ARG:HD2    | 7:UJ:239:ILE:HD12   | 2.02                     | 0.41              |
| 7:UJ:1203:LYS:HB2   | 7:UJ:1258:LEU:HA    | 2.02                     | 0.41              |
| 7:UJ:1260:SER:HA    | 7:UJ:1290:ARG:HD3   | 2.03                     | 0.41              |
| 7:UJ:1345:ASP:OD1   | 7:UJ:1345:ASP:N     | 2.52                     | 0.41              |
| 10:UM:794:VAL:HA    | 10:UM:797:VAL:HG12  | 2.03                     | 0.41              |
| 12:UO:34:LYS:HE2    | 12:UO:89:ARG:HH21   | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:UO:210:TYR:HA   | 12:UO:234:PRO:HB3  | 2.03                     | 0.41              |
| 13:UQ:578:LYS:HE3  | 13:UQ:578:LYS:HB2  | 1.92                     | 0.41              |
| 13:UQ:658:LEU:HD21 | 55:UE:32:ARG:HD2   | 2.02                     | 0.41              |
| 14:UR:345:ARG:HB2  | 50:C1:75:G:H5'     | 2.02                     | 0.41              |
| 28:CM:28:ALA:HB3   | 28:CM:31:LEU:HD13  | 2.02                     | 0.41              |
| 29:CN:103:PRO:HG3  | 29:CO:232:LEU:HD21 | 2.03                     | 0.41              |
| 32:CR:28:VAL:HG21  | 32:CR:193:LEU:HD13 | 2.02                     | 0.41              |
| 32:CR:337:LYS:H    | 32:CR:341:ASP:HB2  | 1.86                     | 0.41              |
| 32:CS:122:MET:SD   | 32:CS:148:LEU:HB2  | 2.61                     | 0.41              |
| 32:CS:514:SER:HA   | 32:CS:652:LYS:HE2  | 2.02                     | 0.41              |
| 34:Ca:23:PRO:O     | 34:Ca:27:LYS:HG2   | 2.20                     | 0.41              |
| 34:Ca:121:ILE:HB   | 34:Ca:141:ALA:HB3  | 2.03                     | 0.41              |
| 36:Cc:40:ILE:HG22  | 36:Cc:42:ASP:H     | 1.86                     | 0.41              |
| 42:Ci:49:ARG:NH1   | 50:C1:1504:A:N3    | 2.68                     | 0.41              |
| 51:C2:137:U:H2'    | 51:C2:138:A:H8     | 1.85                     | 0.41              |
| 52:CW:303:ARG:NH2  | 52:CW:319:GLN:OE1  | 2.51                     | 0.41              |
| 53:UT:813:ALA:O    | 53:UT:817:ILE:HD12 | 2.21                     | 0.41              |
| 53:UT:1940:ARG:HD3 | 53:UT:2042:MET:HE3 | 2.02                     | 0.41              |
| 1:UA:467:HIS:O     | 26:CK:135:ARG:NH2  | 2.53                     | 0.41              |
| 1:UA:541:GLU:O     | 1:UA:543:GLN:N     | 2.54                     | 0.41              |
| 2:UB:526:PHE:HA    | 2:UB:529:VAL:HG12  | 2.02                     | 0.41              |
| 4:UD:1:MET:HE3     | 4:UD:3:ILE:HD11    | 2.03                     | 0.41              |
| 7:UJ:524:ALA:HB1   | 7:UJ:530:ASP:HB3   | 2.01                     | 0.41              |
| 7:UJ:750:ARG:HA    | 7:UJ:796:LEU:HD21  | 2.03                     | 0.41              |
| 7:UJ:757:ALA:N     | 7:UJ:802:ARG:HH22  | 2.19                     | 0.41              |
| 7:UJ:1001:PRO:O    | 7:UJ:1005:ASN:ND2  | 2.43                     | 0.41              |
| 7:UJ:1556:LYS:O    | 7:UJ:1559:GLU:HG2  | 2.21                     | 0.41              |
| 7:UJ:1576:ILE:HD12 | 7:UJ:1580:PHE:HE2  | 1.86                     | 0.41              |
| 7:UJ:1622:ALA:O    | 7:UJ:1626:VAL:HG13 | 2.20                     | 0.41              |
| 9:UL:195:ASP:N     | 9:UL:195:ASP:OD1   | 2.46                     | 0.41              |
| 10:UM:759:VAL:HG22 | 10:UM:797:VAL:HG21 | 2.02                     | 0.41              |
| 12:UO:255:ILE:HG12 | 12:UO:279:LEU:HD21 | 2.02                     | 0.41              |
| 13:UQ:395:LEU:HD12 | 13:UQ:399:ILE:HD11 | 2.02                     | 0.41              |
| 15:UU:692:VAL:HG12 | 15:UU:699:THR:HA   | 2.03                     | 0.41              |
| 17:UZ:85:LEU:HD11  | 17:UZ:231:ALA:HB2  | 2.03                     | 0.41              |
| 18:CA:235:GLN:HG2  | 18:CA:255:ILE:HD11 | 2.03                     | 0.41              |
| 19:CC:209:LEU:HD12 | 19:CC:209:LEU:HA   | 1.94                     | 0.41              |
| 21:CE:35:LYS:HB2   | 21:CE:102:SER:HB3  | 2.03                     | 0.41              |
| 21:CE:41:THR:HG23  | 21:CE:102:SER:HB2  | 2.03                     | 0.41              |
| 24:CI:929:LYS:NZ   | 50:C1:2071:G:O6    | 2.47                     | 0.41              |
| 28:CM:264:ILE:HB   | 28:CM:279:GLN:HB2  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 28:CM:284:ALA:HB3  | 28:CM:304:ASP:H     | 1.84                     | 0.41              |
| 28:CM:423:ARG:NH1  | 28:CM:428:LYS:O     | 2.54                     | 0.41              |
| 31:CQ:245:TYR:CE2  | 31:CQ:249:ARG:HD2   | 2.56                     | 0.41              |
| 32:CS:308:SER:HA   | 32:CS:367:GLN:HG2   | 2.01                     | 0.41              |
| 34:Ca:138:PHE:HB2  | 34:Ca:214:LYS:HB3   | 2.02                     | 0.41              |
| 36:Cc:107:ILE:HD13 | 36:Cc:179:GLU:HG3   | 2.03                     | 0.41              |
| 38:Ce:61:LYS:HE3   | 38:Ce:95:HIS:CD2    | 2.56                     | 0.41              |
| 41:Ch:92:ILE:HD13  | 41:Ch:122:ILE:HD13  | 2.02                     | 0.41              |
| 41:Ch:110:ASP:OD1  | 41:Ch:114:ARG:NH1   | 2.54                     | 0.41              |
| 50:C1:803:A:C4     | 53:UT:1363:LYS:HE2  | 2.56                     | 0.41              |
| 50:C1:1727:A:N1    | 50:C1:2228:G:O2'    | 2.52                     | 0.41              |
| 53:UT:190:VAL:O    | 53:UT:194:MET:N     | 2.54                     | 0.41              |
| 53:UT:652:ILE:O    | 53:UT:656:ILE:HG12  | 2.21                     | 0.41              |
| 53:UT:736:GLY:HA2  | 53:UT:739:THR:HG22  | 2.03                     | 0.41              |
| 53:UT:870:PHE:HA   | 53:UT:873:THR:HG22  | 2.01                     | 0.41              |
| 53:UT:1616:TYR:CE2 | 53:UT:1648:LEU:HD11 | 2.56                     | 0.41              |
| 54:UH:12:VAL:HG22  | 54:UH:410:VAL:HG12  | 2.02                     | 0.41              |
| 54:UH:301:THR:OG1  | 54:UH:318:SER:OG    | 2.31                     | 0.41              |
| 57:Cl:26:GLN:HG2   | 57:Cl:30:TYR:CD2    | 2.55                     | 0.41              |
| 55:UI:229:LEU:HD22 | 55:UI:235:LEU:HD22  | 2.03                     | 0.41              |
| 7:UJ:290:THR:HG23  | 7:UJ:319:ARG:HD2    | 2.03                     | 0.41              |
| 7:UJ:1349:ALA:O    | 7:UJ:1353:THR:HG23  | 2.21                     | 0.41              |
| 9:UL:597:LEU:HB2   | 49:CU:98:VAL:HG11   | 2.03                     | 0.41              |
| 18:CB:292:LEU:HD12 | 18:CB:299:HIS:HB3   | 2.02                     | 0.41              |
| 20:CD:164:MET:HG3  | 20:CD:281:ARG:HH12  | 1.85                     | 0.41              |
| 26:CK:88:VAL:O     | 26:CK:114:ALA:HA    | 2.20                     | 0.41              |
| 28:CM:282:HIS:CE1  | 28:CM:302:SER:HB2   | 2.56                     | 0.41              |
| 32:CR:126:GLN:O    | 32:CR:154:LYS:NZ    | 2.54                     | 0.41              |
| 32:CR:767:GLN:HG3  | 32:CR:769:GLY:H     | 1.85                     | 0.41              |
| 34:Ca:143:THR:HG23 | 34:Ca:205:TYR:CE2   | 2.50                     | 0.41              |
| 35:Cb:82:TYR:HA    | 35:Cb:83:PRO:HD3    | 1.97                     | 0.41              |
| 36:Cc:50:GLN:HE22  | 36:Cc:53:ALA:HB3    | 1.85                     | 0.41              |
| 39:Cf:62:SER:HA    | 39:Cf:77:ARG:HA     | 2.03                     | 0.41              |
| 43:Cj:122:ARG:HD2  | 50:C1:2167:G:C8     | 2.56                     | 0.41              |
| 50:C1:346:C:O2'    | 50:C1:347:C:O5'     | 2.33                     | 0.41              |
| 50:C1:685:C:O2     | 50:C1:686:A:N6      | 2.52                     | 0.41              |
| 53:UT:2121:THR:O   | 53:UT:2125:THR:OG1  | 2.31                     | 0.41              |
| 53:UT:2133:ASP:HA  | 53:UT:2136:ARG:HE   | 1.86                     | 0.41              |
| 54:UH:346:TYR:HA   | 54:UH:355:LEU:O     | 2.21                     | 0.41              |
| 54:UH:755:TYR:CZ   | 55:UI:204:MET:HG2   | 2.56                     | 0.41              |
| 1:UA:808:ASN:O     | 1:UA:812:VAL:HG22   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:UJ:534:PHE:HA    | 7:UJ:537:THR:HG23  | 2.03                     | 0.40              |
| 7:UJ:867:HIS:HA    | 7:UJ:870:ILE:HG22  | 2.03                     | 0.40              |
| 7:UJ:1288:GLU:O    | 7:UJ:1334:LYS:NZ   | 2.51                     | 0.40              |
| 12:UO:546:MET:SD   | 55:UE:219:GLN:HG2  | 2.61                     | 0.40              |
| 16:UX:68:THR:HG21  | 16:UX:75:LEU:HD13  | 2.02                     | 0.40              |
| 20:CD:261:ALA:HA   | 20:CD:264:VAL:HG12 | 2.03                     | 0.40              |
| 22:CG:108:LEU:HD23 | 22:CG:108:LEU:HA   | 1.89                     | 0.40              |
| 22:CG:269:ARG:HG2  | 22:CG:285:THR:HG22 | 2.03                     | 0.40              |
| 27:CL:63:PHE:HE1   | 27:CL:70:LEU:HD13  | 1.86                     | 0.40              |
| 30:CP:40:MET:HA    | 30:CP:78:MET:O     | 2.22                     | 0.40              |
| 32:CS:38:ILE:HG22  | 32:CS:41:LEU:HD12  | 2.03                     | 0.40              |
| 35:Cb:42:MET:HA    | 35:Cb:43:PRO:HD3   | 1.94                     | 0.40              |
| 38:Ce:87:LEU:O     | 38:Ce:91:PHE:HB3   | 2.21                     | 0.40              |
| 40:Cg:55:ARG:NH1   | 40:Cg:59:THR:HB    | 2.35                     | 0.40              |
| 46:Cn:46:SER:OG    | 46:Cn:48:HIS:O     | 2.35                     | 0.40              |
| 50:C1:468:C:O2'    | 50:C1:469:G:O4'    | 2.39                     | 0.40              |
| 56:US:125:LEU:HA   | 56:US:128:MET:HE3  | 2.03                     | 0.40              |
| 59:CY:18:LEU:HD22  | 60:CZ:365:LYS:HE3  | 2.03                     | 0.40              |
| 55:UI:256:LEU:HD23 | 55:UI:256:LEU:HA   | 1.97                     | 0.40              |
| 7:UJ:435:GLY:HA2   | 7:UJ:438:ILE:HG22  | 2.03                     | 0.40              |
| 10:UM:11:PHE:HB2   | 10:UM:689:LEU:HD21 | 2.03                     | 0.40              |
| 10:UM:887:THR:O    | 10:UM:891:MET:HG3  | 2.21                     | 0.40              |
| 13:UQ:499:LEU:HD11 | 13:UQ:519:THR:HG21 | 2.04                     | 0.40              |
| 15:UU:39:ARG:HH21  | 15:UU:72:GLN:NE2   | 2.19                     | 0.40              |
| 15:UU:465:ILE:HG23 | 15:UU:513:THR:HG23 | 2.03                     | 0.40              |
| 20:CD:12:GLY:HA3   | 20:CD:49:ALA:O     | 2.20                     | 0.40              |
| 23:CH:256:TYR:HB3  | 50:C1:1711:G:C8    | 2.55                     | 0.40              |
| 26:CK:185:SER:HA   | 50:C1:2206:C:H4'   | 2.03                     | 0.40              |
| 30:CP:58:VAL:HA    | 30:CP:112:LEU:HD21 | 2.02                     | 0.40              |
| 32:CR:373:ARG:HA   | 32:CR:374:PRO:HD3  | 1.94                     | 0.40              |
| 32:CR:389:ASP:OD1  | 32:CR:390:GLU:N    | 2.54                     | 0.40              |
| 32:CS:765:PRO:HG3  | 32:CS:775:LEU:HD22 | 2.03                     | 0.40              |
| 50:C1:5:G:H2'      | 50:C1:6:G:H8       | 1.86                     | 0.40              |
| 1:UA:216:ASP:OD1   | 1:UA:216:ASP:N     | 2.53                     | 0.40              |
| 2:UB:512:HIS:O     | 2:UB:519:ASN:ND2   | 2.42                     | 0.40              |
| 2:UB:714:SER:O     | 2:UB:718:THR:HG23  | 2.21                     | 0.40              |
| 3:UC:608:TYR:CG    | 40:Cg:30:GLY:HA3   | 2.57                     | 0.40              |
| 6:UG:434:ASN:HB3   | 6:UG:437:GLU:HB3   | 2.03                     | 0.40              |
| 7:UJ:527:SER:HB3   | 7:UJ:530:ASP:HB2   | 2.02                     | 0.40              |
| 7:UJ:1079:LEU:HA   | 7:UJ:1082:PHE:HB2  | 2.03                     | 0.40              |
| 7:UJ:1532:LEU:O    | 7:UJ:1536:VAL:HG12 | 2.22                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:UM:33:ARG:HA     | 10:UM:33:ARG:HD2    | 1.87                     | 0.40              |
| 15:UU:201:VAL:O     | 15:UU:208:VAL:HA    | 2.22                     | 0.40              |
| 15:UU:329:PRO:HA    | 15:UU:330:PRO:HD3   | 1.97                     | 0.40              |
| 18:CA:191:ARG:HH21  | 19:CC:171:HIS:CE1   | 2.39                     | 0.40              |
| 20:CD:215:GLY:HA2   | 20:CD:254:TYR:CZ    | 2.56                     | 0.40              |
| 21:CE:58:ASP:O      | 21:CE:60:GLN:NE2    | 2.55                     | 0.40              |
| 25:CJ:50:LEU:HD21   | 27:CL:630:LEU:HD23  | 2.04                     | 0.40              |
| 30:CP:42:LEU:HD23   | 34:Ca:115:ARG:NH1   | 2.37                     | 0.40              |
| 32:CS:314:SER:OG    | 32:CS:316:SER:O     | 2.40                     | 0.40              |
| 32:CS:751:ALA:HB1   | 32:CS:756:GLY:HA2   | 2.03                     | 0.40              |
| 32:CS:790:LEU:HD23  | 32:CS:794:PHE:HB2   | 2.04                     | 0.40              |
| 39:Cf:92:ARG:NH2    | 52:CW:198:SER:O     | 2.54                     | 0.40              |
| 53:UT:76:SER:O      | 53:UT:80:GLN:HB2    | 2.22                     | 0.40              |
| 53:UT:260:ALA:HA    | 53:UT:263:MET:HE2   | 2.03                     | 0.40              |
| 53:UT:348:VAL:HG12  | 53:UT:804:LEU:HB2   | 2.02                     | 0.40              |
| 53:UT:1102:LEU:HD13 | 53:UT:1137:ALA:HB3  | 2.03                     | 0.40              |
| 54:UH:304:SER:O     | 54:UH:346:TYR:OH    | 2.38                     | 0.40              |
| 54:UH:742:LEU:HD23  | 54:UH:742:LEU:HA    | 1.93                     | 0.40              |
| 59:CY:107:LEU:HB2   | 59:CY:110:GLN:NE2   | 2.36                     | 0.40              |
| 2:UB:654:VAL:HG12   | 2:UB:657:MET:H      | 1.86                     | 0.40              |
| 4:UD:707:LEU:HB3    | 4:UD:829:THR:HG22   | 2.02                     | 0.40              |
| 4:UD:867:LEU:HD23   | 4:UD:867:LEU:HA     | 1.91                     | 0.40              |
| 7:UJ:659:VAL:HG11   | 7:UJ:681:ALA:HB2    | 2.04                     | 0.40              |
| 7:UJ:1390:LEU:HA    | 7:UJ:1393:ALA:HB3   | 2.02                     | 0.40              |
| 7:UJ:1633:LEU:HD22  | 7:UJ:1678:VAL:HB    | 2.03                     | 0.40              |
| 8:UK:24:ARG:NH2     | 33:CT:199:ALA:O     | 2.52                     | 0.40              |
| 10:UM:585:HIS:CE1   | 10:UM:625:LYS:HG3   | 2.56                     | 0.40              |
| 23:CH:110:ILE:HD12  | 23:CH:110:ILE:HA    | 1.91                     | 0.40              |
| 24:CI:757:TYR:HE1   | 24:CI:768:VAL:HG12  | 1.86                     | 0.40              |
| 29:CN:43:ASN:HB2    | 29:CN:209:MET:HE3   | 2.03                     | 0.40              |
| 30:CP:48:GLU:OE2    | 30:CP:73:ILE:HG23   | 2.22                     | 0.40              |
| 30:CP:90:ALA:HB3    | 42:CI:116:ARG:HH21  | 1.86                     | 0.40              |
| 30:CP:92:ILE:HD12   | 30:CP:92:ILE:HA     | 1.95                     | 0.40              |
| 30:CP:152:LYS:HE2   | 30:CP:152:LYS:HB2   | 1.88                     | 0.40              |
| 32:CS:535:LYS:HD3   | 32:CS:578:ARG:HH22  | 1.87                     | 0.40              |
| 34:Ca:86:LEU:HB3    | 34:Ca:98:THR:HB     | 2.03                     | 0.40              |
| 44:Ck:60:ASP:OD1    | 44:Ck:60:ASP:N      | 2.55                     | 0.40              |
| 50:C1:2358:U:H3     | 50:C1:2369:G:H1     | 1.69                     | 0.40              |
| 53:UT:1739:ILE:HA   | 53:UT:1742:ILE:HG12 | 2.03                     | 0.40              |
| 53:UT:2016:VAL:HG13 | 53:UT:2017:LYS:HG3  | 2.03                     | 0.40              |
| 57:Cl:80:LYS:CD     | 57:Cl:81:ILE:H      | 2.30                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:CY:57:PHE:CD2   | 59:CY:85:VAL:HG21  | 2.56                     | 0.40              |
| 4:UD:546:ASP:N     | 4:UD:546:ASP:OD1   | 2.54                     | 0.40              |
| 5:UF:30:LYS:HE3    | 5:UF:30:LYS:HB2    | 1.94                     | 0.40              |
| 7:UJ:1362:GLN:NE2  | 7:UJ:1368:ARG:HE   | 2.20                     | 0.40              |
| 7:UJ:1757:LEU:HB2  | 7:UJ:1792:LYS:HZ2  | 1.86                     | 0.40              |
| 10:UM:114:VAL:HA   | 10:UM:130:ALA:HA   | 2.04                     | 0.40              |
| 12:UO:99:ASP:HA    | 57:CI:25:LYS:HD3   | 2.03                     | 0.40              |
| 12:UO:162:SER:O    | 12:UO:169:VAL:HA   | 2.22                     | 0.40              |
| 19:CC:88:GLN:OE1   | 50:C1:454:C:O2'    | 2.30                     | 0.40              |
| 20:CD:12:GLY:HA2   | 20:CD:51:PHE:CZ    | 2.57                     | 0.40              |
| 21:CF:27:GLN:HE21  | 21:CF:31:TYR:HE2   | 1.68                     | 0.40              |
| 22:CG:297:ARG:NE   | 22:CG:340:GLY:O    | 2.42                     | 0.40              |
| 23:CH:154:ARG:HA   | 23:CH:158:LEU:HD12 | 2.04                     | 0.40              |
| 27:CL:78:LEU:HD23  | 27:CL:78:LEU:HA    | 1.93                     | 0.40              |
| 27:CL:563:ASP:OD1  | 27:CL:563:ASP:N    | 2.55                     | 0.40              |
| 31:CQ:89:PRO:HB3   | 31:CQ:120:LYS:NZ   | 2.37                     | 0.40              |
| 32:CR:537:LEU:HA   | 32:CR:540:MET:HG2  | 2.04                     | 0.40              |
| 32:CR:742:PHE:HB3  | 32:CR:762:MET:HB3  | 2.03                     | 0.40              |
| 32:CS:531:PRO:HG2  | 60:CZ:289:ALA:HB2  | 2.02                     | 0.40              |
| 44:Ck:127:MET:HB3  | 44:Ck:148:LEU:HD12 | 2.02                     | 0.40              |
| 50:C1:413:C:H2'    | 50:C1:414:U:O4'    | 2.22                     | 0.40              |
| 51:C2:240:C:H2'    | 51:C2:241:G:H8     | 1.87                     | 0.40              |
| 52:CW:1:MET:SD     | 52:CW:14:VAL:HG12  | 2.62                     | 0.40              |
| 52:CW:280:LEU:HD23 | 52:CW:280:LEU:HA   | 1.94                     | 0.40              |
| 53:UT:448:GLU:HA   | 53:UT:451:LYS:HG3  | 2.04                     | 0.40              |
| 53:UT:658:ASN:ND2  | 53:UT:670:SER:HB3  | 2.37                     | 0.40              |
| 53:UT:716:VAL:O    | 53:UT:720:ILE:HG13 | 2.21                     | 0.40              |
| 54:UH:196:SER:O    | 54:UH:200:ARG:HB2  | 2.21                     | 0.40              |
| 59:CY:290:GLU:HA   | 59:CY:293:LYS:HG2  | 2.02                     | 0.40              |
| 60:CZ:330:ARG:HA   | 60:CZ:333:LYS:HG3  | 2.03                     | 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   | UA    | 834/904 (92%)   | 804 (96%)  | 30 (4%) | 0        | 100         | 100 |
| 2   | UB    | 556/907 (61%)   | 538 (97%)  | 18 (3%) | 0        | 100         | 100 |
| 3   | UC    | 201/648 (31%)   | 196 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 4   | UD    | 761/884 (86%)   | 731 (96%)  | 30 (4%) | 0        | 100         | 100 |
| 5   | UF    | 325/414 (78%)   | 317 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 6   | UG    | 475/558 (85%)   | 455 (96%)  | 19 (4%) | 1 (0%)   | 43          | 72  |
| 7   | UJ    | 1599/1802 (89%) | 1525 (95%) | 72 (4%) | 2 (0%)   | 48          | 77  |
| 8   | UK    | 211/270 (78%)   | 209 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 9   | UL    | 767/962 (80%)   | 732 (95%)  | 35 (5%) | 0        | 100         | 100 |
| 10  | UM    | 835/912 (92%)   | 809 (97%)  | 26 (3%) | 0        | 100         | 100 |
| 11  | UN    | 171/716 (24%)   | 169 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 12  | UO    | 497/557 (89%)   | 479 (96%)  | 17 (3%) | 1 (0%)   | 43          | 72  |
| 13  | UQ    | 775/960 (81%)   | 735 (95%)  | 40 (5%) | 0        | 100         | 100 |
| 14  | UR    | 436/618 (71%)   | 421 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 15  | UU    | 896/1049 (85%)  | 857 (96%)  | 39 (4%) | 0        | 100         | 100 |
| 16  | UX    | 188/193 (97%)   | 180 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 17  | UZ    | 229/391 (59%)   | 215 (94%)  | 14 (6%) | 0        | 100         | 100 |
| 18  | CA    | 238/313 (76%)   | 223 (94%)  | 14 (6%) | 1 (0%)   | 30          | 60  |
| 18  | CB    | 235/313 (75%)   | 222 (94%)  | 13 (6%) | 0        | 100         | 100 |
| 19  | CC    | 383/523 (73%)   | 372 (97%)  | 11 (3%) | 0        | 100         | 100 |
| 20  | CD    | 444/582 (76%)   | 430 (97%)  | 14 (3%) | 0        | 100         | 100 |
| 21  | CE    | 119/127 (94%)   | 116 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 21  | CF    | 118/127 (93%)   | 114 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 22  | CG    | 402/630 (64%)   | 385 (96%)  | 17 (4%) | 0        | 100         | 100 |
| 23  | CH    | 383/411 (93%)   | 371 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 24  | CI    | 829/1163 (71%)  | 801 (97%)  | 27 (3%) | 1 (0%)   | 48          | 77  |
| 25  | CJ    | 177/183 (97%)   | 175 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 26  | CK    | 295/297 (99%)   | 285 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 27  | CL    | 310/785 (40%)   | 293 (94%)  | 16 (5%) | 1 (0%)   | 36          | 66  |
| 28  | CM    | 443/446 (99%)   | 428 (97%)  | 15 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29  | CN    | 222/252 (88%)   | 212 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 29  | CO    | 211/252 (84%)   | 204 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 55  |
| 30  | CP    | 227/322 (70%)   | 216 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 31  | CQ    | 178/259 (69%)   | 175 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 32  | CR    | 836/1073 (78%)  | 806 (96%)  | 29 (4%)  | 1 (0%)   | 48          | 77  |
| 32  | CS    | 826/1073 (77%)  | 783 (95%)  | 43 (5%)  | 0        | 100         | 100 |
| 33  | CT    | 127/203 (63%)   | 122 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 34  | Ca    | 223/255 (88%)   | 212 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 35  | Cb    | 230/264 (87%)   | 219 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 36  | Cc    | 188/212 (89%)   | 183 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 37  | Cd    | 224/239 (94%)   | 220 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 38  | Ce    | 155/203 (76%)   | 141 (91%)  | 14 (9%)  | 0        | 100         | 100 |
| 39  | Cf    | 170/202 (84%)   | 165 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 40  | Cg    | 157/190 (83%)   | 154 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 41  | Ch    | 64/151 (42%)    | 64 (100%)  | 0        | 0        | 100         | 100 |
| 42  | Ci    | 113/150 (75%)   | 109 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 43  | Cj    | 124/143 (87%)   | 118 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 44  | Ck    | 127/161 (79%)   | 121 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 45  | Cm    | 122/130 (94%)   | 119 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 46  | Cn    | 92/145 (63%)    | 90 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 47  | Co    | 90/136 (66%)    | 79 (88%)   | 10 (11%) | 1 (1%)   | 11          | 36  |
| 48  | Cp    | 59/68 (87%)     | 58 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 49  | CU    | 168/311 (54%)   | 163 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 52  | CW    | 381/668 (57%)   | 367 (96%)  | 14 (4%)  | 0        | 100         | 100 |
| 53  | UT    | 1981/2612 (76%) | 1875 (95%) | 103 (5%) | 3 (0%)   | 43          | 72  |
| 54  | UH    | 787/930 (85%)   | 768 (98%)  | 18 (2%)  | 1 (0%)   | 48          | 77  |
| 55  | UE    | 172/410 (42%)   | 155 (90%)  | 17 (10%) | 0        | 100         | 100 |
| 55  | UI    | 126/410 (31%)   | 124 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 56  | US    | 443/549 (81%)   | 428 (97%)  | 14 (3%)  | 1 (0%)   | 43          | 72  |
| 57  | Cl    | 78/156 (50%)    | 71 (91%)   | 7 (9%)   | 0        | 100         | 100 |
| 58  | CX    | 265/480 (55%)   | 249 (94%)  | 16 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 59  | CY    | 258/381 (68%)     | 253 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 60  | CZ    | 279/609 (46%)     | 268 (96%)   | 11 (4%)  | 0        | 100         | 100 |
| 61  | UP    | 52/364 (14%)      | 49 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| All | All   | 23887/32608 (73%) | 22927 (96%) | 945 (4%) | 15 (0%)  | 49          | 77  |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 29  | CO    | 166  | PRO  |
| 32  | CR    | 211  | ILE  |
| 6   | UG    | 56   | PRO  |
| 7   | UJ    | 1263 | GLU  |
| 12  | UO    | 130  | GLN  |
| 27  | CL    | 640  | PRO  |
| 53  | UT    | 457  | TRP  |
| 53  | UT    | 28   | GLU  |
| 24  | CI    | 367  | VAL  |
| 53  | UT    | 1724 | PRO  |
| 54  | UH    | 754  | ARG  |
| 7   | UJ    | 1298 | ASP  |
| 18  | CA    | 312  | GLU  |
| 47  | Co    | 367  | SER  |
| 56  | US    | 241  | GLU  |

### 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   | UA    | 662/774 (86%) | 662 (100%) | 0        | 100         | 100 |
| 2   | UB    | 474/788 (60%) | 473 (100%) | 1 (0%)   | 87          | 96  |
| 3   | UC    | 176/536 (33%) | 176 (100%) | 0        | 100         | 100 |
| 4   | UD    | 657/738 (89%) | 657 (100%) | 0        | 100         | 100 |
| 5   | UF    | 250/341 (73%) | 250 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 6   | UG    | 386/474 (81%)   | 386 (100%)  | 0        | 100         | 100 |
| 7   | UJ    | 1364/1526 (89%) | 1364 (100%) | 0        | 100         | 100 |
| 8   | UK    | 161/227 (71%)   | 161 (100%)  | 0        | 100         | 100 |
| 9   | UL    | 667/821 (81%)   | 667 (100%)  | 0        | 100         | 100 |
| 10  | UM    | 712/770 (92%)   | 712 (100%)  | 0        | 100         | 100 |
| 11  | UN    | 146/583 (25%)   | 146 (100%)  | 0        | 100         | 100 |
| 12  | UO    | 403/456 (88%)   | 403 (100%)  | 0        | 100         | 100 |
| 13  | UQ    | 650/817 (80%)   | 650 (100%)  | 0        | 100         | 100 |
| 14  | UR    | 359/523 (69%)   | 359 (100%)  | 0        | 100         | 100 |
| 15  | UU    | 677/863 (78%)   | 677 (100%)  | 0        | 100         | 100 |
| 16  | UX    | 152/167 (91%)   | 152 (100%)  | 0        | 100         | 100 |
| 17  | UZ    | 186/329 (56%)   | 186 (100%)  | 0        | 100         | 100 |
| 18  | CA    | 175/228 (77%)   | 175 (100%)  | 0        | 100         | 100 |
| 18  | CB    | 195/228 (86%)   | 195 (100%)  | 0        | 100         | 100 |
| 19  | CC    | 287/435 (66%)   | 287 (100%)  | 0        | 100         | 100 |
| 20  | CD    | 344/489 (70%)   | 344 (100%)  | 0        | 100         | 100 |
| 21  | CE    | 91/108 (84%)    | 91 (100%)   | 0        | 100         | 100 |
| 21  | CF    | 88/108 (82%)    | 88 (100%)   | 0        | 100         | 100 |
| 22  | CG    | 331/525 (63%)   | 331 (100%)  | 0        | 100         | 100 |
| 23  | CH    | 303/320 (95%)   | 301 (99%)   | 2 (1%)   | 76          | 91  |
| 24  | CI    | 681/1009 (68%)  | 681 (100%)  | 0        | 100         | 100 |
| 25  | CJ    | 147/169 (87%)   | 147 (100%)  | 0        | 100         | 100 |
| 26  | CK    | 245/266 (92%)   | 245 (100%)  | 0        | 100         | 100 |
| 27  | CL    | 251/642 (39%)   | 251 (100%)  | 0        | 100         | 100 |
| 28  | CM    | 364/383 (95%)   | 364 (100%)  | 0        | 100         | 100 |
| 29  | CN    | 202/223 (91%)   | 202 (100%)  | 0        | 100         | 100 |
| 29  | CO    | 193/223 (86%)   | 193 (100%)  | 0        | 100         | 100 |
| 30  | CP    | 202/287 (70%)   | 202 (100%)  | 0        | 100         | 100 |
| 31  | CQ    | 151/215 (70%)   | 151 (100%)  | 0        | 100         | 100 |
| 32  | CR    | 731/916 (80%)   | 731 (100%)  | 0        | 100         | 100 |
| 32  | CS    | 722/916 (79%)   | 722 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 33  | CT    | 108/167 (65%)     | 108 (100%)   | 0        | 100         | 100 |
| 34  | Ca    | 198/223 (89%)     | 198 (100%)   | 0        | 100         | 100 |
| 35  | Cb    | 199/221 (90%)     | 199 (100%)   | 0        | 100         | 100 |
| 36  | Cc    | 149/178 (84%)     | 149 (100%)   | 0        | 100         | 100 |
| 37  | Cd    | 192/204 (94%)     | 192 (100%)   | 0        | 100         | 100 |
| 38  | Ce    | 137/177 (77%)     | 137 (100%)   | 0        | 100         | 100 |
| 39  | Cf    | 139/164 (85%)     | 139 (100%)   | 0        | 100         | 100 |
| 40  | Cg    | 123/162 (76%)     | 123 (100%)   | 0        | 100         | 100 |
| 41  | Ch    | 58/130 (45%)      | 58 (100%)    | 0        | 100         | 100 |
| 42  | Ci    | 78/117 (67%)      | 78 (100%)    | 0        | 100         | 100 |
| 43  | Cj    | 92/115 (80%)      | 92 (100%)    | 0        | 100         | 100 |
| 44  | Ck    | 117/143 (82%)     | 117 (100%)   | 0        | 100         | 100 |
| 45  | Cm    | 103/113 (91%)     | 103 (100%)   | 0        | 100         | 100 |
| 46  | Cn    | 70/116 (60%)      | 70 (100%)    | 0        | 100         | 100 |
| 47  | Co    | 79/115 (69%)      | 79 (100%)    | 0        | 100         | 100 |
| 48  | Cp    | 47/61 (77%)       | 47 (100%)    | 0        | 100         | 100 |
| 49  | CU    | 137/260 (53%)     | 137 (100%)   | 0        | 100         | 100 |
| 52  | CW    | 310/587 (53%)     | 310 (100%)   | 0        | 100         | 100 |
| 53  | UT    | 1725/2276 (76%)   | 1725 (100%)  | 0        | 100         | 100 |
| 54  | UH    | 674/788 (86%)     | 674 (100%)   | 0        | 100         | 100 |
| 55  | UE    | 148/346 (43%)     | 148 (100%)   | 0        | 100         | 100 |
| 55  | UI    | 108/346 (31%)     | 108 (100%)   | 0        | 100         | 100 |
| 56  | US    | 404/493 (82%)     | 404 (100%)   | 0        | 100         | 100 |
| 57  | Cl    | 71/135 (53%)      | 71 (100%)    | 0        | 100         | 100 |
| 58  | CX    | 227/411 (55%)     | 226 (100%)   | 1 (0%)   | 84          | 94  |
| 59  | CY    | 225/322 (70%)     | 225 (100%)   | 0        | 100         | 100 |
| 60  | CZ    | 238/519 (46%)     | 238 (100%)   | 0        | 100         | 100 |
| 61  | UP    | 44/314 (14%)      | 44 (100%)    | 0        | 100         | 100 |
| All | All   | 19985/27626 (72%) | 19981 (100%) | 4 (0%)   | 100         | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | UB    | 43  | GLN  |
| 23  | CH    | 269 | GLN  |
| 23  | CH    | 405 | ASN  |
| 58  | CX    | 380 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | UA    | 9    | ASN  |
| 1   | UA    | 110  | HIS  |
| 1   | UA    | 147  | HIS  |
| 1   | UA    | 230  | HIS  |
| 1   | UA    | 268  | ASN  |
| 1   | UA    | 524  | GLN  |
| 1   | UA    | 592  | ASN  |
| 1   | UA    | 705  | GLN  |
| 1   | UA    | 801  | HIS  |
| 1   | UA    | 808  | ASN  |
| 2   | UB    | 483  | GLN  |
| 2   | UB    | 606  | HIS  |
| 2   | UB    | 663  | ASN  |
| 4   | UD    | 198  | ASN  |
| 5   | UF    | 59   | ASN  |
| 6   | UG    | 96   | GLN  |
| 6   | UG    | 127  | GLN  |
| 6   | UG    | 190  | GLN  |
| 6   | UG    | 196  | GLN  |
| 6   | UG    | 331  | ASN  |
| 6   | UG    | 391  | GLN  |
| 6   | UG    | 464  | ASN  |
| 7   | UJ    | 184  | GLN  |
| 7   | UJ    | 349  | HIS  |
| 7   | UJ    | 379  | ASN  |
| 7   | UJ    | 909  | GLN  |
| 7   | UJ    | 996  | GLN  |
| 7   | UJ    | 1276 | ASN  |
| 7   | UJ    | 1311 | GLN  |
| 7   | UJ    | 1365 | GLN  |
| 7   | UJ    | 1460 | ASN  |
| 7   | UJ    | 1718 | HIS  |
| 7   | UJ    | 1723 | ASN  |
| 7   | UJ    | 1745 | GLN  |
| 9   | UL    | 274  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | UL    | 359 | GLN  |
| 9   | UL    | 446 | ASN  |
| 9   | UL    | 504 | ASN  |
| 9   | UL    | 832 | ASN  |
| 9   | UL    | 835 | GLN  |
| 10  | UM    | 244 | GLN  |
| 10  | UM    | 274 | HIS  |
| 10  | UM    | 466 | ASN  |
| 10  | UM    | 527 | GLN  |
| 10  | UM    | 743 | GLN  |
| 12  | UO    | 24  | GLN  |
| 12  | UO    | 145 | GLN  |
| 12  | UO    | 253 | ASN  |
| 12  | UO    | 271 | ASN  |
| 12  | UO    | 284 | GLN  |
| 12  | UO    | 480 | ASN  |
| 12  | UO    | 522 | GLN  |
| 13  | UQ    | 328 | ASN  |
| 13  | UQ    | 368 | ASN  |
| 13  | UQ    | 474 | ASN  |
| 13  | UQ    | 785 | GLN  |
| 14  | UR    | 264 | GLN  |
| 14  | UR    | 301 | HIS  |
| 14  | UR    | 407 | GLN  |
| 15  | UU    | 72  | GLN  |
| 15  | UU    | 81  | ASN  |
| 15  | UU    | 113 | ASN  |
| 15  | UU    | 236 | GLN  |
| 15  | UU    | 634 | ASN  |
| 15  | UU    | 636 | HIS  |
| 15  | UU    | 774 | GLN  |
| 15  | UU    | 894 | GLN  |
| 16  | UX    | 57  | ASN  |
| 16  | UX    | 88  | ASN  |
| 17  | UZ    | 90  | ASN  |
| 17  | UZ    | 234 | HIS  |
| 17  | UZ    | 280 | ASN  |
| 18  | CA    | 235 | GLN  |
| 18  | CA    | 249 | GLN  |
| 18  | CA    | 270 | GLN  |
| 18  | CA    | 308 | GLN  |
| 18  | CB    | 277 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 18  | CB    | 289  | GLN  |
| 19  | CC    | 137  | HIS  |
| 19  | CC    | 394  | ASN  |
| 19  | CC    | 410  | GLN  |
| 20  | CD    | 204  | ASN  |
| 20  | CD    | 256  | ASN  |
| 21  | CF    | 19   | GLN  |
| 21  | CF    | 46   | ASN  |
| 21  | CF    | 106  | ASN  |
| 22  | CG    | 329  | HIS  |
| 22  | CG    | 341  | GLN  |
| 23  | CH    | 244  | ASN  |
| 23  | CH    | 255  | GLN  |
| 24  | CI    | 282  | GLN  |
| 24  | CI    | 287  | HIS  |
| 24  | CI    | 374  | GLN  |
| 24  | CI    | 749  | GLN  |
| 24  | CI    | 767  | GLN  |
| 24  | CI    | 930  | ASN  |
| 24  | CI    | 1011 | GLN  |
| 25  | CJ    | 68   | ASN  |
| 26  | CK    | 169  | ASN  |
| 26  | CK    | 225  | ASN  |
| 26  | CK    | 286  | GLN  |
| 27  | CL    | 88   | GLN  |
| 27  | CL    | 138  | GLN  |
| 27  | CL    | 667  | GLN  |
| 27  | CL    | 778  | GLN  |
| 28  | CM    | 239  | HIS  |
| 29  | CN    | 23   | GLN  |
| 31  | CQ    | 112  | GLN  |
| 32  | CR    | 309  | ASN  |
| 32  | CR    | 339  | HIS  |
| 32  | CR    | 557  | GLN  |
| 32  | CR    | 641  | ASN  |
| 32  | CR    | 819  | ASN  |
| 32  | CR    | 890  | GLN  |
| 32  | CR    | 902  | ASN  |
| 32  | CS    | 52   | GLN  |
| 32  | CS    | 134  | ASN  |
| 32  | CS    | 360  | ASN  |
| 32  | CS    | 485  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | CS    | 515  | GLN  |
| 32  | CS    | 554  | ASN  |
| 32  | CS    | 655  | GLN  |
| 33  | CT    | 92   | ASN  |
| 33  | CT    | 107  | GLN  |
| 36  | Cc    | 50   | GLN  |
| 36  | Cc    | 114  | GLN  |
| 36  | Cc    | 115  | ASN  |
| 36  | Cc    | 145  | GLN  |
| 37  | Cd    | 7    | HIS  |
| 37  | Cd    | 56   | ASN  |
| 37  | Cd    | 116  | GLN  |
| 37  | Cd    | 200  | GLN  |
| 38  | Ce    | 74   | GLN  |
| 38  | Ce    | 95   | HIS  |
| 38  | Ce    | 197  | GLN  |
| 39  | Cf    | 44   | HIS  |
| 44  | Ck    | 18   | HIS  |
| 44  | Ck    | 143  | ASN  |
| 47  | Co    | 346  | ASN  |
| 47  | Co    | 353  | GLN  |
| 47  | Co    | 382  | GLN  |
| 49  | CU    | 223  | GLN  |
| 49  | CU    | 251  | ASN  |
| 52  | CW    | 94   | HIS  |
| 52  | CW    | 116  | GLN  |
| 52  | CW    | 177  | GLN  |
| 52  | CW    | 284  | GLN  |
| 52  | CW    | 374  | ASN  |
| 53  | UT    | 202  | HIS  |
| 53  | UT    | 334  | GLN  |
| 53  | UT    | 393  | ASN  |
| 53  | UT    | 492  | GLN  |
| 53  | UT    | 495  | GLN  |
| 53  | UT    | 701  | GLN  |
| 53  | UT    | 833  | GLN  |
| 53  | UT    | 1017 | HIS  |
| 53  | UT    | 1201 | ASN  |
| 53  | UT    | 1233 | ASN  |
| 53  | UT    | 1236 | ASN  |
| 53  | UT    | 1345 | GLN  |
| 53  | UT    | 1366 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 53  | UT    | 1386 | GLN  |
| 53  | UT    | 1396 | ASN  |
| 53  | UT    | 1416 | ASN  |
| 53  | UT    | 1437 | ASN  |
| 53  | UT    | 1551 | GLN  |
| 53  | UT    | 1571 | HIS  |
| 53  | UT    | 1874 | GLN  |
| 53  | UT    | 1985 | ASN  |
| 53  | UT    | 2141 | GLN  |
| 53  | UT    | 2156 | GLN  |
| 53  | UT    | 2192 | GLN  |
| 54  | UH    | 14   | HIS  |
| 54  | UH    | 306  | GLN  |
| 54  | UH    | 329  | ASN  |
| 54  | UH    | 366  | ASN  |
| 54  | UH    | 373  | GLN  |
| 54  | UH    | 740  | ASN  |
| 55  | UE    | 269  | GLN  |
| 56  | US    | 225  | ASN  |
| 56  | US    | 266  | GLN  |
| 56  | US    | 372  | HIS  |
| 56  | US    | 464  | GLN  |
| 56  | US    | 488  | ASN  |
| 60  | CZ    | 383  | GLN  |
| 55  | UI    | 174  | GLN  |
| 61  | UP    | 309  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 50  | C1    | 1549/2348 (65%) | 316 (20%)         | 22 (1%)         |
| 51  | C2    | 225/274 (82%)   | 53 (23%)          | 1 (0%)          |
| All | All   | 1774/2622 (67%) | 369 (20%)         | 23 (1%)         |

All (369) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | C1    | 5   | G    |
| 50  | C1    | 14  | G    |
| 50  | C1    | 16  | U    |
| 50  | C1    | 17  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | C1    | 18  | G    |
| 50  | C1    | 23  | G    |
| 50  | C1    | 26  | C    |
| 50  | C1    | 40  | A    |
| 50  | C1    | 41  | G    |
| 50  | C1    | 59  | U    |
| 50  | C1    | 60  | A    |
| 50  | C1    | 61  | G    |
| 50  | C1    | 64  | C    |
| 50  | C1    | 71  | A    |
| 50  | C1    | 72  | U    |
| 50  | C1    | 74  | C    |
| 50  | C1    | 75  | G    |
| 50  | C1    | 77  | C    |
| 50  | C1    | 86  | C    |
| 50  | C1    | 90  | A    |
| 50  | C1    | 93  | G    |
| 50  | C1    | 96  | C    |
| 50  | C1    | 97  | C    |
| 50  | C1    | 104 | U    |
| 50  | C1    | 105 | A    |
| 50  | C1    | 107 | C    |
| 50  | C1    | 126 | C    |
| 50  | C1    | 127 | C    |
| 50  | C1    | 128 | G    |
| 50  | C1    | 134 | C    |
| 50  | C1    | 136 | C    |
| 50  | C1    | 143 | A    |
| 50  | C1    | 152 | G    |
| 50  | C1    | 159 | C    |
| 50  | C1    | 160 | C    |
| 50  | C1    | 162 | G    |
| 50  | C1    | 167 | C    |
| 50  | C1    | 183 | C    |
| 50  | C1    | 185 | G    |
| 50  | C1    | 193 | U    |
| 50  | C1    | 202 | A    |
| 50  | C1    | 203 | C    |
| 50  | C1    | 207 | U    |
| 50  | C1    | 209 | A    |
| 50  | C1    | 210 | G    |
| 50  | C1    | 224 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | C1    | 234 | G    |
| 50  | C1    | 236 | C    |
| 50  | C1    | 242 | U    |
| 50  | C1    | 243 | U    |
| 50  | C1    | 244 | G    |
| 50  | C1    | 257 | G    |
| 50  | C1    | 259 | U    |
| 50  | C1    | 267 | U    |
| 50  | C1    | 269 | G    |
| 50  | C1    | 272 | A    |
| 50  | C1    | 273 | G    |
| 50  | C1    | 276 | C    |
| 50  | C1    | 277 | U    |
| 50  | C1    | 278 | A    |
| 50  | C1    | 281 | U    |
| 50  | C1    | 282 | C    |
| 50  | C1    | 283 | A    |
| 50  | C1    | 285 | A    |
| 50  | C1    | 291 | C    |
| 50  | C1    | 292 | G    |
| 50  | C1    | 306 | G    |
| 50  | C1    | 310 | G    |
| 50  | C1    | 312 | G    |
| 50  | C1    | 319 | U    |
| 50  | C1    | 320 | A    |
| 50  | C1    | 323 | G    |
| 50  | C1    | 333 | C    |
| 50  | C1    | 346 | C    |
| 50  | C1    | 347 | C    |
| 50  | C1    | 349 | C    |
| 50  | C1    | 351 | U    |
| 50  | C1    | 382 | U    |
| 50  | C1    | 383 | G    |
| 50  | C1    | 384 | C    |
| 50  | C1    | 386 | G    |
| 50  | C1    | 398 | C    |
| 50  | C1    | 402 | U    |
| 50  | C1    | 403 | G    |
| 50  | C1    | 416 | U    |
| 50  | C1    | 435 | A    |
| 50  | C1    | 436 | A    |
| 50  | C1    | 440 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | C1    | 441 | A    |
| 50  | C1    | 459 | C    |
| 50  | C1    | 468 | C    |
| 50  | C1    | 469 | G    |
| 50  | C1    | 472 | G    |
| 50  | C1    | 483 | U    |
| 50  | C1    | 484 | G    |
| 50  | C1    | 491 | G    |
| 50  | C1    | 495 | G    |
| 50  | C1    | 499 | G    |
| 50  | C1    | 500 | C    |
| 50  | C1    | 501 | U    |
| 50  | C1    | 583 | A    |
| 50  | C1    | 584 | U    |
| 50  | C1    | 589 | A    |
| 50  | C1    | 594 | G    |
| 50  | C1    | 595 | U    |
| 50  | C1    | 597 | G    |
| 50  | C1    | 604 | C    |
| 50  | C1    | 609 | A    |
| 50  | C1    | 613 | A    |
| 50  | C1    | 614 | U    |
| 50  | C1    | 621 | G    |
| 50  | C1    | 628 | A    |
| 50  | C1    | 638 | A    |
| 50  | C1    | 652 | A    |
| 50  | C1    | 653 | U    |
| 50  | C1    | 655 | A    |
| 50  | C1    | 661 | U    |
| 50  | C1    | 662 | A    |
| 50  | C1    | 663 | U    |
| 50  | C1    | 680 | U    |
| 50  | C1    | 685 | C    |
| 50  | C1    | 686 | A    |
| 50  | C1    | 690 | A    |
| 50  | C1    | 691 | A    |
| 50  | C1    | 700 | C    |
| 50  | C1    | 702 | U    |
| 50  | C1    | 715 | A    |
| 50  | C1    | 719 | U    |
| 50  | C1    | 720 | A    |
| 50  | C1    | 723 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | C1    | 725 | A    |
| 50  | C1    | 737 | G    |
| 50  | C1    | 743 | U    |
| 50  | C1    | 744 | C    |
| 50  | C1    | 755 | A    |
| 50  | C1    | 760 | C    |
| 50  | C1    | 762 | G    |
| 50  | C1    | 763 | A    |
| 50  | C1    | 764 | A    |
| 50  | C1    | 772 | A    |
| 50  | C1    | 775 | U    |
| 50  | C1    | 776 | C    |
| 50  | C1    | 777 | G    |
| 50  | C1    | 786 | G    |
| 50  | C1    | 798 | U    |
| 50  | C1    | 801 | A    |
| 50  | C1    | 802 | A    |
| 50  | C1    | 803 | A    |
| 50  | C1    | 806 | C    |
| 50  | C1    | 807 | A    |
| 50  | C1    | 808 | A    |
| 50  | C1    | 810 | G    |
| 50  | C1    | 816 | C    |
| 50  | C1    | 841 | A    |
| 50  | C1    | 845 | C    |
| 50  | C1    | 849 | A    |
| 50  | C1    | 850 | A    |
| 50  | C1    | 861 | U    |
| 50  | C1    | 871 | G    |
| 50  | C1    | 897 | U    |
| 50  | C1    | 900 | A    |
| 50  | C1    | 904 | U    |
| 50  | C1    | 913 | G    |
| 50  | C1    | 921 | G    |
| 50  | C1    | 922 | C    |
| 50  | C1    | 934 | A    |
| 50  | C1    | 936 | A    |
| 50  | C1    | 942 | U    |
| 50  | C1    | 943 | A    |
| 50  | C1    | 972 | A    |
| 50  | C1    | 984 | A    |
| 50  | C1    | 985 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | C1    | 986  | C    |
| 50  | C1    | 999  | C    |
| 50  | C1    | 1000 | A    |
| 50  | C1    | 1002 | G    |
| 50  | C1    | 1003 | G    |
| 50  | C1    | 1007 | G    |
| 50  | C1    | 1017 | C    |
| 50  | C1    | 1018 | G    |
| 50  | C1    | 1023 | U    |
| 50  | C1    | 1024 | U    |
| 50  | C1    | 1025 | A    |
| 50  | C1    | 1027 | C    |
| 50  | C1    | 1028 | C    |
| 50  | C1    | 1029 | A    |
| 50  | C1    | 1039 | C    |
| 50  | C1    | 1043 | G    |
| 50  | C1    | 1044 | A    |
| 50  | C1    | 1052 | A    |
| 50  | C1    | 1059 | A    |
| 50  | C1    | 1061 | A    |
| 50  | C1    | 1069 | A    |
| 50  | C1    | 1076 | U    |
| 50  | C1    | 1077 | U    |
| 50  | C1    | 1078 | U    |
| 50  | C1    | 1079 | C    |
| 50  | C1    | 1080 | G    |
| 50  | C1    | 1085 | U    |
| 50  | C1    | 1086 | U    |
| 50  | C1    | 1088 | U    |
| 50  | C1    | 1089 | A    |
| 50  | C1    | 1096 | A    |
| 50  | C1    | 1098 | G    |
| 50  | C1    | 1099 | A    |
| 50  | C1    | 1103 | C    |
| 50  | C1    | 1116 | U    |
| 50  | C1    | 1122 | A    |
| 50  | C1    | 1123 | G    |
| 50  | C1    | 1124 | G    |
| 50  | C1    | 1125 | A    |
| 50  | C1    | 1126 | A    |
| 50  | C1    | 1129 | A    |
| 50  | C1    | 1148 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | C1    | 1149 | C    |
| 50  | C1    | 1154 | A    |
| 50  | C1    | 1158 | G    |
| 50  | C1    | 1159 | C    |
| 50  | C1    | 1163 | A    |
| 50  | C1    | 1164 | A    |
| 50  | C1    | 1165 | U    |
| 50  | C1    | 1166 | U    |
| 50  | C1    | 1167 | C    |
| 50  | C1    | 1169 | A    |
| 50  | C1    | 1171 | C    |
| 50  | C1    | 1178 | A    |
| 50  | C1    | 1179 | G    |
| 50  | C1    | 1218 | G    |
| 50  | C1    | 1219 | A    |
| 50  | C1    | 1223 | U    |
| 50  | C1    | 1254 | G    |
| 50  | C1    | 1256 | G    |
| 50  | C1    | 1257 | C    |
| 50  | C1    | 1258 | A    |
| 50  | C1    | 1259 | C    |
| 50  | C1    | 1260 | U    |
| 50  | C1    | 1265 | G    |
| 50  | C1    | 1444 | A    |
| 50  | C1    | 1448 | A    |
| 50  | C1    | 1449 | U    |
| 50  | C1    | 1466 | G    |
| 50  | C1    | 1481 | U    |
| 50  | C1    | 1483 | A    |
| 50  | C1    | 1491 | A    |
| 50  | C1    | 1497 | U    |
| 50  | C1    | 1498 | G    |
| 50  | C1    | 1499 | G    |
| 50  | C1    | 1518 | A    |
| 50  | C1    | 1519 | C    |
| 50  | C1    | 1520 | U    |
| 50  | C1    | 1527 | G    |
| 50  | C1    | 1529 | A    |
| 50  | C1    | 1544 | U    |
| 50  | C1    | 1551 | A    |
| 50  | C1    | 1555 | A    |
| 50  | C1    | 1613 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | C1    | 1614 | U    |
| 50  | C1    | 1624 | A    |
| 50  | C1    | 1625 | G    |
| 50  | C1    | 1628 | A    |
| 50  | C1    | 1632 | G    |
| 50  | C1    | 1642 | A    |
| 50  | C1    | 1643 | U    |
| 50  | C1    | 1645 | U    |
| 50  | C1    | 1665 | A    |
| 50  | C1    | 1667 | G    |
| 50  | C1    | 1668 | A    |
| 50  | C1    | 1710 | G    |
| 50  | C1    | 1711 | G    |
| 50  | C1    | 1712 | C    |
| 50  | C1    | 1713 | U    |
| 50  | C1    | 1735 | A    |
| 50  | C1    | 1742 | C    |
| 50  | C1    | 1743 | C    |
| 50  | C1    | 1744 | A    |
| 50  | C1    | 1759 | U    |
| 50  | C1    | 2055 | C    |
| 50  | C1    | 2056 | U    |
| 50  | C1    | 2069 | G    |
| 50  | C1    | 2076 | C    |
| 50  | C1    | 2077 | C    |
| 50  | C1    | 2078 | C    |
| 50  | C1    | 2085 | G    |
| 50  | C1    | 2086 | A    |
| 50  | C1    | 2087 | G    |
| 50  | C1    | 2088 | A    |
| 50  | C1    | 2107 | A    |
| 50  | C1    | 2118 | U    |
| 50  | C1    | 2119 | G    |
| 50  | C1    | 2120 | C    |
| 50  | C1    | 2121 | U    |
| 50  | C1    | 2156 | A    |
| 50  | C1    | 2157 | G    |
| 50  | C1    | 2158 | G    |
| 50  | C1    | 2167 | G    |
| 50  | C1    | 2173 | G    |
| 50  | C1    | 2177 | G    |
| 50  | C1    | 2178 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | C1    | 2184 | G    |
| 50  | C1    | 2185 | C    |
| 50  | C1    | 2197 | A    |
| 50  | C1    | 2199 | G    |
| 50  | C1    | 2201 | C    |
| 50  | C1    | 2202 | C    |
| 50  | C1    | 2205 | G    |
| 50  | C1    | 2214 | A    |
| 50  | C1    | 2220 | C    |
| 50  | C1    | 2227 | C    |
| 50  | C1    | 2234 | A    |
| 50  | C1    | 2237 | G    |
| 50  | C1    | 2351 | G    |
| 50  | C1    | 2362 | U    |
| 50  | C1    | 2363 | G    |
| 50  | C1    | 2364 | A    |
| 50  | C1    | 2373 | A    |
| 50  | C1    | 2374 | G    |
| 51  | C2    | 15   | A    |
| 51  | C2    | 26   | U    |
| 51  | C2    | 28   | U    |
| 51  | C2    | 29   | A    |
| 51  | C2    | 31   | A    |
| 51  | C2    | 33   | U    |
| 51  | C2    | 34   | A    |
| 51  | C2    | 37   | U    |
| 51  | C2    | 39   | U    |
| 51  | C2    | 48   | G    |
| 51  | C2    | 58   | A    |
| 51  | C2    | 62   | A    |
| 51  | C2    | 63   | G    |
| 51  | C2    | 81   | G    |
| 51  | C2    | 90   | C    |
| 51  | C2    | 91   | G    |
| 51  | C2    | 92   | A    |
| 51  | C2    | 103  | G    |
| 51  | C2    | 104  | C    |
| 51  | C2    | 105  | C    |
| 51  | C2    | 111  | G    |
| 51  | C2    | 125  | U    |
| 51  | C2    | 126  | U    |
| 51  | C2    | 127  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | C2    | 128 | C    |
| 51  | C2    | 136 | C    |
| 51  | C2    | 142 | G    |
| 51  | C2    | 153 | G    |
| 51  | C2    | 160 | U    |
| 51  | C2    | 162 | C    |
| 51  | C2    | 163 | C    |
| 51  | C2    | 165 | C    |
| 51  | C2    | 166 | G    |
| 51  | C2    | 167 | U    |
| 51  | C2    | 170 | C    |
| 51  | C2    | 178 | U    |
| 51  | C2    | 179 | A    |
| 51  | C2    | 181 | A    |
| 51  | C2    | 182 | G    |
| 51  | C2    | 187 | U    |
| 51  | C2    | 189 | G    |
| 51  | C2    | 190 | C    |
| 51  | C2    | 199 | G    |
| 51  | C2    | 200 | U    |
| 51  | C2    | 201 | A    |
| 51  | C2    | 244 | G    |
| 51  | C2    | 247 | G    |
| 51  | C2    | 255 | U    |
| 51  | C2    | 256 | G    |
| 51  | C2    | 259 | A    |
| 51  | C2    | 260 | G    |
| 51  | C2    | 261 | U    |
| 51  | C2    | 262 | C    |

All (23) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | C1    | 89  | G    |
| 50  | C1    | 135 | A    |
| 50  | C1    | 150 | C    |
| 50  | C1    | 209 | A    |
| 50  | C1    | 259 | U    |
| 50  | C1    | 277 | U    |
| 50  | C1    | 281 | U    |
| 50  | C1    | 397 | U    |
| 50  | C1    | 593 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 50  | C1    | 684  | U    |
| 50  | C1    | 689  | A    |
| 50  | C1    | 771  | G    |
| 50  | C1    | 802  | A    |
| 50  | C1    | 1001 | A    |
| 50  | C1    | 1017 | C    |
| 50  | C1    | 1068 | C    |
| 50  | C1    | 1087 | G    |
| 50  | C1    | 1163 | A    |
| 50  | C1    | 1734 | G    |
| 50  | C1    | 2156 | A    |
| 50  | C1    | 2177 | G    |
| 50  | C1    | 2219 | C    |
| 51  | C2    | 255  | U    |

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | SEP  | UR    | 139  | 14   | 8,9,10       | 1.50 | 1 (12%)  | 8,12,14     | 1.46 | 2 (25%)  |
| 1   | SEP  | UA    | 646  | 1    | 8,9,10       | 1.50 | 1 (12%)  | 8,12,14     | 1.40 | 2 (25%)  |
| 50  | A2M  | C1    | 1004 | 50   | 22,25,26     | 3.41 | 9 (40%)  | 31,36,39    | 2.67 | 9 (29%)  |
| 50  | OMC  | C1    | 998  | 50   | 19,22,23     | 2.98 | 8 (42%)  | 26,31,34    | 0.69 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 14  | SEP  | UR    | 139 | 14   | -       | 0/5/8/10 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | SEP  | UA    | 646  | 1    | -       | 2/5/8/10  | -       |
| 50  | A2M  | C1    | 1004 | 50   | -       | 0/9/27/28 | 0/3/3/3 |
| 50  | OMC  | C1    | 998  | 50   | -       | 0/9/27/28 | 0/2/2/2 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 50  | C1    | 1004 | A2M  | C2'-C1' | -8.59 | 1.31        | 1.53     |
| 50  | C1    | 1004 | A2M  | O4'-C1' | 8.49  | 1.62        | 1.42     |
| 50  | C1    | 1004 | A2M  | O4'-C4' | -6.35 | 1.30        | 1.45     |
| 50  | C1    | 998  | OMC  | C2-N3   | 6.22  | 1.49        | 1.36     |
| 50  | C1    | 998  | OMC  | C6-C5   | 6.00  | 1.49        | 1.35     |
| 50  | C1    | 998  | OMC  | C4-N3   | 5.01  | 1.44        | 1.34     |
| 50  | C1    | 998  | OMC  | C4-N4   | 4.86  | 1.45        | 1.33     |
| 50  | C1    | 1004 | A2M  | C6-N6   | 4.40  | 1.45        | 1.34     |
| 50  | C1    | 998  | OMC  | C2-N1   | 4.32  | 1.49        | 1.40     |
| 1   | UA    | 646  | SEP  | P-O1P   | 3.31  | 1.61        | 1.50     |
| 14  | UR    | 139  | SEP  | P-O1P   | 3.26  | 1.61        | 1.50     |
| 50  | C1    | 998  | OMC  | C6-N1   | 3.19  | 1.45        | 1.38     |
| 50  | C1    | 1004 | A2M  | O3'-C3' | -2.99 | 1.35        | 1.43     |
| 50  | C1    | 1004 | A2M  | C5-C4   | -2.84 | 1.33        | 1.39     |
| 50  | C1    | 998  | OMC  | O2-C2   | -2.80 | 1.18        | 1.23     |
| 50  | C1    | 1004 | A2M  | O2'-C2' | 2.79  | 1.49        | 1.42     |
| 50  | C1    | 1004 | A2M  | C5-N7   | -2.64 | 1.34        | 1.39     |
| 50  | C1    | 998  | OMC  | C5-C4   | 2.41  | 1.48        | 1.42     |
| 50  | C1    | 1004 | A2M  | C8-N9   | -2.09 | 1.33        | 1.37     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 50  | C1    | 1004 | A2M  | N6-C6-N1 | -7.00 | 103.03      | 118.35   |
| 50  | C1    | 1004 | A2M  | C5-C6-N6 | 6.18  | 136.88      | 123.43   |
| 50  | C1    | 1004 | A2M  | N3-C2-N1 | -5.54 | 119.93      | 128.60   |
| 50  | C1    | 1004 | A2M  | C5-C4-N3 | -5.28 | 119.86      | 126.75   |
| 50  | C1    | 1004 | A2M  | N9-C8-N7 | -4.25 | 108.10      | 113.91   |
| 50  | C1    | 1004 | A2M  | C2-N3-C4 | 3.56  | 120.17      | 111.75   |
| 50  | C1    | 1004 | A2M  | N3-C4-N9 | 3.20  | 132.36      | 127.08   |
| 50  | C1    | 1004 | A2M  | C5-N7-C8 | 3.08  | 107.88      | 103.51   |
| 1   | UA    | 646  | SEP  | P-OG-CB  | -2.80 | 110.58      | 118.30   |
| 14  | UR    | 139  | SEP  | P-OG-CB  | -2.67 | 110.94      | 118.30   |
| 14  | UR    | 139  | SEP  | OG-CB-CA | 2.44  | 110.52      | 108.14   |
| 1   | UA    | 646  | SEP  | OG-CB-CA | 2.17  | 110.26      | 108.14   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 50  | C1    | 1004 | A2M  | C4-N9-C8 | 2.13 | 108.03      | 105.73   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | UA    | 646 | SEP  | CB-OG-P-O2P |
| 1   | UA    | 646 | SEP  | CB-OG-P-O3P |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | UR    | 139  | SEP  | 1       | 0            |
| 50  | C1    | 1004 | A2M  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 65  | ADP  | CS    | 1101 | -    | 27,29,29     | 2.92 | 8 (29%)     | 42,45,45    | 2.15 | 14 (33%)    |
| 63  | GTP  | CI    | 1201 | 64   | 30,34,34     | 0.87 | 0           | 46,54,54    | 1.69 | 10 (21%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 65  | ADP  | CS    | 1101 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 63  | GTP  | CI    | 1201 | 64   | -       | 5/22/38/38 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 65  | CS    | 1101 | ADP  | O4'-C1' | 8.48  | 1.62        | 1.42     |
| 65  | CS    | 1101 | ADP  | C2'-C1' | -7.00 | 1.31        | 1.53     |
| 65  | CS    | 1101 | ADP  | O4'-C4' | -6.24 | 1.31        | 1.45     |
| 65  | CS    | 1101 | ADP  | C6-N6   | 4.54  | 1.45        | 1.34     |
| 65  | CS    | 1101 | ADP  | O2'-C2' | 2.98  | 1.50        | 1.43     |
| 65  | CS    | 1101 | ADP  | O3'-C3' | -2.90 | 1.36        | 1.43     |
| 65  | CS    | 1101 | ADP  | C5-C4   | -2.66 | 1.34        | 1.39     |
| 65  | CS    | 1101 | ADP  | C5-N7   | -2.46 | 1.34        | 1.39     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 65  | CS    | 1101 | ADP  | N3-C2-N1    | -5.57 | 119.89      | 128.60   |
| 65  | CS    | 1101 | ADP  | C5-C4-N3    | -5.37 | 119.74      | 126.75   |
| 63  | CI    | 1201 | GTP  | C5-C4-N3    | -4.81 | 120.66      | 128.46   |
| 63  | CI    | 1201 | GTP  | C2-N3-C4    | 4.37  | 120.08      | 112.30   |
| 65  | CS    | 1101 | ADP  | N9-C8-N7    | -4.19 | 108.18      | 113.91   |
| 65  | CS    | 1101 | ADP  | C2-N3-C4    | 3.66  | 120.39      | 111.75   |
| 65  | CS    | 1101 | ADP  | N6-C6-N1    | -3.49 | 110.71      | 118.35   |
| 65  | CS    | 1101 | ADP  | C4-N9-C1'   | -3.41 | 118.48      | 126.59   |
| 65  | CS    | 1101 | ADP  | N3-C4-N9    | 3.24  | 132.42      | 127.08   |
| 65  | CS    | 1101 | ADP  | C5-N7-C8    | 3.10  | 107.91      | 103.51   |
| 63  | CI    | 1201 | GTP  | PB-O3B-PG   | -3.04 | 122.40      | 132.83   |
| 63  | CI    | 1201 | GTP  | N9-C4-N3    | 2.99  | 131.95      | 125.94   |
| 65  | CS    | 1101 | ADP  | C1'-N9-C8   | 2.84  | 133.55      | 127.14   |
| 63  | CI    | 1201 | GTP  | C2-N1-C6    | -2.80 | 119.99      | 125.10   |
| 65  | CS    | 1101 | ADP  | C3'-C2'-C1' | 2.69  | 106.54      | 101.43   |
| 63  | CI    | 1201 | GTP  | N9-C8-N7    | -2.64 | 108.42      | 113.39   |
| 65  | CS    | 1101 | ADP  | C5-C6-N6    | 2.56  | 128.99      | 123.43   |
| 63  | CI    | 1201 | GTP  | C5-C6-N1    | 2.50  | 119.54      | 113.19   |
| 63  | CI    | 1201 | GTP  | C8-N7-C5    | 2.49  | 108.75      | 104.24   |
| 65  | CS    | 1101 | ADP  | PA-O3A-PB   | -2.46 | 124.37      | 132.83   |
| 63  | CI    | 1201 | GTP  | PA-O3A-PB   | -2.36 | 124.72      | 132.83   |
| 63  | CI    | 1201 | GTP  | O6-C6-C5    | -2.31 | 120.47      | 126.60   |
| 65  | CS    | 1101 | ADP  | C4-N9-C8    | 2.08  | 107.98      | 105.73   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 65  | CS    | 1101 | ADP  | C4-C5-N7 | -2.07 | 108.10      | 110.62   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

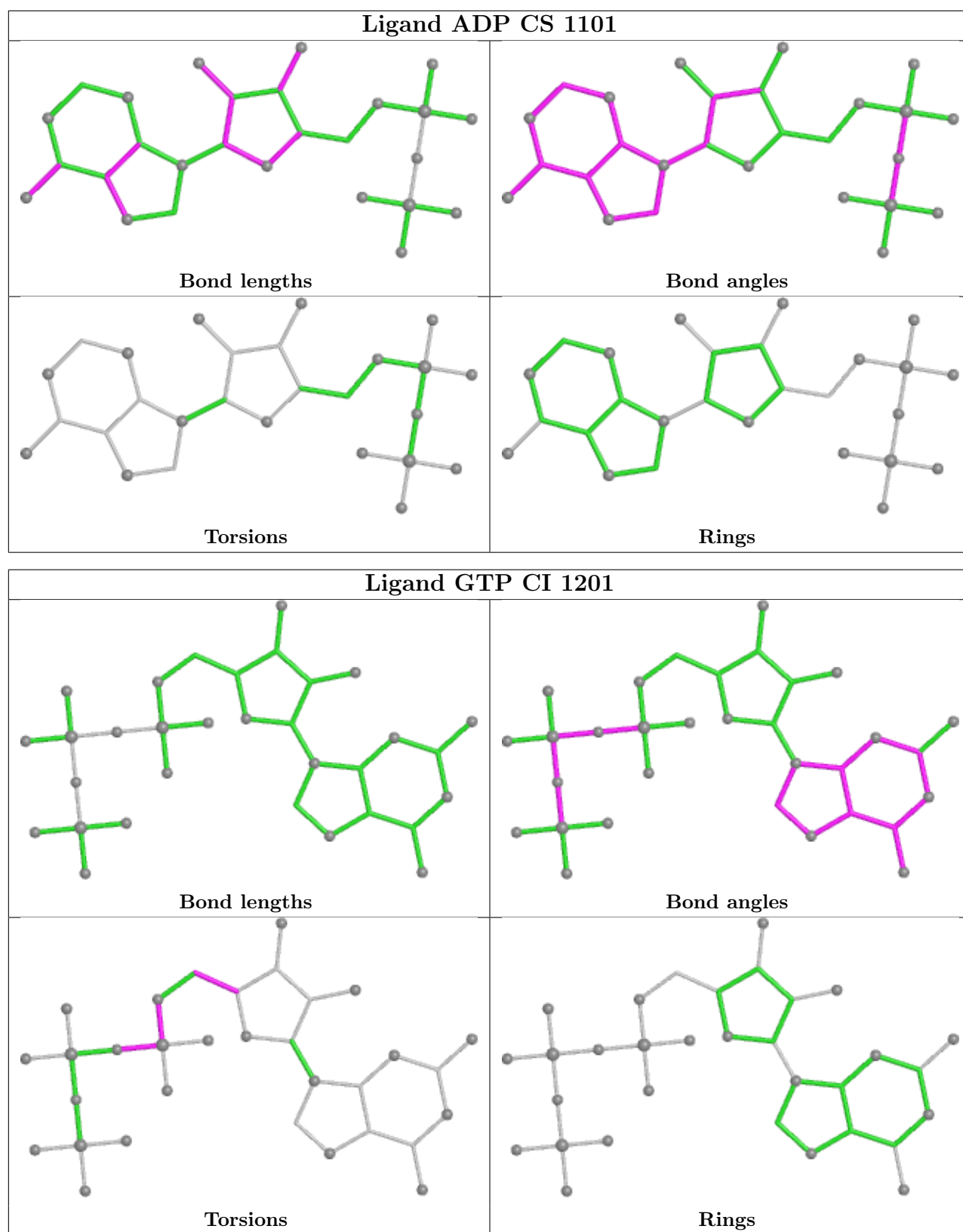
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 63  | CI    | 1201 | GTP  | C5'-O5'-PA-O3A  |
| 63  | CI    | 1201 | GTP  | O4'-C4'-C5'-O5' |
| 63  | CI    | 1201 | GTP  | PB-O3A-PA-O1A   |
| 63  | CI    | 1201 | GTP  | C5'-O5'-PA-O2A  |
| 63  | CI    | 1201 | GTP  | C5'-O5'-PA-O1A  |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 65  | CS    | 1101 | ADP  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

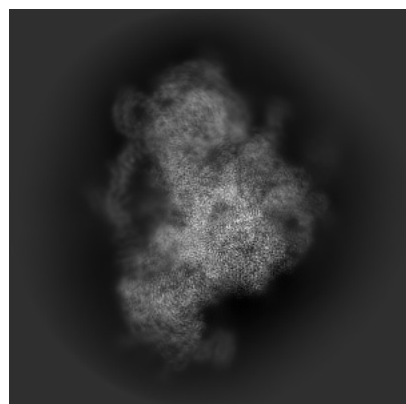
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66686. These allow visual inspection of the internal detail of the map and identification of artifacts.

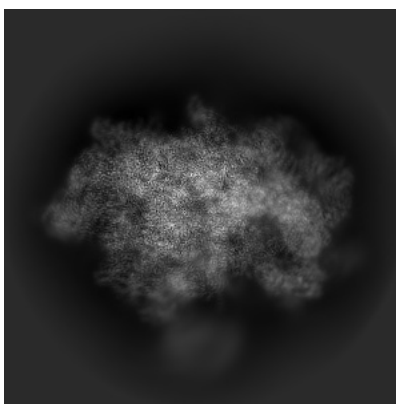
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

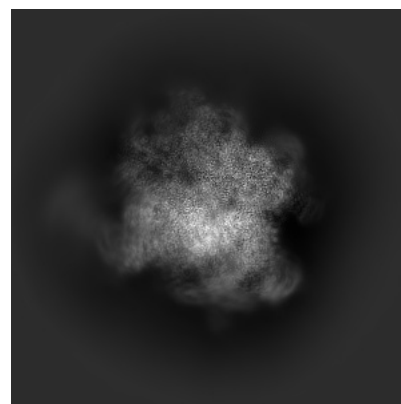
#### 6.1.1 Primary map



X

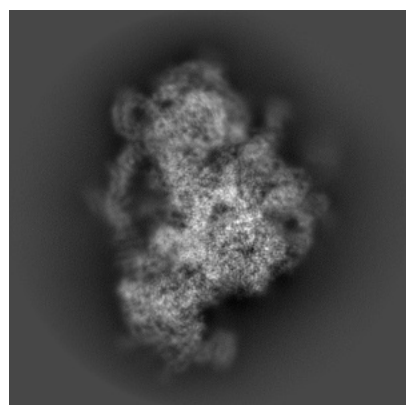


Y

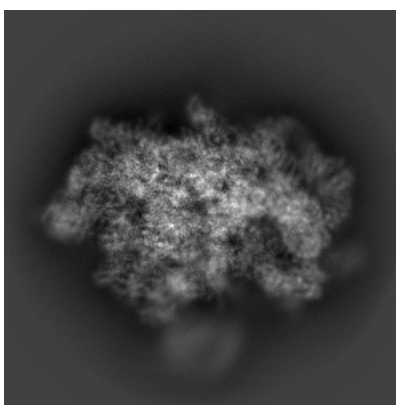


Z

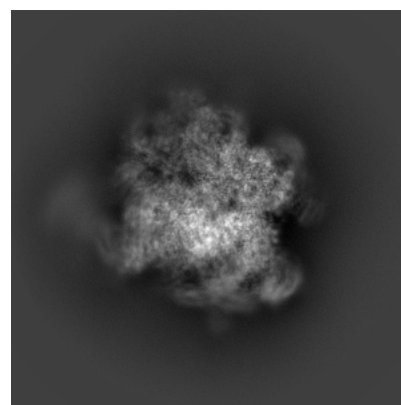
#### 6.1.2 Raw map



X



Y

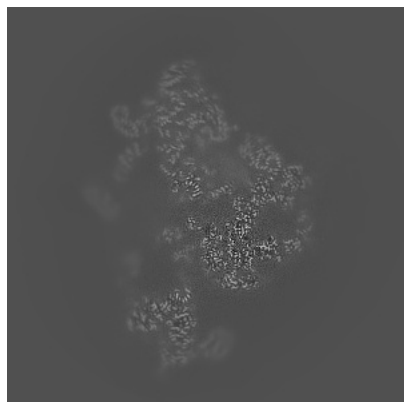


Z

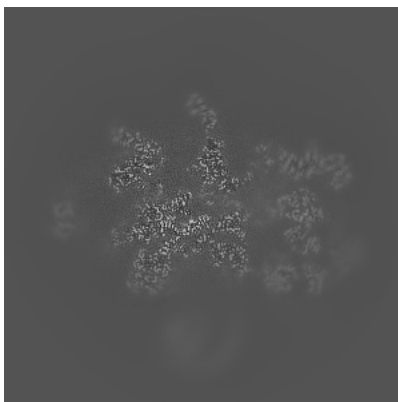
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

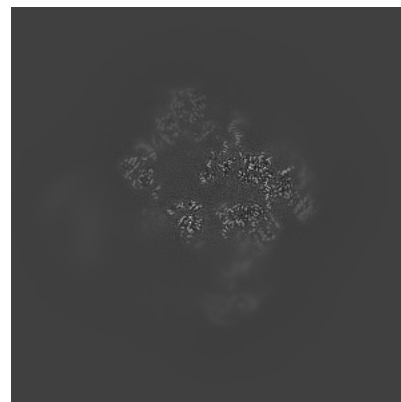
### 6.2.1 Primary map



X Index: 240

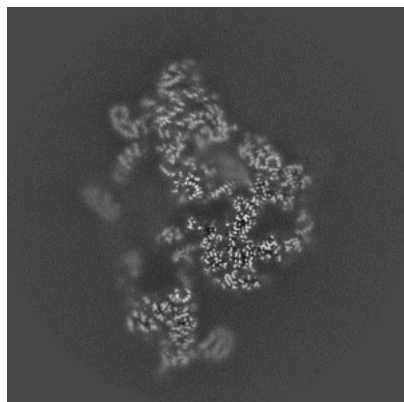


Y Index: 240

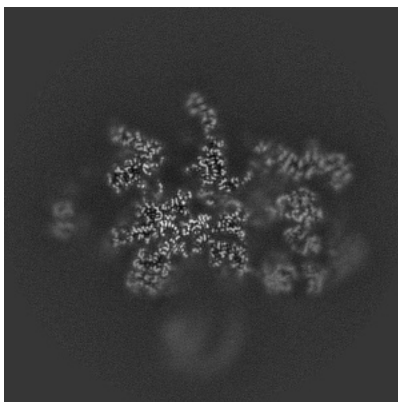


Z Index: 240

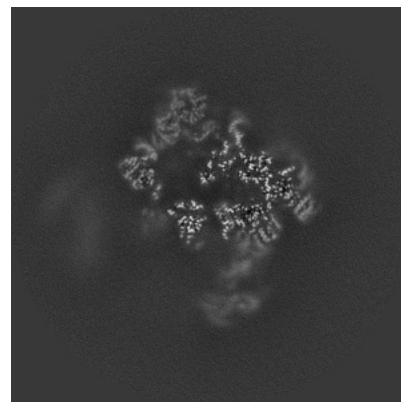
### 6.2.2 Raw map



X Index: 240



Y Index: 240

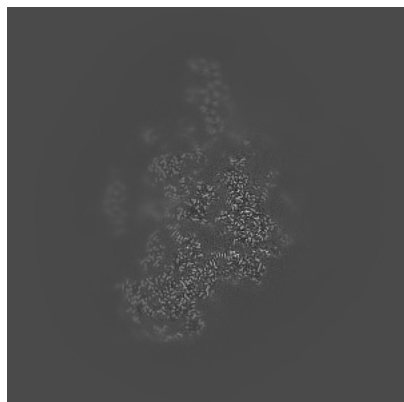


Z Index: 240

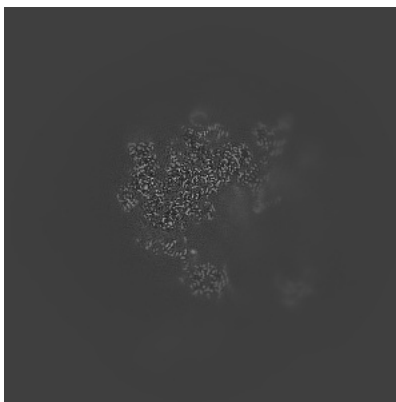
The images above show central slices of the map in three orthogonal directions.

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

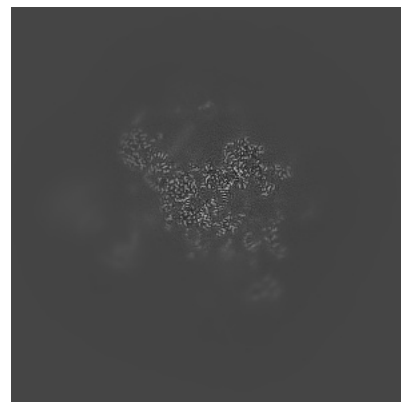
### 6.3.1 Primary map



X Index: 282

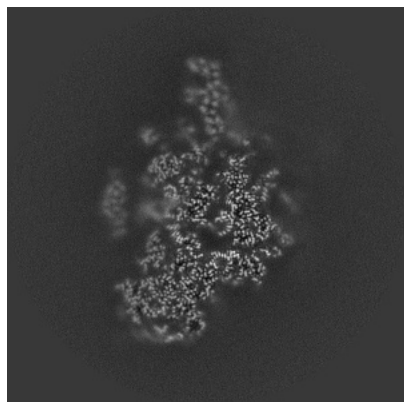


Y Index: 282

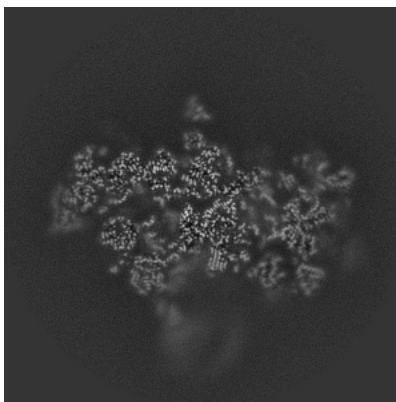


Z Index: 217

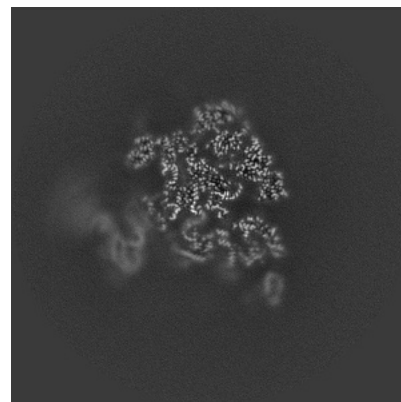
### 6.3.2 Raw map



X Index: 282



Y Index: 225

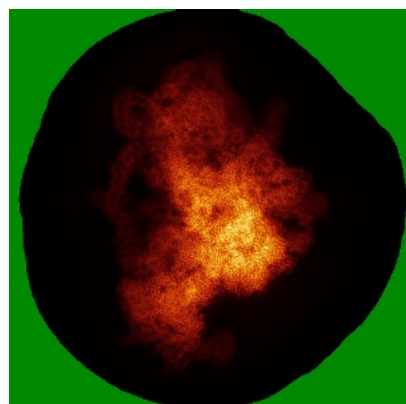


Z Index: 202

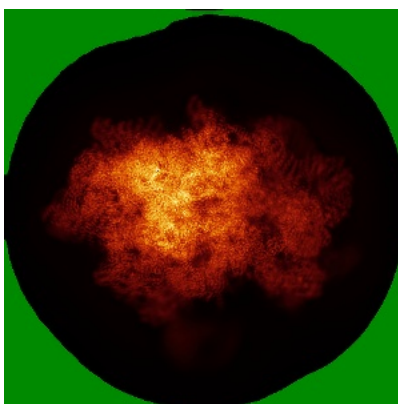
The images above show the largest variance slices of the map in three orthogonal directions.

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

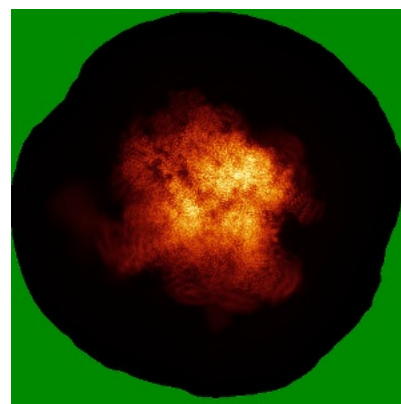
### 6.4.1 Primary map



X

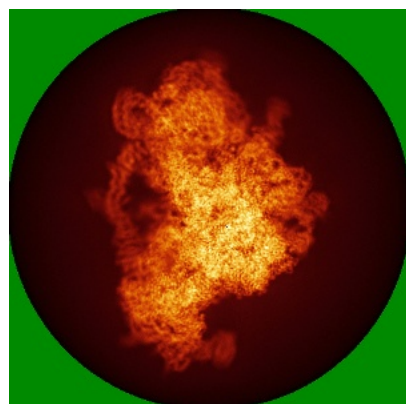


Y

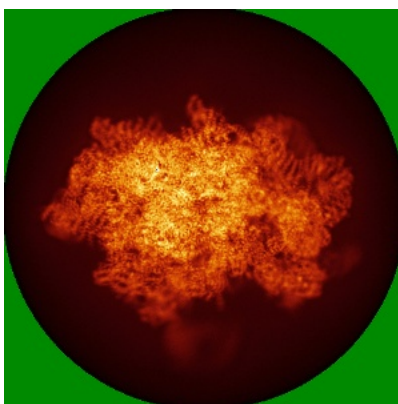


Z

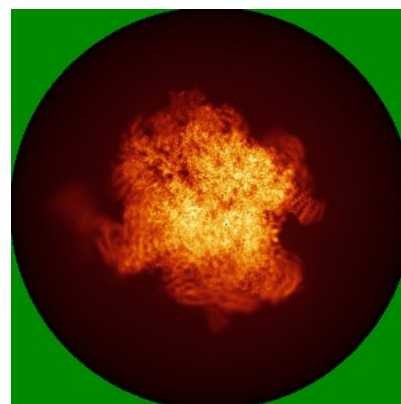
### 6.4.2 Raw map



X



Y

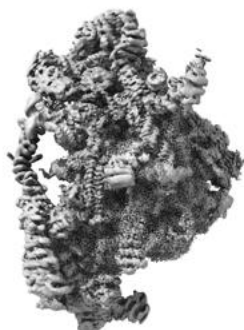


Z

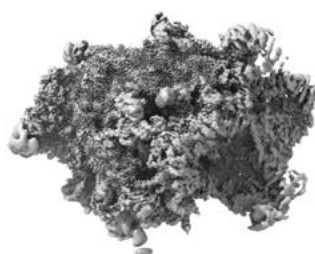
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

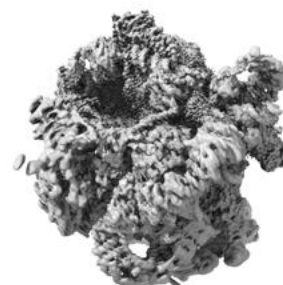
### 6.5.1 Primary map



X



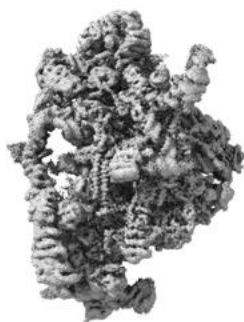
Y



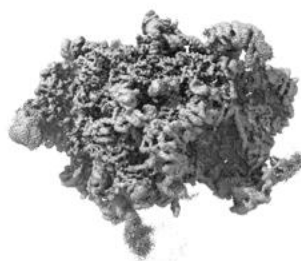
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

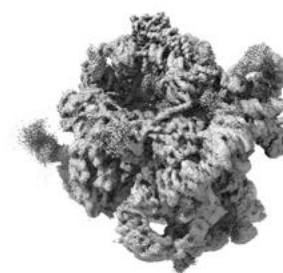
### 6.5.2 Raw map



X



Y



Z

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

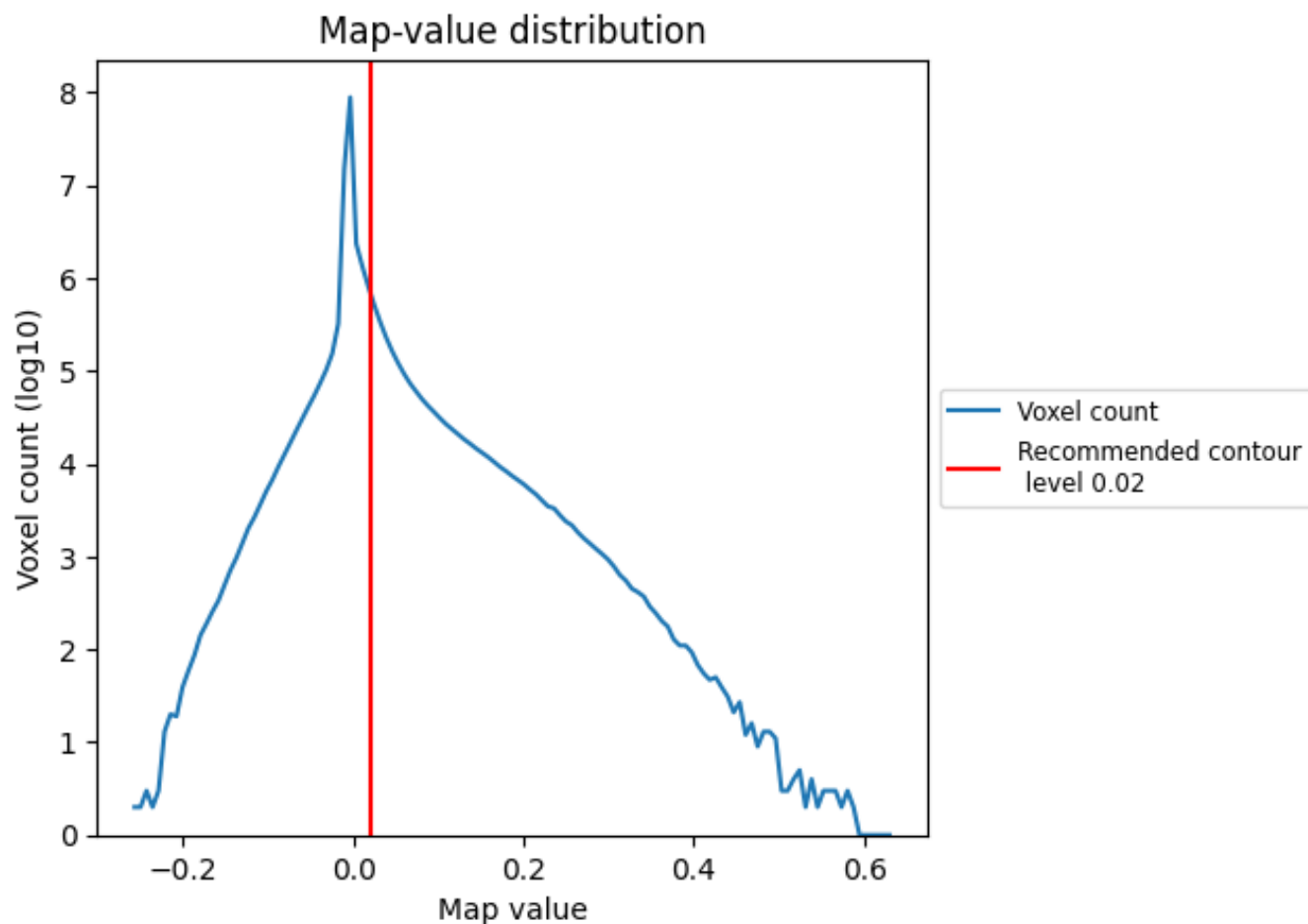
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

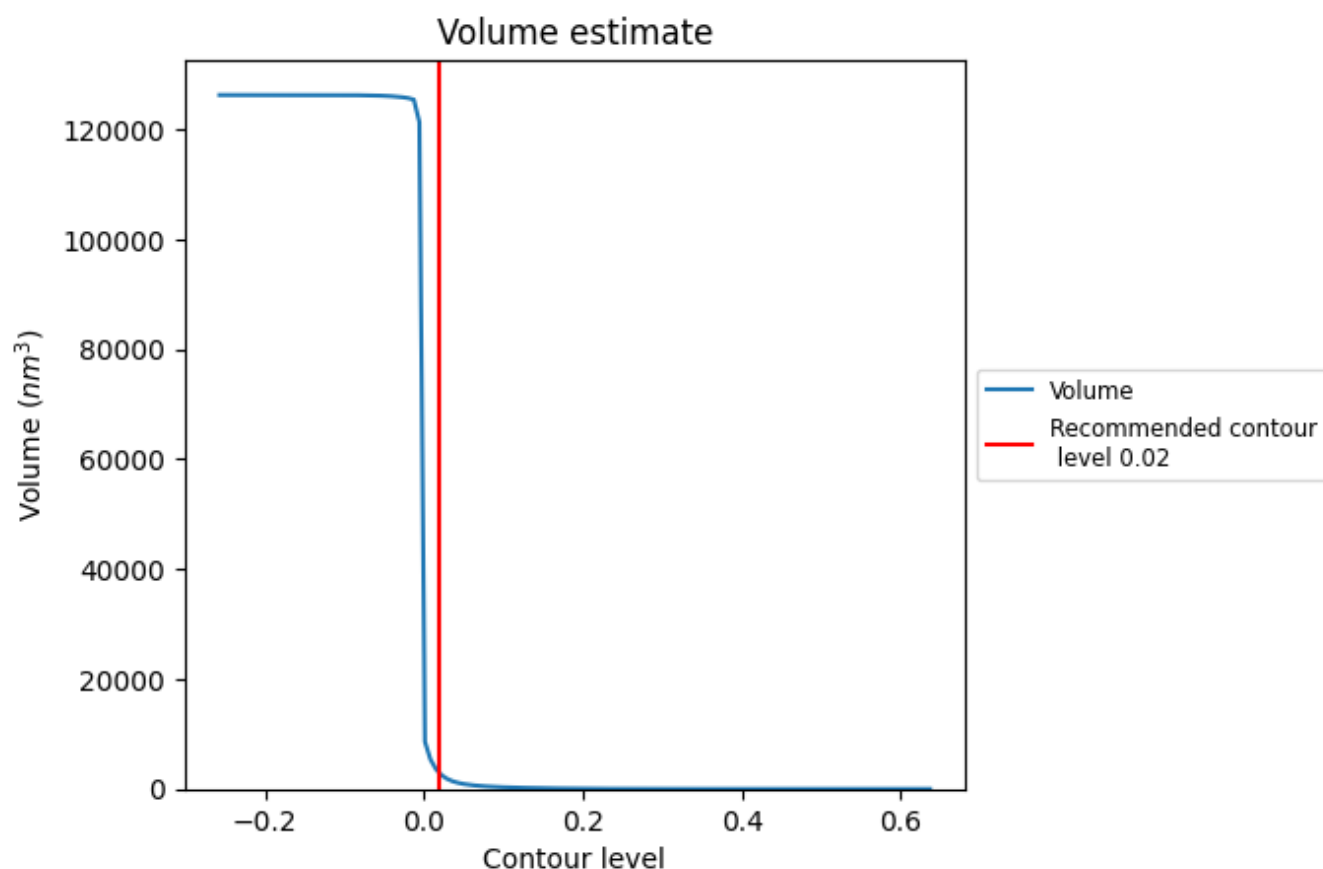
This section contains the results of statistical analysis of the map.

### 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.

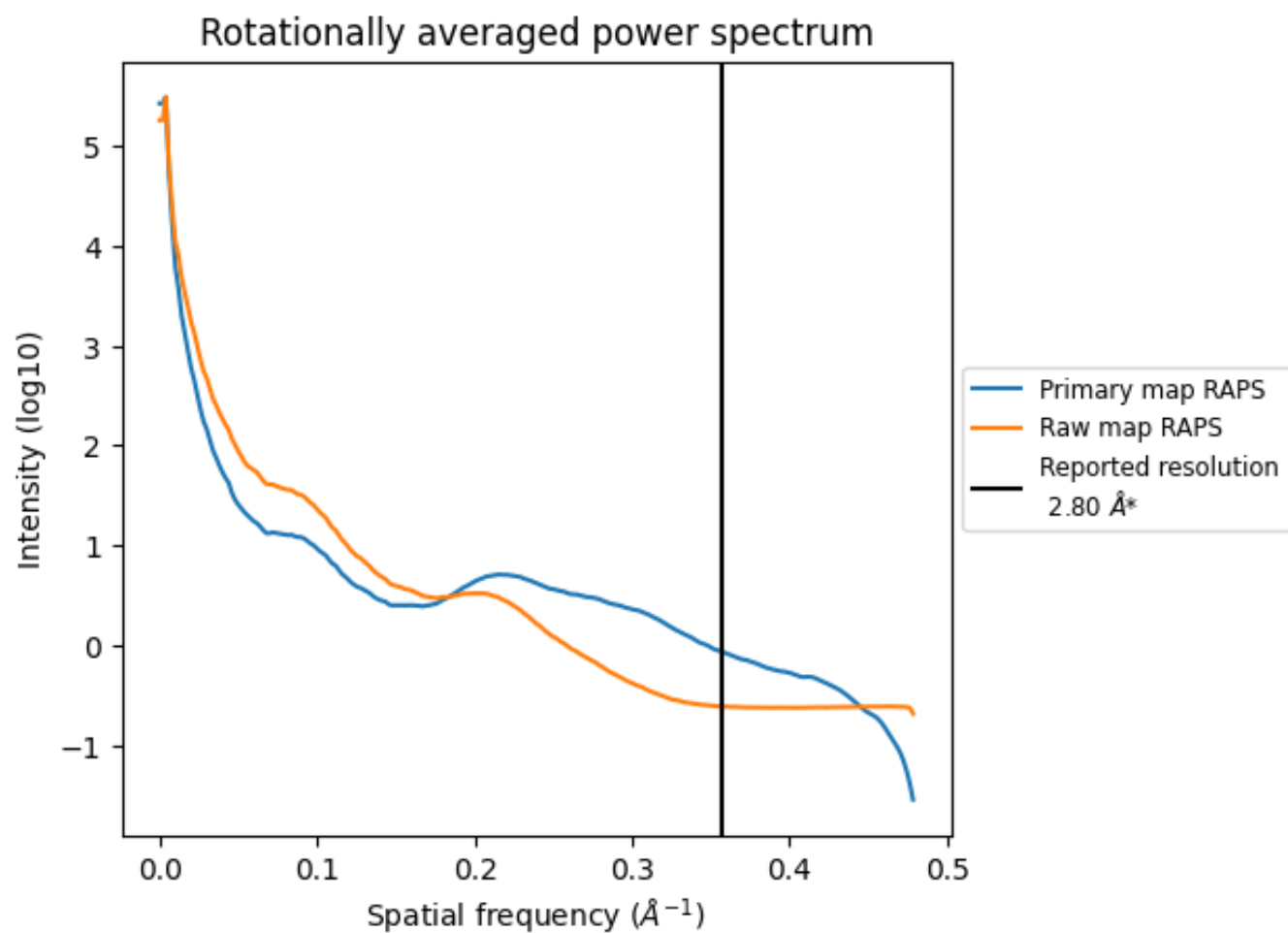
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2859  $\text{nm}^3$ ; this corresponds to an approximate mass of 2583 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 ⓘ

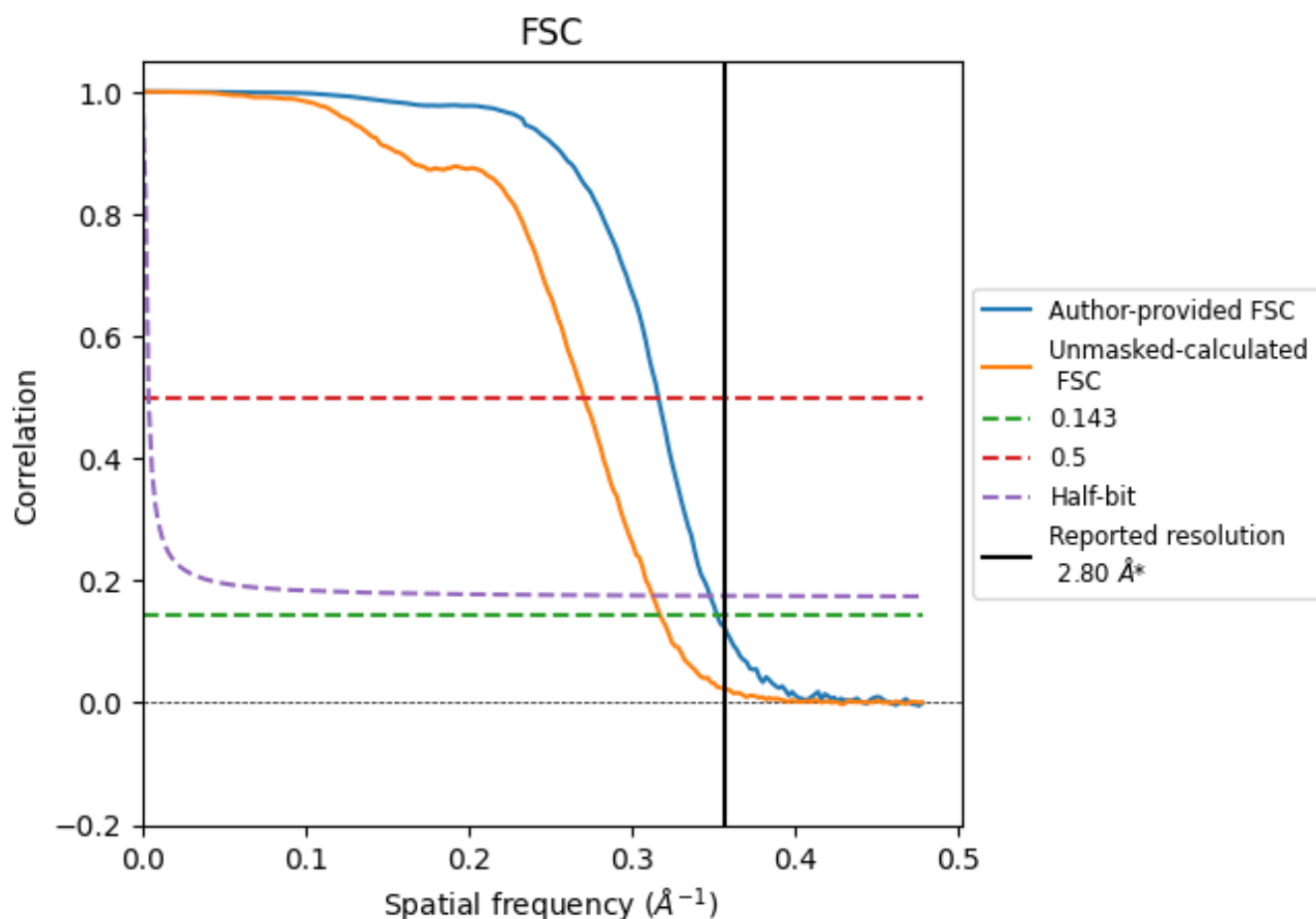


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

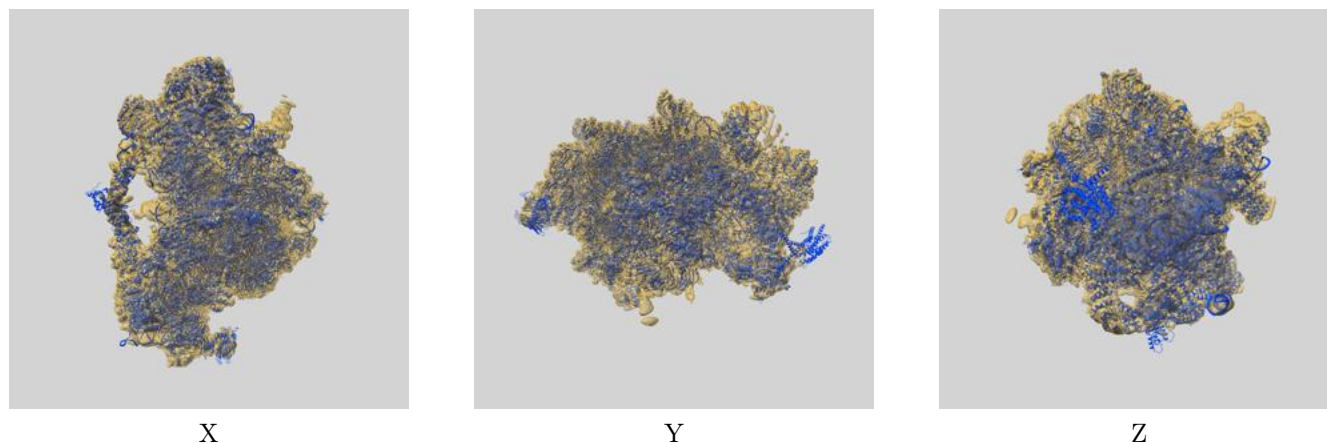
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.80                               | -    | -        |
| Author-provided FSC curve | 2.84                               | 3.16 | 2.87     |
| Unmasked-calculated*      | 3.15                               | 3.69 | 3.19     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.8 by more than 10 %

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

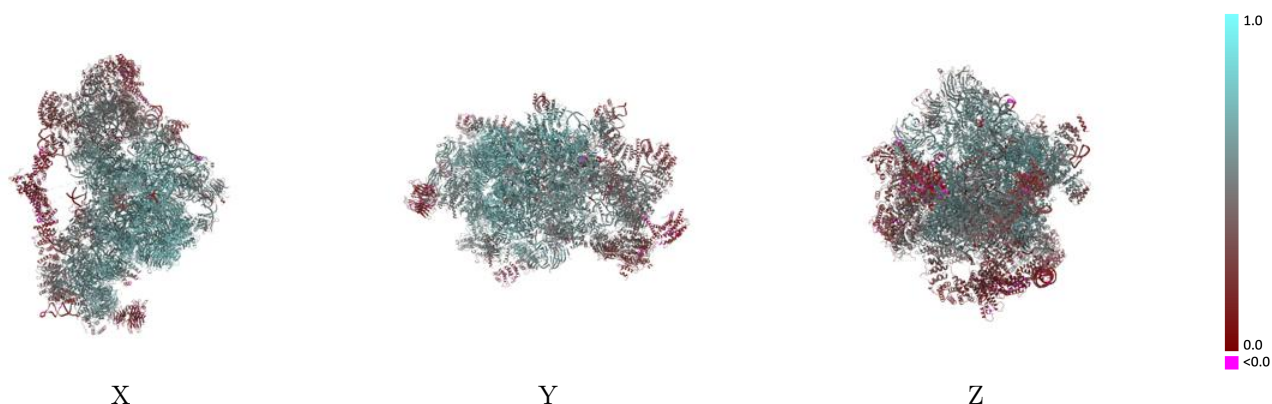
This section contains information regarding the fit between EMDB map EMD-66686 and PDB model 9XAG. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



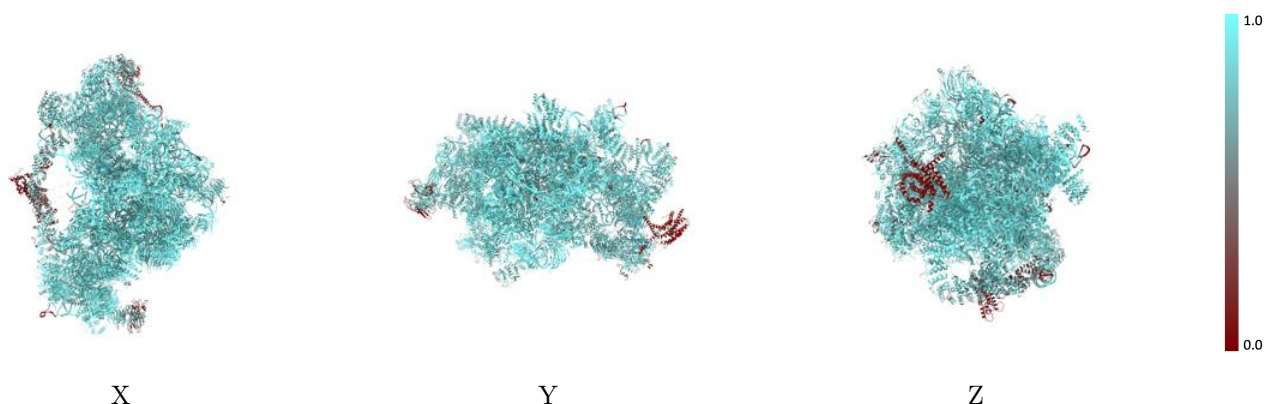
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



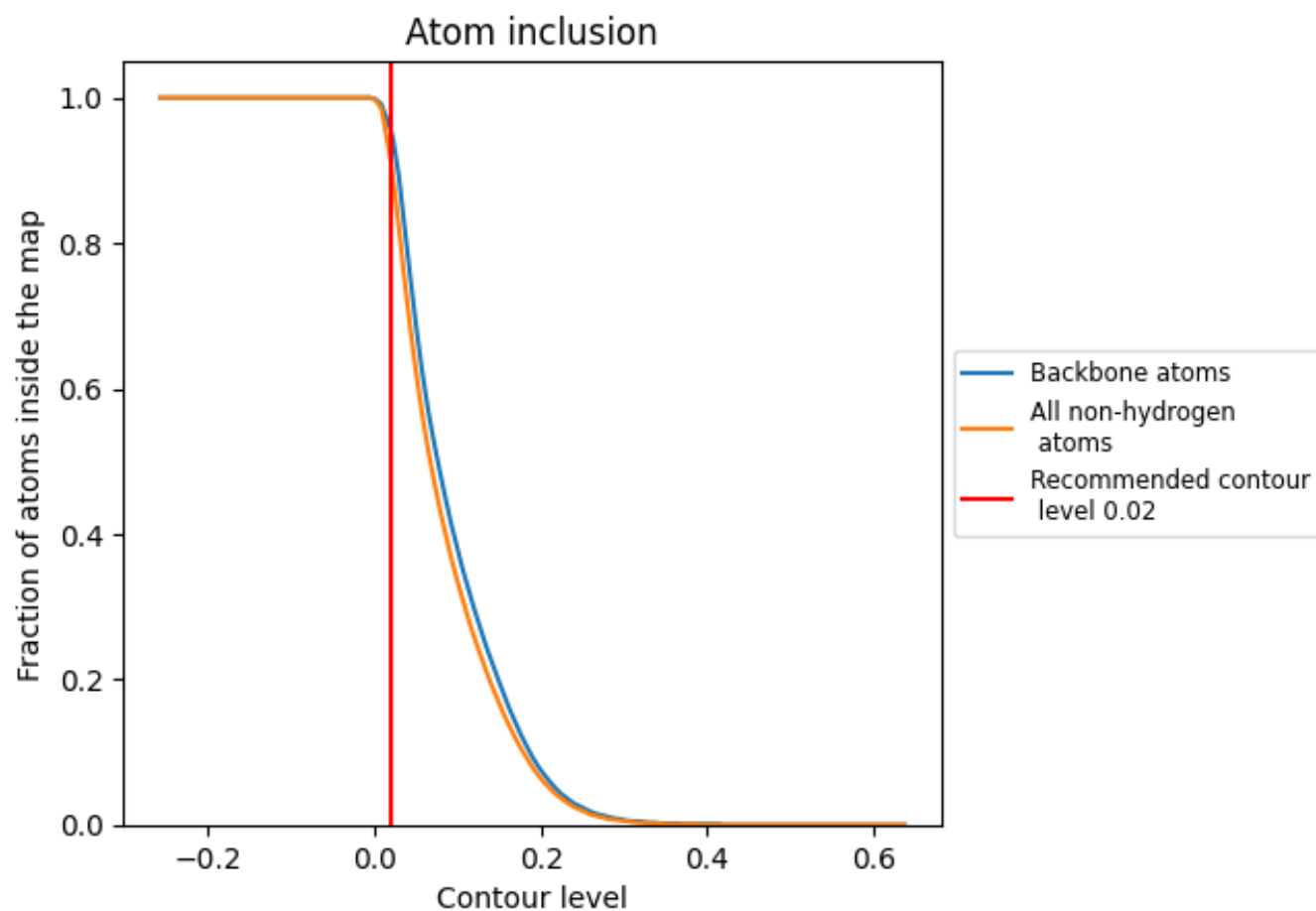
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9110   |  0.5280   |
| C1    |  0.9660   |  0.5570   |
| C2    |  0.9160   |  0.4990   |
| CA    |  0.9890   |  0.6970   |
| CB    |  0.9310   |  0.5340   |
| CC    |  0.9630   |  0.5860   |
| CD    |  0.9340   |  0.5520   |
| CE    |  0.9840   |  0.6620   |
| CF    |  0.9930   |  0.6180   |
| CG    |  0.9570   |  0.5490   |
| CH    |  0.9900   |  0.6310   |
| CI    |  0.9750   |  0.6360   |
| CJ    |  0.9980   |  0.7560   |
| CK    |  0.9930   |  0.7100   |
| CL    |  0.7330  |  0.5170  |
| CM    |  0.9920 |  0.7100 |
| CN    |  0.9740 |  0.5900 |
| CO    |  0.9170 |  0.4860 |
| CP    |  0.9420 |  0.5630 |
| CQ    |  0.9550 |  0.5420 |
| CR    |  0.8770 |  0.4330 |
| CS    |  0.8080 |  0.3200 |
| CT    |  0.9840 |  0.6670 |
| CU    |  0.9670 |  0.6150 |
| CW    |  0.9250 |  0.4890 |
| CX    |  0.7870 |  0.1690 |
| CY    |  0.4530 |  0.2880 |
| CZ    |  0.1920 |  0.1680 |
| Ca    |  0.9610 |  0.5610 |
| Cb    |  0.9520 |  0.4730 |
| Cc    |  0.9900 |  0.6800 |
| Cd    |  0.9470 |  0.5160 |
| Ce    |  0.8980 |  0.4520 |
| Cf    |  0.9490 |  0.4980 |
| Cg    |  0.9930 |  0.6530 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Ch    |  0.8750   |  0.4370   |
| Ci    |  0.9890   |  0.6000   |
| Cj    |  0.9920   |  0.7140   |
| Ck    |  0.9480   |  0.4460   |
| Cl    |  0.9160   |  0.4780   |
| Cm    |  0.9790   |  0.6210   |
| Cn    |  0.9970   |  0.6890   |
| Co    |  0.9580   |  0.4620   |
| Cp    |  0.9890   |  0.6640   |
| UA    |  0.9940   |  0.7230   |
| UB    |  0.9470   |  0.5130   |
| UC    |  0.4140   |  0.3460   |
| UD    |  0.9770   |  0.6080   |
| UE    |  0.9740   |  0.5750   |
| UF    |  0.9520   |  0.5750   |
| UG    |  0.9880   |  0.7120   |
| UH    |  0.6920   |  0.3220   |
| UI    |  0.9310   |  0.4830   |
| UJ    |  0.7650   |  0.3340   |
| UK    |  0.9780  |  0.6620  |
| UL    |  0.9770 |  0.5930 |
| UM    |  0.8980 |  0.5130 |
| UN    |  0.9660 |  0.6360 |
| UO    |  0.9870 |  0.6400 |
| UP    |  0.9580 |  0.5720 |
| UQ    |  0.9740 |  0.6090 |
| UR    |  0.9890 |  0.6870 |
| US    |  0.9440 |  0.5110 |
| UT    |  0.8520 |  0.3630 |
| UU    |  0.9900 |  0.6960 |
| UX    |  0.9920 |  0.6870 |
| UZ    |  0.9560 |  0.5000 |