



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:39 AM UTC

PDB ID : 6HIV / pdb\_00006hiv  
EMDB ID : EMD-0229  
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the complete mitoribosome  
Authors : Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boehringer, D.; Schneider, A.; Ban, N.  
Deposited on : 2018-08-31  
Resolution : 7.80 Å(reported)

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

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

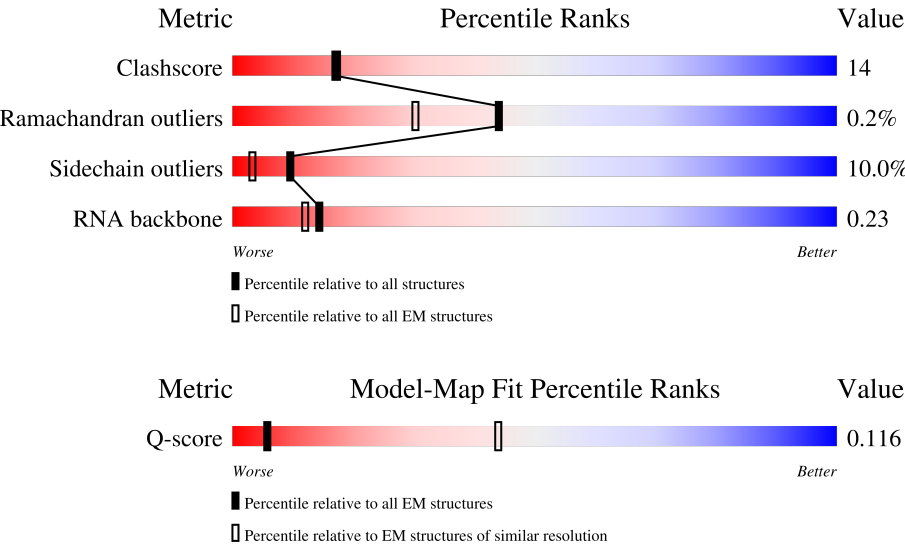
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 7.80 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                       | 370 ( 7.30 - 8.30 )                                      |

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   | DA    | 1788   | <div> <div>11%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>•</div> <div>13%</div> </div> </div> |
| 2   | DD    | 812    | <div> <div>20%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>•</div> <div>•</div> </div> </div>   |
| 3   | DI    | 407    | <div> <div>9%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>•</div> <div>•</div> </div> </div>    |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | DL    | 307    |                  |
| 5   | DM    | 294    |                  |
| 6   | DN    | 293    |                  |
| 7   | DO    | 282    |                  |
| 8   | DP    | 274    |                  |
| 9   | DQ    | 268    |                  |
| 10  | DR    | 270    |                  |
| 11  | DS    | 261    |                  |
| 12  | DU    | 228    |                  |
| 13  | DZ    | 94     |                  |
| 14  | Da    | 64     |                  |
| 15  | DB    | 1181   |                  |
| 16  | DC    | 1165   |                  |
| 17  | DE    | 746    |                  |
| 18  | DF    | 666    |                  |
| 19  | DG    | 631    |                  |
| 20  | DH    | 581    |                  |
| 21  | DJ    | 396    |                  |
| 22  | DK    | 324    |                  |
| 23  | DT    | 247    |                  |
| 24  | DV    | 183    |                  |
| 25  | DW    | 179    |                  |
| 26  | DX    | 169    |                  |
| 27  | DY    | 163    |                  |
| 28  | CC    | 74     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | CE    | 435    |                  |
| 30  | CF    | 160    |                  |
| 31  | CH    | 282    |                  |
| 32  | CI    | 443    |                  |
| 33  | CJ    | 817    |                  |
| 34  | CK    | 326    |                  |
| 35  | CL    | 87     |                  |
| 36  | CN    | 166    |                  |
| 37  | CO    | 429    |                  |
| 38  | CP    | 188    |                  |
| 39  | CQ    | 307    |                  |
| 40  | CR    | 320    |                  |
| 41  | CS    | 244    |                  |
| 42  | CU    | 193    |                  |
| 43  | CZ    | 360    |                  |
| 44  | Ca    | 602    |                  |
| 45  | Cb    | 324    |                  |
| 46  | Cd    | 440    |                  |
| 47  | Cg    | 498    |                  |
| 48  | Ci    | 181    |                  |
| 49  | Cj    | 257    |                  |
| 50  | Ck    | 874    |                  |
| 51  | Cm    | 215    |                  |
| 52  | Cn    | 250    |                  |
| 53  | Cp    | 187    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | Cq    | 263    |                  |
| 55  | Cr    | 439    |                  |
| 56  | Cv    | 1211   |                  |
| 57  | CA    | 621    |                  |
| 58  | UO    | 5      |                  |
| 59  | UP    | 7      |                  |
| 59  | UW    | 7      |                  |
| 60  | UQ    | 32     |                  |
| 61  | UR    | 8      |                  |
| 61  | UV    | 8      |                  |
| 61  | UX    | 8      |                  |
| 62  | US    | 54     |                  |
| 63  | UT    | 44     |                  |
| 64  | A0    | 185    |                  |
| 65  | A1    | 241    |                  |
| 66  | A2    | 471    |                  |
| 67  | A3    | 218    |                  |
| 68  | A4    | 183    |                  |
| 69  | A5    | 80     |                  |
| 70  | A6    | 114    |                  |
| 71  | A8    | 181    |                  |
| 72  | A9    | 184    |                  |
| 73  | AE    | 473    |                  |
| 74  | AF    | 459    |                  |
| 75  | AI    | 263    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 76  | AJ    | 177    |                  |
| 77  | AK    | 342    |                  |
| 78  | AN    | 202    |                  |
| 79  | AP    | 374    |                  |
| 80  | AQ    | 167    |                  |
| 81  | AR    | 301    |                  |
| 82  | AT    | 144    |                  |
| 83  | AU    | 213    |                  |
| 84  | AV    | 188    |                  |
| 85  | AW    | 278    |                  |
| 86  | AX    | 246    |                  |
| 87  | AY    | 378    |                  |
| 88  | Ab    | 507    |                  |
| 89  | Ad    | 289    |                  |
| 90  | Ae    | 197    |                  |
| 91  | Af    | 189    |                  |
| 92  | Ag    | 260    |                  |
| 93  | Aj    | 296    |                  |
| 94  | Al    | 218    |                  |
| 95  | Ao    | 259    |                  |
| 96  | Ap    | 309    |                  |
| 97  | At    | 154    |                  |
| 98  | Av    | 242    |                  |
| 99  | AB    | 56     |                  |
| 100 | AC    | 28     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 100 | AD    | 28     | 96%<br>          |
| 101 | AG    | 27     | 100%<br>         |
| 102 | AA    | 1179   | 96%<br>          |
| 103 | BA    | 831    | 11%<br>          |
| 104 | BB    | 541    | 16%<br>          |
| 105 | BC    | 523    | 24%<br>          |
| 106 | BD    | 547    | 55%<br>          |
| 107 | BE    | 449    | 23%<br>          |
| 108 | BF    | 541    | 18%<br>          |
| 109 | BG    | 378    | 16%<br>          |
| 110 | BH    | 349    | 54%<br>          |
| 111 | BI    | 449    | 24%<br>          |
| 112 | BJ    | 343    | 19%<br>          |
| 113 | BK    | 386    | 12%<br>          |
| 114 | BL    | 312    | 55%<br>          |
| 115 | BM    | 283    | 26%<br>          |
| 116 | BN    | 302    | 34%<br>          |
| 117 | BO    | 262    | 68%<br>          |
| 118 | BP    | 266    | 7%<br>           |
| 119 | BQ    | 231    | 58%<br>          |
| 120 | BR    | 205    | 26%<br>          |
| 121 | BS    | 160    | 5%<br>           |
| 122 | BT    | 191    | 27%<br>          |
| 123 | BU    | 185    | 16%<br>          |
| 124 | BV    | 190    | 29%<br>          |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 125 | BW    | 188    |                  |
| 126 | BX    | 190    |                  |
| 127 | BY    | 172    |                  |
| 128 | BZ    | 190    |                  |
| 129 | Ba    | 139    |                  |
| 130 | Bb    | 162    |                  |
| 131 | Bc    | 146    |                  |
| 132 | Bd    | 144    |                  |
| 133 | Be    | 113    |                  |
| 134 | Bf    | 113    |                  |
| 135 | Bg    | 105    |                  |
| 136 | Bh    | 92     |                  |
| 137 | UA    | 46     |                  |
| 138 | UB    | 40     |                  |
| 139 | UC    | 12     |                  |
| 139 | UH    | 12     |                  |
| 140 | UD    | 177    |                  |
| 141 | UE    | 22     |                  |
| 142 | UF    | 24     |                  |
| 142 | UG    | 24     |                  |
| 142 | UN    | 24     |                  |
| 143 | UI    | 17     |                  |
| 144 | UK    | 10     |                  |
| 145 | UL    | 15     |                  |
| 146 | UM    | 6      |                  |

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| Mol | Chain | Length | Quality of chain                                                 |
|-----|-------|--------|------------------------------------------------------------------|
| 147 | UU    | 11     | <div><div></div><div>64%</div><div>55%</div><div>45%</div></div> |

## 2 Entry composition

There are 156 unique types of molecules in this entry. The entry contains 311240 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 ms48.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | DA    | 1557     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 12482 | 7881 | 2226 | 2337 | 38 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DA    | 894     | HIS      | ASN    | conflict | UNP Q57UJ2 |
| DA    | 1181    | THR      | ILE    | conflict | UNP Q57UJ2 |
| DA    | 1333    | ALA      | VAL    | conflict | UNP Q57UJ2 |
| DA    | 1700    | ARG      | HIS    | conflict | UNP Q57UJ2 |
| DA    | 1761    | LYS      | ARG    | conflict | UNP Q57UJ2 |

- Molecule 2 is a protein called ms51.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | DD    | 791      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6523  | 4127 | 1184 | 1171 | 41 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DD    | 371     | PRO      | SER    | conflict | UNP Q385L8 |
| DD    | 599     | ALA      | VAL    | conflict | UNP Q385L8 |

- Molecule 3 is a protein called ms56.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | DI    | 390      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3182  | 2020 | 554 | 594 | 14 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DI    | 92      | GLU      | GLY    | conflict | UNP Q587C2 |
| DI    | 116     | ASP      | GLU    | conflict | UNP Q587C2 |

- Molecule 4 is a protein called ms59.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | DL    | 283      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2287  | 1451 | 423 | 401 | 12 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DL    | 274     | THR      | ALA    | conflict | UNP Q38BS2 |

- Molecule 5 is a protein called ms60.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | DM    | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2430  | 1533 | 459 | 426 | 12 |         |       |

- Molecule 6 is a protein called ms61.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | DN    | 257      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2091  | 1331 | 379 | 371 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DN    | 51      | GLY      | SER    | conflict | UNP Q38D60 |

- Molecule 7 is a protein called ms62.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | DO    | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1804  | 1127 | 327 | 340 | 10 |         |       |

- Molecule 8 is a protein called ms63.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | DP    | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1760  | 1132 | 312 | 307 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DP    | 3       | HIS      | ARG    | conflict | UNP Q38F25 |

- Molecule 9 is a protein called ms64.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | DQ    | 256      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2061  | 1293 | 389 | 370 | 9 |         |       |

- Molecule 10 is a protein called ms65.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | DR    | 251      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2025  | 1304 | 369 | 342 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DR    | 128     | PRO      | SER    | conflict | UNP C9ZPP1 |

- Molecule 11 is a protein called ms66.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | DS    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1904  | 1185 | 356 | 348 | 15 |         |       |

- Molecule 12 is a protein called ms68.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | DU    | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1754  | 1103 | 310 | 335 | 6 |         |       |

- Molecule 13 is a protein called ms73.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | DZ    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 697   | 457 | 113 | 123 | 4 |         |       |

- Molecule 14 is a protein called ms74.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 14  | Da    | 55       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 501   | 315 | 109 | 74 | 3 |         |       |

- Molecule 15 is a protein called ms49.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 15  | DB    | 1111     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9148  | 5691 | 1717 | 1711 | 29 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DB    | 359     | ILE      | THR    | conflict | UNP C9ZJE4 |

- Molecule 16 is a protein called ms50.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 16  | DC    | 1095     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8748  | 5519 | 1544 | 1654 | 31 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DC    | 373     | GLY      | GLU    | conflict | UNP C9ZSK8 |
| DC    | 671     | ARG      | CYS    | conflict | UNP C9ZSK8 |
| DC    | 696     | VAL      | ALA    | conflict | UNP C9ZSK8 |

- Molecule 17 is a protein called mS52.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | DE    | 590      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3075 | 874 | 863 | 19 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DE    | 378     | UNK      | LYS    | conflict | UNP Q386Q7 |
| DE    | 384     | UNK      | THR    | conflict | UNP Q386Q7 |
| DE    | ?       | -        | SER    | deletion | UNP Q386Q7 |

- Molecule 18 is a protein called ms53.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | DF    | 590      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4747  | 2979 | 896 | 847 | 25 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DF    | 18      | THR      | ALA    | conflict | UNP Q38ET1 |
| DF    | 258     | ASP      | ASN    | conflict | UNP Q38ET1 |
| DF    | 372     | ASN      | ASP    | conflict | UNP Q38ET1 |
| DF    | 406     | ASN      | SER    | conflict | UNP Q38ET1 |
| DF    | 510     | ASP      | GLY    | conflict | UNP Q38ET1 |
| DF    | 577     | ALA      | VAL    | conflict | UNP Q38ET1 |
| DF    | 636     | UNK      | GLY    | conflict | UNP Q38ET1 |
| DF    | 638     | LYS      | ARG    | conflict | UNP Q38ET1 |

- Molecule 19 is a protein called ms54.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | DG    | 566      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4575  | 2875 | 835 | 834 | 31 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DG    | 428     | ASN      | SER    | conflict | UNP Q57ZP8 |
| DG    | 429     | GLY      | SER    | conflict | UNP Q57ZP8 |

- Molecule 20 is a protein called ms55.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | DH    | 564      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4578  | 2872 | 850 | 834 | 22 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DH    | 191     | HIS      | GLN    | conflict | UNP Q580V1 |
| DH    | 194     | PRO      | ARG    | conflict | UNP Q580V1 |
| DH    | 488     | GLY      | SER    | conflict | UNP Q580V1 |

- Molecule 21 is a protein called ms57.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | DJ    | 315      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2572  | 1646 | 452 | 460 | 14 |         |       |

- Molecule 22 is a protein called ms58.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | DK    | 255      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2007  | 1260 | 365 | 377 | 5 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DK    | 61      | SER      | PRO    | conflict | UNP Q38BP1 |
| DK    | 257     | GLY      | SER    | conflict | UNP Q38BP1 |

- Molecule 23 is a protein called ms67.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | DT    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2058  | 1321 | 364 | 362 | 11 |         |       |

- Molecule 24 is a protein called ms69.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | DV    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 855 | 252 | 235 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DV    | 163     | ALA      | THR    | conflict | UNP Q57UZ6 |

- Molecule 25 is a protein called ms70.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | DW    | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1359  | 866 | 260 | 228 | 5 |         |       |

- Molecule 26 is a protein called ms71.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | DX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1196  | 762 | 226 | 201 | 7 |         |       |

- Molecule 27 is a protein called ms72.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | DY    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1293  | 827 | 245 | 216 | 5 |         |       |

- Molecule 28 is a protein called uS3m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | CC    | 74       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 646   | 451 | 96 | 98 | 1 |         |       |

There are 38 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CC    | 4       | MET      | -      | initiating methionine | UNP E0A3K1 |
| CC    | 5       | PHE      | -      | expression tag        | UNP E0A3K1 |
| CC    | 6       | LEU      | -      | expression tag        | UNP E0A3K1 |
| CC    | 7       | ILE      | -      | expression tag        | UNP E0A3K1 |
| CC    | 8       | HIS      | -      | expression tag        | UNP E0A3K1 |
| CC    | 9       | PHE      | -      | expression tag        | UNP E0A3K1 |
| CC    | 10      | VAL      | -      | expression tag        | UNP E0A3K1 |
| CC    | 11      | HIS      | -      | expression tag        | UNP E0A3K1 |
| CC    | 12      | TYR      | -      | expression tag        | UNP E0A3K1 |
| CC    | 13      | LYS      | -      | expression tag        | UNP E0A3K1 |
| CC    | 14      | THR      | -      | expression tag        | UNP E0A3K1 |
| CC    | 15      | ILE      | -      | expression tag        | UNP E0A3K1 |
| CC    | 16      | LEU      | -      | expression tag        | UNP E0A3K1 |
| CC    | 17      | GLN      | -      | expression tag        | UNP E0A3K1 |
| CC    | 18      | LYS      | -      | expression tag        | UNP E0A3K1 |
| CC    | 20      | THR      | LYS    | conflict              | UNP E0A3K1 |
| CC    | 21      | PHE      | ILE    | conflict              | UNP E0A3K1 |
| CC    | 24      | LYS      | ILE    | conflict              | UNP E0A3K1 |
| CC    | 25      | HIS      | PHE    | conflict              | UNP E0A3K1 |
| CC    | 26      | ILE      | ASN    | conflict              | UNP E0A3K1 |
| CC    | 27      | PHE      | LEU    | conflict              | UNP E0A3K1 |
| CC    | 28      | LEU      | TYR    | conflict              | UNP E0A3K1 |
| CC    | 29      | SER      | CYS    | conflict              | UNP E0A3K1 |
| CC    | 32      | LYS      | ASN    | conflict              | UNP E0A3K1 |
| CC    | 36      | LEU      | ILE    | conflict              | UNP E0A3K1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| CC    | 37      | PHE      | TYR    | conflict       | UNP E0A3K1 |
| CC    | 40      | ILE      | LEU    | conflict       | UNP E0A3K1 |
| CC    | 41      | SER      | ASN    | conflict       | UNP E0A3K1 |
| CC    | 45      | ILE      | LEU    | conflict       | UNP E0A3K1 |
| CC    | 50      | ILE      | LEU    | conflict       | UNP E0A3K1 |
| CC    | 57      | ILE      | VAL    | conflict       | UNP E0A3K1 |
| CC    | 62      | PHE      | LEU    | conflict       | UNP E0A3K1 |
| CC    | 65      | ILE      | LEU    | conflict       | UNP E0A3K1 |
| CC    | 68      | PHE      | LEU    | conflict       | UNP E0A3K1 |
| CC    | 74      | LEU      | -      | expression tag | UNP E0A3K1 |
| CC    | 75      | ILE      | -      | expression tag | UNP E0A3K1 |
| CC    | 76      | SER      | -      | expression tag | UNP E0A3K1 |
| CC    | 77      | THR      | -      | expression tag | UNP E0A3K1 |

- Molecule 29 is a protein called uS55m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | CE    | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3399  | 2151 | 632 | 600 | 16 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CE    | 341     | ARG      | LYS    | conflict | UNP Q38AX6 |

- Molecule 30 is a protein called bS6m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | CF    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1292  | 821 | 228 | 237 | 6 |         |       |

- Molecule 31 is a protein called uS8m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 31  | CH    | 273      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2228  | 1387 | 432 | 398 | 11 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CH    | 74      | ASN      | SER    | conflict | UNP Q388R7 |

- Molecule 32 is a protein called uS9m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32  | CI    | 424      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3386  | 2136 | 611 | 622 | 17 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CI    | 370     | ALA      | VAL    | conflict | UNP Q57W62 |

- Molecule 33 is a protein called uS10m.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 33  | CJ    | 800      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6516  | 4119 | 1151 | 1216 | 30 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CJ    | 311     | LEU      | TYR    | conflict | UNP Q57Z45 |
| CJ    | 484     | HIS      | ARG    | conflict | UNP Q57Z45 |
| CJ    | 488     | SER      | ASN    | conflict | UNP Q57Z45 |
| CJ    | 594     | GLU      | VAL    | conflict | UNP Q57Z45 |
| CJ    | 629     | ARG      | LYS    | conflict | UNP Q57Z45 |

- Molecule 34 is a protein called uS11m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | CK    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2418  | 1506 | 458 | 437 | 17 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CK    | 3       | ARG      | GLN    | conflict | UNP Q389T7 |
| CK    | 138     | UNK      | ILE    | conflict | UNP Q389T7 |

- Molecule 35 is a protein called uS12.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 35  | CL    | 87       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 733   | 503 | 113 | 107 | 10 |         |       |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| CL    | 54      | LEU      | -      | expression tag | UNP A0A0E3J9R6 |
| CL    | 55      | PHE      | -      | expression tag | UNP A0A0E3J9R6 |
| CL    | 56      | PHE      | -      | expression tag | UNP A0A0E3J9R6 |
| CL    | 57      | LEU      | -      | expression tag | UNP A0A0E3J9R6 |
| CL    | 58      | ARG      | -      | expression tag | UNP A0A0E3J9R6 |
| CL    | 103     | MET      | LEU    | conflict       | UNP A0A0E3J9R6 |
| CL    | ?       | -        | VAL    | deletion       | UNP A0A0E3J9R6 |
| CL    | 112     | ILE      | PHE    | conflict       | UNP A0A0E3J9R6 |
| CL    | 115     | VAL      | HIS    | conflict       | UNP A0A0E3J9R6 |
| CL    | 116     | MET      | LEU    | conflict       | UNP A0A0E3J9R6 |
| CL    | 132     | VAL      | ILE    | conflict       | UNP A0A0E3J9R6 |
| CL    | 138     | ILE      | MET    | conflict       | UNP A0A0E3J9R6 |
| CL    | 139     | VAL      | -      | expression tag | UNP A0A0E3J9R6 |
| CL    | 140     | SER      | -      | expression tag | UNP A0A0E3J9R6 |

- Molecule 36 is a protein called uS14m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | CN    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1322  | 843 | 251 | 220 | 8 |         |       |

- Molecule 37 is a protein called uS15m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | CO    | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3003  | 1907 | 560 | 520 | 16 |         |       |

- Molecule 38 is a protein called bS16m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | CP    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1489  | 956 | 274 | 250 | 9 |         |       |

- Molecule 39 is a protein called uS17m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | CQ    | 190      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1584  | 1015 | 302 | 259 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CQ    | 138     | ALA      | VAL    | conflict | UNP Q38DP8 |

- Molecule 40 is a protein called bS18m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | CR    | 314      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2567  | 1623 | 471 | 465 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CR    | 8       | ILE      | VAL    | conflict | UNP Q38AS2 |

- Molecule 41 is a protein called uS19m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | CS    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1175  | 761 | 210 | 198 | 6 |         |       |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CS    | -71     | MET      | -      | initiating methionine | UNP Q584T8 |
| CS    | -70     | ALA      | -      | expression tag        | UNP Q584T8 |
| CS    | -69     | PHE      | -      | expression tag        | UNP Q584T8 |
| CS    | -68     | ARG      | -      | expression tag        | UNP Q584T8 |
| CS    | -67     | ASN      | -      | expression tag        | UNP Q584T8 |
| CS    | -66     | THR      | -      | expression tag        | UNP Q584T8 |
| CS    | -65     | PHE      | -      | expression tag        | UNP Q584T8 |
| CS    | -64     | THR      | -      | expression tag        | UNP Q584T8 |
| CS    | -63     | THR      | -      | expression tag        | UNP Q584T8 |
| CS    | -62     | PRO      | -      | expression tag        | UNP Q584T8 |
| CS    | -61     | GLY      | -      | expression tag        | UNP Q584T8 |
| CS    | -60     | LYS      | -      | expression tag        | UNP Q584T8 |
| CS    | -59     | PHE      | -      | expression tag        | UNP Q584T8 |
| CS    | -58     | SER      | -      | expression tag        | UNP Q584T8 |
| CS    | -57     | THR      | -      | expression tag        | UNP Q584T8 |
| CS    | -56     | VAL      | -      | expression tag        | UNP Q584T8 |
| CS    | -55     | SER      | -      | expression tag        | UNP Q584T8 |
| CS    | -54     | LYS      | -      | expression tag        | UNP Q584T8 |
| CS    | -53     | ASN      | -      | expression tag        | UNP Q584T8 |
| CS    | -52     | ILE      | -      | expression tag        | UNP Q584T8 |
| CS    | -51     | VAL      | -      | expression tag        | UNP Q584T8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| CS    | -50     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -49     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -48     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -47     | ILE      | -      | expression tag | UNP Q584T8 |
| CS    | -46     | TRP      | -      | expression tag | UNP Q584T8 |
| CS    | -45     | ARG      | -      | expression tag | UNP Q584T8 |
| CS    | -44     | VAL      | -      | expression tag | UNP Q584T8 |
| CS    | -43     | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | -42     | VAL      | -      | expression tag | UNP Q584T8 |
| CS    | -41     | PHE      | -      | expression tag | UNP Q584T8 |
| CS    | -40     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -39     | ARG      | -      | expression tag | UNP Q584T8 |
| CS    | -38     | ALA      | -      | expression tag | UNP Q584T8 |
| CS    | -37     | GLU      | -      | expression tag | UNP Q584T8 |
| CS    | -36     | GLY      | -      | expression tag | UNP Q584T8 |
| CS    | -35     | PHE      | -      | expression tag | UNP Q584T8 |
| CS    | -34     | ALA      | -      | expression tag | UNP Q584T8 |
| CS    | -33     | HIS      | -      | expression tag | UNP Q584T8 |
| CS    | -32     | SER      | -      | expression tag | UNP Q584T8 |
| CS    | -31     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -30     | VAL      | -      | expression tag | UNP Q584T8 |
| CS    | -29     | MET      | -      | expression tag | UNP Q584T8 |
| CS    | -28     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -27     | PRO      | -      | expression tag | UNP Q584T8 |
| CS    | -26     | VAL      | -      | expression tag | UNP Q584T8 |
| CS    | -25     | SER      | -      | expression tag | UNP Q584T8 |
| CS    | -24     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -23     | TYR      | -      | expression tag | UNP Q584T8 |
| CS    | -22     | SER      | -      | expression tag | UNP Q584T8 |
| CS    | -21     | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | -20     | ILE      | -      | expression tag | UNP Q584T8 |
| CS    | -19     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -18     | LEU      | -      | expression tag | UNP Q584T8 |
| CS    | -17     | CYS      | -      | expression tag | UNP Q584T8 |
| CS    | -16     | ASP      | -      | expression tag | UNP Q584T8 |
| CS    | -15     | VAL      | -      | expression tag | UNP Q584T8 |
| CS    | -14     | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | -13     | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | -12     | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | -11     | ILE      | -      | expression tag | UNP Q584T8 |
| CS    | -10     | VAL      | -      | expression tag | UNP Q584T8 |
| CS    | -9      | TYR      | -      | expression tag | UNP Q584T8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| CS    | -8      | PHE      | -      | expression tag | UNP Q584T8 |
| CS    | -7      | HIS      | -      | expression tag | UNP Q584T8 |
| CS    | -6      | CYS      | -      | expression tag | UNP Q584T8 |
| CS    | -5      | CYS      | -      | expression tag | UNP Q584T8 |
| CS    | -4      | THR      | -      | expression tag | UNP Q584T8 |
| CS    | -3      | ARG      | -      | expression tag | UNP Q584T8 |
| CS    | -2      | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | -1      | LYS      | -      | expression tag | UNP Q584T8 |
| CS    | 0       | SER      | -      | expression tag | UNP Q584T8 |

- Molecule 42 is a protein called bS12m.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 42  | CU    | 184      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1538  | 965 | 307 | 254 | 12 |         |       |

- Molecule 43 is a protein called mt-IF-3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | CZ    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1212  | 759 | 231 | 215 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CZ    | 30      | THR      | ILE    | conflict | UNP C9ZRZ4 |

- Molecule 44 is a protein called mS22.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | Ca    | 592      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5004  | 3201 | 898 | 882 | 23 |         |       |

- Molecule 45 is a protein called mS23.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45  | Cb    | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2056  | 1300 | 368 | 380 | 8 |         |       |

There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| Cb    | 244     | SER      | ASN    | conflict       | UNP Q57VB2 |
| Cb    | ?       | -        | GLU    | deletion       | UNP Q57VB2 |
| Cb    | 312     | CYS      | -      | expression tag | UNP Q57VB2 |
| Cb    | 313     | SER      | -      | expression tag | UNP Q57VB2 |
| Cb    | 314     | ARG      | -      | expression tag | UNP Q57VB2 |
| Cb    | 315     | ASP      | -      | expression tag | UNP Q57VB2 |
| Cb    | 316     | GLY      | -      | expression tag | UNP Q57VB2 |
| Cb    | 317     | PHE      | -      | expression tag | UNP Q57VB2 |
| Cb    | 318     | ALA      | -      | expression tag | UNP Q57VB2 |
| Cb    | 319     | LEU      | -      | expression tag | UNP Q57VB2 |
| Cb    | 320     | MET      | -      | expression tag | UNP Q57VB2 |
| Cb    | 321     | LYS      | -      | expression tag | UNP Q57VB2 |
| Cb    | 322     | ALA      | -      | expression tag | UNP Q57VB2 |
| Cb    | 323     | ASN      | -      | expression tag | UNP Q57VB2 |
| Cb    | 324     | LYS      | -      | expression tag | UNP Q57VB2 |

- Molecule 46 is a protein called mS26.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | Cd    | 291      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2389  | 1491 | 442 | 446 | 10 |         |       |

- Molecule 47 is a protein called mS29.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | Cg    | 482      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3904  | 2499 | 684 | 701 | 20 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| Cg    | 181     | VAL      | ALA    | conflict       | UNP Q585C2 |
| Cg    | 498     | ARG      | -      | expression tag | UNP Q585C2 |

- Molecule 48 is a protein called mS33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Ci    | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1348  | 848 | 247 | 244 | 9 |         |       |

- Molecule 49 is a protein called mS34.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | Cj    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1792  | 1138 | 310 | 340 | 4 |         |       |

- Molecule 50 is a protein called mS35.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 50  | Ck    | 703      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5596  | 3503 | 1017 | 1050 | 26 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Ck    | 107     | SER      | LEU    | conflict | UNP Q387C7 |
| Ck    | 144     | PHE      | LEU    | conflict | UNP Q387C7 |
| Ck    | 253     | TYR      | PHE    | conflict | UNP Q387C7 |
| Ck    | 339     | GLU      | VAL    | conflict | UNP Q387C7 |
| Ck    | 871     | GLY      | GLU    | conflict | UNP Q387C7 |

- Molecule 51 is a protein called mS37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | Cm    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1577  | 975 | 304 | 289 | 9 |         |       |

- Molecule 52 is a protein called mS38.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Cn    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 912   | 585 | 181 | 143 | 3 |         |       |

- Molecule 53 is a protein called ms34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | Cp    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1483  | 937 | 268 | 273 | 5 |         |       |

- Molecule 54 is a protein called ms42.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | Cq    | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2005  | 1285 | 342 | 369 | 9 |         |       |



- Molecule 55 is a protein called mS43.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | Cr    | 257      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1999  | 1261 | 368 | 356 | 14 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Cr    | 351     | LYS      | GLU    | conflict | UNP Q585I1 |

- Molecule 56 is a protein called mS47.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 56  | Cv    | 1059     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8557  | 5387 | 1535 | 1596 | 39 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Cv    | 16      | CYS      | PRO    | conflict | UNP Q383R4 |
| Cv    | 718     | THR      | ALA    | conflict | UNP Q383R4 |
| Cv    | 1179    | GLU      | GLY    | conflict | UNP Q383R4 |

- Molecule 57 is a RNA chain called 9s rRNA.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 57  | CA    | 621      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 13122 | 5906 | 2227 | 4368 | 621 |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference |
|-------|---------|----------|--------|----------------|-----------|
| CA    | 298     | U        | C      | conflict       | GB 343546 |
| CA    | 473     | U        | G      | conflict       | GB 343546 |
| CA    | 614     | U        | -      | expression tag | GB 343546 |
| CA    | 615     | U        | -      | expression tag | GB 343546 |
| CA    | 616     | U        | -      | expression tag | GB 343546 |
| CA    | 617     | U        | -      | expression tag | GB 343546 |
| CA    | 618     | U        | -      | expression tag | GB 343546 |
| CA    | 619     | U        | -      | expression tag | GB 343546 |
| CA    | 620     | U        | -      | expression tag | GB 343546 |
| CA    | 621     | U        | -      | expression tag | GB 343546 |

- Molecule 58 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |   |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 58  | UO    | 5        | Total | C  | N | O | 0       | 0     |
|     |       |          | 30    | 20 | 5 | 5 |         |       |

- Molecule 59 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |   |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 59  | UP    | 7        | Total | C  | N | O | 0       | 0     |
|     |       |          | 42    | 28 | 7 | 7 |         |       |
| 59  | UW    | 7        | Total | C  | N | O | 0       | 0     |
|     |       |          | 42    | 28 | 7 | 7 |         |       |

- Molecule 60 is a protein called UNK.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 60  | UQ    | 32       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 192   | 128 | 32 | 32 |         |       |

- Molecule 61 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |   |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 61  | UR    | 8        | Total | C  | N | O | 0       | 0     |
|     |       |          | 48    | 32 | 8 | 8 |         |       |
| 61  | UV    | 8        | Total | C  | N | O | 0       | 0     |
|     |       |          | 48    | 32 | 8 | 8 |         |       |
| 61  | UX    | 8        | Total | C  | N | O | 0       | 0     |
|     |       |          | 48    | 32 | 8 | 8 |         |       |

- Molecule 62 is a protein called UNK.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 62  | US    | 54       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 324   | 216 | 54 | 54 |         |       |

- Molecule 63 is a protein called UNK.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 63  | UT    | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 264   | 176 | 44 | 44 |         |       |

- Molecule 64 is a protein called bL27m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | A0    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1269  | 801 | 236 | 227 | 5 |         |       |

- Molecule 65 is a protein called bL28m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | A1    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1788  | 1138 | 324 | 317 | 9 |         |       |

- Molecule 66 is a protein called uL29m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 66  | A2    | 449      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3638  | 2324 | 631 | 670 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A2    | 238     | GLY      | ALA    | conflict | UNP Q38EM7 |

- Molecule 67 is a protein called uL30m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | A3    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1215  | 776 | 234 | 199 | 6 |         |       |

- Molecule 68 is a protein called bL31m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | A4    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1387  | 880 | 262 | 240 | 5 |         |       |

- Molecule 69 is a protein called bL32m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 69  | A5    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 483   | 311 | 90 | 76 | 6 |         |       |

- Molecule 70 is a protein called bL33m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | A6    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 568   | 361 | 102 | 101 | 4 |         |       |

- Molecule 71 is a protein called bL35m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | A8    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 753 | 243 | 198 | 9 |         |       |

- Molecule 72 is a protein called bL36m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 72  | A9    | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 288 | 85 | 78 | 8 |         |       |

- Molecule 73 is a protein called uL3m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 73  | AE    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1543 | 395 | 440 | 12 |         |       |

- Molecule 74 is a protein called uL4m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 74  | AF    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3597  | 2294 | 624 | 654 | 25 |         |       |

- Molecule 75 is a protein called bL9m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 75  | AI    | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1790  | 1153 | 316 | 312 | 9 |         |       |

- Molecule 76 is a protein called uL10m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | AJ    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 965   | 606 | 191 | 165 | 3 |         |       |

- Molecule 77 is a protein called uL11m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 77  | AK    | 323      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2676  | 1703 | 485 | 469 | 19 |         |       |

- Molecule 78 is a protein called 50S ribosomal protein L13, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | AN    | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 973 | 275 | 251 | 9 |         |       |

- Molecule 79 is a protein called uL15m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 79  | AP    | 352      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2904  | 1846 | 538 | 507 | 13 |         |       |

- Molecule 80 is a protein called 50S ribosomal protein L16, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | AQ    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1020  | 658 | 183 | 175 | 4 |         |       |

- Molecule 81 is a protein called 50S ribosomal protein L17, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 81  | AR    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1912  | 1211 | 356 | 332 | 13 |         |       |

- Molecule 82 is a protein called bL19m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 82  | AT    | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 287   | 180 | 61 | 45 | 1 |         |       |

- Molecule 83 is a protein called bL20m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | AU    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 895 | 280 | 243 | 5 |         |       |

- Molecule 84 is a protein called bL21m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | AV    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1424  | 909 | 257 | 252 | 6 |         |       |

- Molecule 85 is a protein called uL22m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 85  | AW    | 276      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2235  | 1416 | 415 | 391 | 13 |         |       |

- Molecule 86 is a protein called uL23m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 86  | AX    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1416  | 913 | 253 | 245 | 5 |         |       |

- Molecule 87 is a protein called uL24m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 87  | AY    | 340      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1689 | 493 | 517 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AY    | 345     | GLU      | VAL    | conflict | UNP C9ZK52 |

- Molecule 88 is a protein called mL38.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 88  | Ab    | 453      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3545  | 2252 | 621 | 657 | 15 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Ab    | 290     | SER      | PHE    | conflict | UNP Q381T7 |
| Ab    | 299     | GLU      | LYS    | conflict | UNP Q381T7 |
| Ab    | 471     | ASN      | ILE    | conflict | UNP Q381T7 |

- Molecule 89 is a protein called mL40.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 89  | Ad    | 257      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2122  | 1319 | 386 | 405 | 12 |         |       |

- Molecule 90 is a protein called mL41.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 90  | Ae    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 927   | 594 | 170 | 158 | 5 |         |       |

- Molecule 91 is a protein called mL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 91  | Af    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 630 | 196 | 183 | 4 |         |       |

- Molecule 92 is a protein called mL43.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 92  | Ag    | 259      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2193  | 1368 | 422 | 392 | 11 |         |       |

- Molecule 93 is a protein called mL46.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 93  | Aj    | 279      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2246  | 1408 | 414 | 416 | 8 |         |       |

- Molecule 94 is a protein called mL49.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 94  | Al    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1618  | 1051 | 281 | 279 | 7 |         |       |

- Molecule 95 is a protein called mL52.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 95  | Ao    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1475  | 936 | 272 | 264 | 3 |         |       |

- Molecule 96 is a protein called mL53.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 96  | Ap    | 261      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2143  | 1391 | 372 | 368 | 12 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Ap    | 2       | LEU      | SER    | conflict | UNP Q57YA9 |

- Molecule 97 is a protein called mL63.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 97  | At    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1100  | 690 | 210 | 196 | 4 |         |       |

- Molecule 98 is a protein called mL68.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 98  | Av    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1792  | 1138 | 333 | 308 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Av    | 164     | ARG      | GLN    | conflict | UNP Q383B7 |

- Molecule 99 is a protein called bL12m.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 99  | AB    | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 280   | 168 | 56 | 56 |         |       |

- Molecule 100 is a protein called bL12m.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 100 | AC    | 28       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 140   | 84 | 28 | 28 |         |       |
| 100 | AD    | 28       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 140   | 84 | 28 | 28 |         |       |

- Molecule 101 is a protein called bL12m.



| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 101 | AG    | 27       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 135   | 81 | 27 | 27 |         |       |

- Molecule 102 is a RNA chain called 12S rRNA.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 102 | AA    | 591      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 12491 | 5628 | 2125 | 4147 | 591 |         |       |

There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference |
|-------|---------|----------|--------|----------|-----------|
| AA    | 448     | A        | U      | conflict | GB 343546 |
| AA    | 454     | U        | G      | conflict | GB 343546 |
| AA    | 455     | U        | G      | conflict | GB 343546 |
| AA    | 622     | A        | U      | conflict | GB 343546 |
| AA    | 636     | A        | G      | conflict | GB 343546 |
| AA    | 702     | G        | A      | conflict | GB 343546 |
| AA    | 706     | C        | U      | conflict | GB 343546 |
| AA    | 743     | C        | G      | conflict | GB 343546 |
| AA    | 752     | G        | A      | conflict | GB 343546 |
| AA    | 757     | U        | A      | conflict | GB 343546 |
| AA    | 760     | U        | G      | conflict | GB 343546 |
| AA    | 762     | U        | G      | conflict | GB 343546 |
| AA    | 789     | G        | C      | conflict | GB 343546 |
| AA    | 793     | G        | U      | conflict | GB 343546 |
| AA    | 877     | A        | UNK    | conflict | GB 343546 |

- Molecule 103 is a protein called mL67.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 103 | BA    | 679      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5384  | 3422 | 948 | 981 | 33 |         |       |

- Molecule 104 is a protein called mL68.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 104 | BB    | 389      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3050  | 1883 | 535 | 619 | 13 |         |       |

There are 77 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BB    | 264     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 265     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 267     | SER      | HIS    | conflict | UNP Q38CI0 |
| BB    | 268     | SER      | GLY    | conflict | UNP Q38CI0 |
| BB    | 269     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 270     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 271     | SER      | THR    | conflict | UNP Q38CI0 |
| BB    | 272     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 273     | SER      | ASP    | conflict | UNP Q38CI0 |
| BB    | 274     | SER      | ASP    | conflict | UNP Q38CI0 |
| BB    | 275     | SER      | VAL    | conflict | UNP Q38CI0 |
| BB    | 276     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 277     | SER      | HIS    | conflict | UNP Q38CI0 |
| BB    | 278     | SER      | GLN    | conflict | UNP Q38CI0 |
| BB    | 279     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 280     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 281     | SER      | VAL    | conflict | UNP Q38CI0 |
| BB    | 282     | SER      | ARG    | conflict | UNP Q38CI0 |
| BB    | 283     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 284     | SER      | TYR    | conflict | UNP Q38CI0 |
| BB    | 285     | SER      | ARG    | conflict | UNP Q38CI0 |
| BB    | 286     | SER      | ASP    | conflict | UNP Q38CI0 |
| BB    | 287     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 288     | SER      | MET    | conflict | UNP Q38CI0 |
| BB    | 289     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 290     | SER      | LYS    | conflict | UNP Q38CI0 |
| BB    | 291     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 292     | SER      | ASP    | conflict | UNP Q38CI0 |
| BB    | 293     | SER      | MET    | conflict | UNP Q38CI0 |
| BB    | 294     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 295     | SER      | VAL    | conflict | UNP Q38CI0 |
| BB    | 296     | SER      | MET    | conflict | UNP Q38CI0 |
| BB    | 297     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 298     | SER      | GLY    | conflict | UNP Q38CI0 |
| BB    | 299     | SER      | ASN    | conflict | UNP Q38CI0 |
| BB    | 300     | SER      | GLY    | conflict | UNP Q38CI0 |
| BB    | 301     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 302     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 303     | SER      | ILE    | conflict | UNP Q38CI0 |
| BB    | 304     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 305     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 306     | SER      | MET    | conflict | UNP Q38CI0 |
| BB    | 307     | SER      | ASP    | conflict | UNP Q38CI0 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BB    | 308     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 309     | SER      | ARG    | conflict | UNP Q38CI0 |
| BB    | 310     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 311     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 312     | SER      | PHE    | conflict | UNP Q38CI0 |
| BB    | 313     | SER      | HIS    | conflict | UNP Q38CI0 |
| BB    | 314     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 316     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 317     | SER      | ASN    | conflict | UNP Q38CI0 |
| BB    | 318     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 319     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 320     | SER      | ARG    | conflict | UNP Q38CI0 |
| BB    | 321     | SER      | MET    | conflict | UNP Q38CI0 |
| BB    | 322     | SER      | LYS    | conflict | UNP Q38CI0 |
| BB    | 323     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 324     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 326     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 327     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 330     | SER      | TRP    | conflict | UNP Q38CI0 |
| BB    | 331     | SER      | ARG    | conflict | UNP Q38CI0 |
| BB    | 332     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 333     | SER      | VAL    | conflict | UNP Q38CI0 |
| BB    | 334     | SER      | ARG    | conflict | UNP Q38CI0 |
| BB    | 335     | SER      | GLY    | conflict | UNP Q38CI0 |
| BB    | 336     | SER      | MET    | conflict | UNP Q38CI0 |
| BB    | 337     | SER      | LEU    | conflict | UNP Q38CI0 |
| BB    | 338     | SER      | ALA    | conflict | UNP Q38CI0 |
| BB    | 339     | SER      | PRO    | conflict | UNP Q38CI0 |
| BB    | 340     | SER      | VAL    | conflict | UNP Q38CI0 |
| BB    | 341     | SER      | GLN    | conflict | UNP Q38CI0 |
| BB    | 342     | SER      | GLU    | conflict | UNP Q38CI0 |
| BB    | 343     | SER      | VAL    | conflict | UNP Q38CI0 |
| BB    | 361     | ALA      | VAL    | conflict | UNP Q38CI0 |
| BB    | 403     | THR      | ARG    | conflict | UNP Q38CI0 |

- Molecule 105 is a protein called mL69.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 105 | BC    | 478      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3821  | 2451 | 670 | 680 | 20 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BC    | 29      | PRO      | SER    | conflict | UNP Q584V5 |
| BC    | 42      | GLY      | SER    | conflict | UNP Q584V5 |

- Molecule 106 is a protein called mL70.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 106 | BD    | 417      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2063  | 1229 | 417 | 417 |         |       |

There are 56 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BD    | 47      | CYS      | LEU    | conflict | UNP C9ZR91 |
| BD    | 49      | CYS      | LEU    | conflict | UNP C9ZR91 |
| BD    | 50      | LEU      | SER    | conflict | UNP C9ZR91 |
| BD    | 51      | TRP      | LEU    | conflict | UNP C9ZR91 |
| BD    | 52      | SER      | VAL    | conflict | UNP C9ZR91 |
| BD    | 53      | ILE      | HIS    | conflict | UNP C9ZR91 |
| BD    | 55      | LEU      | PRO    | conflict | UNP C9ZR91 |
| BD    | 56      | SER      | GLN    | conflict | UNP C9ZR91 |
| BD    | 57      | PHE      | LEU    | conflict | UNP C9ZR91 |
| BD    | 58      | ARG      | PRO    | conflict | UNP C9ZR91 |
| BD    | 59      | CYS      | VAL    | conflict | UNP C9ZR91 |
| BD    | 60      | PHE      | LEU    | conflict | UNP C9ZR91 |
| BD    | 61      | CYS      | LEU    | conflict | UNP C9ZR91 |
| BD    | 63      | ARG      | SER    | conflict | UNP C9ZR91 |
| BD    | 64      | SER      | PHE    | conflict | UNP C9ZR91 |
| BD    | 65      | TYR      | LEU    | conflict | UNP C9ZR91 |
| BD    | 66      | ALA      | CYS    | conflict | UNP C9ZR91 |
| BD    | 67      | ILE      | ASP    | conflict | UNP C9ZR91 |
| BD    | 68      | MET      | HIS    | conflict | UNP C9ZR91 |
| BD    | 69      | LEU      | ALA    | conflict | UNP C9ZR91 |
| BD    | ?       | -        | THR    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | THR    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | PHE    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | PHE    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | SER    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | ASP    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | ASN    | deletion | UNP C9ZR91 |
| BD    | ?       | -        | SER    | deletion | UNP C9ZR91 |
| BD    | 71      | LEU      | ASP    | conflict | UNP C9ZR91 |
| BD    | 73      | SER      | HIS    | conflict | UNP C9ZR91 |
| BD    | 76      | THR      | PHE    | conflict | UNP C9ZR91 |

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| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| BD    | 80      | SER      | ALA    | conflict  | UNP C9ZR91 |
| BD    | 81      | ILE      | ASN    | conflict  | UNP C9ZR91 |
| BD    | 82      | PHE      | TYR    | conflict  | UNP C9ZR91 |
| BD    | 83      | LEU      | TYR    | conflict  | UNP C9ZR91 |
| BD    | 84      | SER      | LEU    | conflict  | UNP C9ZR91 |
| BD    | 86      | LYS      | -      | insertion | UNP C9ZR91 |
| BD    | 87      | LEU      | -      | insertion | UNP C9ZR91 |
| BD    | 88      | PRO      | -      | insertion | UNP C9ZR91 |
| BD    | 89      | ILE      | -      | insertion | UNP C9ZR91 |
| BD    | 90      | THR      | -      | insertion | UNP C9ZR91 |
| BD    | 93      | LEU      | SER    | conflict  | UNP C9ZR91 |
| BD    | 95      | SER      | -      | insertion | UNP C9ZR91 |
| BD    | 96      | PRO      | PHE    | conflict  | UNP C9ZR91 |
| BD    | 99      | VAL      | CYS    | conflict  | UNP C9ZR91 |
| BD    | 100     | PHE      | VAL    | conflict  | UNP C9ZR91 |
| BD    | 101     | VAL      | CYS    | conflict  | UNP C9ZR91 |
| BD    | 102     | PHE      | LEU    | conflict  | UNP C9ZR91 |
| BD    | 103     | VAL      | ARG    | conflict  | UNP C9ZR91 |
| BD    | 104     | PHE      | TYR    | conflict  | UNP C9ZR91 |
| BD    | 105     | ALA      | SER    | conflict  | UNP C9ZR91 |
| BD    | 106     | ILE      | LEU    | conflict  | UNP C9ZR91 |
| BD    | 107     | ARG      | LEU    | conflict  | UNP C9ZR91 |
| BD    | 108     | TYR      | TRP    | conflict  | UNP C9ZR91 |
| BD    | 109     | CYS      | VAL    | conflict  | UNP C9ZR91 |
| BD    | 110     | GLY      | THR    | conflict  | UNP C9ZR91 |

- Molecule 107 is a protein called mL71.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 107 | BE    | 392      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3105  | 1970 | 540 | 582 | 13 |         |       |

- Molecule 108 is a protein called mL72.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 108 | BF    | 345      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2838  | 1797 | 517 | 511 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BF    | 296     | ILE      | THR    | conflict | UNP C9ZR63 |

- Molecule 109 is a protein called mL73.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 109 | BG    | 319      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2503  | 1578 | 449 | 459 | 17 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BG    | 185     | PHE      | LEU    | conflict | UNP Q57Y49 |

- Molecule 110 is a protein called mL74.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 110 | BH    | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1729  | 1110 | 301 | 315 | 3 |         |       |

- Molecule 111 is a protein called mL75.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 111 | BI    | 319      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2609  | 1664 | 473 | 456 | 16 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| BI    | 227     | ASN      | ASP    | conflict       | UNP Q38CK0 |
| BI    | 319     | ARG      | GLN    | conflict       | UNP Q38CK0 |
| BI    | 343     | ALA      | -      | expression tag | UNP Q38CK0 |

- Molecule 112 is a protein called mL76.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 112 | BJ    | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1339  | 832 | 262 | 239 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BJ    | 329     | GLU      | ALA    | conflict | UNP Q383M2 |

- Molecule 113 is a protein called mL77.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 113 | BK    | 258      | Total<br>1998 | C<br>1239 | N<br>383 | O<br>368 | S<br>8 | 0       | 0     |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BK    | 234     | SER      | GLU    | conflict | UNP C9ZQR6 |
| BK    | 235     | SER      | GLY    | conflict | UNP C9ZQR6 |
| BK    | 236     | SER      | ASP    | conflict | UNP C9ZQR6 |
| BK    | 237     | SER      | ASP    | conflict | UNP C9ZQR6 |
| BK    | 238     | SER      | GLY    | conflict | UNP C9ZQR6 |
| BK    | 240     | SER      | PRO    | conflict | UNP C9ZQR6 |
| BK    | 241     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 242     | SER      | GLY    | conflict | UNP C9ZQR6 |
| BK    | 243     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 244     | SER      | GLU    | conflict | UNP C9ZQR6 |
| BK    | 245     | SER      | GLU    | conflict | UNP C9ZQR6 |
| BK    | 247     | SER      | ILE    | conflict | UNP C9ZQR6 |
| BK    | 248     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 249     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 250     | SER      | VAL    | conflict | UNP C9ZQR6 |
| BK    | 251     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 252     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 253     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 254     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 255     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 256     | SER      | GLU    | conflict | UNP C9ZQR6 |
| BK    | 257     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 258     | SER      | PHE    | conflict | UNP C9ZQR6 |
| BK    | 259     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 260     | SER      | GLU    | conflict | UNP C9ZQR6 |
| BK    | 261     | SER      | LYS    | conflict | UNP C9ZQR6 |
| BK    | 262     | SER      | VAL    | conflict | UNP C9ZQR6 |
| BK    | 263     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 264     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 265     | SER      | GLN    | conflict | UNP C9ZQR6 |
| BK    | 266     | SER      | TYR    | conflict | UNP C9ZQR6 |
| BK    | 267     | SER      | GLY    | conflict | UNP C9ZQR6 |
| BK    | 268     | SER      | PRO    | conflict | UNP C9ZQR6 |
| BK    | 269     | SER      | GLY    | conflict | UNP C9ZQR6 |
| BK    | 270     | SER      | MET    | conflict | UNP C9ZQR6 |
| BK    | 271     | SER      | LEU    | conflict | UNP C9ZQR6 |
| BK    | 272     | SER      | ARG    | conflict | UNP C9ZQR6 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BK    | 273     | SER      | HIS    | conflict | UNP C9ZQR6 |
| BK    | 274     | SER      | ALA    | conflict | UNP C9ZQR6 |
| BK    | 275     | SER      | ARG    | conflict | UNP C9ZQR6 |
| BK    | 276     | SER      | VAL    | conflict | UNP C9ZQR6 |
| BK    | 277     | SER      | TYR    | conflict | UNP C9ZQR6 |
| BK    | 278     | SER      | THR    | conflict | UNP C9ZQR6 |
| BK    | 280     | SER      | LEU    | conflict | UNP C9ZQR6 |
| BK    | 348     | VAL      | LEU    | conflict | UNP C9ZQR6 |

- Molecule 114 is a protein called mL78.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 114 | BL    | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1887  | 1158 | 370 | 349 | 10 |         |       |

- Molecule 115 is a protein called mL79.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 115 | BM    | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2015  | 1280 | 370 | 356 | 9 |         |       |

- Molecule 116 is a protein called mL80.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 116 | BN    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1746  | 1079 | 320 | 342 | 5 |         |       |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BN    | 145     | SER      | ALA    | conflict | UNP Q585A3 |
| BN    | 146     | SER      | HIS    | conflict | UNP Q585A3 |
| BN    | 148     | SER      | GLY    | conflict | UNP Q585A3 |
| BN    | 149     | SER      | LEU    | conflict | UNP Q585A3 |
| BN    | 150     | SER      | ARG    | conflict | UNP Q585A3 |
| BN    | 151     | SER      | GLY    | conflict | UNP Q585A3 |
| BN    | 152     | SER      | ALA    | conflict | UNP Q585A3 |
| BN    | 153     | SER      | ALA    | conflict | UNP Q585A3 |
| BN    | 154     | SER      | ALA    | conflict | UNP Q585A3 |
| BN    | 155     | SER      | THR    | conflict | UNP Q585A3 |
| BN    | 156     | SER      | GLU    | conflict | UNP Q585A3 |
| BN    | 157     | SER      | THR    | conflict | UNP Q585A3 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BN    | 159     | SER      | THR    | conflict | UNP Q585A3 |
| BN    | 160     | SER      | TYR    | conflict | UNP Q585A3 |
| BN    | 161     | SER      | ALA    | conflict | UNP Q585A3 |
| BN    | 162     | SER      | GLU    | conflict | UNP Q585A3 |
| BN    | 163     | SER      | LYS    | conflict | UNP Q585A3 |
| BN    | 164     | SER      | PHE    | conflict | UNP Q585A3 |
| BN    | 165     | SER      | ARG    | conflict | UNP Q585A3 |
| BN    | 166     | SER      | GLU    | conflict | UNP Q585A3 |
| BN    | 167     | SER      | MET    | conflict | UNP Q585A3 |
| BN    | 168     | SER      | ASN    | conflict | UNP Q585A3 |
| BN    | 169     | SER      | VAL    | conflict | UNP Q585A3 |
| BN    | 170     | SER      | GLU    | conflict | UNP Q585A3 |
| BN    | 171     | SER      | ALA    | conflict | UNP Q585A3 |
| BN    | 172     | SER      | LYS    | conflict | UNP Q585A3 |
| BN    | 173     | SER      | GLU    | conflict | UNP Q585A3 |
| BN    | 174     | SER      | ALA    | conflict | UNP Q585A3 |

- Molecule 117 is a protein called mL81.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 117 | BO    | 147      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1146  | 719 | 202 | 213 | 12 |         |       |

- Molecule 118 is a protein called mL82.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 118 | BP    | 202      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1550  | 973 | 292 | 276 | 9 |         |       |

- Molecule 119 is a protein called mL83.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 119 | BQ    | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1675  | 1061 | 291 | 315 | 8 |         |       |

- Molecule 120 is a protein called mL84.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 120 | BR    | 195      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1059 | 298 | 284 | 9 |         |       |

- Molecule 121 is a protein called mL85.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 121 | BS    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 493 | 141 | 144 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BS    | 45      | ILE      | VAL    | conflict | UNP Q38FG8 |

- Molecule 122 is a protein called mL86.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 122 | BT    | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1389  | 853 | 270 | 260 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BT    | 70      | ARG      | GLN    | conflict | UNP C9ZPU8 |

- Molecule 123 is a protein called mL87.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 123 | BU    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 436 | 139 | 115 | 4 |         |       |

- Molecule 124 is a protein called mL88.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 124 | BV    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1307  | 832 | 233 | 236 | 6 |         |       |

- Molecule 125 is a protein called mL89.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 125 | BW    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1557  | 987 | 298 | 264 | 8 |         |       |

- Molecule 126 is a protein called mL90.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 126 | BX    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 867   | 552 | 160 | 147 | 8 |         |       |

- Molecule 127 is a protein called mS91.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 127 | BY    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 549 | 171 | 154 | 3 |         |       |

- Molecule 128 is a protein called mL92.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 128 | BZ    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1390  | 878 | 242 | 263 | 7 |         |       |

- Molecule 129 is a protein called mL93.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 129 | Ba    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1224  | 785 | 223 | 209 | 7 |         |       |

- Molecule 130 is a protein called mL94.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 130 | Bb    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 770   | 482 | 144 | 143 | 1 |         |       |

- Molecule 131 is a protein called mL95.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 131 | Bc    | 90       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 781   | 495 | 148 | 138 |         |       |

- Molecule 132 is a protein called mL96.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 132 | Bd    | 140      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1113  | 689 | 209 | 204 | 11 |         |       |

- Molecule 133 is a protein called mL97.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 133 | Be    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 822   | 517 | 152 | 144 | 9 |         |       |

- Molecule 134 is a protein called mL98.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 134 | Bf    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 434   | 279 | 80 | 75 |         |       |

- Molecule 135 is a protein called mL99.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 135 | Bg    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 656   | 412 | 126 | 116 | 2 |         |       |

- Molecule 136 is a protein called mL100.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 136 | Bh    | 91       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 730   | 466 | 129 | 125 | 10 |         |       |

- Molecule 137 is a protein called UNK.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 137 | UA    | 46       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 276   | 184 | 46 | 46 |         |       |

- Molecule 138 is a protein called UNK.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 138 | UB    | 40       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 240   | 160 | 40 | 40 |         |       |

- Molecule 139 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 139 | UC    | 12       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 72    | 48 | 12 | 12 |         |       |
| 139 | UH    | 12       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 72    | 48 | 12 | 12 |         |       |

- Molecule 140 is a protein called UNK.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 140 | UD    | 177      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1062  | 708 | 177 | 177 |         |       |

- Molecule 141 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 141 | UE    | 22       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 132   | 88 | 22 | 22 |         |       |

- Molecule 142 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 142 | UF    | 24       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 144   | 96 | 24 | 24 |         |       |
| 142 | UG    | 24       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 144   | 96 | 24 | 24 |         |       |
| 142 | UN    | 24       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 144   | 96 | 24 | 24 |         |       |

- Molecule 143 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 143 | UI    | 17       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 102   | 68 | 17 | 17 |         |       |

- Molecule 144 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 144 | UK    | 10       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 60    | 40 | 10 | 10 |         |       |

- Molecule 145 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 145 | UL    | 15       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 90    | 60 | 15 | 15 |         |       |

- Molecule 146 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |   |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 146 | UM    | 6        | Total | C  | N | O | 0       | 0     |
|     |       |          | 36    | 24 | 6 | 6 |         |       |

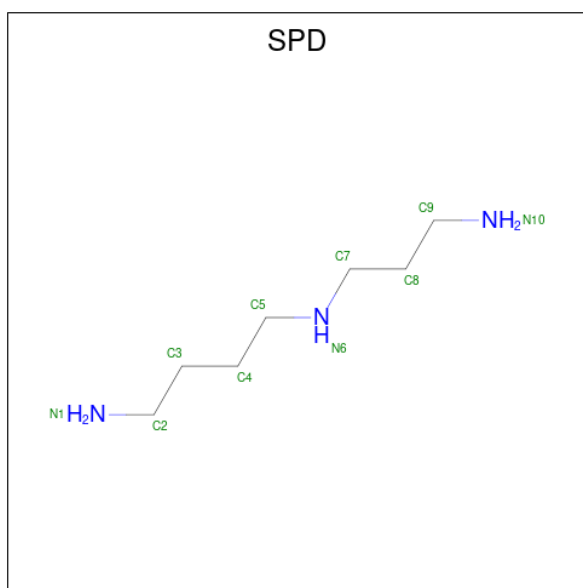
- Molecule 147 is a protein called UNK.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 147 | UU    | 11       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 66    | 44 | 11 | 11 |         |       |

- Molecule 148 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 148 | DA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 148 | DS    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 148 | Cr    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 148 | A5    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 148 | A9    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 148 | BX    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 148 | Be    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 148 | Bh    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 149 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



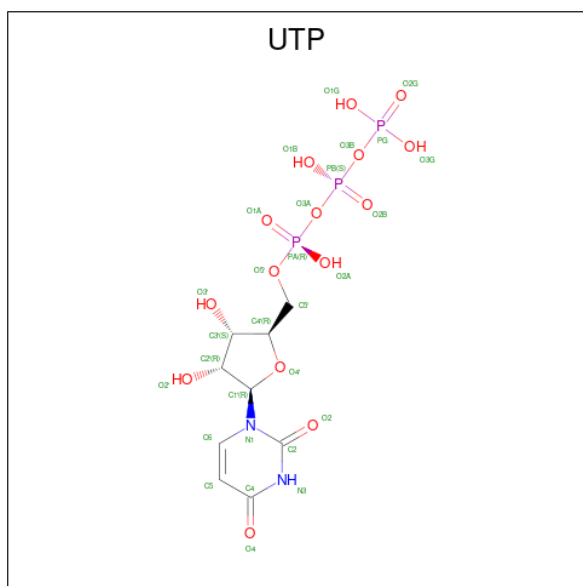
| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 149 | DL    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 149 | CA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 149 | CA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

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| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 149 | CA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 150 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).

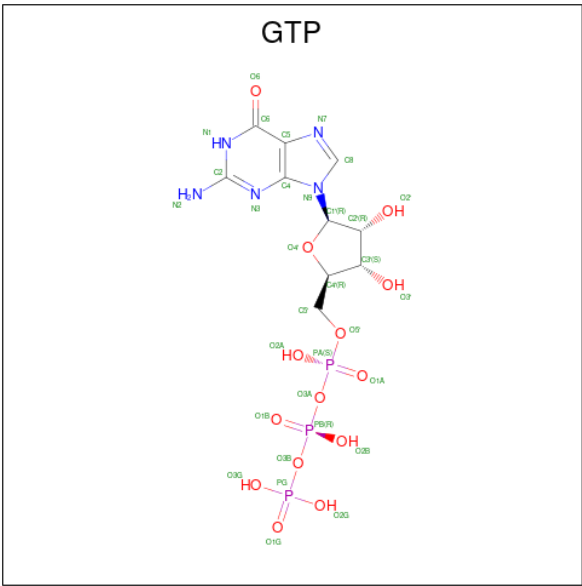


| Mol | Chain | Residues | Atoms |   |   |    |   | AltConf |
|-----|-------|----------|-------|---|---|----|---|---------|
| 150 | DJ    | 1        | Total | C | N | O  | P | 0       |
|     |       |          | 29    | 9 | 2 | 15 | 3 |         |

- Molecule 151 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

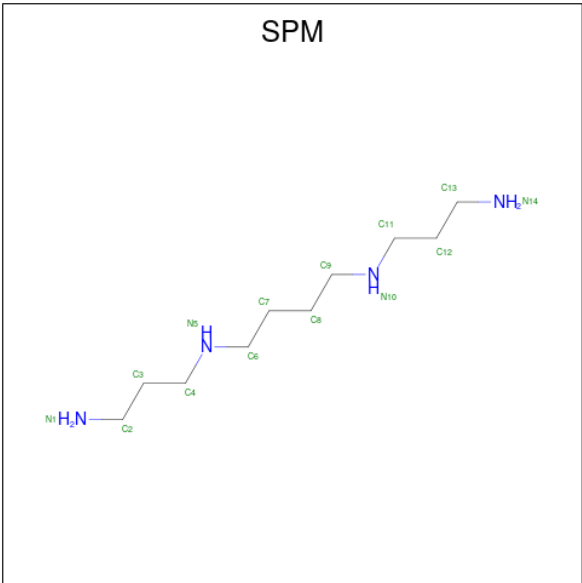
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 151 | CO    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 151 | CQ    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 151 | Ca    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 151 | Cg    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 151 | Cv    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 151 | CA    | 34       | Total | Mg | 0       |
|     |       |          | 34    | 34 |         |
| 151 | AA    | 7        | Total | Mg | 0       |
|     |       |          | 7     | 7  |         |

- Molecule 152 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 152 | Cg    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 153 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).

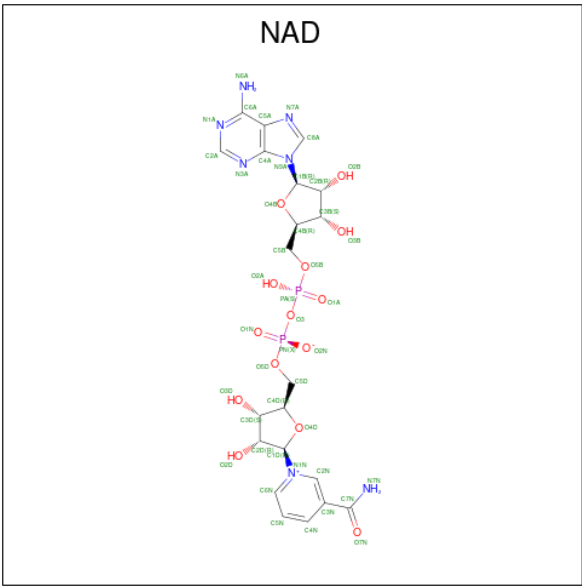


| Mol | Chain | Residues | Atoms |    |   |  | AltConf |
|-----|-------|----------|-------|----|---|--|---------|
| 153 | CA    | 1        | Total | C  | N |  | 0       |
|     |       |          | 14    | 10 | 4 |  |         |

- Molecule 154 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:

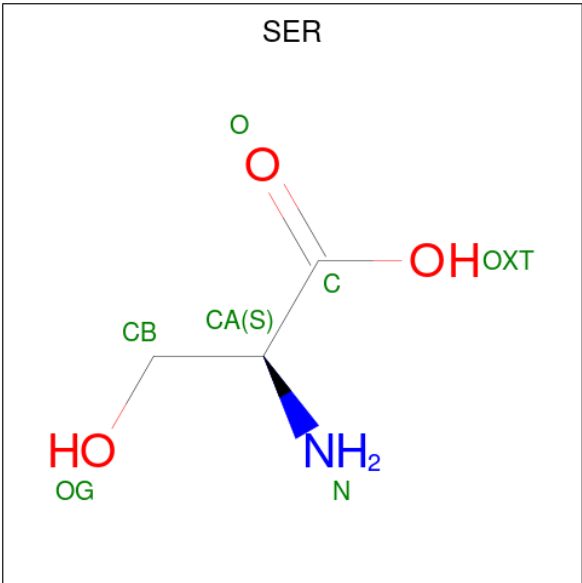


C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 154 | Av    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |

- Molecule 155 is SERINE (CCD ID: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 155 | UB    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

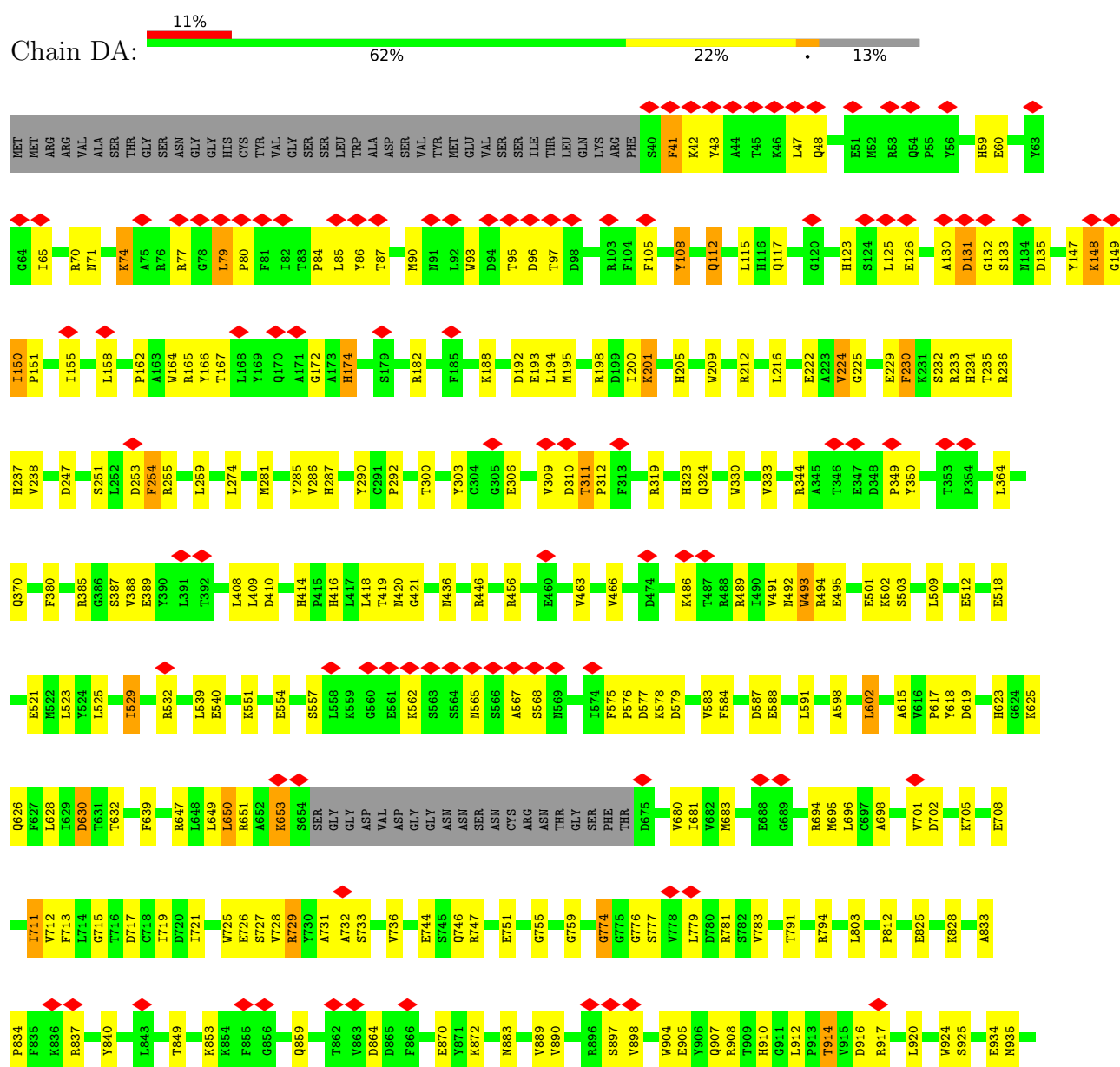
- Molecule 156 is water.

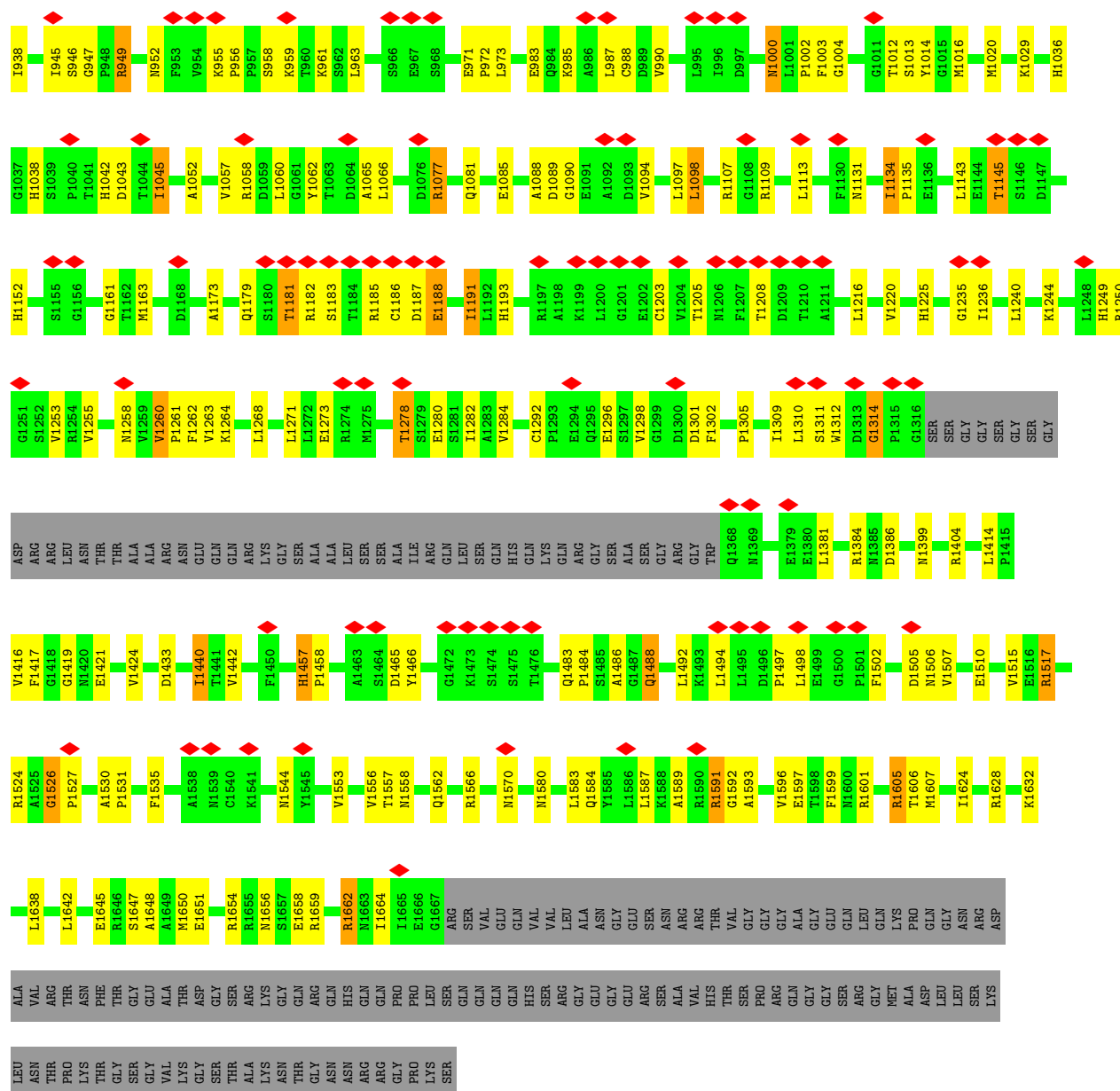
| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 156 | Cg    | 3        | Total<br>3 | O<br>3 | 0       |

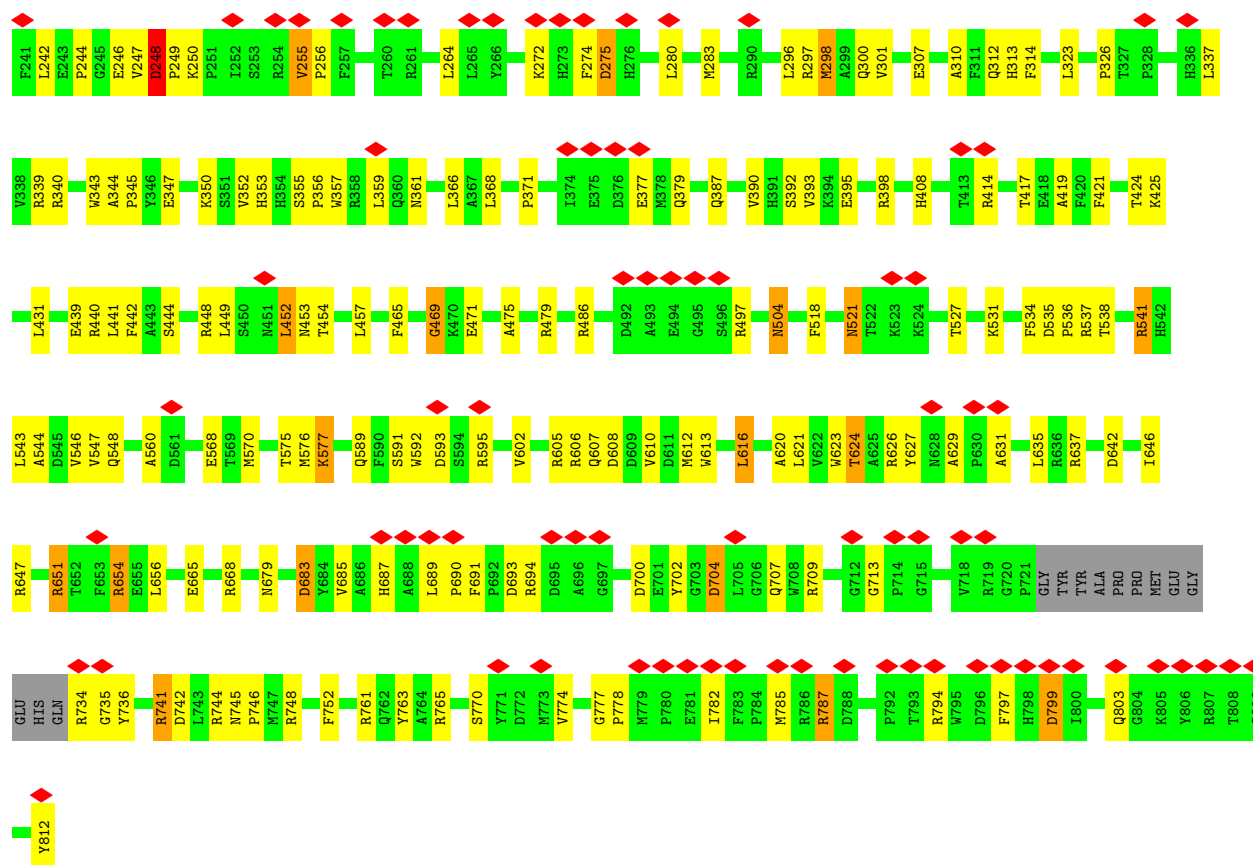
### 3 Residue-property plots

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

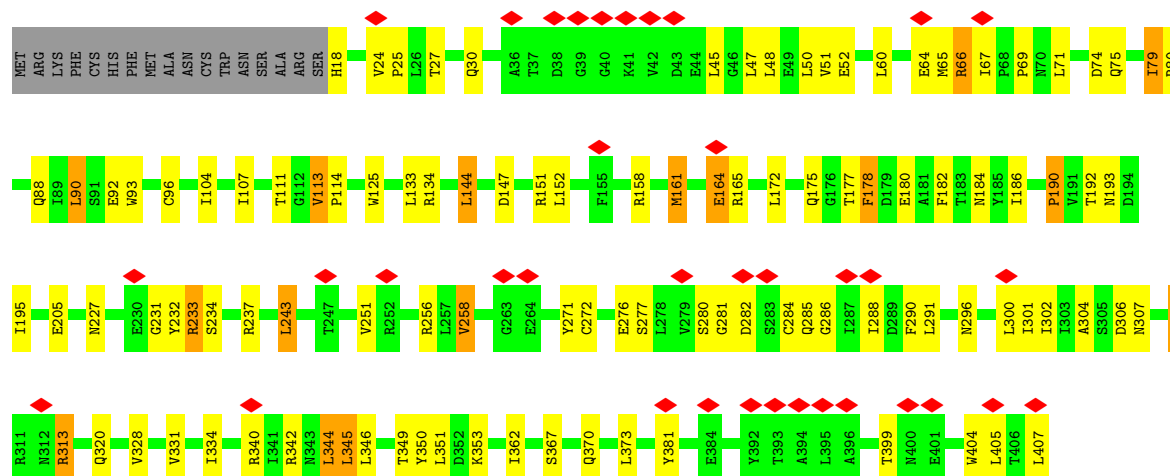
- Molecule 1: ms48



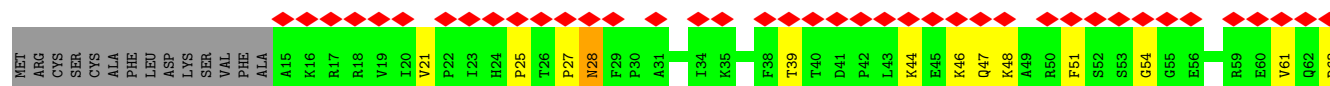


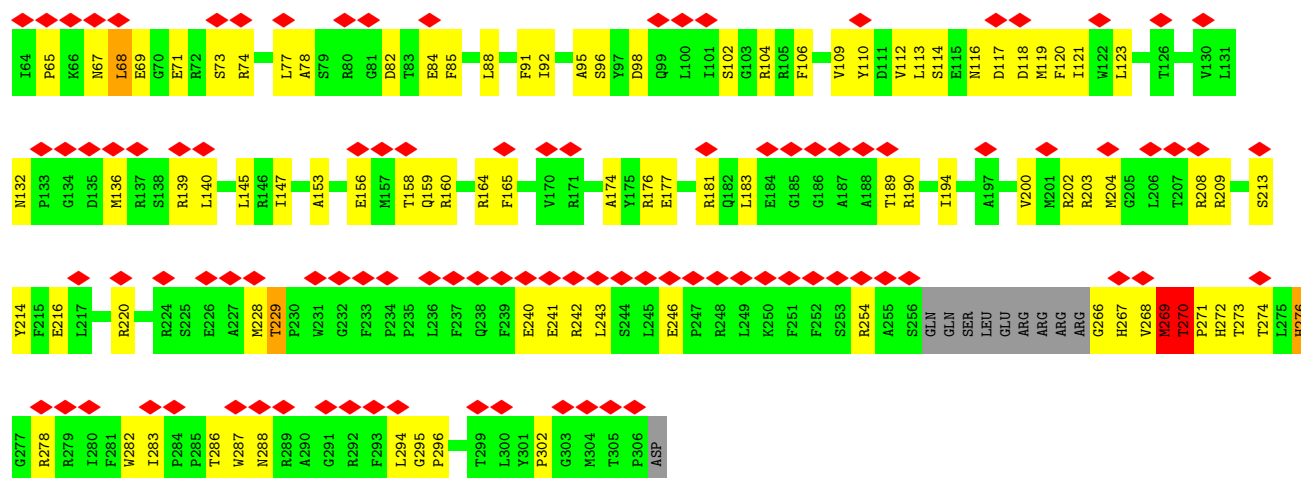


• Molecule 3: ms56

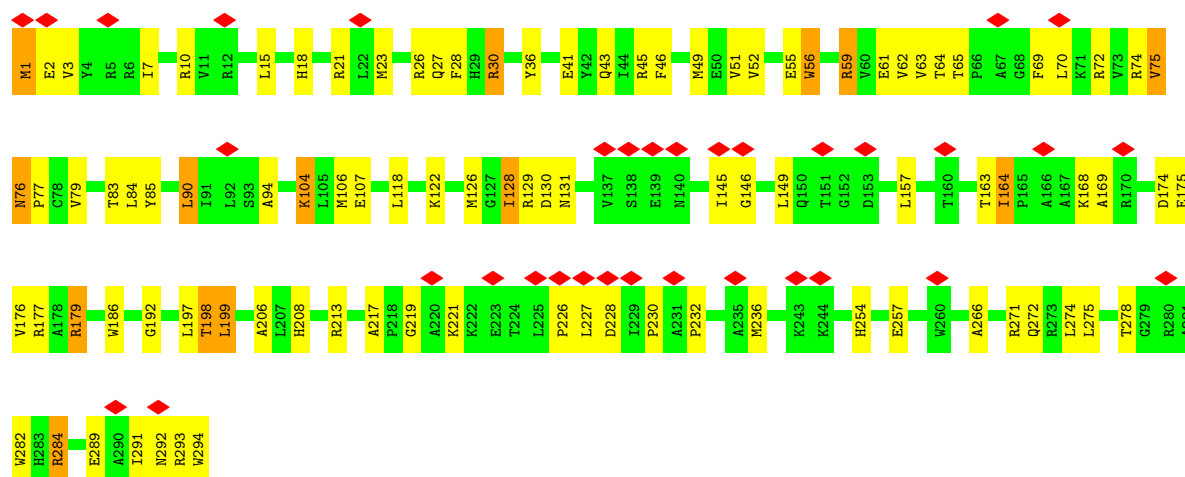


• Molecule 4: ms59

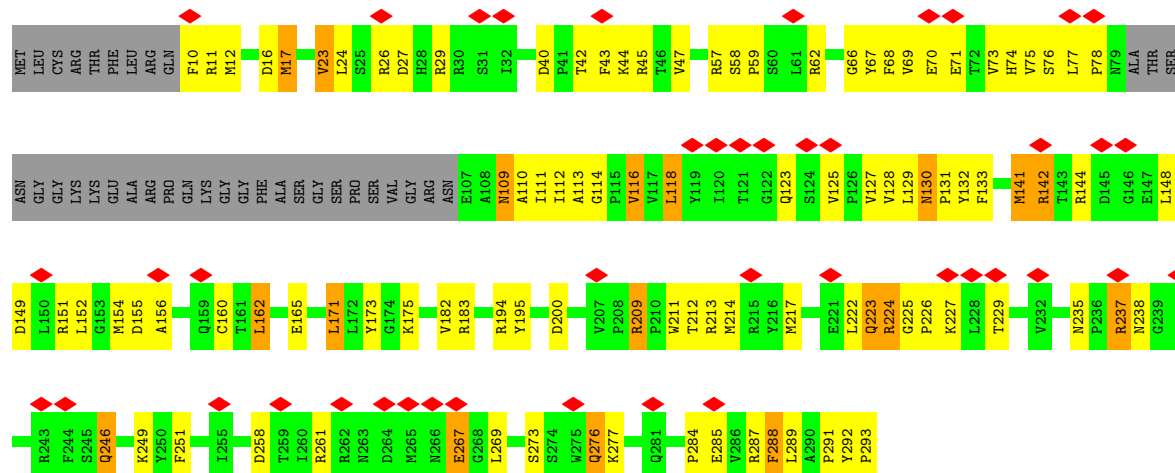




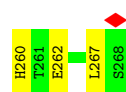
• Molecule 5: ms60



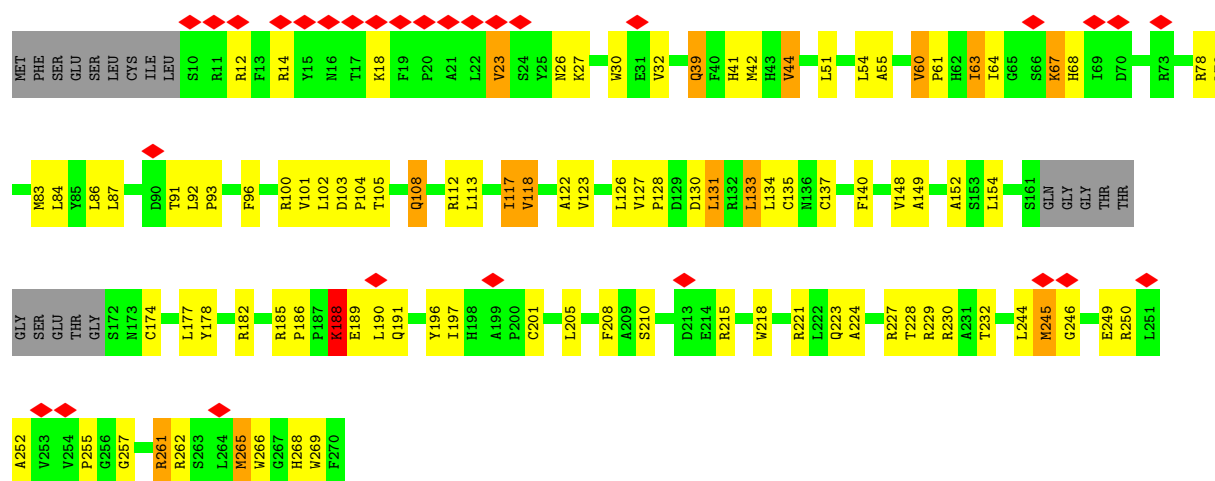
• Molecule 6: ms61



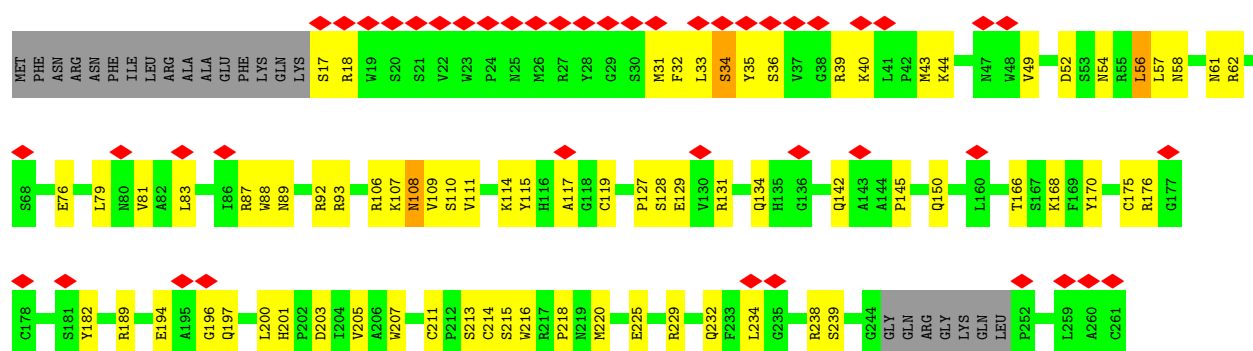




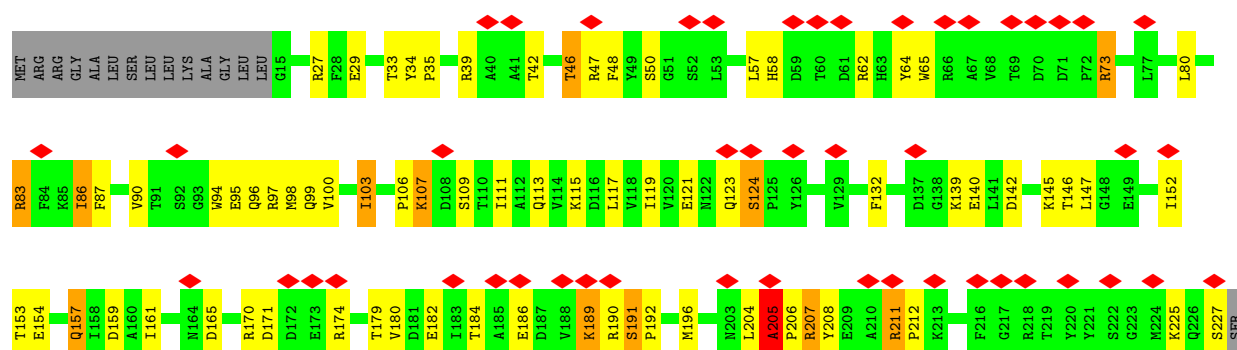
• Molecule 10: ms65



• Molecule 11: ms66

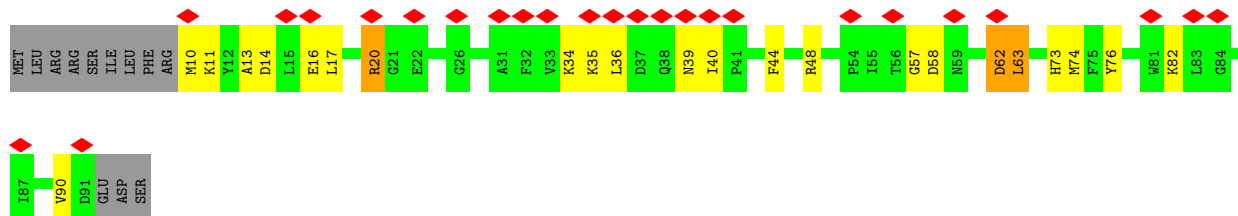


• Molecule 12: ms68

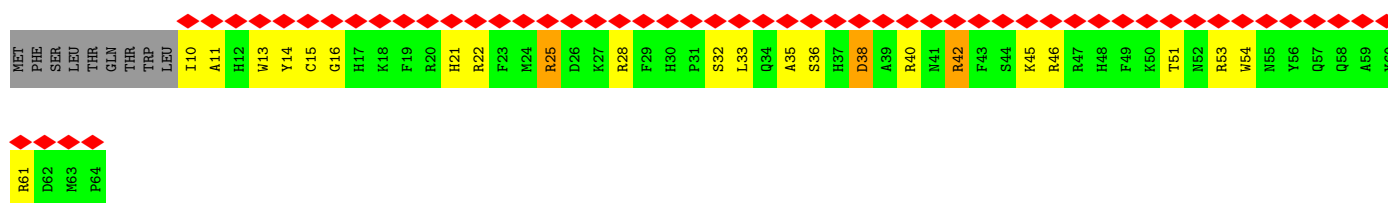
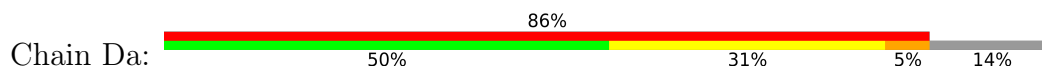




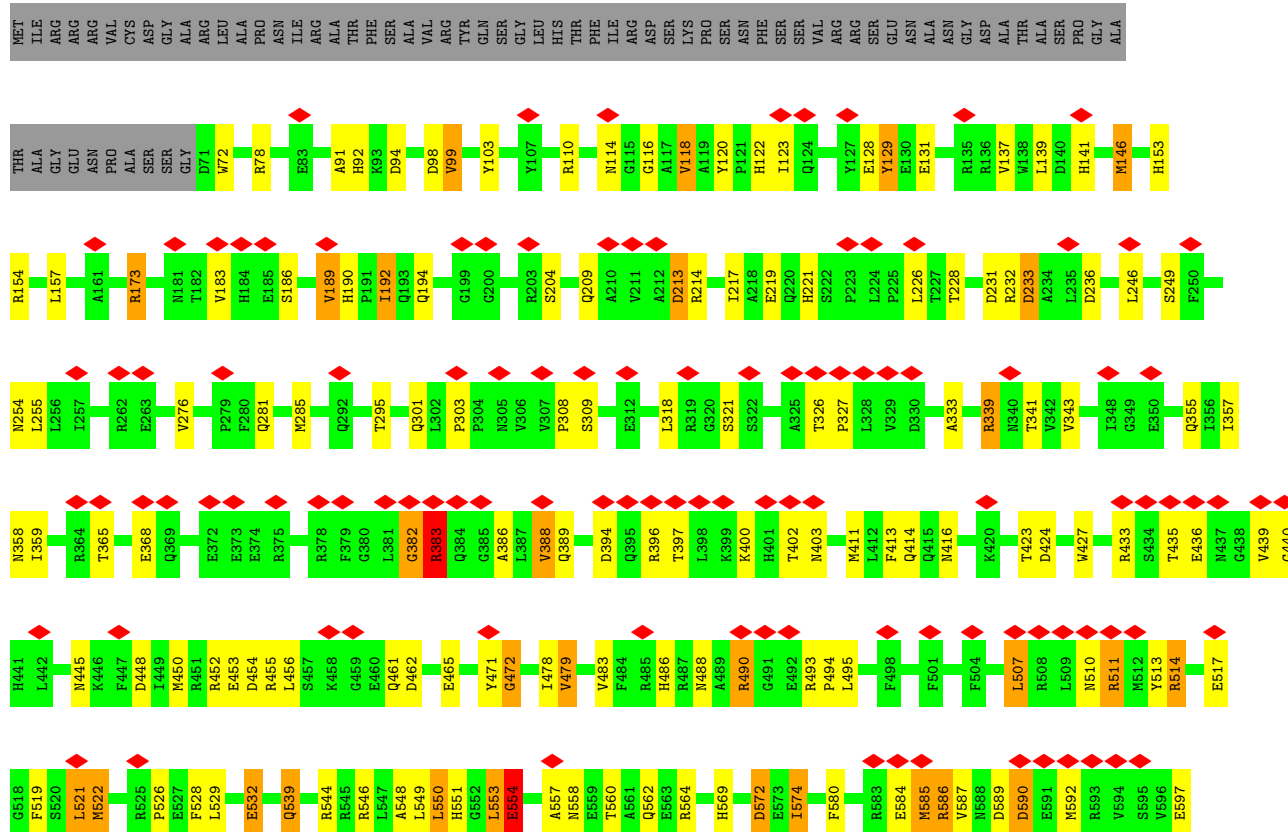
- Molecule 13: ms73

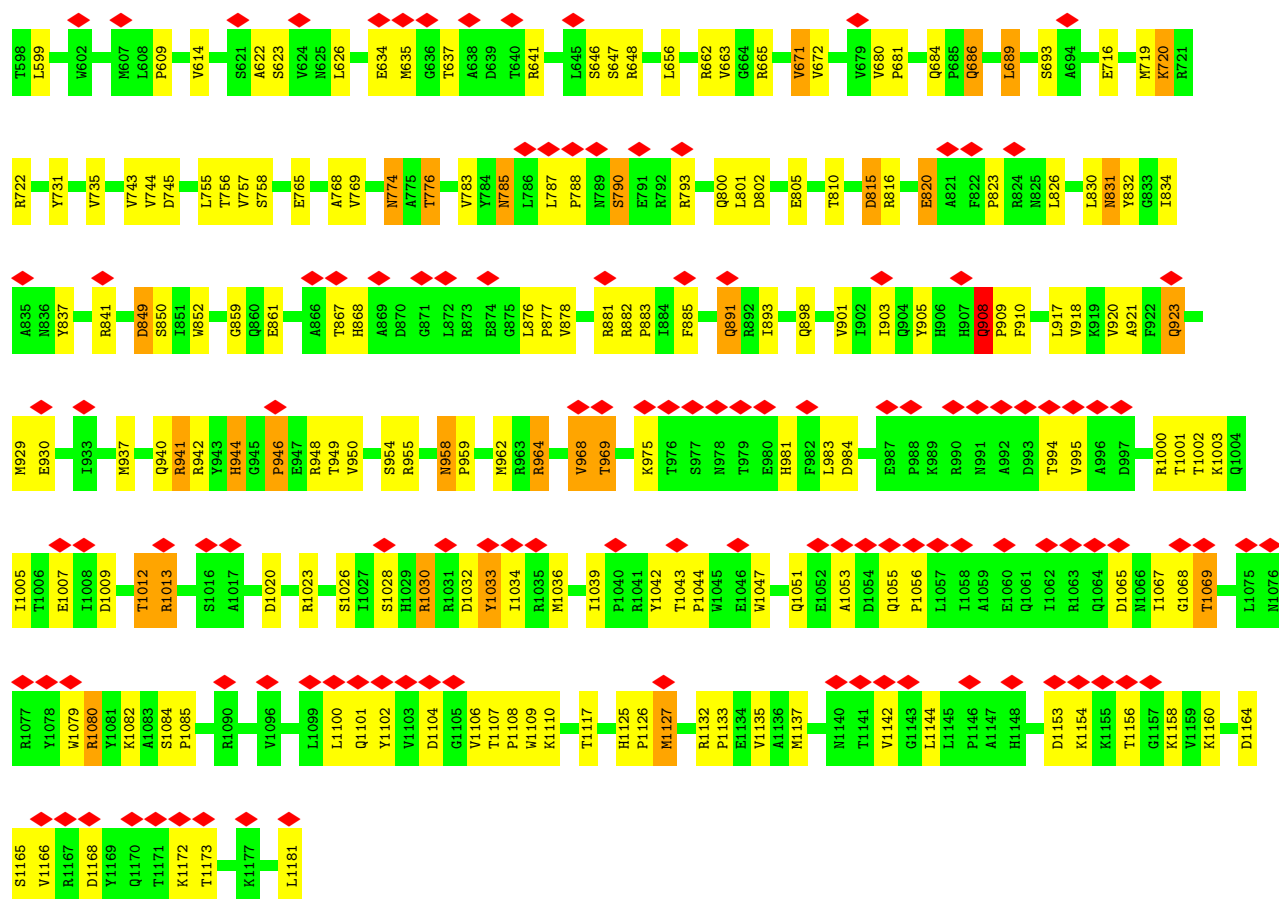


- Molecule 14: ms74

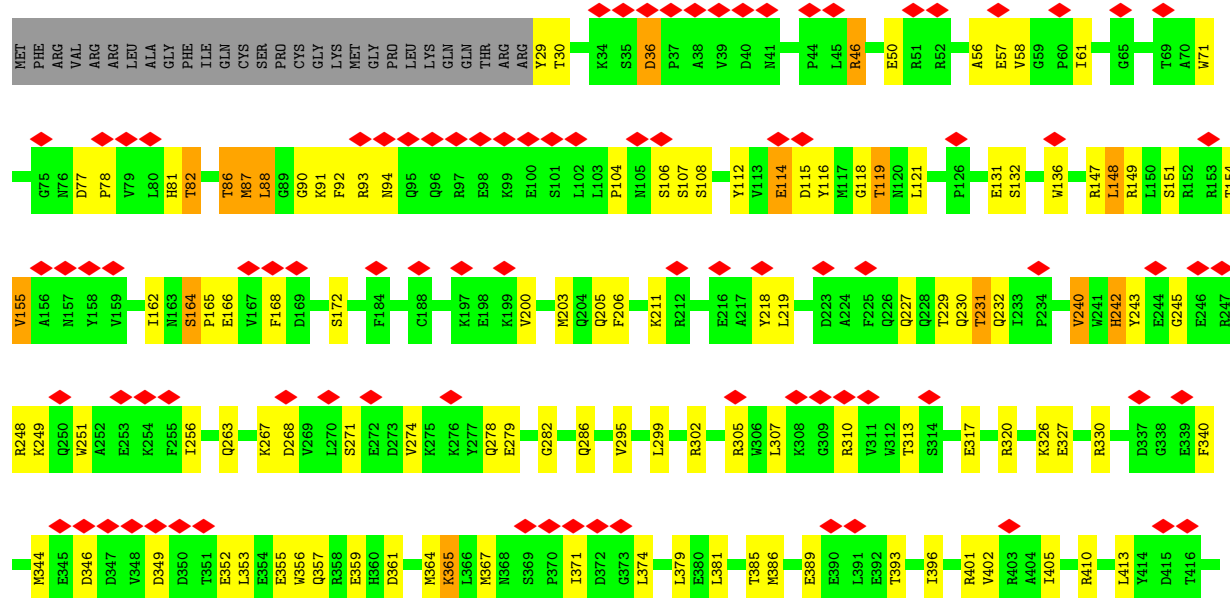


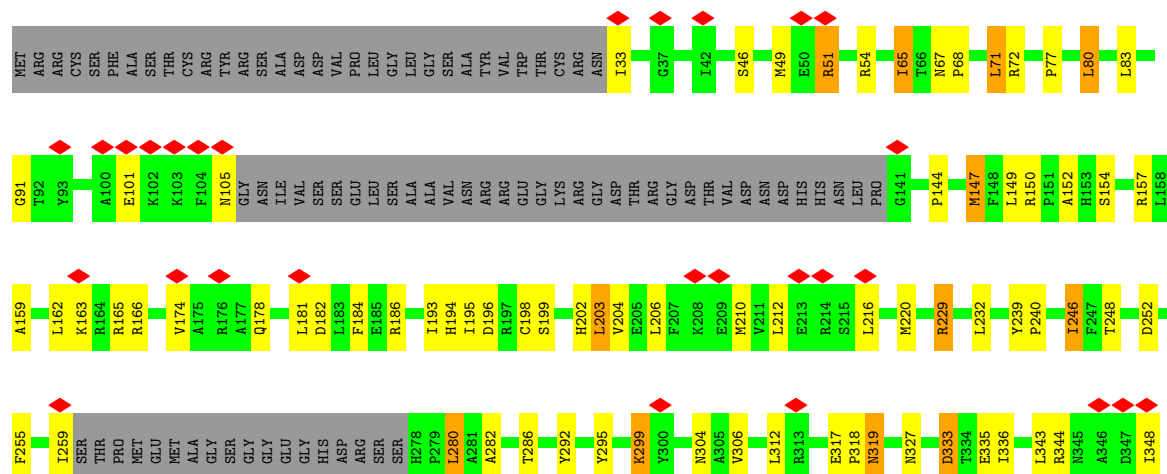
- Molecule 15: ms49

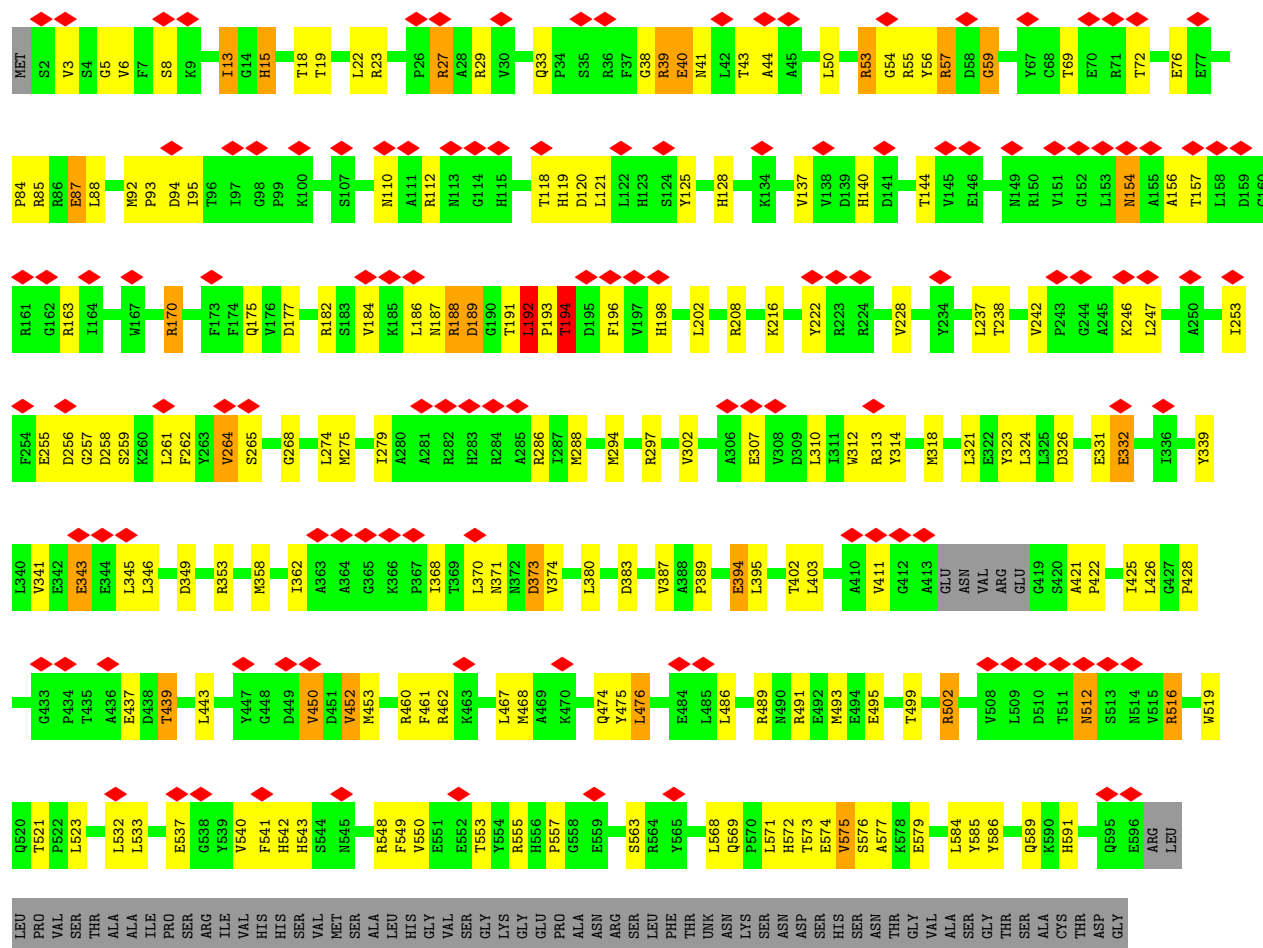




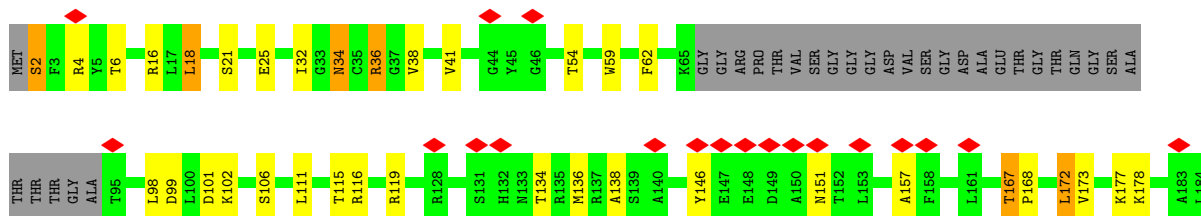
• Molecule 16: ms50

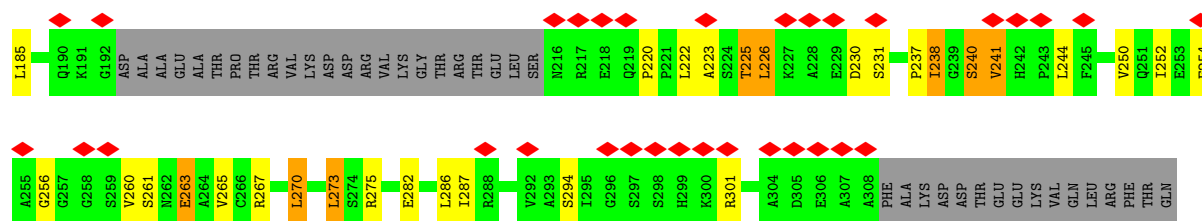




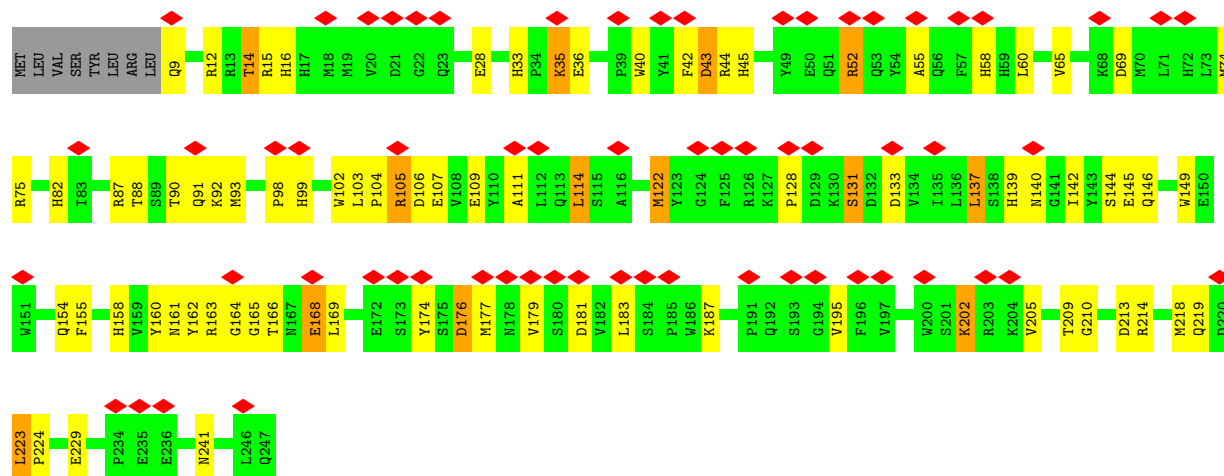




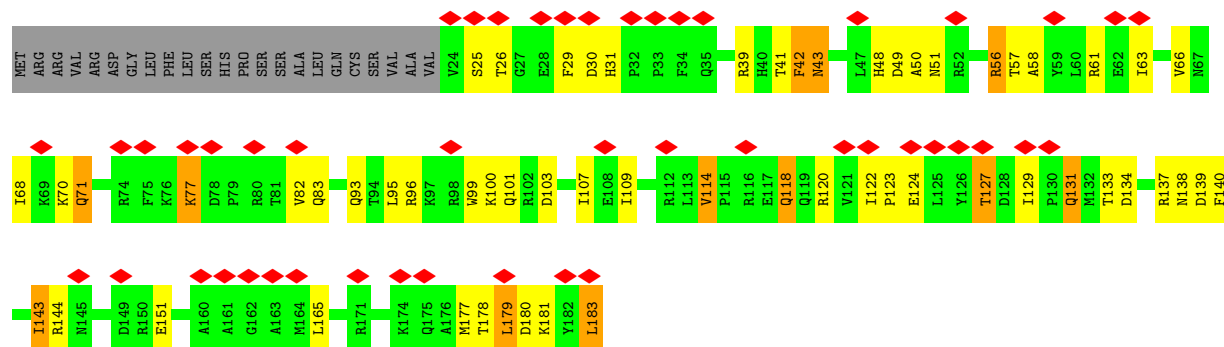




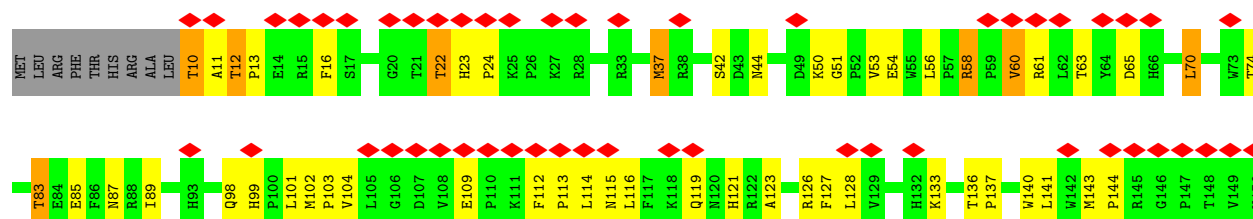
• Molecule 23: ms67

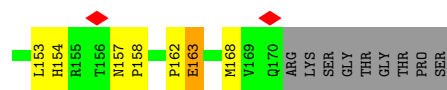


• Molecule 24: ms69

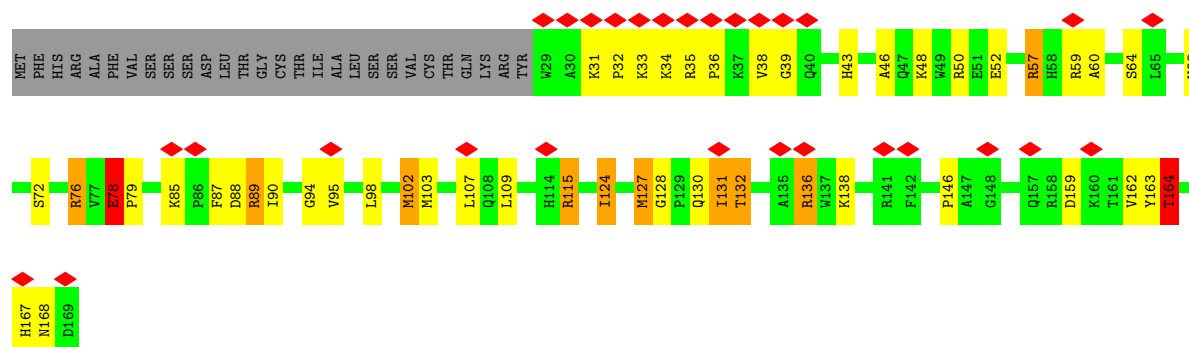


• Molecule 25: ms70

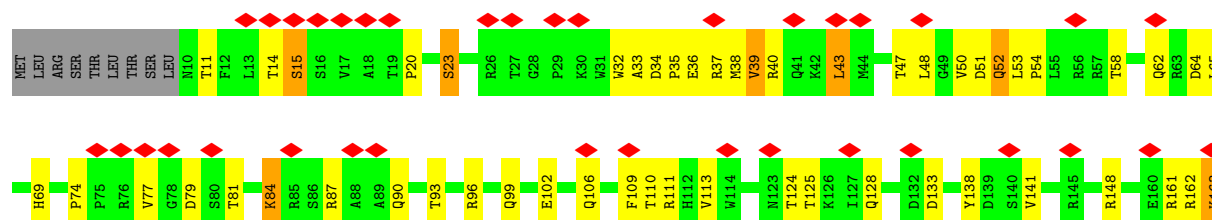




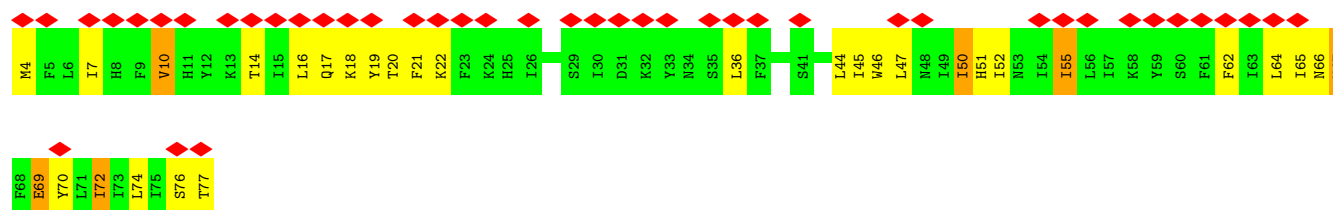
- Molecule 26: ms71



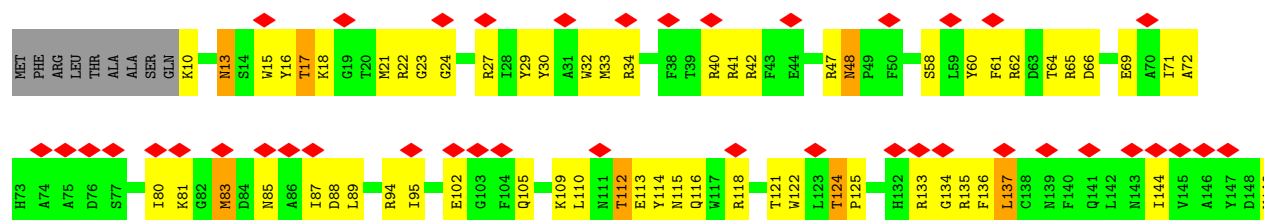
- Molecule 27: ms72



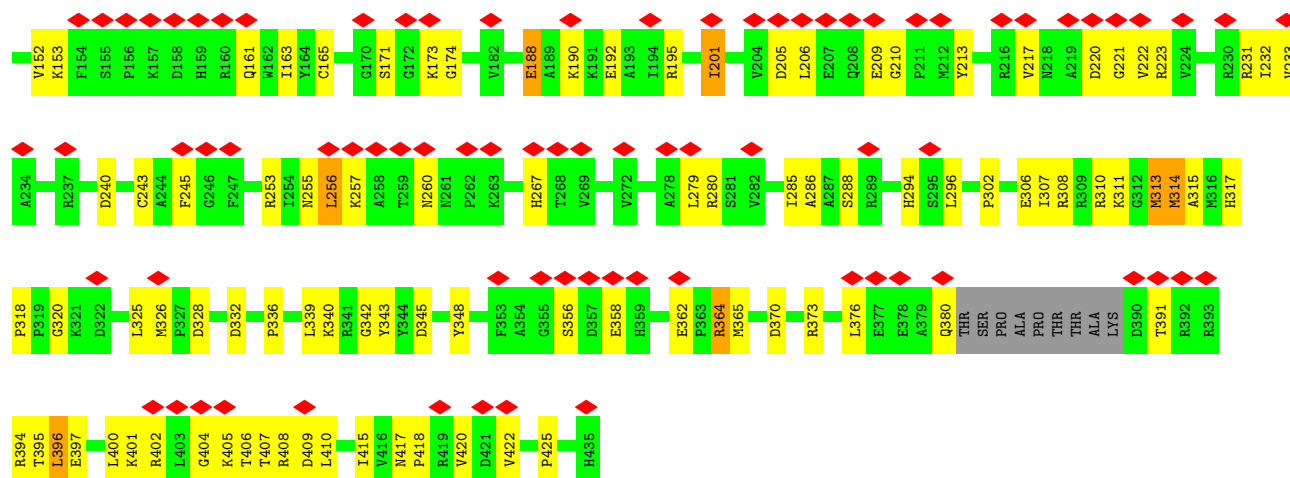
- Molecule 28: uS3m



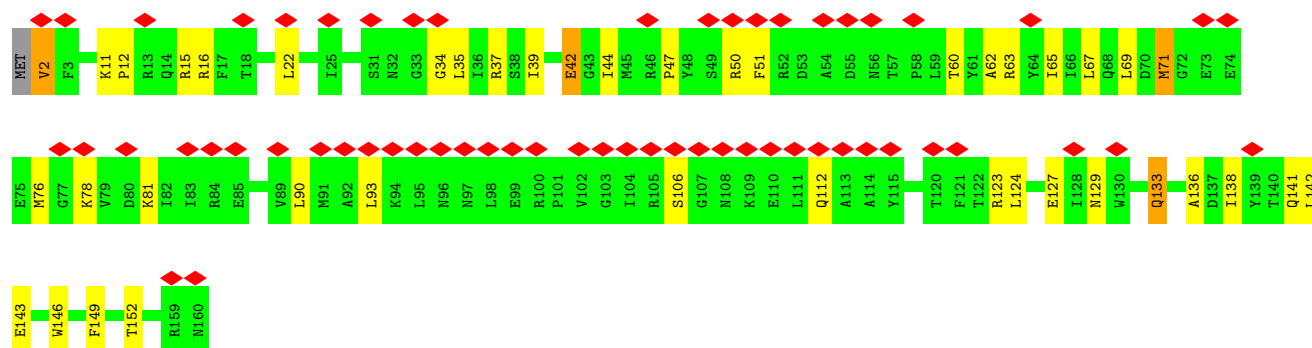
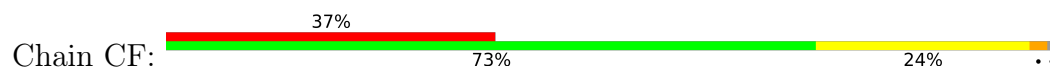
- Molecule 29: uS55m



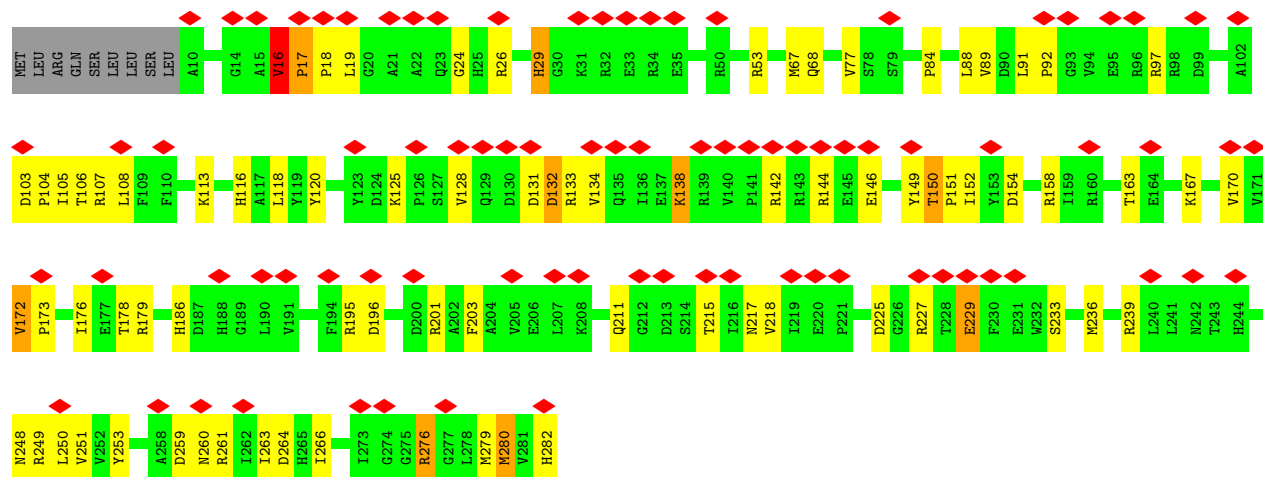




• Molecule 30: bS6m

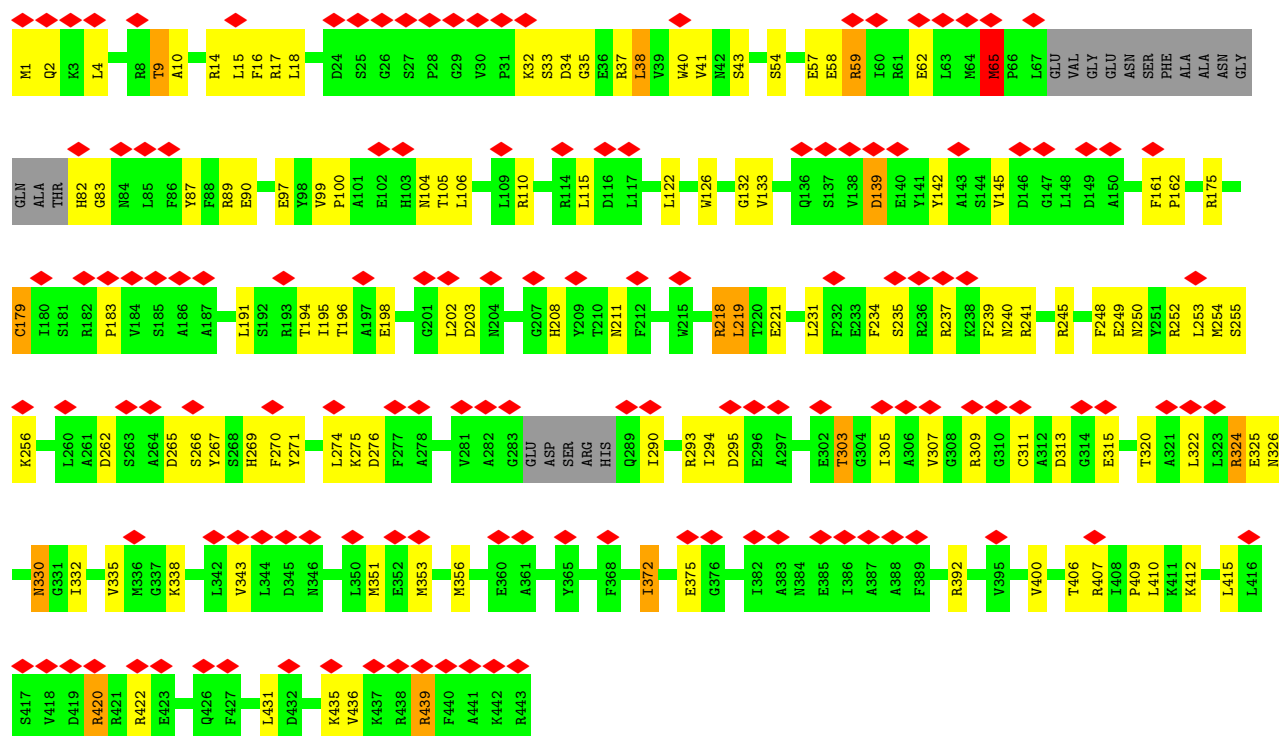


• Molecule 31: uS8m

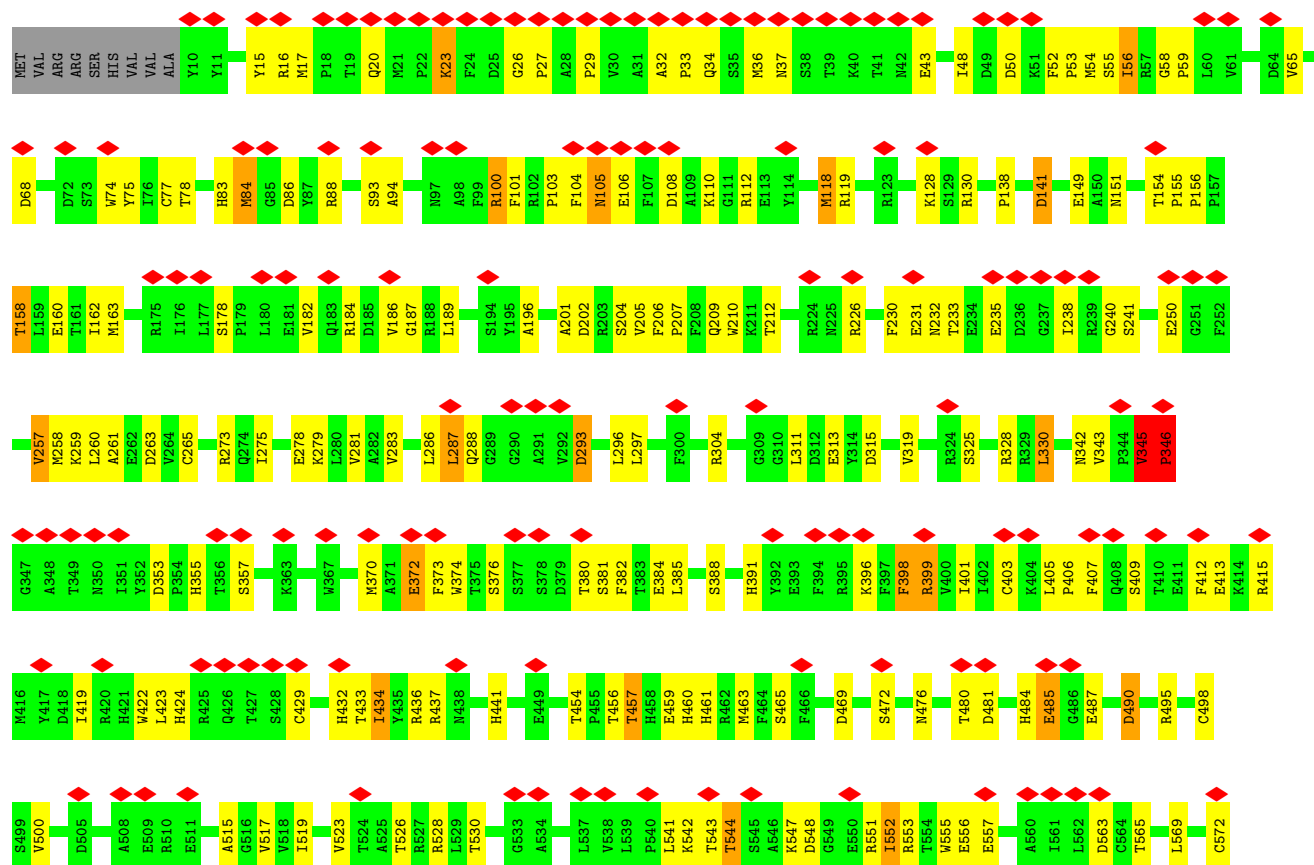


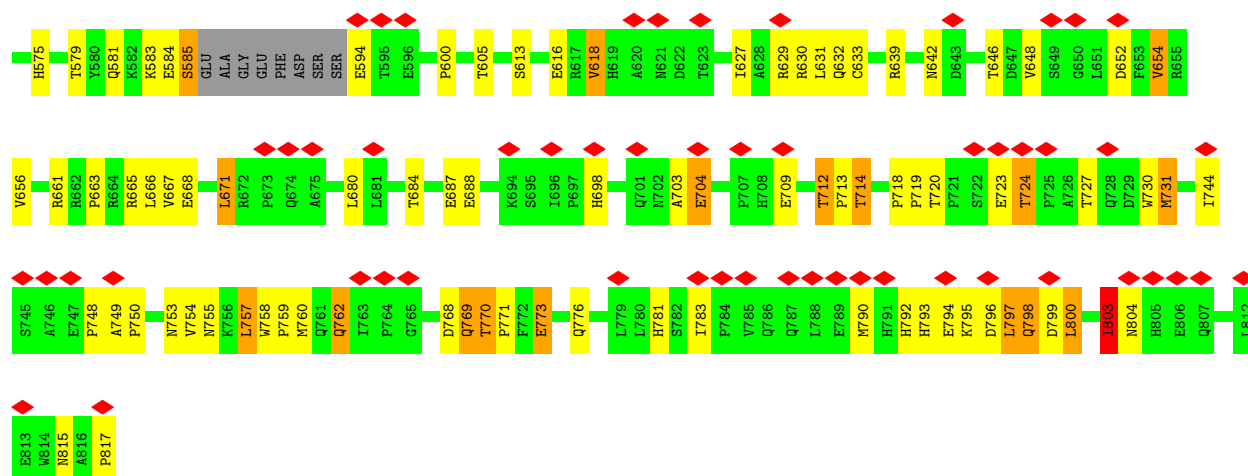
• Molecule 32: uS9m



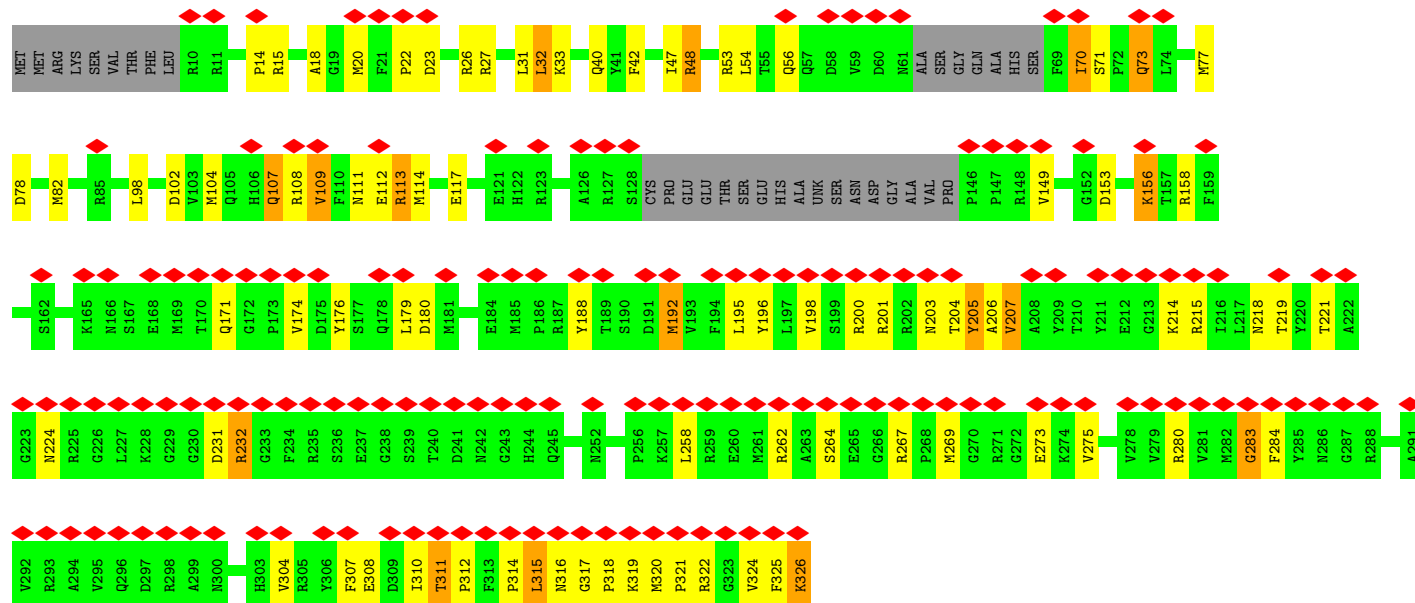


• Molecule 33: uS10m

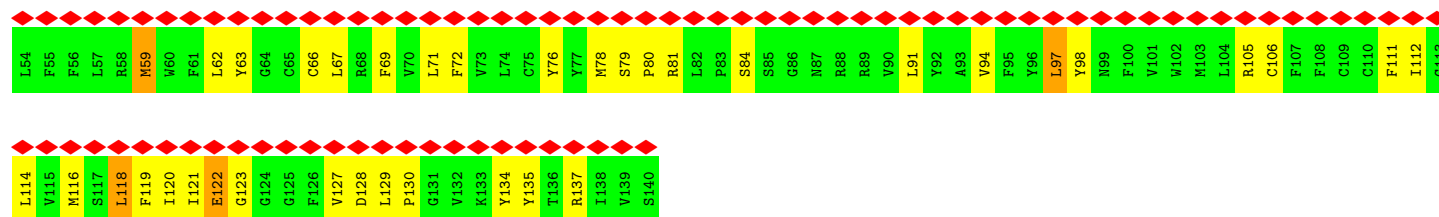




• Molecule 34: uS11m



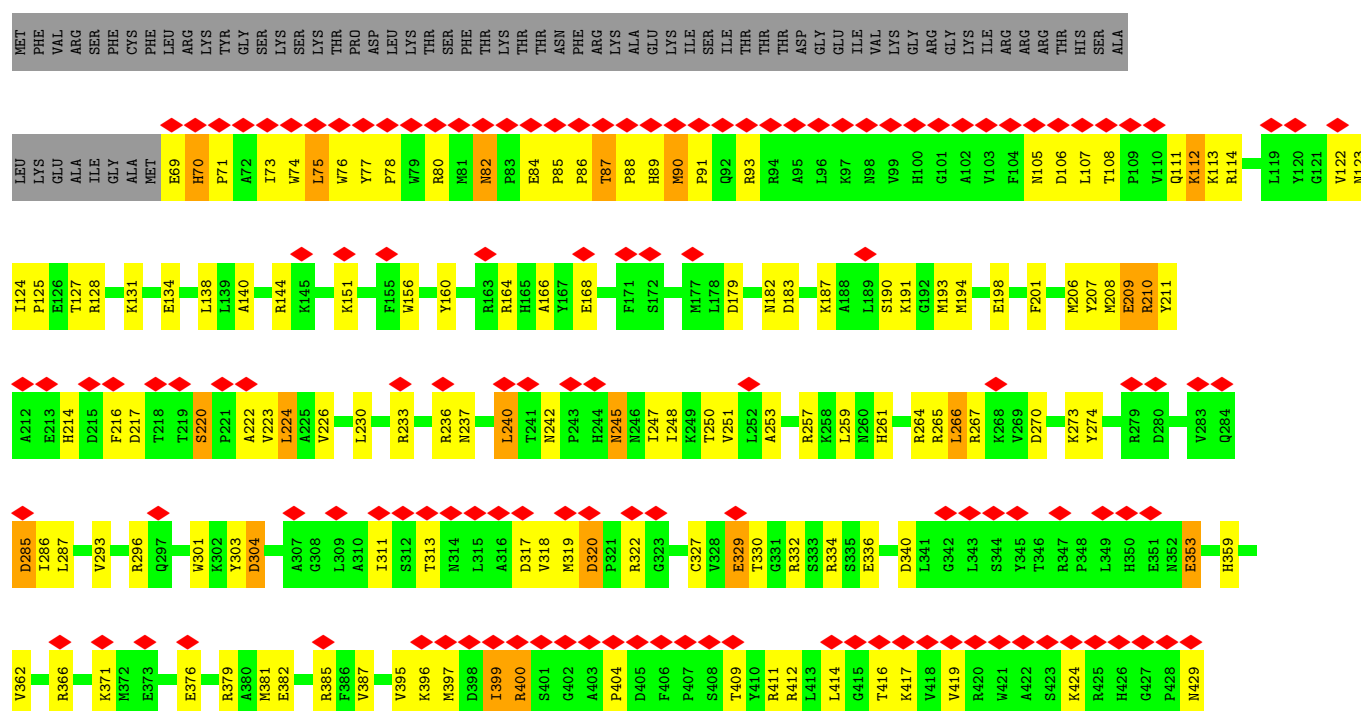
• Molecule 35: uS12



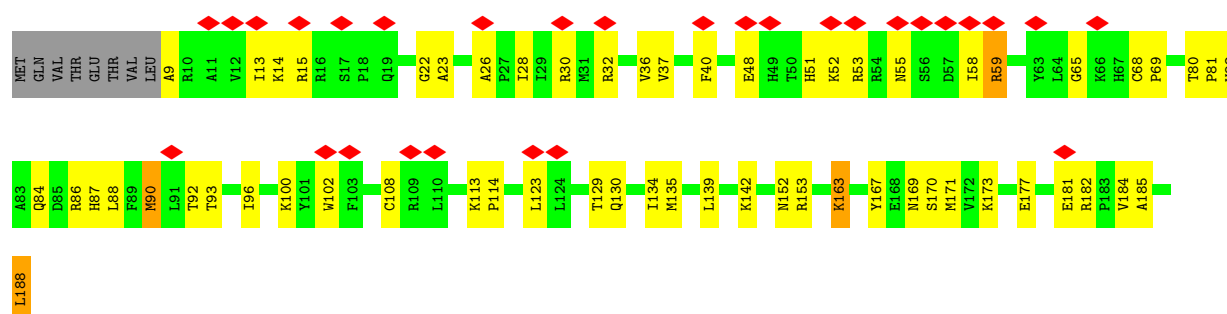
• Molecule 36: uS14m



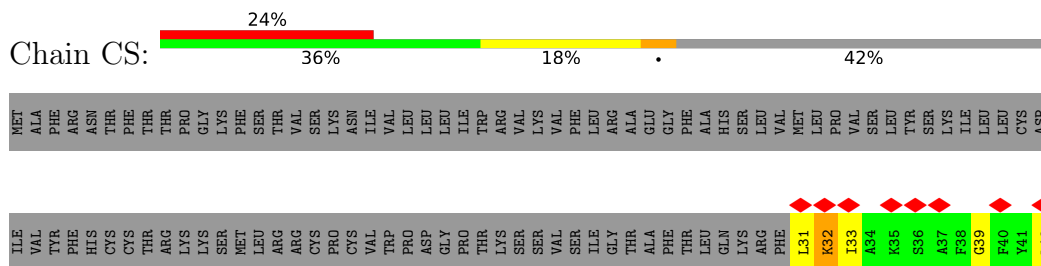
- Molecule 37: uS15m

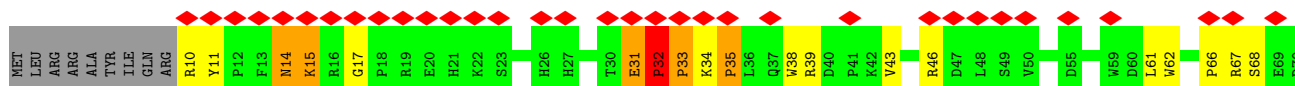


- Molecule 38: bS16m



- Molecule 39: uS17m





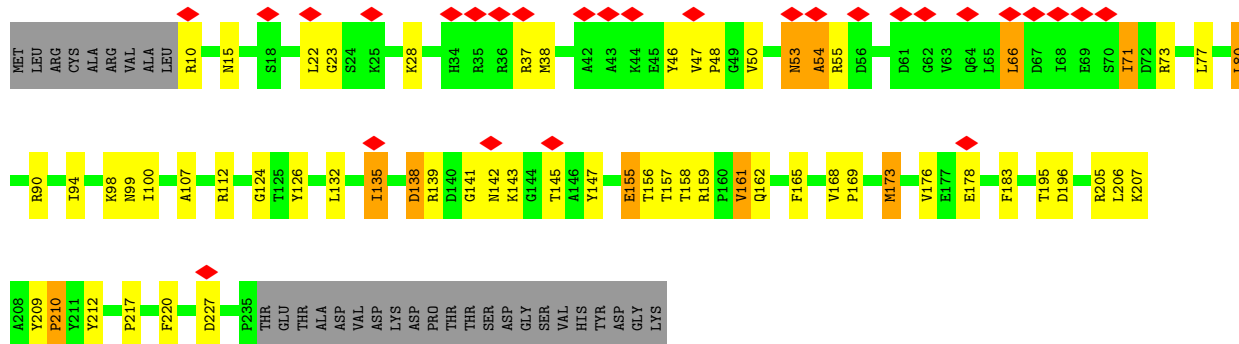




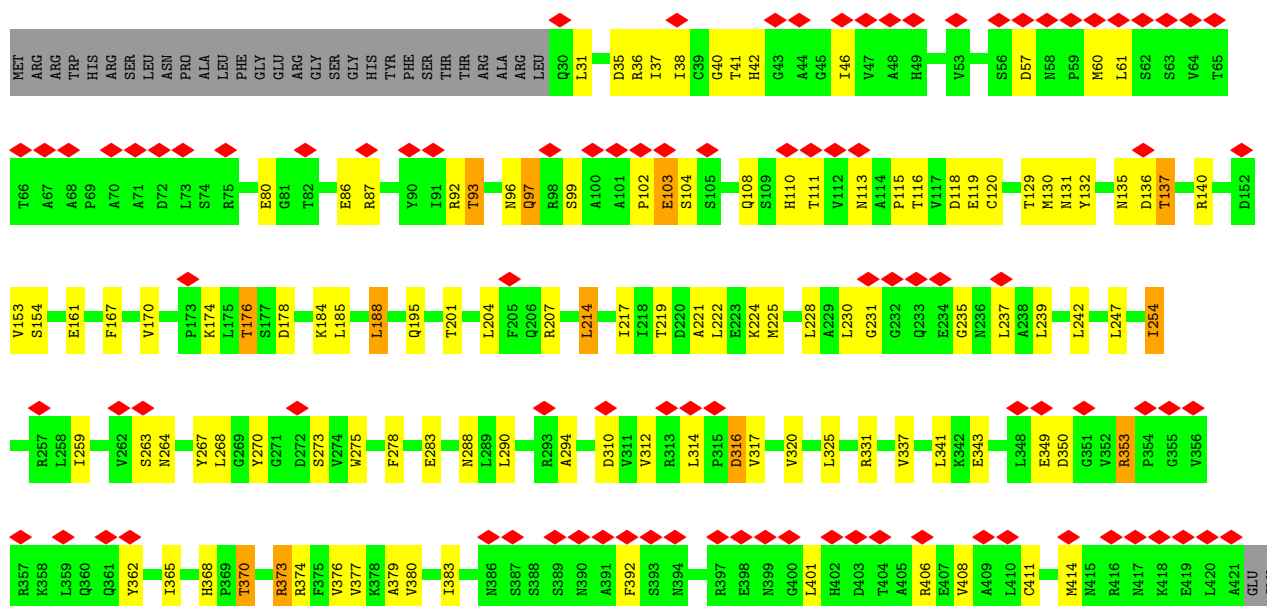


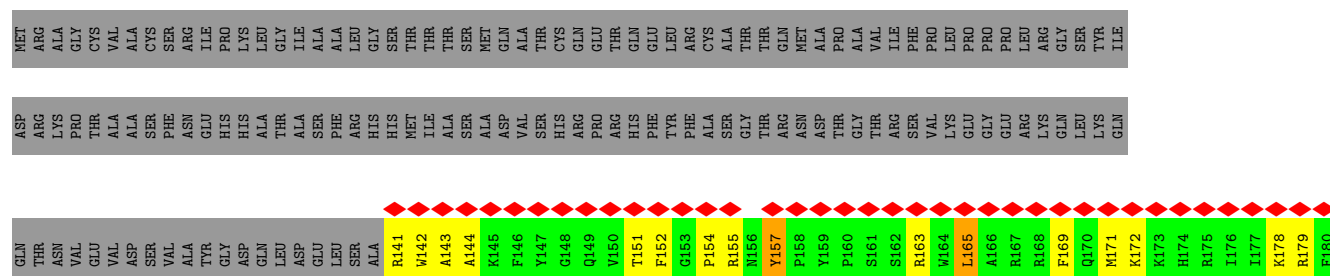


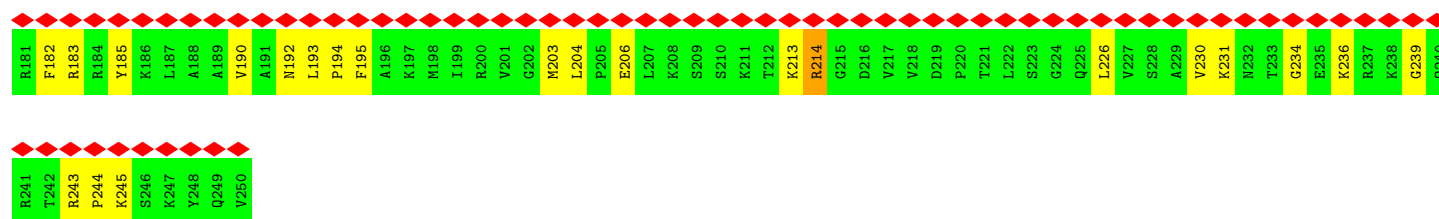
• Molecule 49: mS34



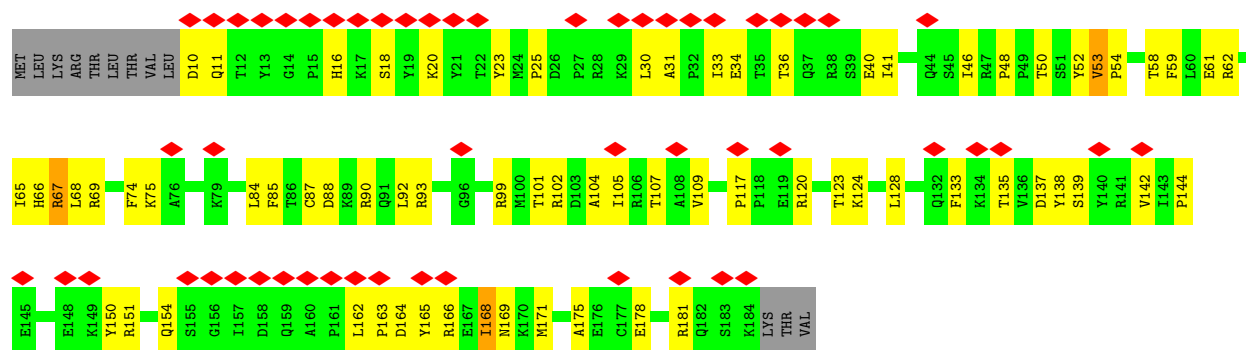
• Molecule 50: mS35



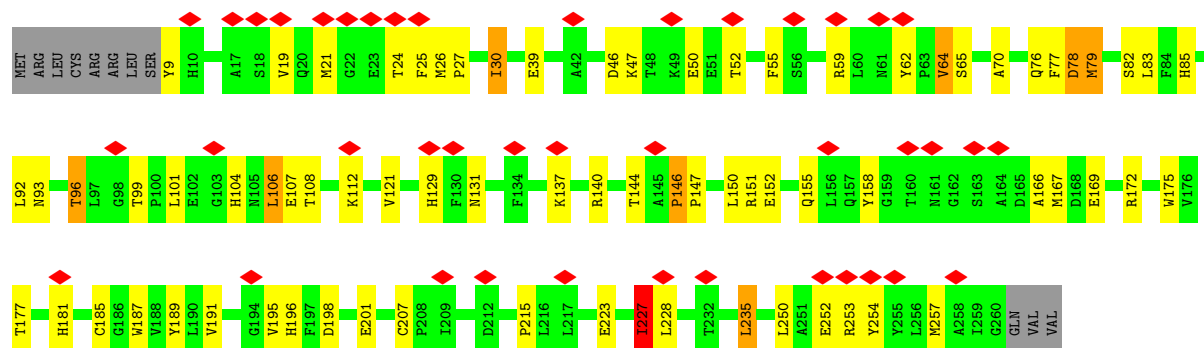




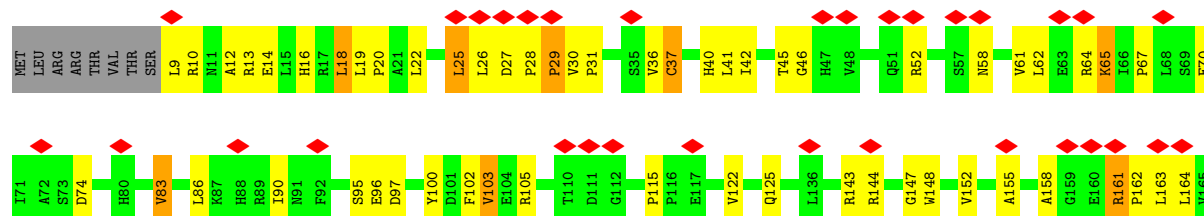
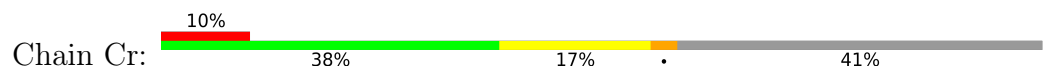
• Molecule 53: ms34

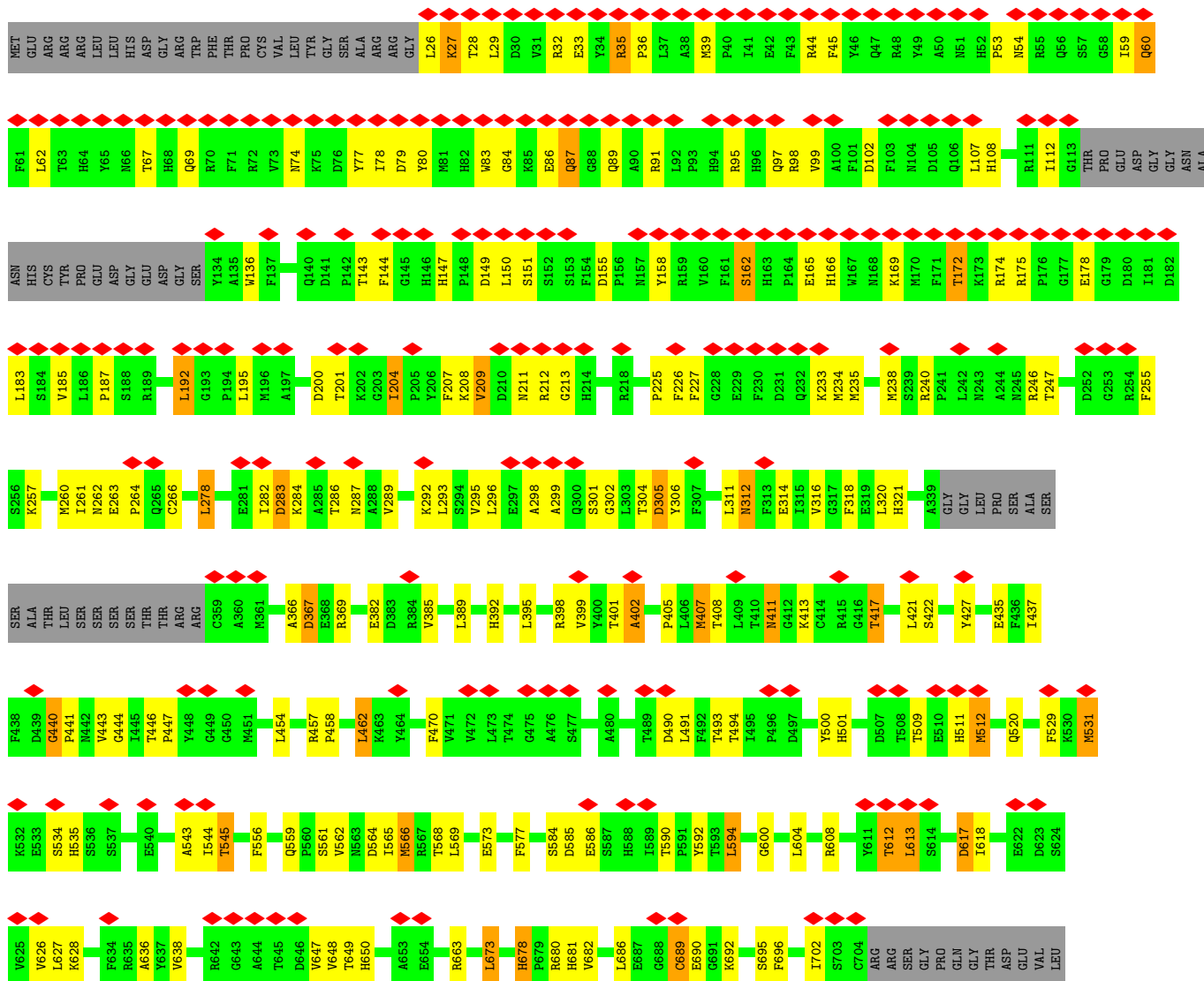


• Molecule 54: ms42

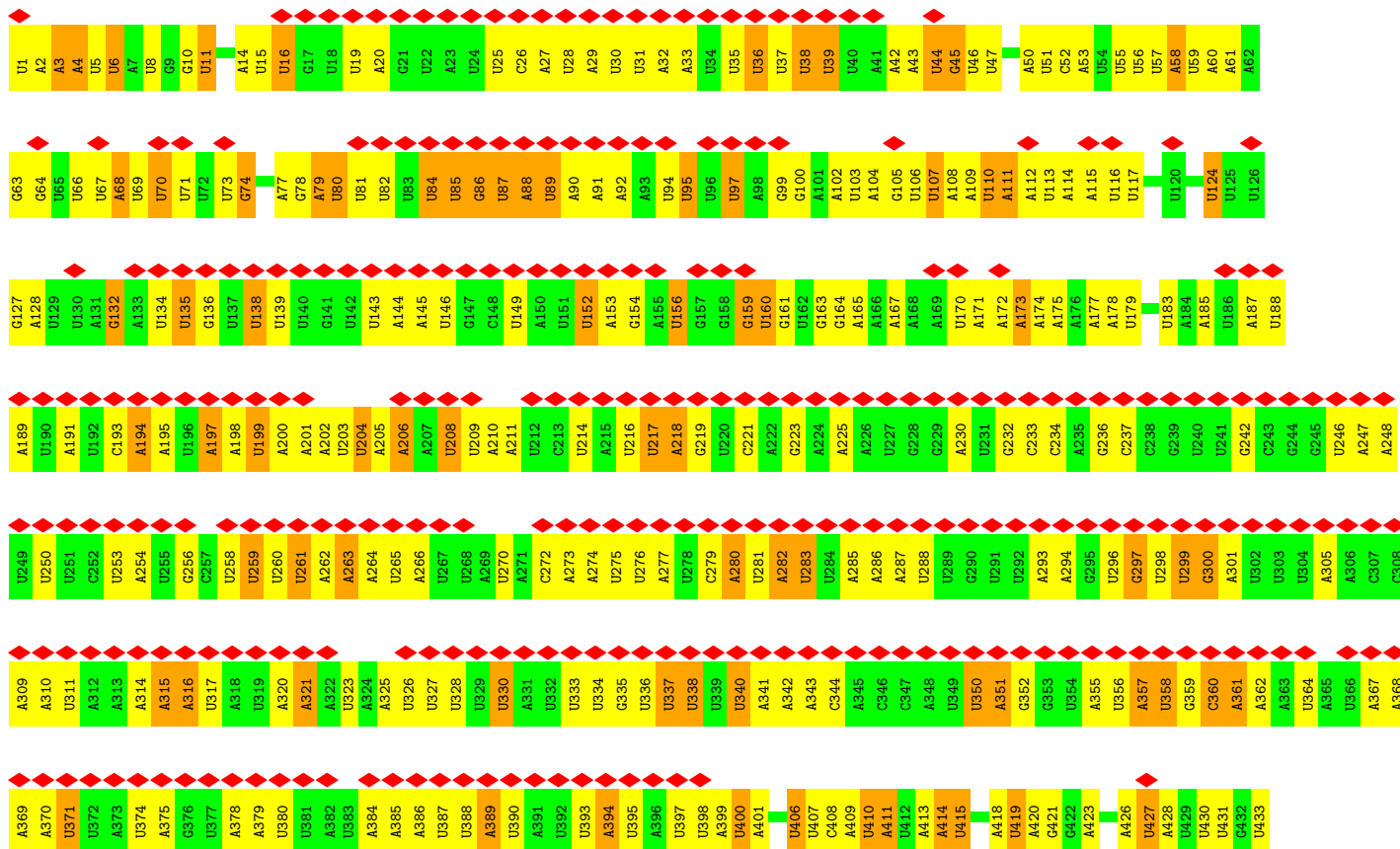


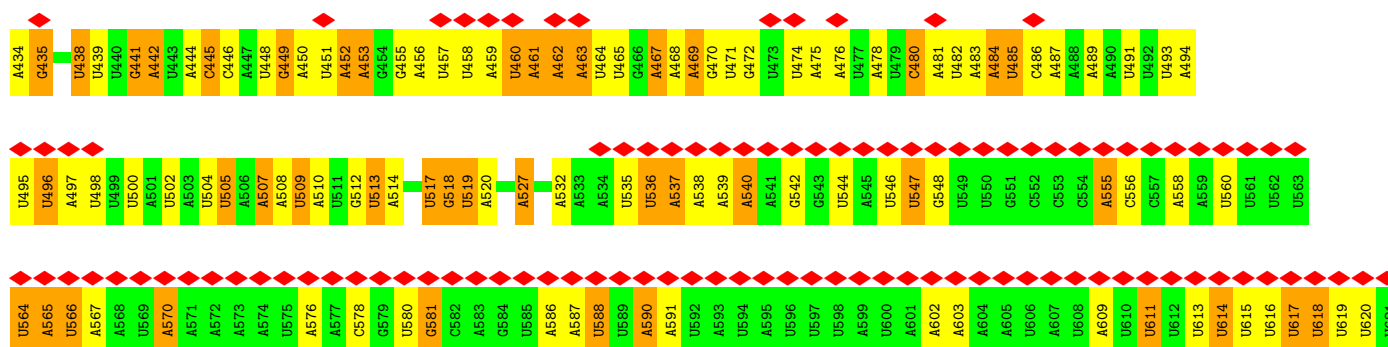
• Molecule 55: mS43



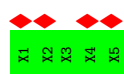
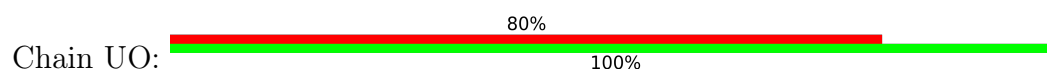


- Molecule 57: 9s rRNA





- Molecule 58: UNK

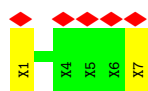
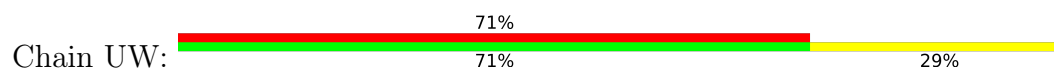


- Molecule 59: UNK

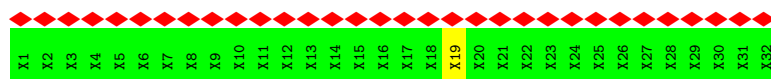


There are no outlier residues recorded for this chain.

- Molecule 59: UNK



- Molecule 60: UNK

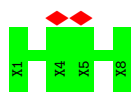


- Molecule 61: UNK

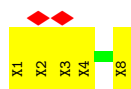
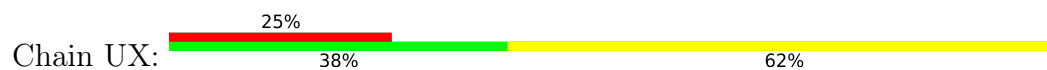


- Molecule 61: UNK

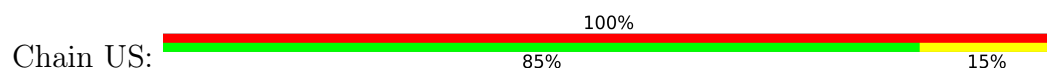




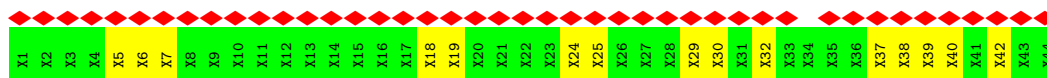
- Molecule 61: UNK



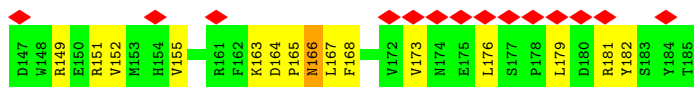
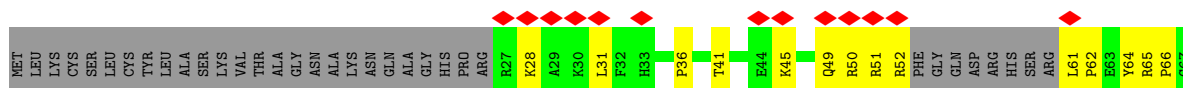
- Molecule 62: UNK



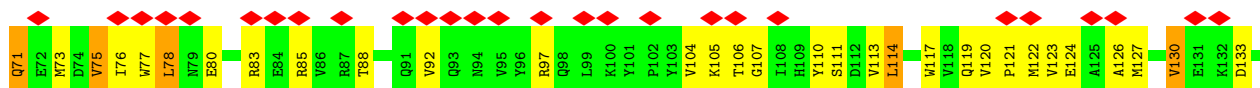
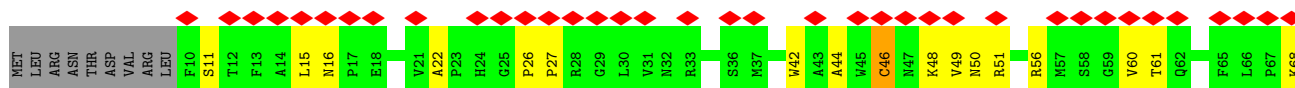
- Molecule 63: UNK

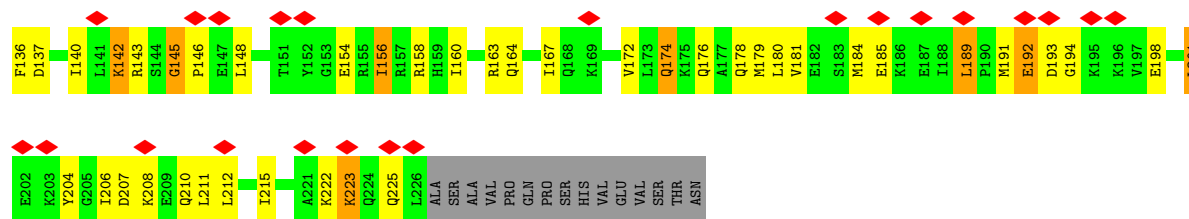


- Molecule 64: bL27m

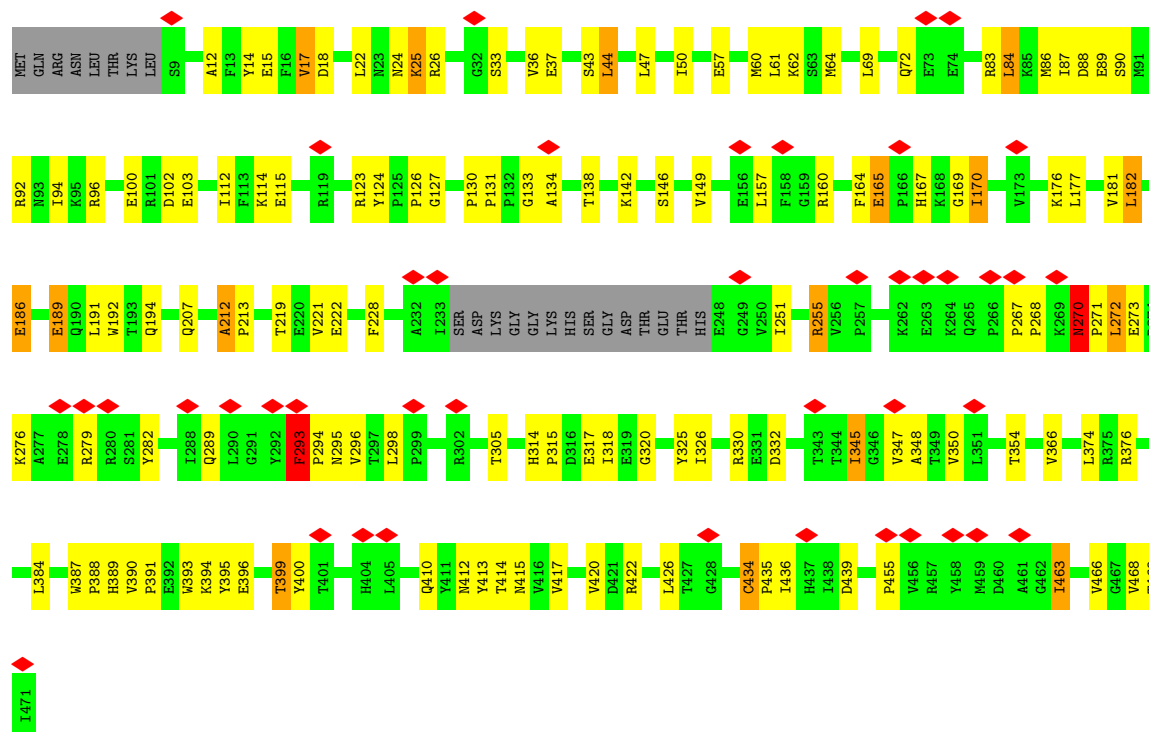


- Molecule 65: bL28m

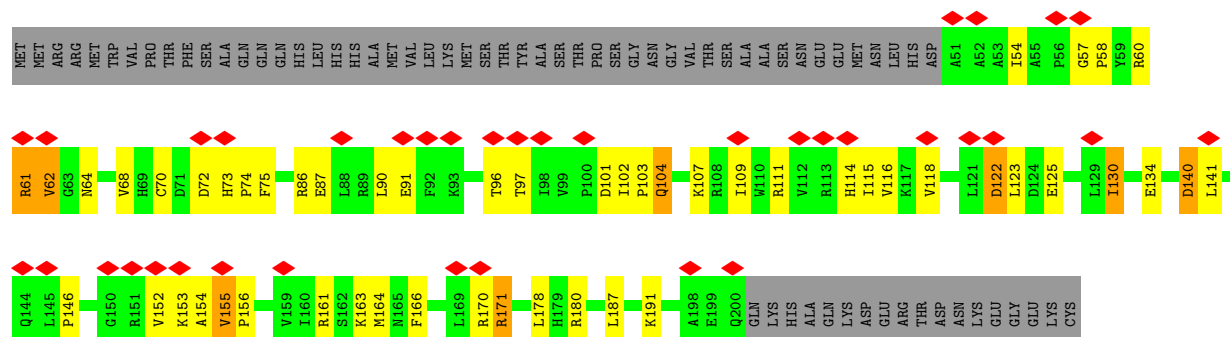
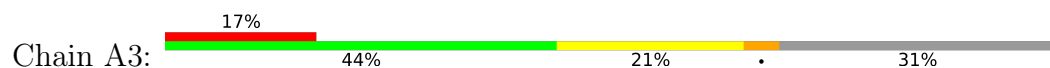




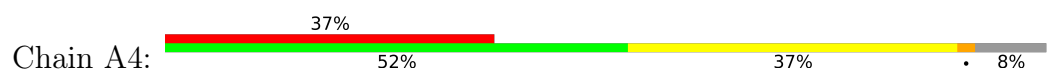
• Molecule 66: uL29m



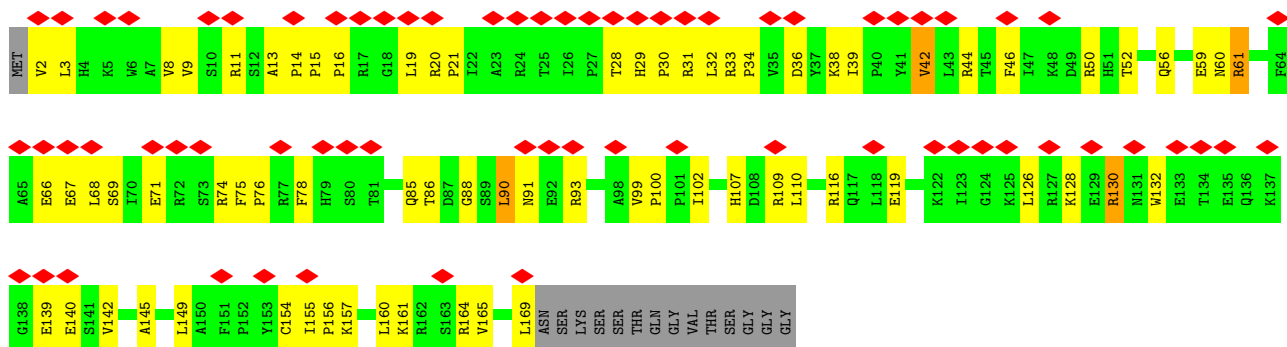
• Molecule 67: uL30m



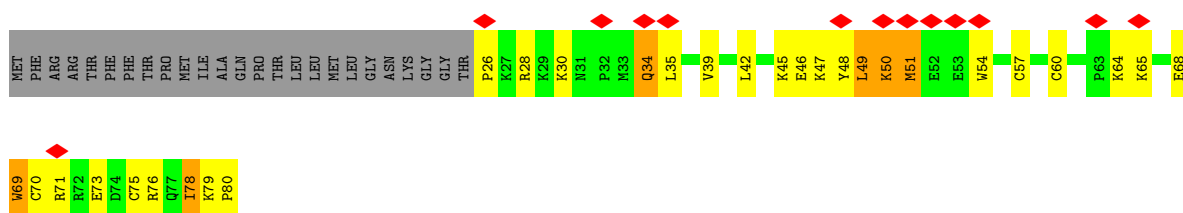
• Molecule 68: bL31m



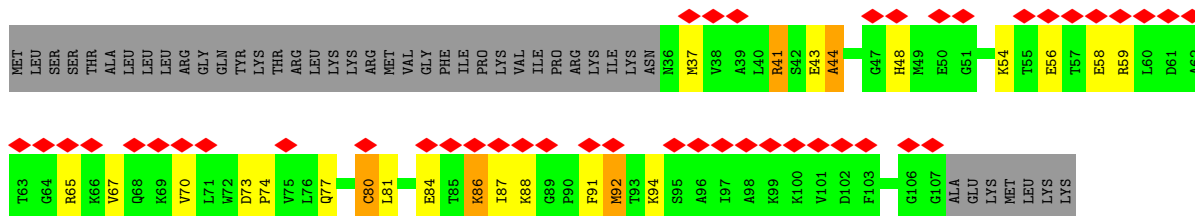
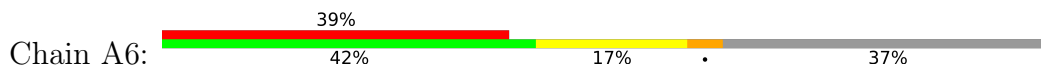




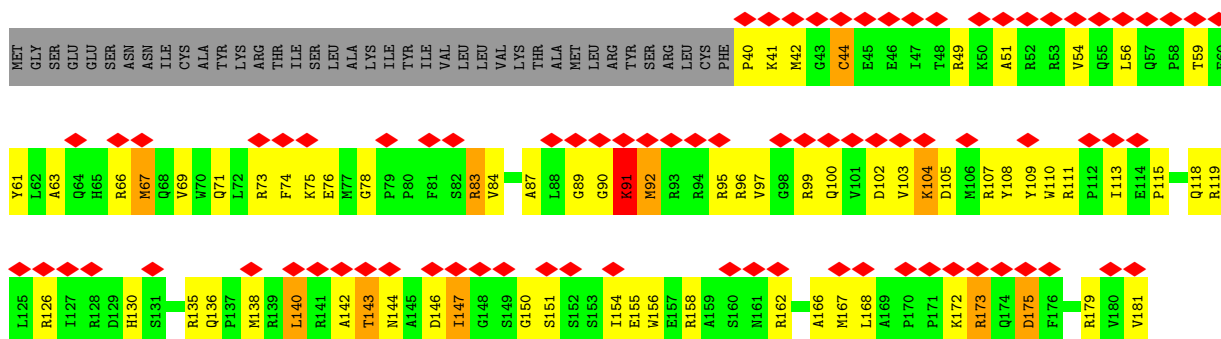
• Molecule 69: bL32m



• Molecule 70: bL33m

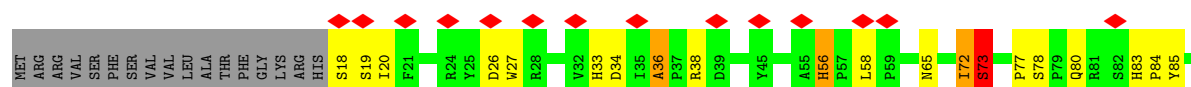


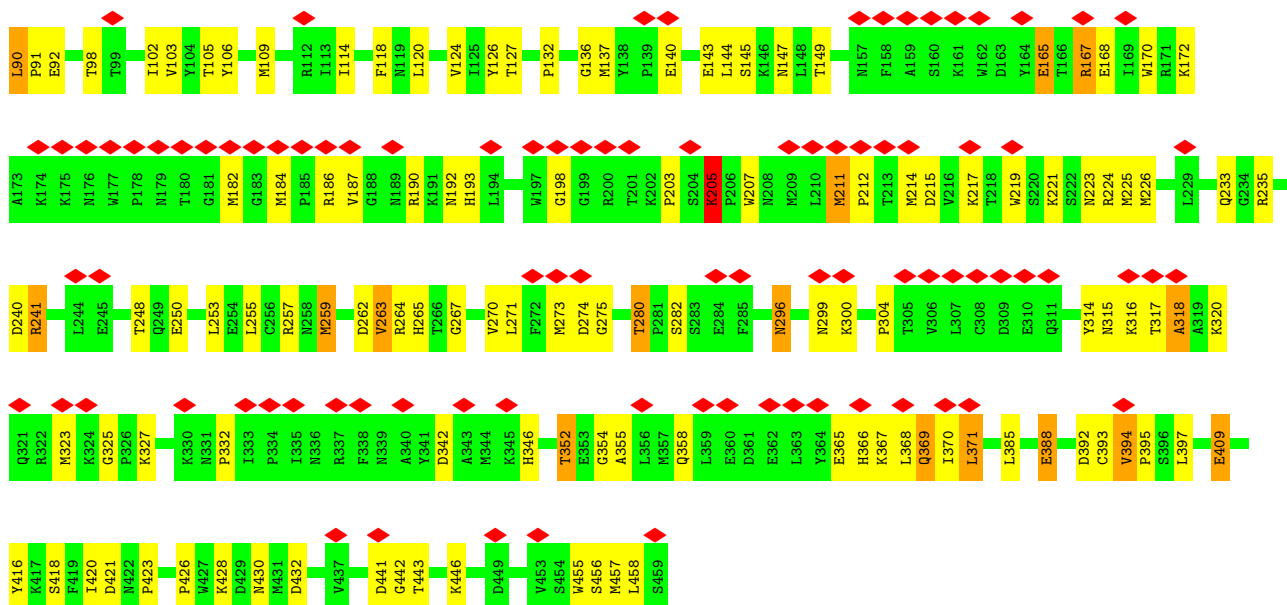
• Molecule 71: bL35m



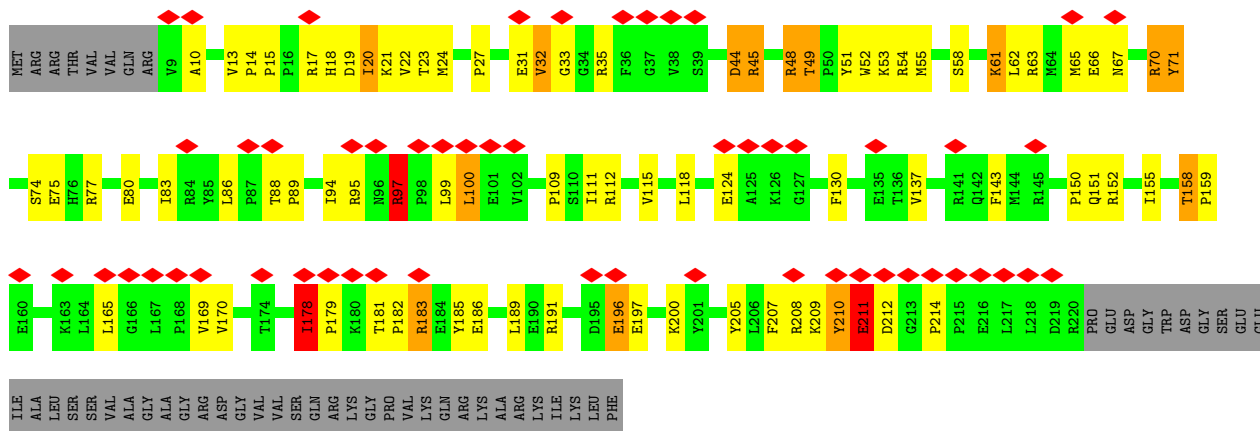
• Molecule 72: bL36m







• Molecule 75: bL9m

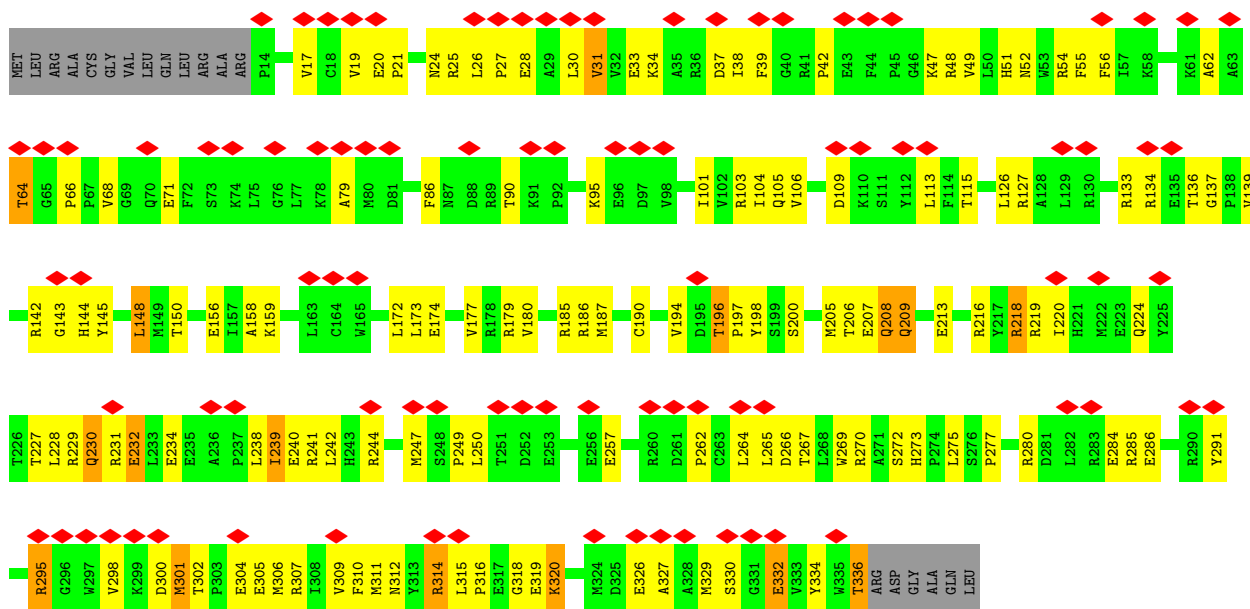


• Molecule 76: uL10m



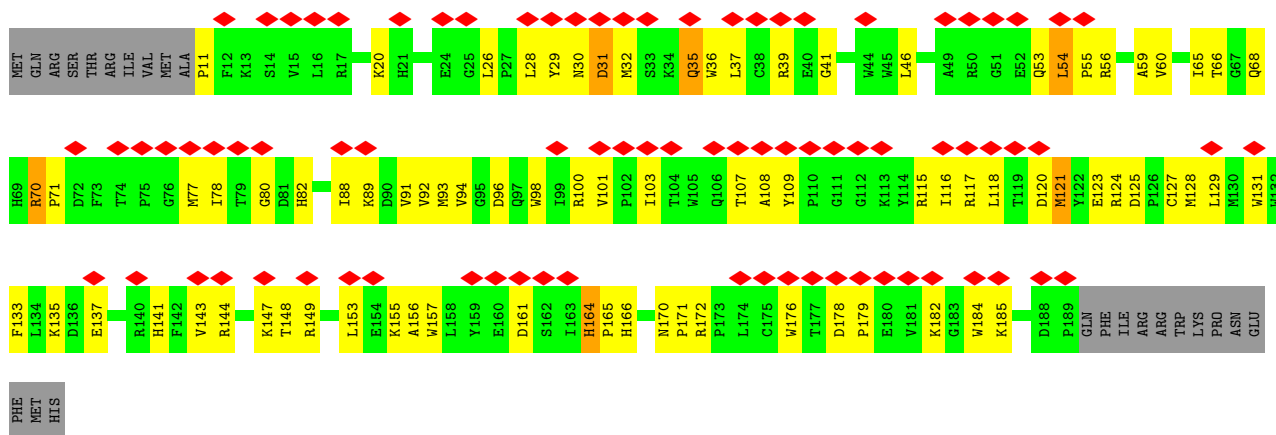
• Molecule 77: uL11m

Chain AK: 



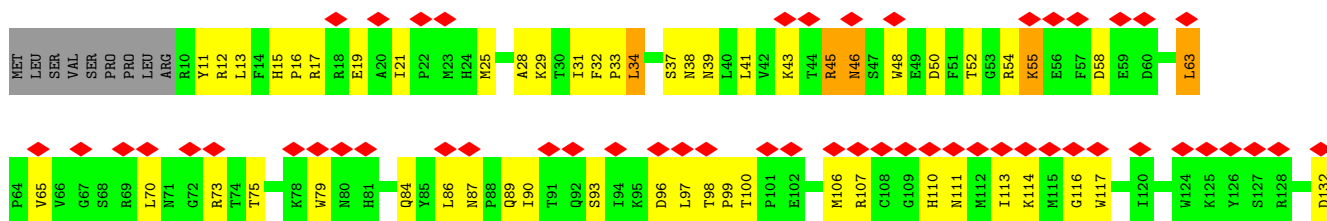
• Molecule 78: 50S ribosomal protein L13, putative

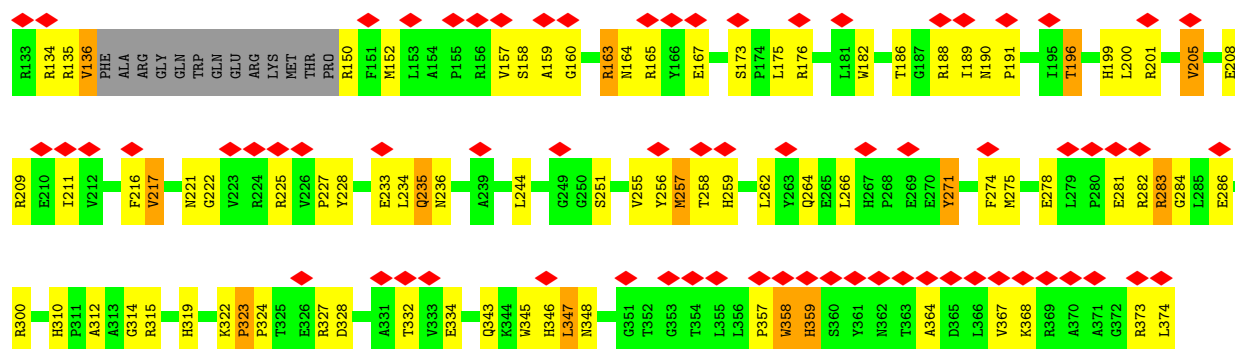
Chain AN: 



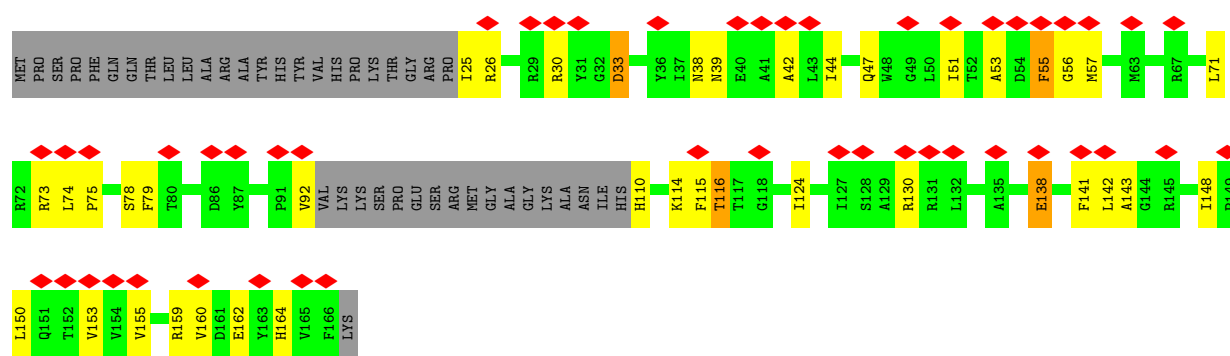
• Molecule 79: uL15m

Chain AP: 

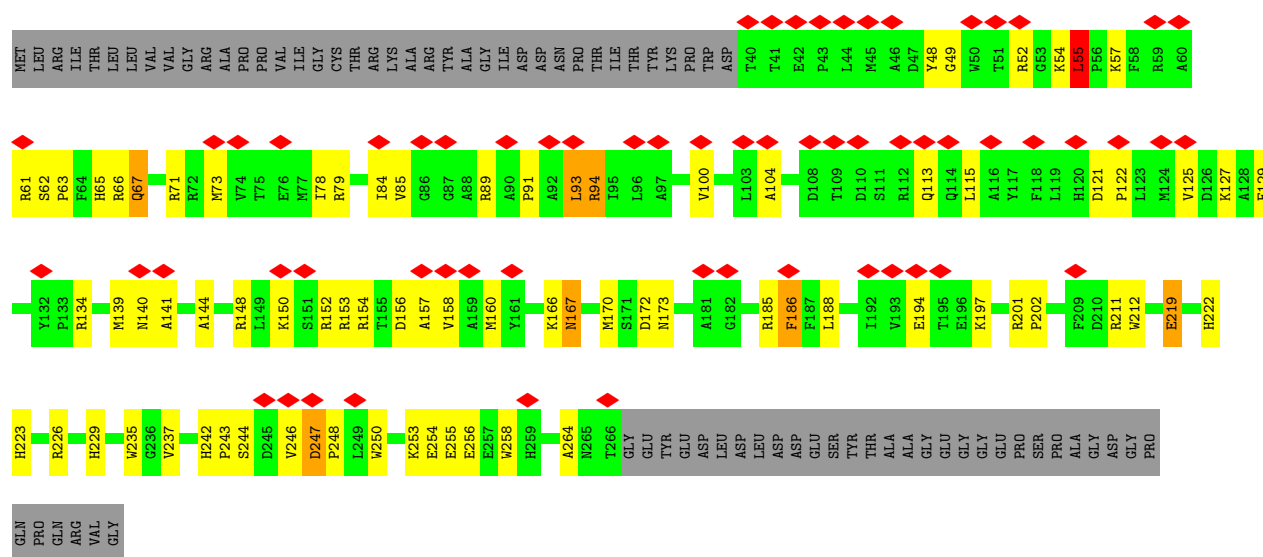




• Molecule 80: 50S ribosomal protein L16, putative

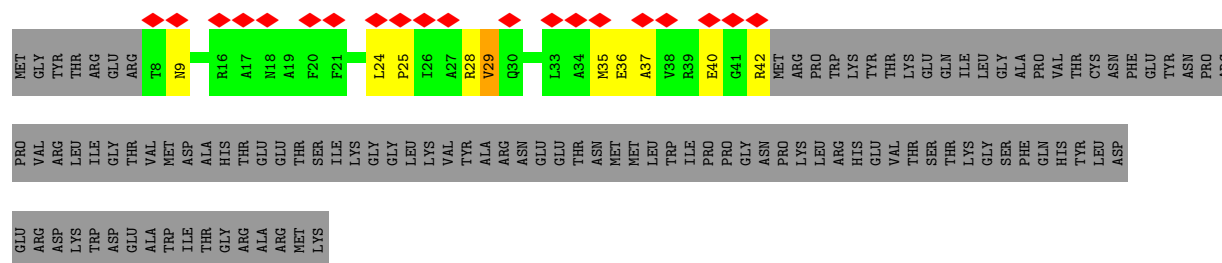


• Molecule 81: 50S ribosomal protein L17, putative

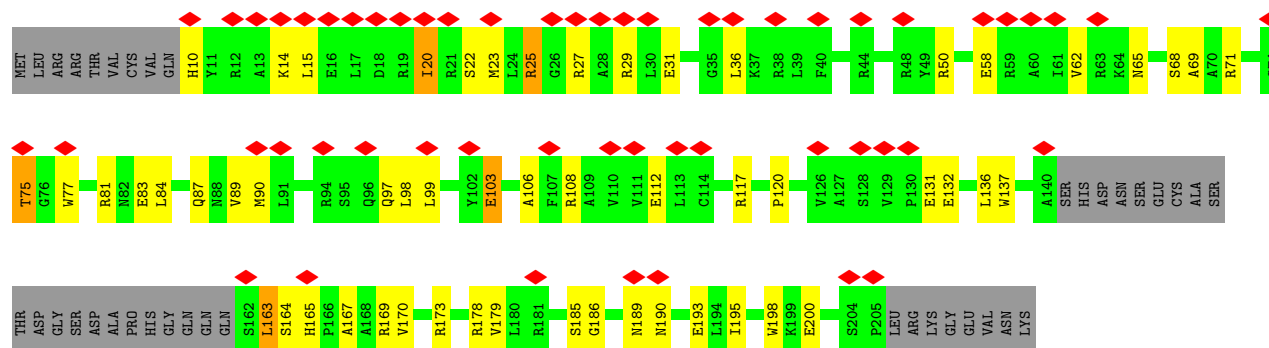


• Molecule 82: bL19m

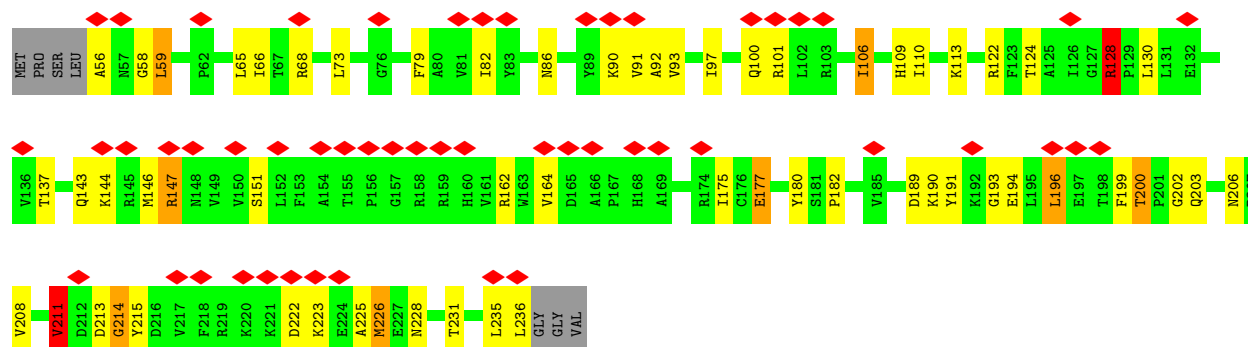




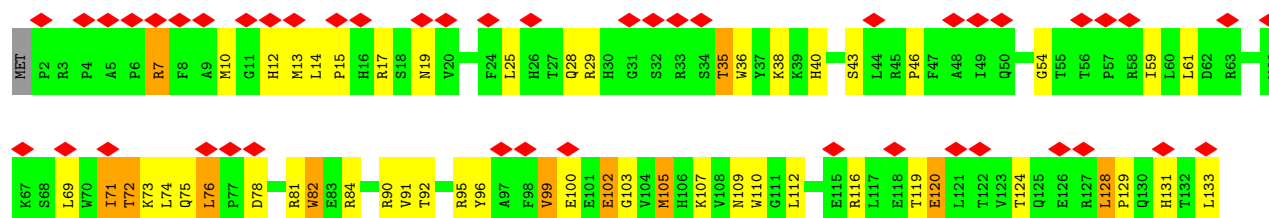
• Molecule 83: bL20m

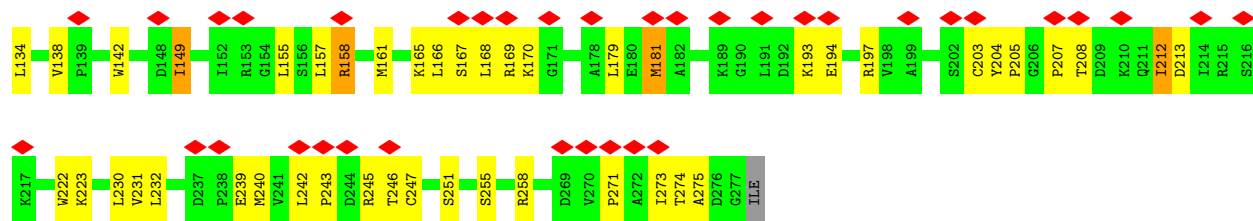


• Molecule 84: bL21m

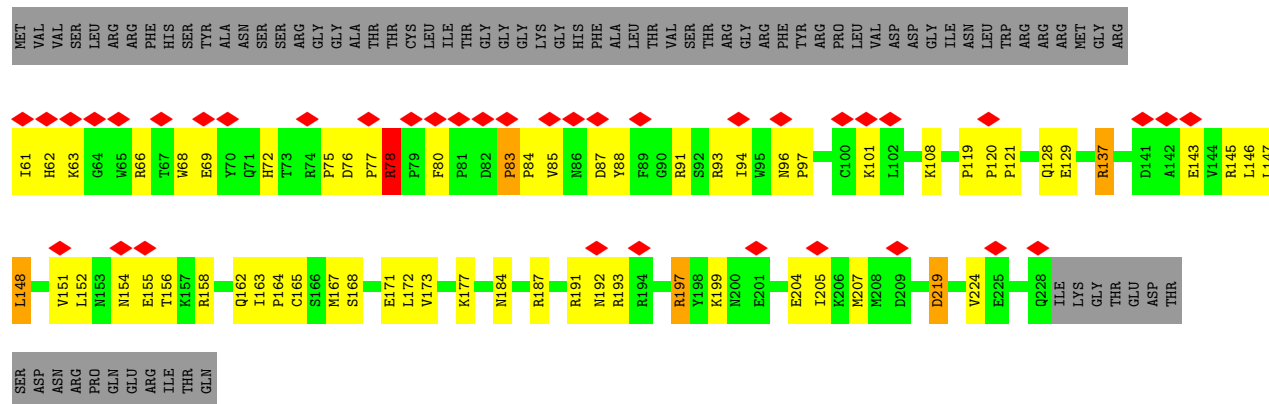
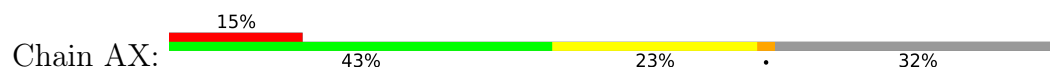


• Molecule 85: uL22m

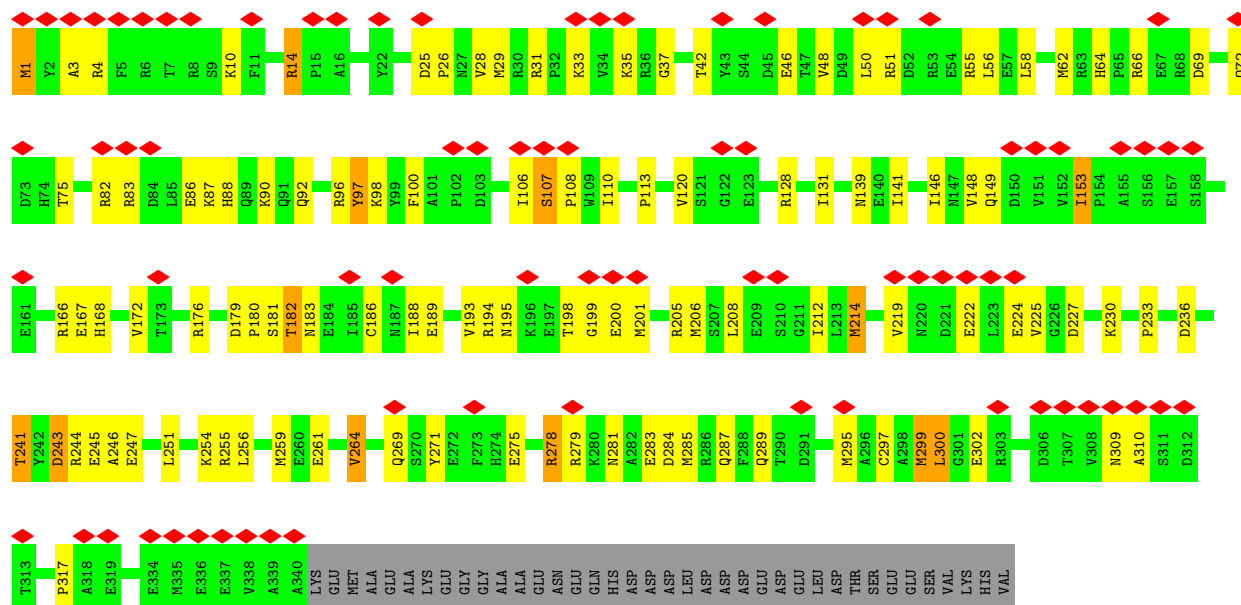




• Molecule 86: uL23m

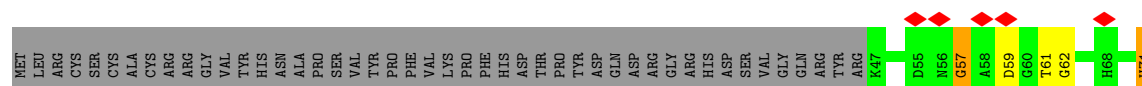


• Molecule 87: uL24m

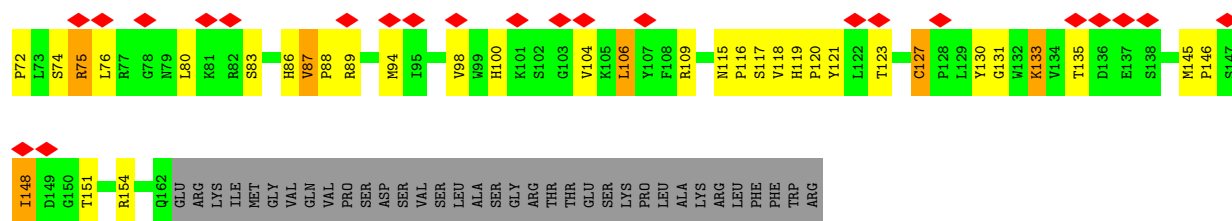


• Molecule 88: mL38

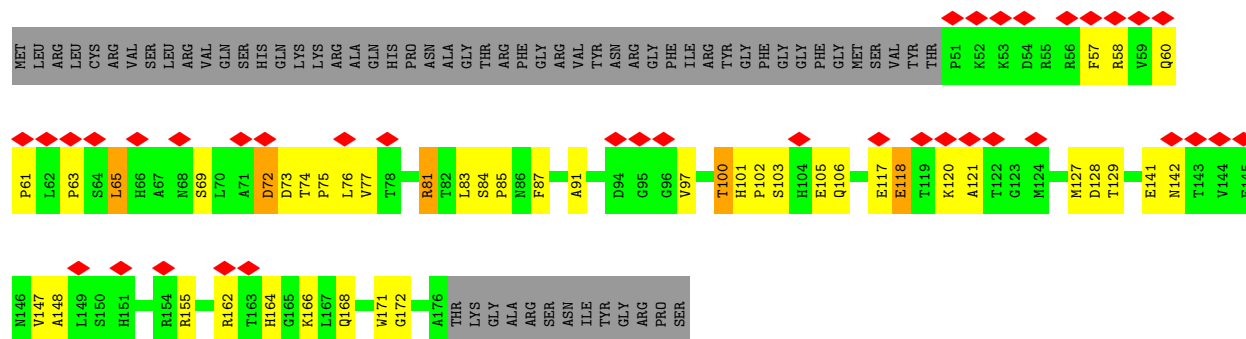
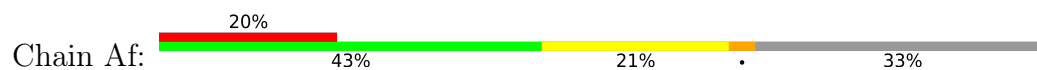




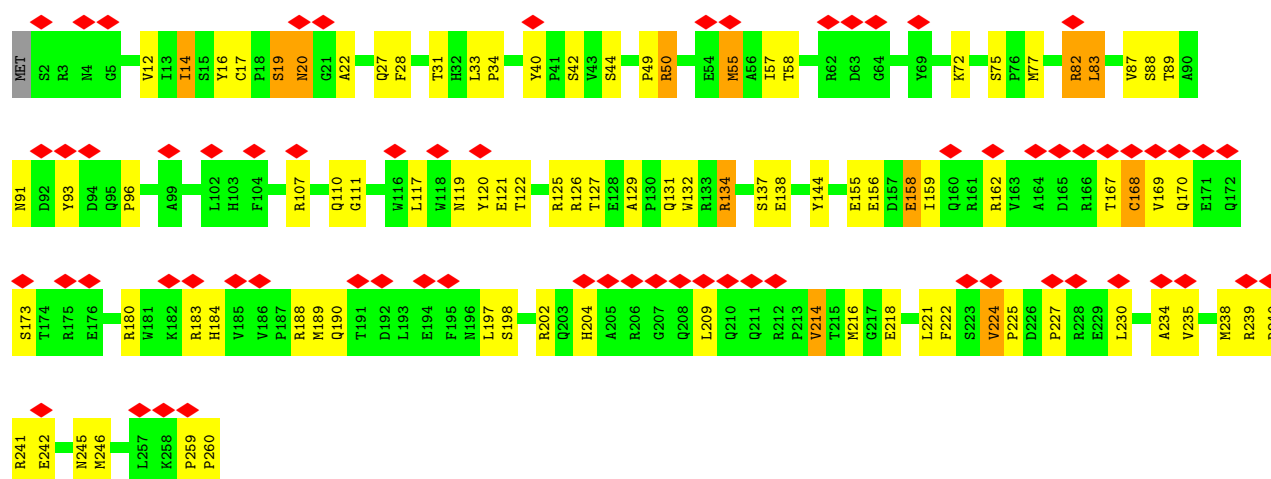




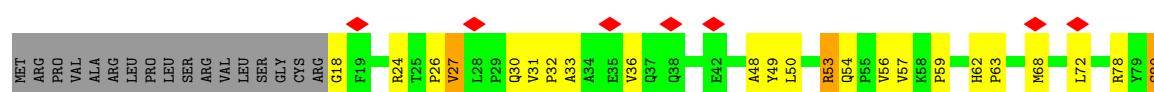
• Molecule 91: mL42

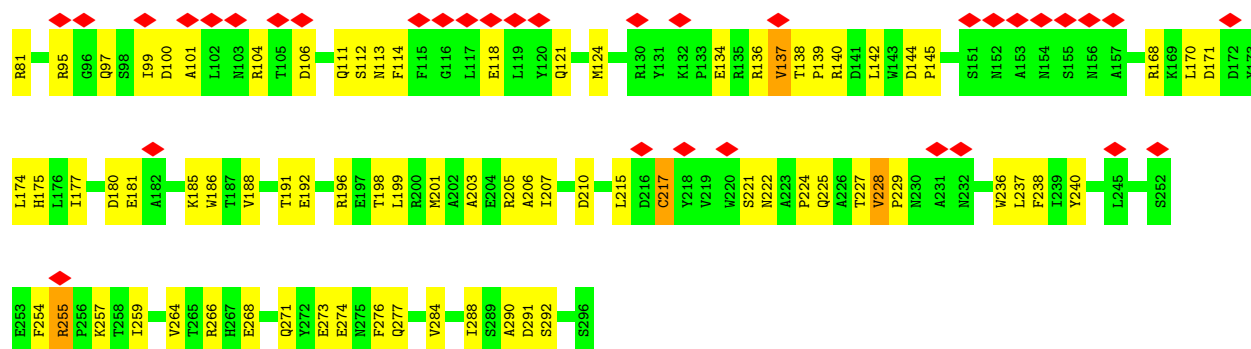


• Molecule 92: mL43

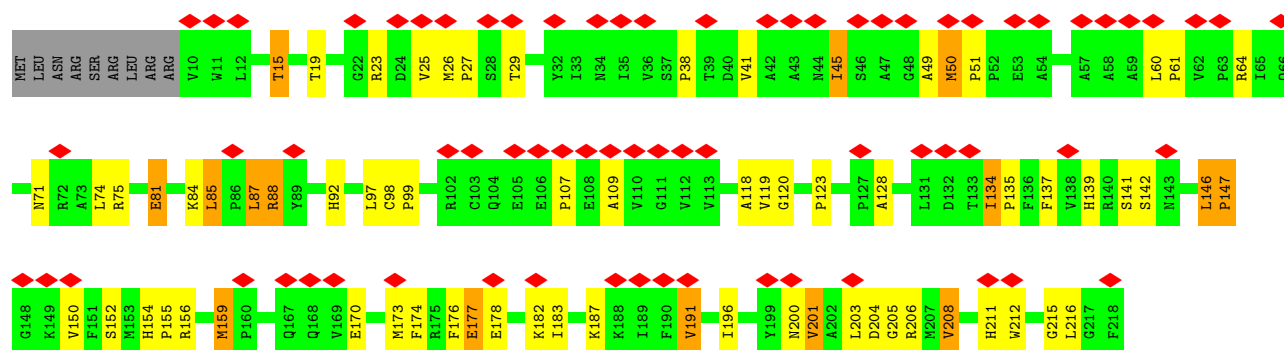


• Molecule 93: mL46

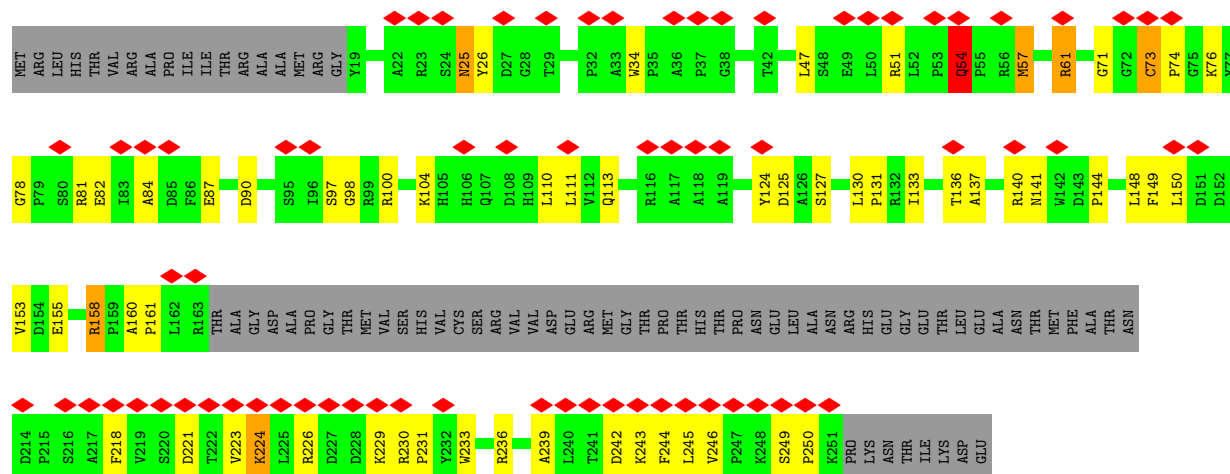




• Molecule 94: mL49

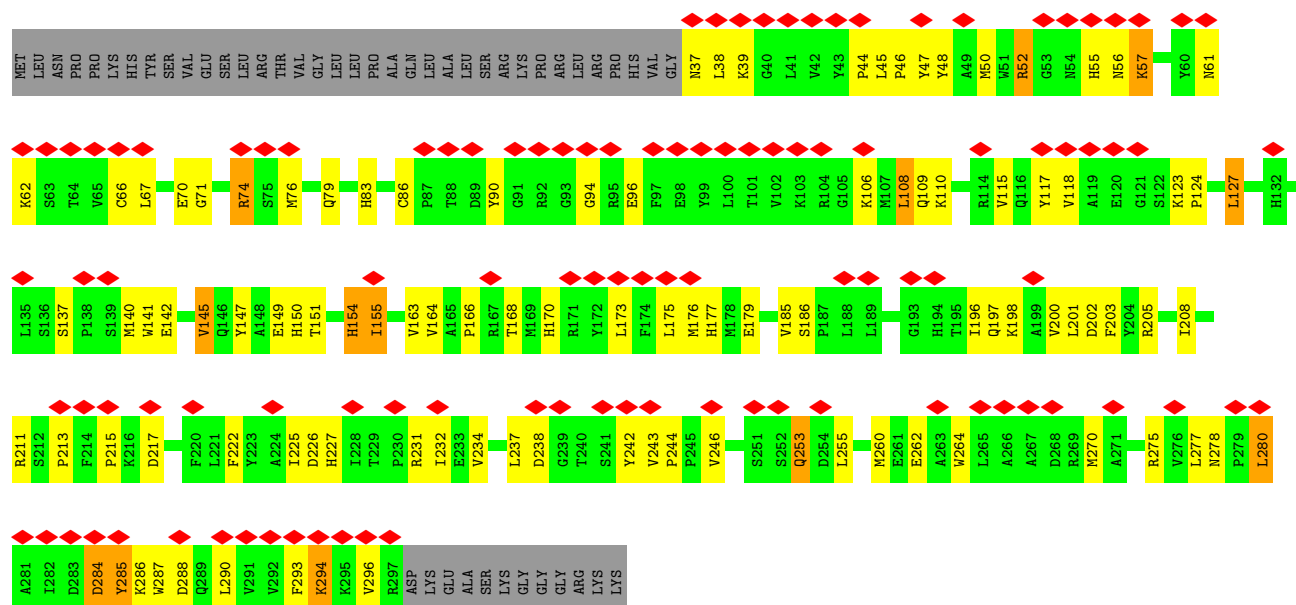


• Molecule 95: mL52

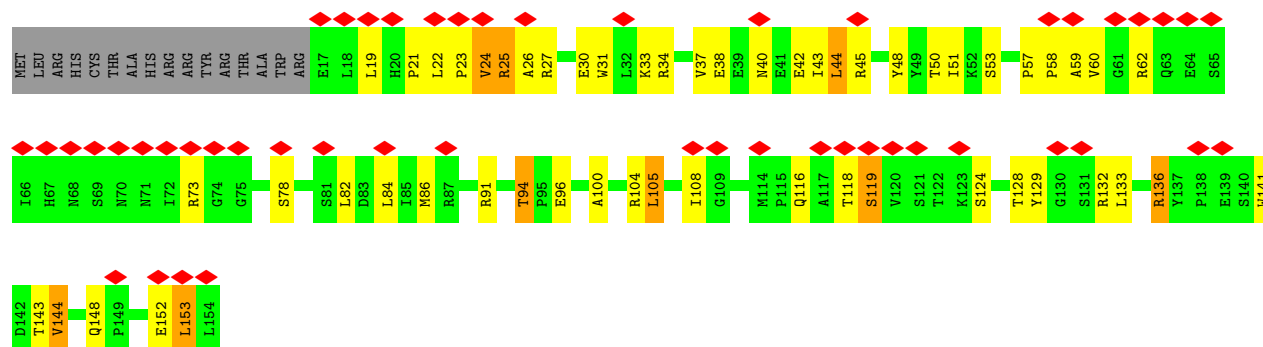


• Molecule 96: mL53

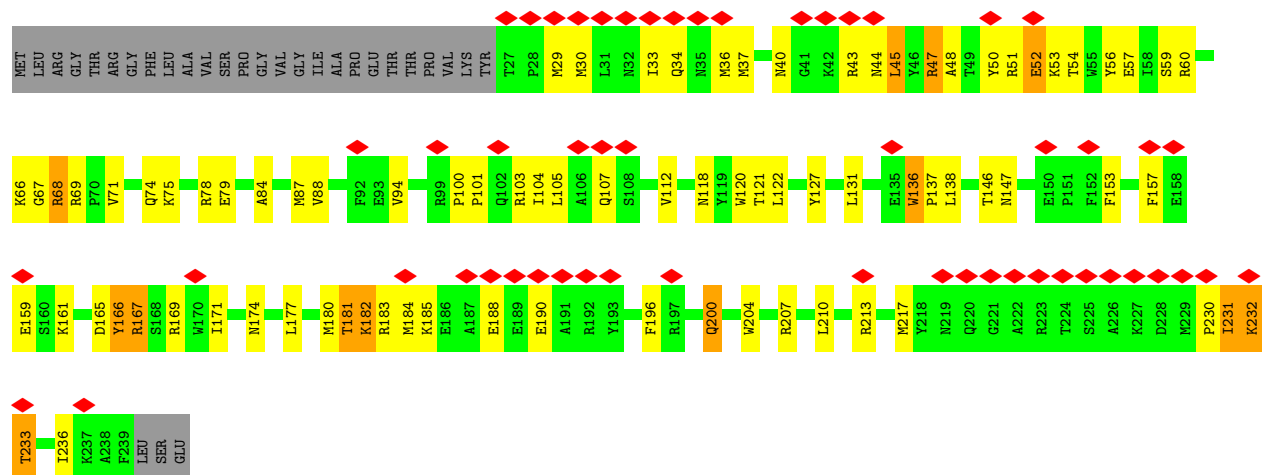




• Molecule 97: mL63

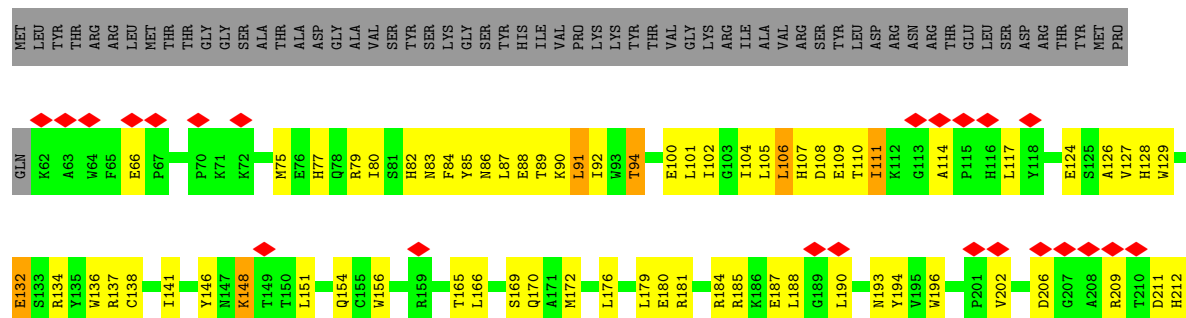


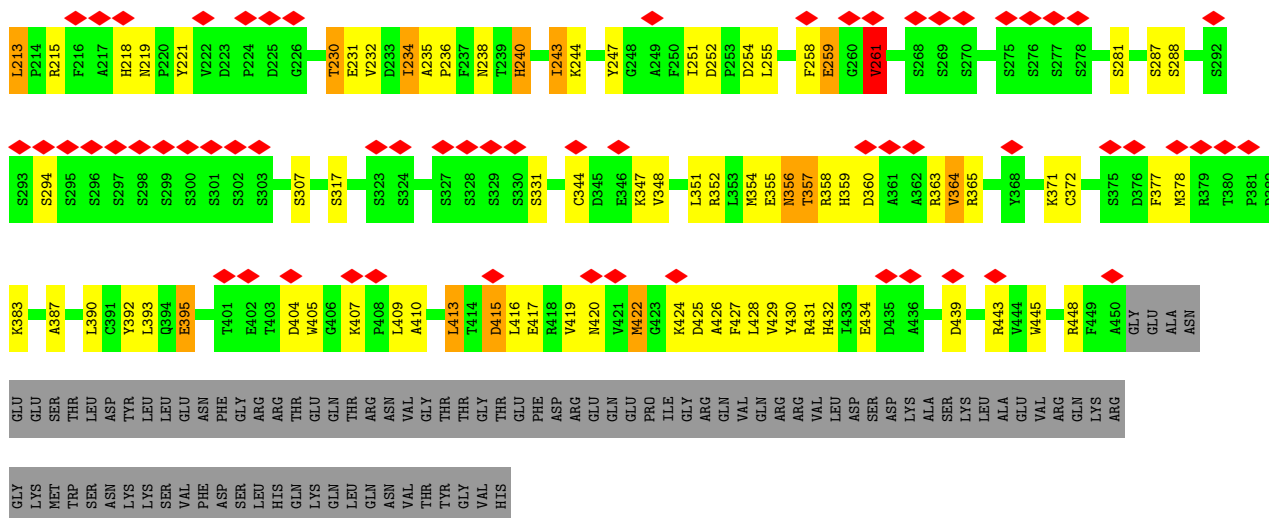
• Molecule 98: mL68



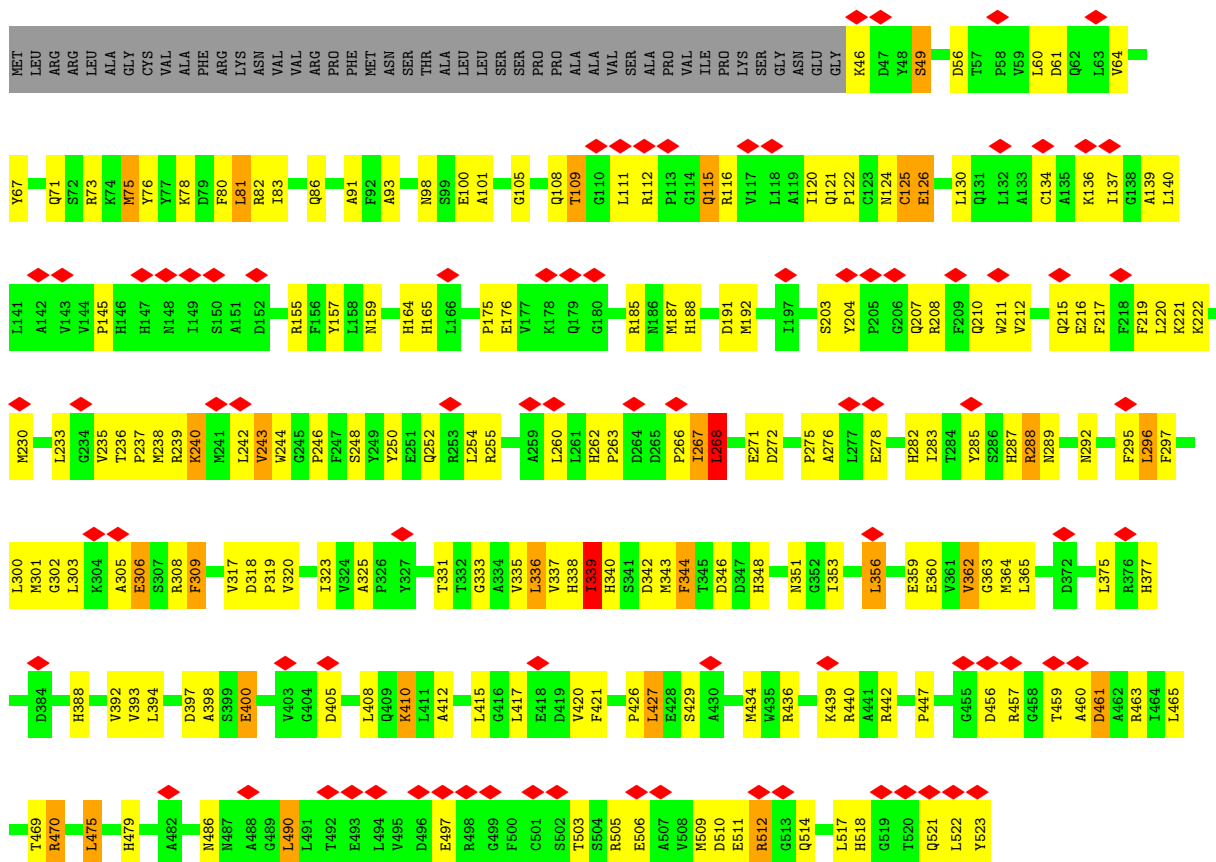




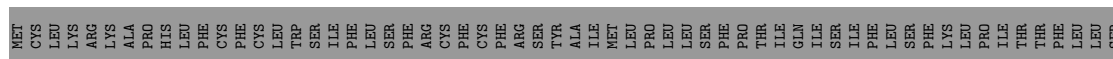


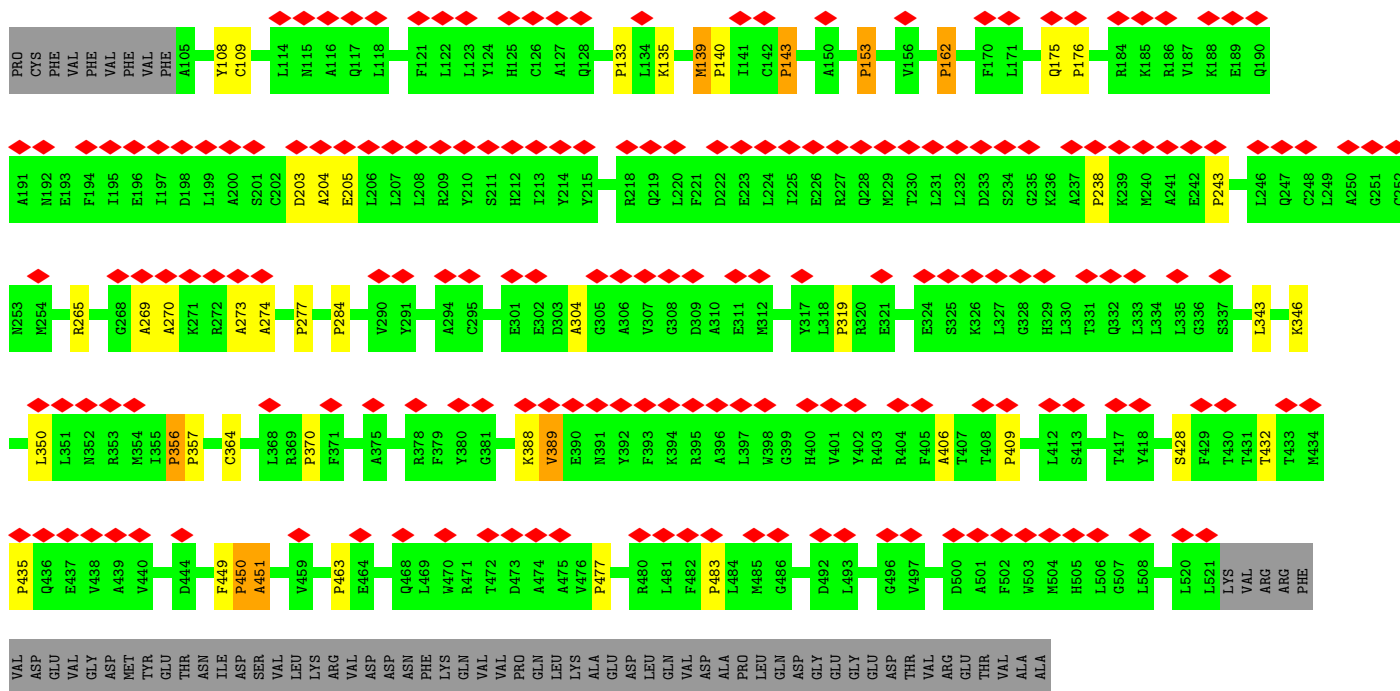


• Molecule 105: mL69

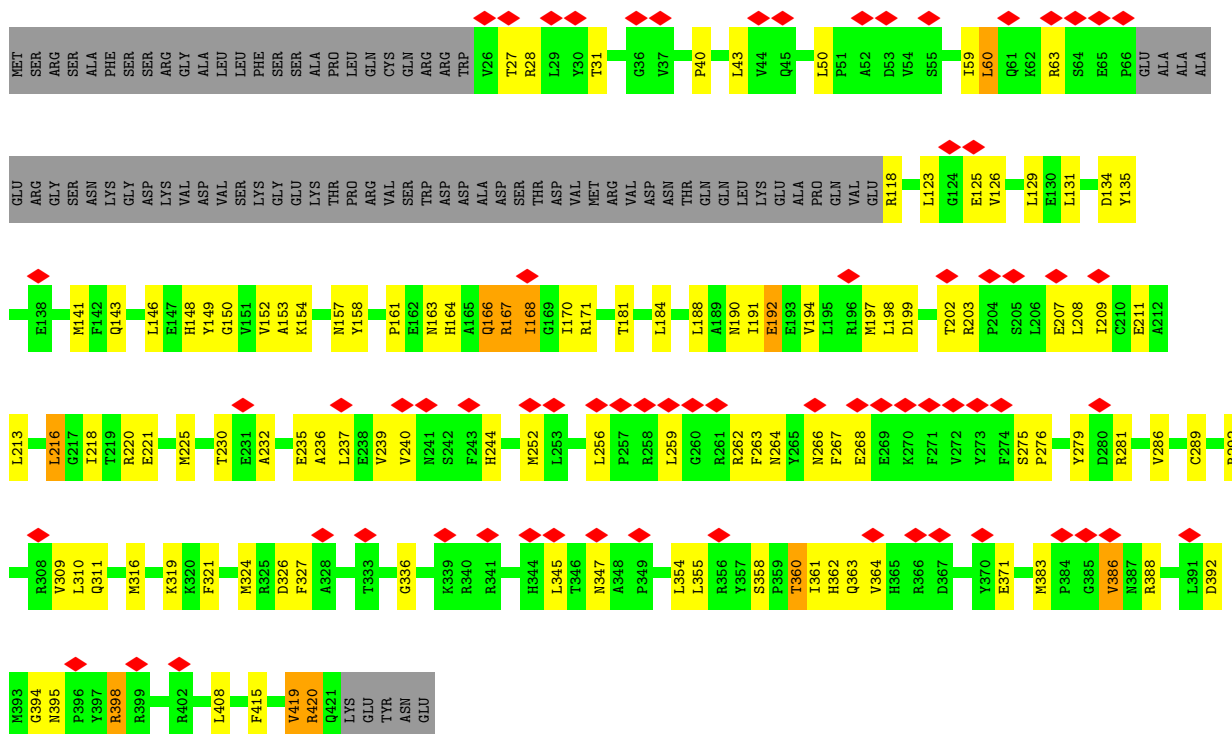


• Molecule 106: mL70

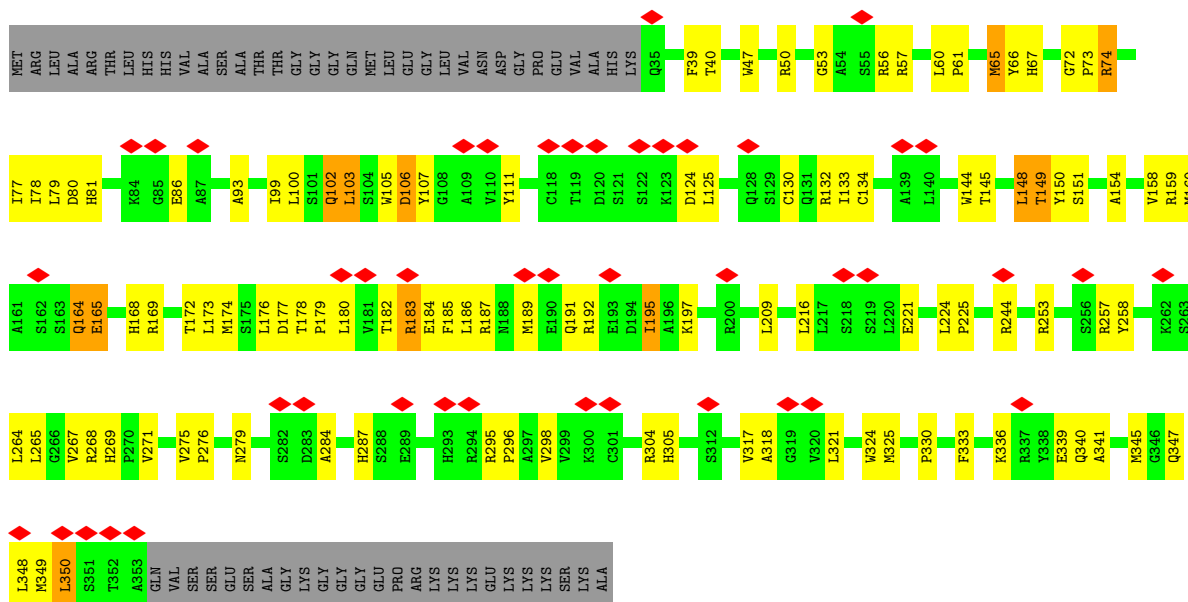






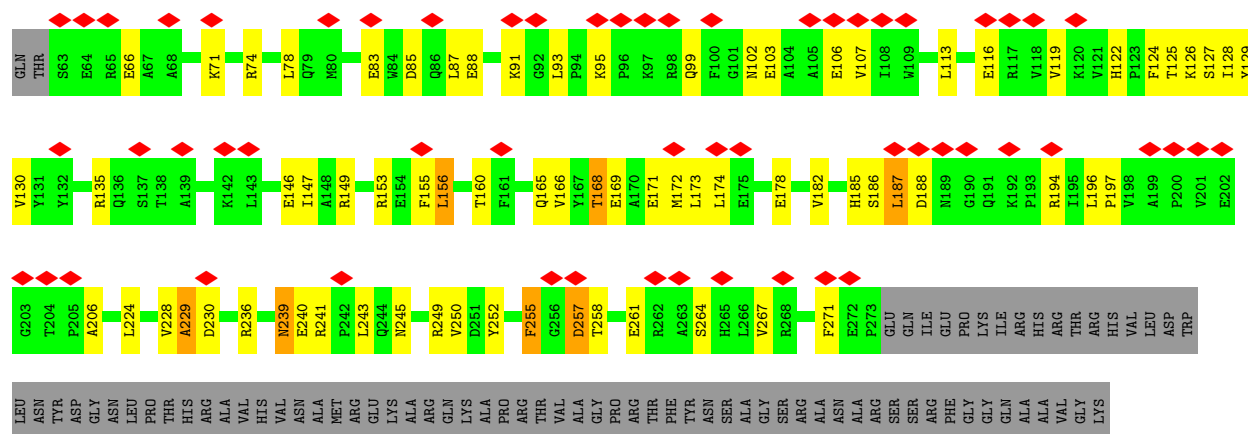


• Molecule 109: mL73



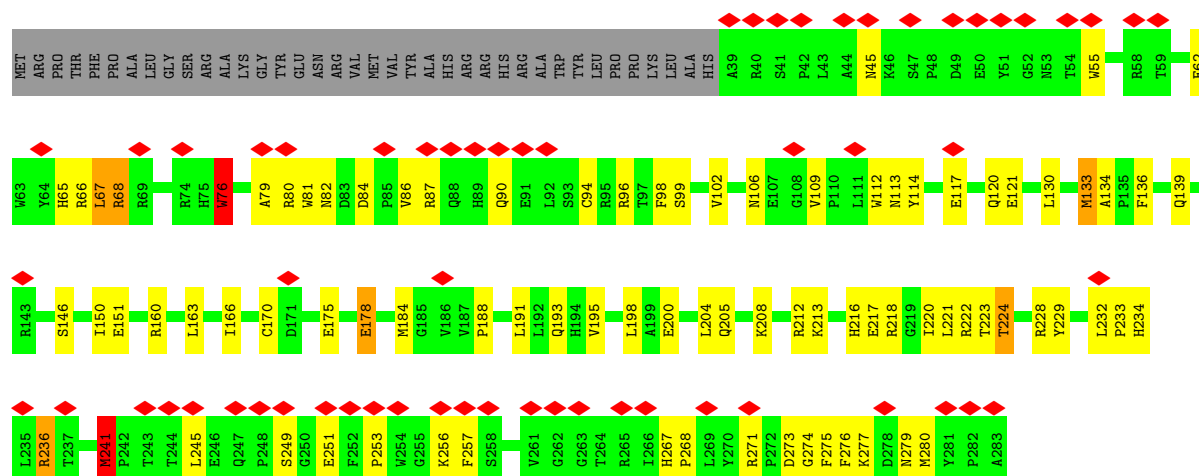
• Molecule 110: mL74



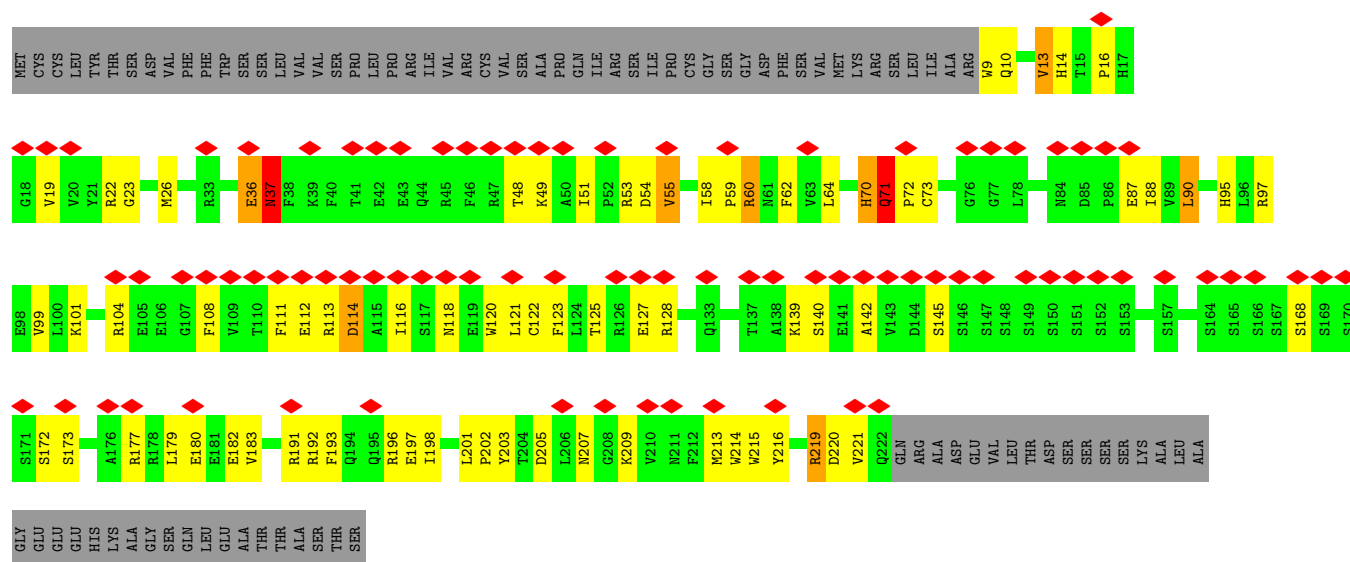




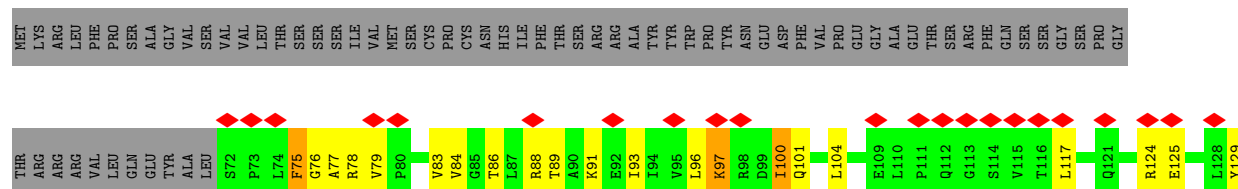
- Molecule 115: mL79

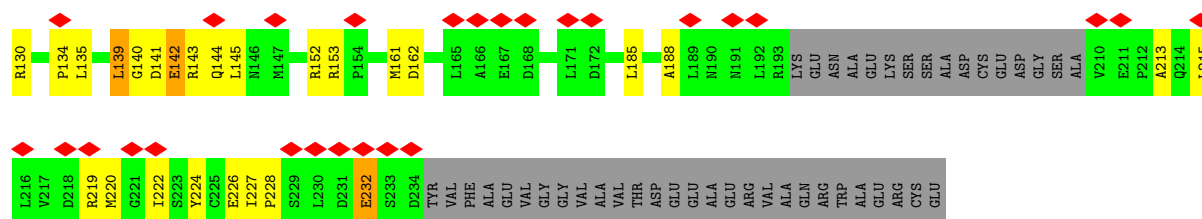


- Molecule 116: mL80

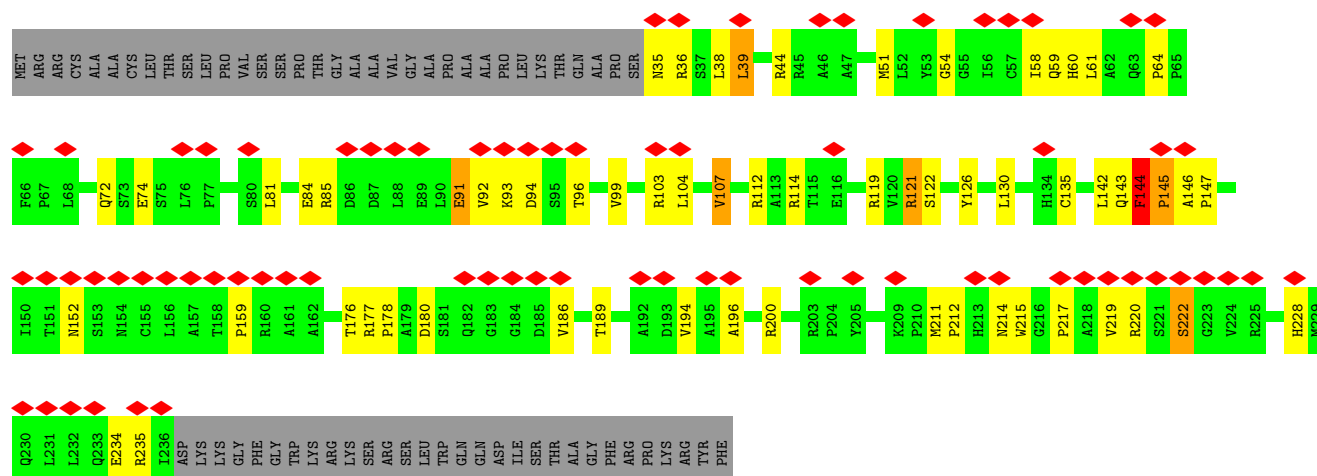


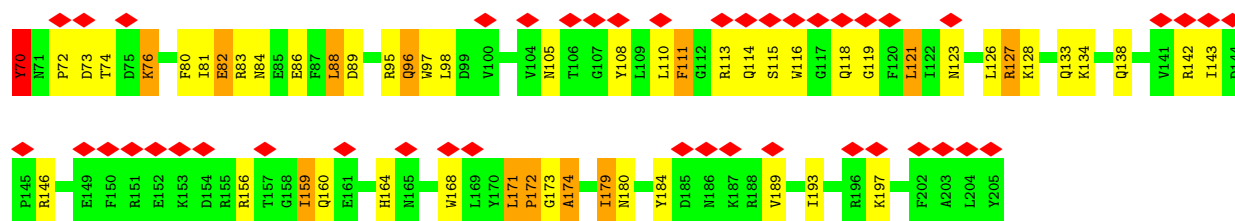
- Molecule 117: mL81



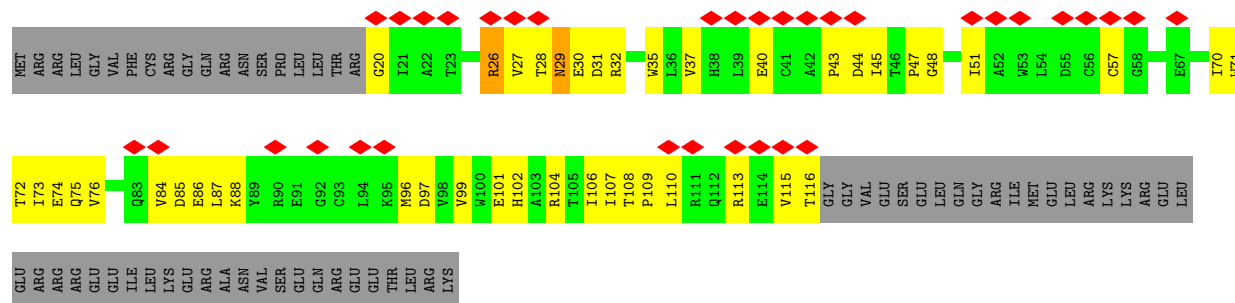


• Molecule 118: mL82

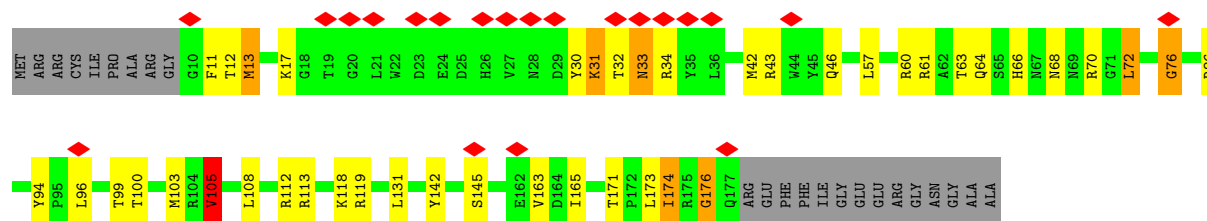




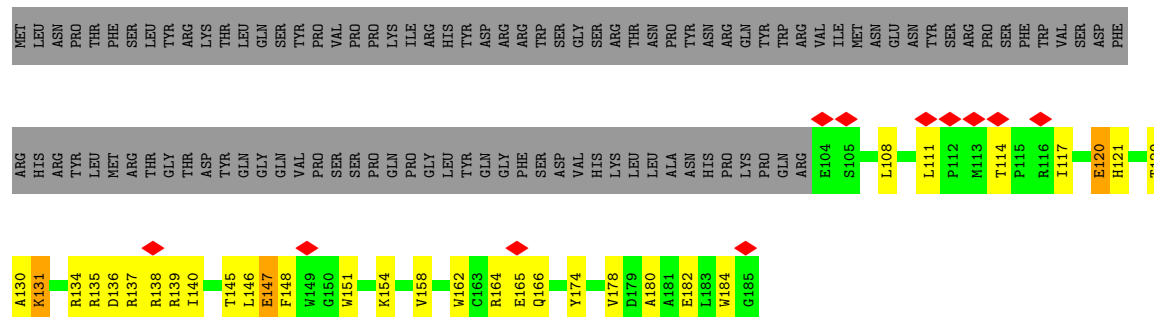
- Molecule 121: mL85



- Molecule 122: mL86

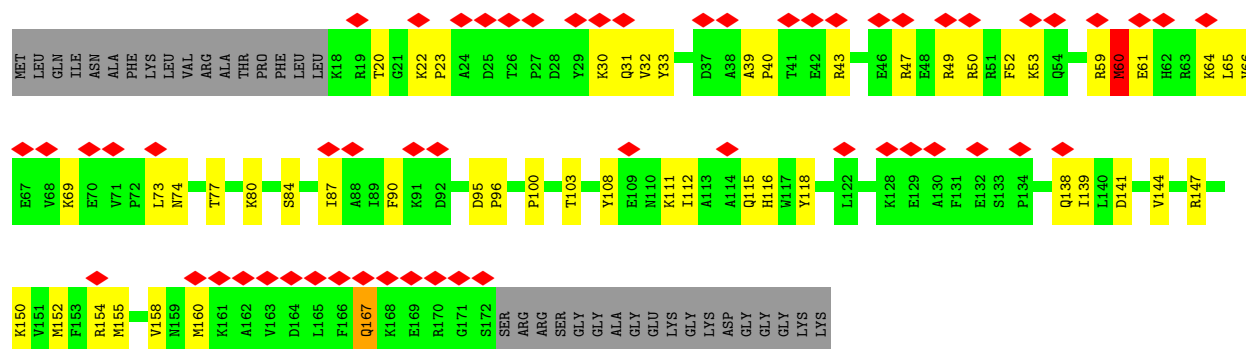


- Molecule 123: mL87

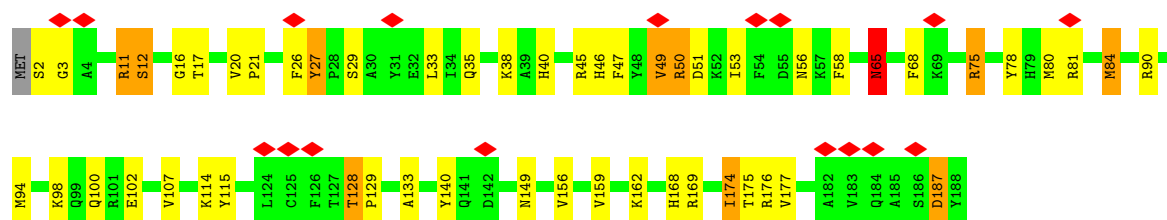


- Molecule 124: mL88

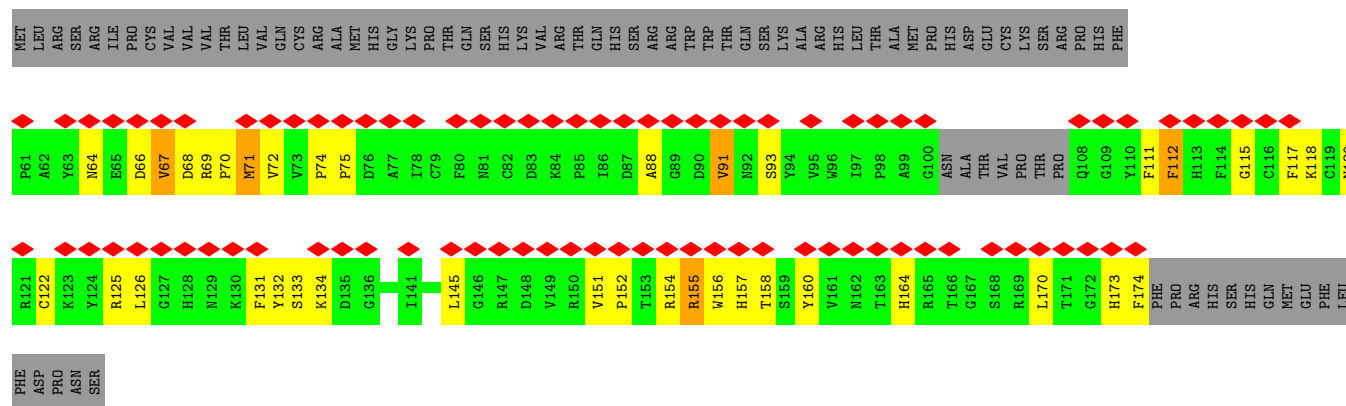




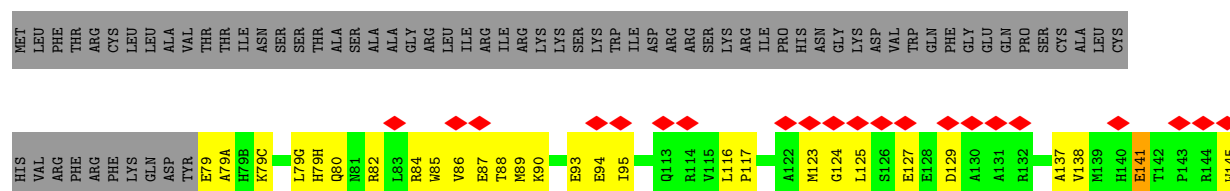
• Molecule 125: mL89

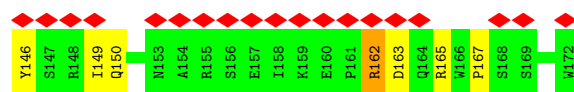


• Molecule 126: mL90

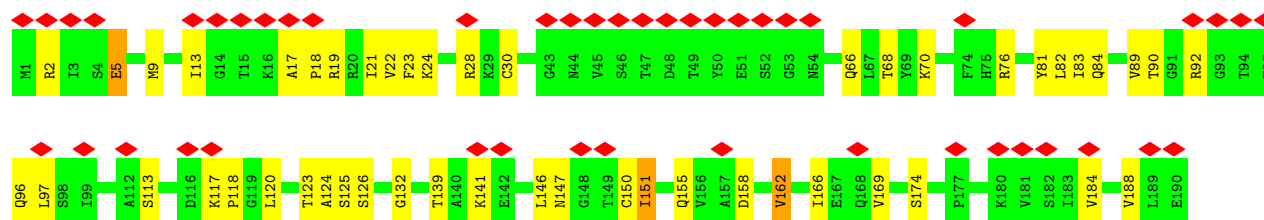
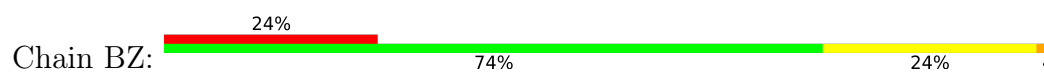


• Molecule 127: mS91

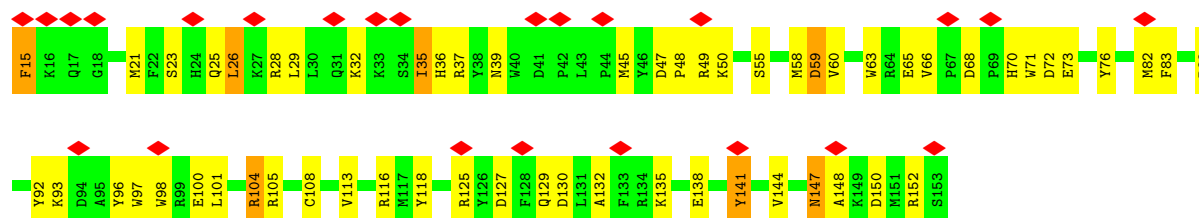




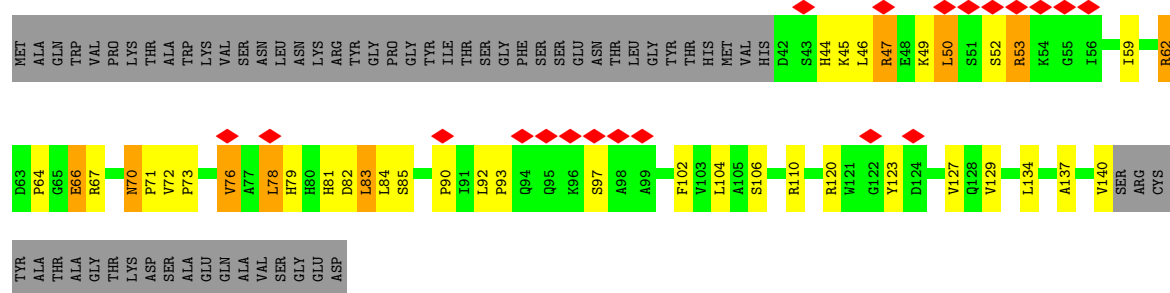
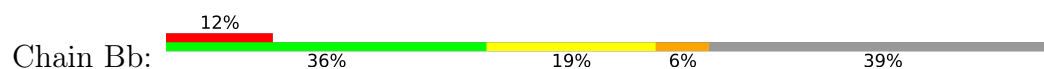
- Molecule 128: mL92



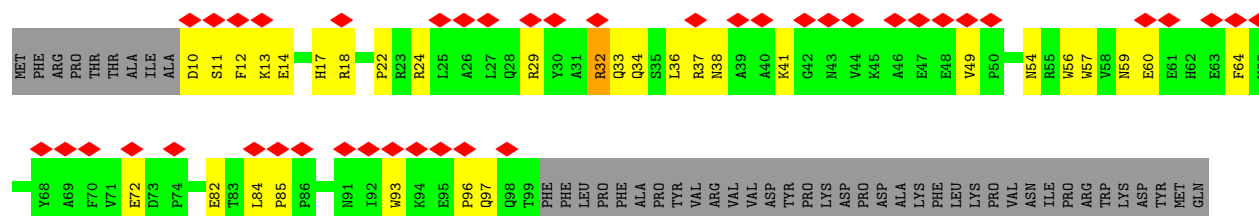
- Molecule 129: mL93



- Molecule 130: mL94



- Molecule 131: mL95

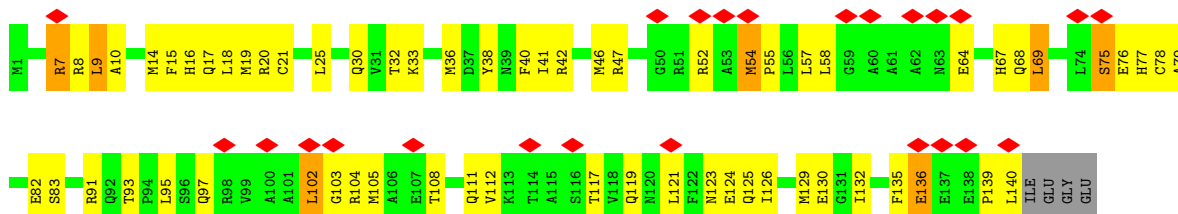




ARG  
THR  
LYS  
PRO  
VAL  
ILE  
PRO  
ARG  
THR  
TRP  
TYR

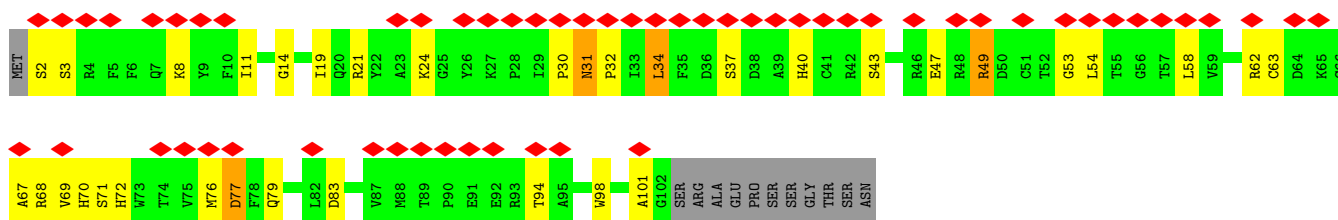
• Molecule 132: mL96

Chain Bd:  17% 53% 40% 5%



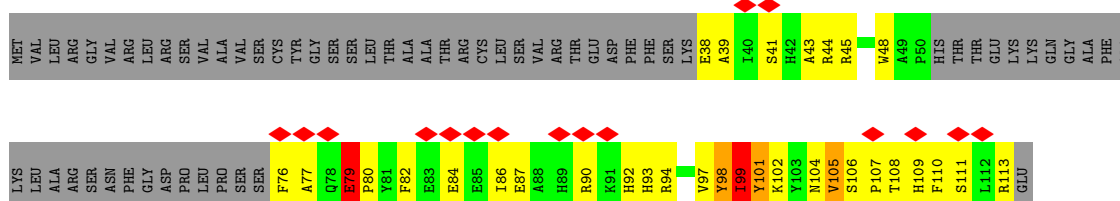
• Molecule 133: mL97

Chain Be:  51% 58% 27% 11%



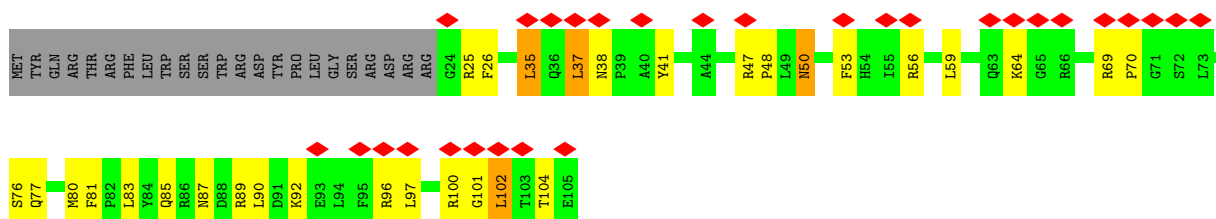
• Molecule 134: mL98

Chain Bf:  14% 15% 25% 56%



• Molecule 135: mL99

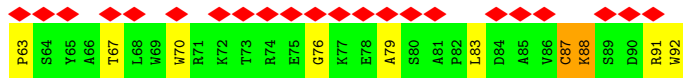
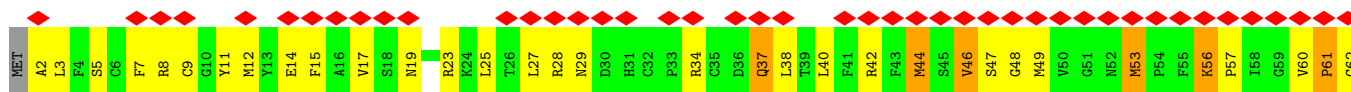
Chain Bg:  28% 49% 26% 22%



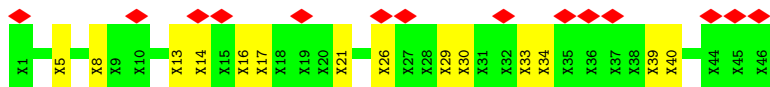
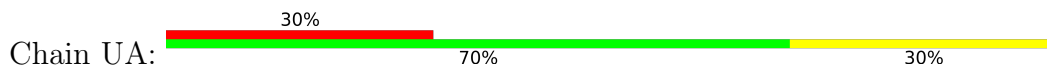
• Molecule 136: mL100

Chain Bh:  72% 52% 38% 9%

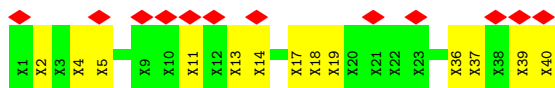




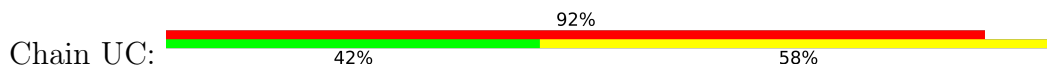
• Molecule 137: UNK



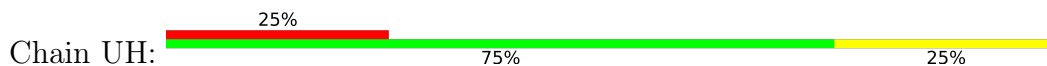
• Molecule 138: UNK



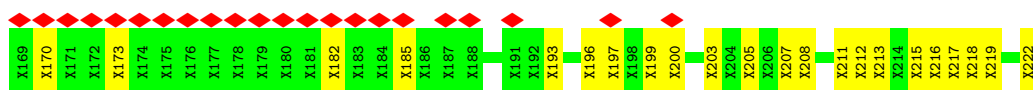
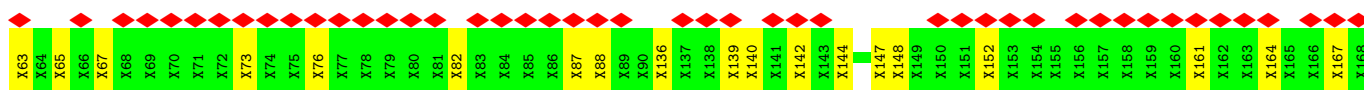
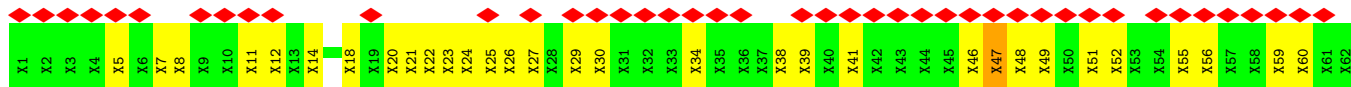
• Molecule 139: UNK



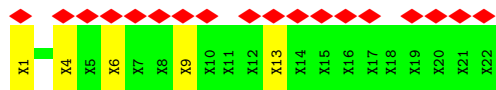
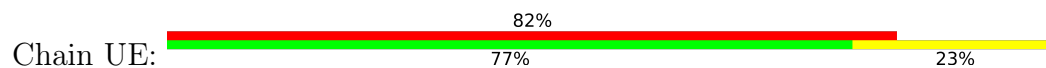
• Molecule 139: UNK



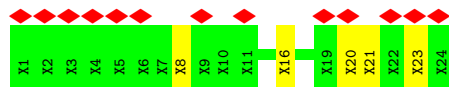
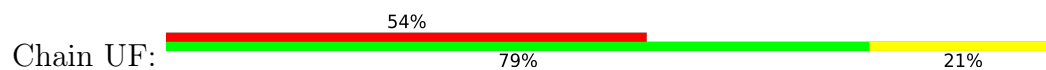
• Molecule 140: UNK



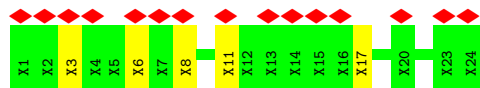
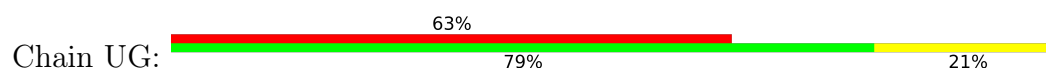
## • Molecule 141: UNK



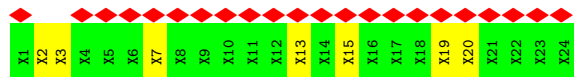
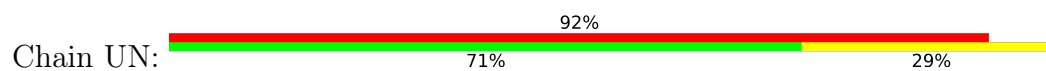
## • Molecule 142: UNK



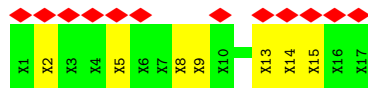
## • Molecule 142: UNK



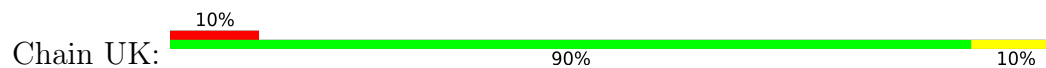
## • Molecule 142: UNK



## • Molecule 143: UNK



## • Molecule 144: UNK



## • Molecule 145: UNK



• Molecule 146: UNK



• Molecule 147: UNK



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 7141                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.183                                   | Depositor |
| Minimum map value                    | -0.090                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.012                                   | Depositor |
| Recommended contour level            | 0.054                                   | Depositor |
| Map size (Å)                         | 556.0, 556.0, 556.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.39, 1.39, 1.39                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UTP, NAD, SPD, SPM, GTP, ZN

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | DA    | 0.48         | 4/12780 (0.0%) | 0.89        | 34/17297 (0.2%) |
| 2   | DD    | 0.48         | 0/6710         | 0.91        | 11/9087 (0.1%)  |
| 3   | DI    | 0.46         | 0/3248         | 0.88        | 3/4401 (0.1%)   |
| 4   | DL    | 0.55         | 0/2346         | 0.97        | 11/3164 (0.3%)  |
| 5   | DM    | 0.50         | 0/2488         | 0.88        | 7/3362 (0.2%)   |
| 6   | DN    | 0.53         | 0/2148         | 0.99        | 10/2916 (0.3%)  |
| 7   | DO    | 0.46         | 0/1840         | 0.89        | 5/2482 (0.2%)   |
| 8   | DP    | 0.58         | 0/1813         | 0.89        | 2/2457 (0.1%)   |
| 9   | DQ    | 0.48         | 0/2111         | 0.92        | 0/2863          |
| 10  | DR    | 0.48         | 0/2090         | 0.92        | 4/2849 (0.1%)   |
| 11  | DS    | 0.44         | 0/1950         | 0.82        | 0/2633          |
| 12  | DU    | 0.46         | 0/1799         | 0.86        | 4/2438 (0.2%)   |
| 13  | DZ    | 0.45         | 0/725          | 0.87        | 2/984 (0.2%)    |
| 14  | Da    | 0.46         | 0/520          | 0.83        | 0/694           |
| 15  | DB    | 0.56         | 0/9369         | 0.98        | 30/12692 (0.2%) |
| 16  | DC    | 0.52         | 0/8952         | 0.93        | 23/12145 (0.2%) |
| 17  | DE    | 0.51         | 0/4955         | 0.97        | 15/6708 (0.2%)  |
| 18  | DF    | 0.57         | 0/4856         | 0.96        | 13/6581 (0.2%)  |
| 19  | DG    | 0.48         | 0/4674         | 0.92        | 5/6333 (0.1%)   |
| 20  | DH    | 0.58         | 0/4684         | 0.96        | 16/6347 (0.3%)  |
| 21  | DJ    | 0.57         | 1/2649 (0.0%)  | 0.97        | 6/3598 (0.2%)   |
| 22  | DK    | 0.58         | 0/2045         | 0.92        | 2/2759 (0.1%)   |
| 23  | DT    | 0.61         | 0/2133         | 1.03        | 7/2889 (0.2%)   |
| 24  | DV    | 0.61         | 0/1382         | 1.06        | 5/1871 (0.3%)   |
| 25  | DW    | 0.51         | 0/1407         | 0.95        | 4/1916 (0.2%)   |
| 26  | DX    | 0.56         | 0/1231         | 1.02        | 9/1654 (0.5%)   |
| 27  | DY    | 0.64         | 0/1334         | 0.98        | 3/1810 (0.2%)   |
| 28  | CC    | 0.63         | 0/666          | 1.09        | 2/900 (0.2%)    |
| 29  | CE    | 0.53         | 0/3484         | 0.90        | 4/4708 (0.1%)   |
| 30  | CF    | 0.46         | 0/1319         | 0.81        | 0/1783          |
| 31  | CH    | 0.52         | 0/2276         | 0.95        | 6/3071 (0.2%)   |
| 32  | CI    | 0.52         | 0/3453         | 0.89        | 2/4655 (0.0%)   |

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 33  | CJ    | 0.67         | 3/6705 (0.0%) | 1.06        | 49/9124 (0.5%)  |
| 34  | CK    | 0.45         | 0/2472        | 0.89        | 1/3315 (0.0%)   |
| 35  | CL    | 0.46         | 0/759         | 0.87        | 2/1026 (0.2%)   |
| 36  | CN    | 0.63         | 0/1361        | 0.99        | 4/1840 (0.2%)   |
| 37  | CO    | 0.48         | 0/3085        | 0.89        | 2/4165 (0.0%)   |
| 38  | CP    | 0.55         | 0/1533        | 0.93        | 5/2074 (0.2%)   |
| 39  | CQ    | 0.56         | 0/1631        | 0.99        | 4/2203 (0.2%)   |
| 40  | CR    | 0.49         | 0/2640        | 0.88        | 3/3572 (0.1%)   |
| 41  | CS    | 0.55         | 0/1209        | 1.05        | 12/1626 (0.7%)  |
| 42  | CU    | 0.45         | 0/1576        | 0.80        | 0/2115          |
| 43  | CZ    | 0.51         | 0/1237        | 0.88        | 1/1659 (0.1%)   |
| 44  | Ca    | 0.49         | 0/5159        | 0.90        | 13/6980 (0.2%)  |
| 45  | Cb    | 0.50         | 0/2105        | 0.88        | 0/2842          |
| 46  | Cd    | 0.50         | 0/2446        | 0.81        | 0/3299          |
| 47  | Cg    | 0.56         | 0/4025        | 1.00        | 15/5467 (0.3%)  |
| 48  | Ci    | 0.67         | 0/1388        | 1.09        | 4/1878 (0.2%)   |
| 49  | Cj    | 0.44         | 0/1842        | 0.87        | 2/2511 (0.1%)   |
| 50  | Ck    | 0.54         | 0/5696        | 0.94        | 6/7705 (0.1%)   |
| 51  | Cm    | 0.53         | 0/1616        | 0.97        | 5/2175 (0.2%)   |
| 52  | Cn    | 0.49         | 0/934         | 0.91        | 3/1248 (0.2%)   |
| 53  | Cp    | 0.44         | 0/1528        | 0.85        | 3/2072 (0.1%)   |
| 54  | Cq    | 0.48         | 0/2066        | 0.85        | 3/2815 (0.1%)   |
| 55  | Cr    | 0.45         | 0/2038        | 0.90        | 7/2759 (0.3%)   |
| 56  | Cv    | 0.46         | 0/8780        | 0.90        | 15/11901 (0.1%) |
| 57  | CA    | 0.30         | 0/14680       | 0.46        | 0/22831         |
| 64  | A0    | 0.45         | 0/1297        | 0.86        | 0/1750          |
| 65  | A1    | 0.48         | 0/1828        | 0.95        | 8/2466 (0.3%)   |
| 66  | A2    | 0.46         | 0/3740        | 0.92        | 5/5094 (0.1%)   |
| 67  | A3    | 0.53         | 0/1241        | 0.95        | 5/1674 (0.3%)   |
| 68  | A4    | 0.40         | 0/1423        | 0.86        | 0/1924          |
| 69  | A5    | 0.47         | 0/498         | 0.85        | 1/663 (0.2%)    |
| 70  | A6    | 0.43         | 0/578         | 0.99        | 4/774 (0.5%)    |
| 71  | A8    | 0.53         | 0/1230        | 1.01        | 3/1645 (0.2%)   |
| 72  | A9    | 0.44         | 0/474         | 0.82        | 0/639           |
| 73  | AE    | 0.49         | 0/2469        | 0.92        | 4/3364 (0.1%)   |
| 74  | AF    | 0.52         | 0/3706        | 0.94        | 14/5029 (0.3%)  |
| 75  | AI    | 0.46         | 0/1850        | 1.00        | 11/2515 (0.4%)  |
| 76  | AJ    | 0.43         | 0/986         | 0.84        | 1/1339 (0.1%)   |
| 77  | AK    | 0.41         | 0/2745        | 0.91        | 6/3705 (0.2%)   |
| 78  | AN    | 0.52         | 0/1561        | 0.93        | 4/2123 (0.2%)   |
| 79  | AP    | 0.51         | 0/2993        | 0.97        | 12/4060 (0.3%)  |
| 80  | AQ    | 0.42         | 0/1046        | 0.90        | 5/1415 (0.4%)   |
| 81  | AR    | 0.48         | 0/1969        | 0.93        | 4/2656 (0.2%)   |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 82  | AT    | 0.41         | 0/292   | 0.74        | 0/390          |
| 83  | AU    | 0.50         | 0/1456  | 0.87        | 1/1971 (0.1%)  |
| 84  | AV    | 0.53         | 0/1453  | 1.00        | 6/1970 (0.3%)  |
| 85  | AW    | 0.50         | 0/2291  | 0.91        | 2/3097 (0.1%)  |
| 86  | AX    | 0.47         | 0/1462  | 0.94        | 4/1986 (0.2%)  |
| 87  | AY    | 0.44         | 0/2763  | 0.89        | 5/3739 (0.1%)  |
| 88  | Ab    | 0.47         | 0/3651  | 0.91        | 10/4988 (0.2%) |
| 89  | Ad    | 0.39         | 0/2171  | 0.80        | 0/2930         |
| 90  | Ae    | 0.49         | 0/960   | 0.95        | 3/1304 (0.2%)  |
| 91  | Af    | 0.46         | 0/1037  | 0.90        | 1/1406 (0.1%)  |
| 92  | Ag    | 0.47         | 0/2253  | 0.88        | 8/3046 (0.3%)  |
| 93  | Aj    | 0.39         | 0/2306  | 0.88        | 7/3136 (0.2%)  |
| 94  | Al    | 0.52         | 0/1665  | 1.02        | 12/2270 (0.5%) |
| 95  | Ao    | 0.48         | 0/1523  | 0.89        | 7/2070 (0.3%)  |
| 96  | Ap    | 0.42         | 0/2213  | 0.95        | 9/3007 (0.3%)  |
| 97  | At    | 0.47         | 0/1128  | 0.91        | 1/1532 (0.1%)  |
| 98  | Av    | 0.46         | 0/1839  | 0.86        | 3/2478 (0.1%)  |
| 99  | AB    | 0.44         | 0/279   | 0.79        | 0/389          |
| 100 | AC    | 0.41         | 0/139   | 0.68        | 0/193          |
| 100 | AD    | 0.52         | 0/139   | 0.72        | 0/193          |
| 101 | AG    | 0.48         | 0/134   | 0.77        | 0/186          |
| 102 | AA    | 0.25         | 0/13972 | 0.43        | 0/21705        |
| 103 | BA    | 0.46         | 0/5501  | 0.91        | 17/7463 (0.2%) |
| 104 | BB    | 0.40         | 0/3122  | 0.87        | 5/4222 (0.1%)  |
| 105 | BC    | 0.48         | 0/3919  | 0.97        | 8/5318 (0.2%)  |
| 106 | BD    | 0.49         | 0/2062  | 1.11        | 21/2872 (0.7%) |
| 107 | BE    | 0.44         | 0/3184  | 0.93        | 19/4308 (0.4%) |
| 108 | BF    | 0.48         | 0/2900  | 0.91        | 5/3909 (0.1%)  |
| 109 | BG    | 0.38         | 0/2561  | 0.88        | 2/3469 (0.1%)  |
| 110 | BH    | 0.42         | 0/1778  | 0.89        | 3/2423 (0.1%)  |
| 111 | BI    | 0.45         | 0/2685  | 0.92        | 6/3633 (0.2%)  |
| 112 | BJ    | 0.40         | 0/1366  | 0.86        | 5/1846 (0.3%)  |
| 113 | BK    | 0.42         | 0/2040  | 0.88        | 4/2757 (0.1%)  |
| 114 | BL    | 0.46         | 0/1924  | 0.90        | 2/2596 (0.1%)  |
| 115 | BM    | 0.46         | 0/2082  | 0.96        | 3/2830 (0.1%)  |
| 116 | BN    | 0.39         | 0/1787  | 0.83        | 4/2415 (0.2%)  |
| 117 | BO    | 0.41         | 0/1160  | 0.81        | 0/1565         |
| 118 | BP    | 0.46         | 0/1593  | 0.98        | 4/2166 (0.2%)  |
| 119 | BQ    | 0.52         | 0/1716  | 1.01        | 11/2324 (0.5%) |
| 120 | BR    | 0.49         | 0/1693  | 1.01        | 8/2284 (0.4%)  |
| 121 | BS    | 0.43         | 0/801   | 0.88        | 0/1090         |
| 122 | BT    | 0.48         | 0/1417  | 0.89        | 3/1907 (0.2%)  |
| 123 | BU    | 0.42         | 0/711   | 0.81        | 0/955          |



| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 124 | BV    | 0.39         | 0/1340          | 0.81        | 0/1802            |
| 125 | BW    | 0.51         | 0/1604          | 0.92        | 4/2167 (0.2%)     |
| 126 | BX    | 0.40         | 0/897           | 0.86        | 2/1215 (0.2%)     |
| 127 | BY    | 0.40         | 0/908           | 0.83        | 0/1231            |
| 128 | BZ    | 0.43         | 0/1416          | 0.92        | 4/1919 (0.2%)     |
| 129 | Ba    | 0.55         | 0/1267          | 0.92        | 2/1711 (0.1%)     |
| 130 | Bb    | 0.42         | 0/785           | 1.01        | 5/1063 (0.5%)     |
| 131 | Bc    | 0.43         | 0/805           | 0.81        | 0/1091            |
| 132 | Bd    | 0.42         | 0/1133          | 0.83        | 0/1528            |
| 133 | Be    | 0.40         | 0/844           | 0.97        | 2/1139 (0.2%)     |
| 134 | Bf    | 0.48         | 0/450           | 1.07        | 5/609 (0.8%)      |
| 135 | Bg    | 0.43         | 0/671           | 0.93        | 2/905 (0.2%)      |
| 136 | Bh    | 0.44         | 0/752           | 0.87        | 0/1015            |
| All | All   | 0.48         | 8/317582 (0.0%) | 0.89        | 726/435817 (0.2%) |

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   | DA    | 0                   | 1                   |
| 2   | DD    | 0                   | 2                   |
| 4   | DL    | 0                   | 2                   |
| 6   | DN    | 0                   | 2                   |
| 7   | DO    | 0                   | 2                   |
| 10  | DR    | 0                   | 1                   |
| 15  | DB    | 0                   | 2                   |
| 16  | DC    | 0                   | 2                   |
| 19  | DG    | 0                   | 2                   |
| 21  | DJ    | 0                   | 1                   |
| 23  | DT    | 0                   | 1                   |
| 26  | DX    | 0                   | 1                   |
| 31  | CH    | 0                   | 1                   |
| 33  | CJ    | 0                   | 1                   |
| 44  | Ca    | 0                   | 1                   |
| 47  | Cg    | 0                   | 1                   |
| 48  | Ci    | 0                   | 1                   |
| 49  | Cj    | 0                   | 1                   |
| 50  | Ck    | 0                   | 1                   |
| 56  | Cv    | 0                   | 2                   |
| 66  | A2    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 67  | A3    | 0                   | 1                   |
| 71  | A8    | 0                   | 2                   |
| 73  | AE    | 0                   | 1                   |
| 74  | AF    | 0                   | 3                   |
| 81  | AR    | 0                   | 3                   |
| 83  | AU    | 0                   | 1                   |
| 84  | AV    | 0                   | 1                   |
| 85  | AW    | 0                   | 1                   |
| 87  | AY    | 0                   | 2                   |
| 88  | Ab    | 0                   | 1                   |
| 98  | Av    | 0                   | 1                   |
| 104 | BB    | 0                   | 1                   |
| 105 | BC    | 0                   | 1                   |
| 107 | BE    | 0                   | 2                   |
| 108 | BF    | 0                   | 1                   |
| 109 | BG    | 0                   | 1                   |
| 110 | BH    | 0                   | 1                   |
| 113 | BK    | 0                   | 2                   |
| 115 | BM    | 0                   | 2                   |
| 116 | BN    | 0                   | 3                   |
| 117 | BO    | 0                   | 1                   |
| 118 | BP    | 0                   | 2                   |
| 120 | BR    | 0                   | 2                   |
| 130 | Bb    | 0                   | 2                   |
| 134 | Bf    | 0                   | 2                   |
| 136 | Bh    | 0                   | 2                   |
| 140 | UD    | 0                   | 1                   |
| 142 | UN    | 0                   | 1                   |
| 147 | UU    | 0                   | 1                   |
| All | All   | 0                   | 75                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 33  | CJ    | 424 | HIS  | CG-CD2  | -12.72 | 1.21        | 1.35     |
| 1   | DA    | 323 | HIS  | CG-CD2  | 10.33  | 1.47        | 1.35     |
| 33  | CJ    | 424 | HIS  | CD2-NE2 | 9.03   | 1.47        | 1.37     |
| 33  | CJ    | 424 | HIS  | CG-ND1  | 7.86   | 1.47        | 1.38     |
| 21  | DJ    | 255 | LYS  | C-O     | 5.87   | 1.30        | 1.24     |
| 1   | DA    | 529 | ILE  | C-O     | 5.86   | 1.30        | 1.24     |
| 1   | DA    | 323 | HIS  | CD2-NE2 | -5.68  | 1.31        | 1.37     |
| 1   | DA    | 323 | HIS  | CB-CG   | -5.28  | 1.42        | 1.50     |

All (726) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 105 | BC    | 302 | GLY  | N-CA-C  | -15.09 | 91.90       | 111.37   |
| 34  | CK    | 283 | GLY  | N-CA-C  | 14.41  | 132.53      | 114.37   |
| 2   | DD    | 255 | VAL  | CA-C-N  | 12.45  | 135.40      | 119.84   |
| 2   | DD    | 255 | VAL  | C-N-CA  | 12.45  | 135.40      | 119.84   |
| 17  | DE    | 327 | ASN  | CA-C-N  | -11.01 | 109.04      | 120.38   |
| 17  | DE    | 327 | ASN  | C-N-CA  | -11.01 | 109.04      | 120.38   |
| 20  | DH    | 133 | CYS  | CA-C-N  | -10.97 | 106.12      | 119.84   |
| 20  | DH    | 133 | CYS  | C-N-CA  | -10.97 | 106.12      | 119.84   |
| 105 | BC    | 400 | GLU  | CA-C-N  | 10.80  | 133.34      | 119.84   |
| 105 | BC    | 400 | GLU  | C-N-CA  | 10.80  | 133.34      | 119.84   |
| 66  | A2    | 124 | TYR  | CA-C-N  | -10.66 | 109.40      | 120.38   |
| 66  | A2    | 124 | TYR  | C-N-CA  | -10.66 | 109.40      | 120.38   |
| 33  | CJ    | 783 | ILE  | CA-C-N  | 10.36  | 130.46      | 120.31   |
| 33  | CJ    | 783 | ILE  | C-N-CA  | 10.36  | 130.46      | 120.31   |
| 47  | Cg    | 16  | ARG  | CA-C-N  | 9.69   | 130.36      | 120.38   |
| 47  | Cg    | 16  | ARG  | C-N-CA  | 9.69   | 130.36      | 120.38   |
| 73  | AE    | 360 | PHE  | CA-C-N  | -9.62  | 107.82      | 119.84   |
| 73  | AE    | 360 | PHE  | C-N-CA  | -9.62  | 107.82      | 119.84   |
| 50  | Ck    | 687 | ARG  | N-CA-C  | 9.48   | 126.01      | 113.30   |
| 81  | AR    | 247 | ASP  | CA-C-N  | 9.32   | 129.40      | 119.89   |
| 81  | AR    | 247 | ASP  | C-N-CA  | 9.32   | 129.40      | 119.89   |
| 106 | BD    | 356 | PRO  | N-CA-CB | 8.89   | 111.70      | 103.08   |
| 28  | CC    | 10  | VAL  | N-CA-C  | 8.85   | 120.61      | 112.29   |
| 87  | AY    | 317 | PRO  | N-CA-CB | 8.75   | 110.96      | 103.35   |
| 33  | CJ    | 712 | THR  | CA-C-N  | -8.65  | 109.03      | 119.84   |
| 33  | CJ    | 712 | THR  | C-N-CA  | -8.65  | 109.03      | 119.84   |
| 120 | BR    | 171 | LEU  | CA-C-N  | -8.63  | 109.06      | 119.84   |
| 120 | BR    | 171 | LEU  | C-N-CA  | -8.63  | 109.06      | 119.84   |
| 32  | CI    | 65  | MET  | CA-C-N  | 8.57   | 128.15      | 119.24   |
| 32  | CI    | 65  | MET  | C-N-CA  | 8.57   | 128.15      | 119.24   |
| 78  | AN    | 164 | HIS  | CA-C-N  | 8.55   | 128.76      | 119.87   |
| 78  | AN    | 164 | HIS  | C-N-CA  | 8.55   | 128.76      | 119.87   |
| 118 | BP    | 144 | PHE  | CA-C-N  | -8.50  | 109.21      | 119.84   |
| 118 | BP    | 144 | PHE  | C-N-CA  | -8.50  | 109.21      | 119.84   |
| 111 | BI    | 48  | PHE  | CA-C-N  | -8.44  | 109.29      | 119.84   |
| 111 | BI    | 48  | PHE  | C-N-CA  | -8.44  | 109.29      | 119.84   |
| 33  | CJ    | 345 | VAL  | CA-C-N  | 8.43   | 128.00      | 119.24   |
| 33  | CJ    | 345 | VAL  | C-N-CA  | 8.43   | 128.00      | 119.24   |
| 70  | A6    | 73  | ASP  | CA-C-N  | 8.41   | 128.38      | 119.05   |
| 70  | A6    | 73  | ASP  | C-N-CA  | 8.41   | 128.38      | 119.05   |
| 106 | BD    | 238 | PRO  | N-CA-CB | 8.37   | 110.33      | 101.88   |
| 15  | DB    | 944 | HIS  | N-CA-C  | 8.34   | 124.04      | 112.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 108 | BF    | 358 | SER  | CA-C-N      | 8.30  | 128.02      | 119.56   |
| 108 | BF    | 358 | SER  | C-N-CA      | 8.30  | 128.02      | 119.56   |
| 106 | BD    | 451 | ALA  | N-CA-C      | 8.22  | 120.15      | 111.03   |
| 20  | DH    | 367 | LEU  | N-CA-C      | -8.20 | 95.81       | 108.76   |
| 44  | Ca    | 32  | PRO  | N-CA-CB     | 8.13  | 110.97      | 103.08   |
| 7   | DO    | 125 | LEU  | CA-C-N      | -8.11 | 110.57      | 119.98   |
| 7   | DO    | 125 | LEU  | C-N-CA      | -8.11 | 110.57      | 119.98   |
| 47  | Cg    | 49  | VAL  | CA-C-N      | -8.07 | 109.75      | 119.84   |
| 47  | Cg    | 49  | VAL  | C-N-CA      | -8.07 | 109.75      | 119.84   |
| 118 | BP    | 159 | PRO  | N-CA-CB     | 8.05  | 110.01      | 101.88   |
| 17  | DE    | 739 | PRO  | CA-C-N      | 8.02  | 128.46      | 119.32   |
| 17  | DE    | 739 | PRO  | C-N-CA      | 8.02  | 128.46      | 119.32   |
| 15  | DB    | 554 | GLU  | CA-C-N      | -8.00 | 111.76      | 119.76   |
| 15  | DB    | 554 | GLU  | C-N-CA      | -8.00 | 111.76      | 119.76   |
| 86  | AX    | 83  | PRO  | CA-C-N      | 7.99  | 127.71      | 119.56   |
| 86  | AX    | 83  | PRO  | C-N-CA      | 7.99  | 127.71      | 119.56   |
| 110 | BH    | 230 | ASP  | CA-C-N      | 7.97  | 127.69      | 119.56   |
| 110 | BH    | 230 | ASP  | C-N-CA      | 7.97  | 127.69      | 119.56   |
| 130 | Bb    | 70  | ASN  | CA-C-N      | 7.89  | 129.70      | 119.84   |
| 130 | Bb    | 70  | ASN  | C-N-CA      | 7.89  | 129.70      | 119.84   |
| 33  | CJ    | 803 | ILE  | CA-C-N      | -7.89 | 111.47      | 123.14   |
| 33  | CJ    | 803 | ILE  | C-N-CA      | -7.89 | 111.47      | 123.14   |
| 17  | DE    | 591 | LEU  | CA-C-N      | -7.88 | 110.54      | 120.23   |
| 17  | DE    | 591 | LEU  | C-N-CA      | -7.88 | 110.54      | 120.23   |
| 33  | CJ    | 424 | HIS  | ND1-CE1-NE2 | 7.86  | 116.26      | 108.40   |
| 92  | Ag    | 20  | ASN  | N-CA-C      | 7.85  | 120.97      | 111.40   |
| 92  | Ag    | 19  | SER  | N-CA-C      | 7.84  | 123.15      | 113.50   |
| 1   | DA    | 311 | THR  | CA-C-N      | 7.81  | 127.45      | 119.56   |
| 1   | DA    | 311 | THR  | C-N-CA      | 7.81  | 127.45      | 119.56   |
| 55  | Cr    | 28  | PRO  | N-CA-CB     | 7.74  | 110.59      | 103.08   |
| 133 | Be    | 31  | ASN  | CA-C-N      | 7.72  | 127.36      | 119.56   |
| 133 | Be    | 31  | ASN  | C-N-CA      | 7.72  | 127.36      | 119.56   |
| 50  | Ck    | 659 | GLY  | CA-C-N      | -7.70 | 112.90      | 120.52   |
| 50  | Ck    | 659 | GLY  | C-N-CA      | -7.70 | 112.90      | 120.52   |
| 67  | A3    | 155 | VAL  | CA-C-N      | 7.69  | 127.59      | 119.05   |
| 67  | A3    | 155 | VAL  | C-N-CA      | 7.69  | 127.59      | 119.05   |
| 84  | AV    | 214 | GLY  | N-CA-C      | -7.66 | 104.75      | 115.32   |
| 17  | DE    | 613 | ILE  | N-CA-C      | 7.64  | 118.23      | 110.82   |
| 10  | DR    | 257 | GLY  | N-CA-C      | -7.64 | 103.32      | 115.08   |
| 15  | DB    | 672 | VAL  | N-CA-C      | 7.63  | 118.38      | 110.36   |
| 103 | BA    | 704 | THR  | CA-C-N      | 7.57  | 127.21      | 119.56   |
| 103 | BA    | 704 | THR  | C-N-CA      | 7.57  | 127.21      | 119.56   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 16  | DC    | 601  | GLU  | N-CA-C  | 7.57  | 119.22      | 110.97   |
| 96  | Ap    | 57   | LYS  | N-CA-C  | 7.56  | 122.19      | 113.19   |
| 135 | Bg    | 38   | ASN  | CA-C-N  | 7.56  | 129.29      | 119.84   |
| 135 | Bg    | 38   | ASN  | C-N-CA  | 7.56  | 129.29      | 119.84   |
| 44  | Ca    | 35   | PRO  | N-CA-CB | 7.54  | 111.17      | 103.25   |
| 107 | BE    | 42   | GLY  | N-CA-C  | 7.53  | 127.70      | 112.34   |
| 15  | DB    | 1033 | TYR  | CA-C-N  | -7.52 | 110.88      | 121.55   |
| 15  | DB    | 1033 | TYR  | C-N-CA  | -7.52 | 110.88      | 121.55   |
| 16  | DC    | 699  | VAL  | CA-C-N  | 7.47  | 127.84      | 119.32   |
| 16  | DC    | 699  | VAL  | C-N-CA  | 7.47  | 127.84      | 119.32   |
| 106 | BD    | 143  | PRO  | N-CA-CB | 7.46  | 111.08      | 103.25   |
| 20  | DH    | 239  | SER  | CA-C-N  | 7.41  | 127.58      | 120.31   |
| 20  | DH    | 239  | SER  | C-N-CA  | 7.41  | 127.58      | 120.31   |
| 33  | CJ    | 32   | ALA  | CA-C-N  | 7.39  | 129.07      | 119.84   |
| 33  | CJ    | 32   | ALA  | C-N-CA  | 7.39  | 129.07      | 119.84   |
| 119 | BQ    | 74   | CYS  | CA-C-N  | -7.39 | 112.14      | 119.90   |
| 119 | BQ    | 74   | CYS  | C-N-CA  | -7.39 | 112.14      | 119.90   |
| 41  | CS    | 130  | SER  | CA-C-N  | 7.38  | 127.65      | 119.90   |
| 41  | CS    | 130  | SER  | C-N-CA  | 7.38  | 127.65      | 119.90   |
| 107 | BE    | 17   | SER  | CA-C-N  | -7.37 | 110.63      | 119.84   |
| 107 | BE    | 17   | SER  | C-N-CA  | -7.37 | 110.63      | 119.84   |
| 26  | DX    | 78   | GLU  | CA-C-N  | 7.36  | 126.99      | 119.19   |
| 26  | DX    | 78   | GLU  | C-N-CA  | 7.36  | 126.99      | 119.19   |
| 44  | Ca    | 33   | PRO  | N-CA-CB | 7.35  | 110.97      | 103.25   |
| 31  | CH    | 17   | PRO  | CA-C-N  | 7.35  | 127.39      | 119.90   |
| 31  | CH    | 17   | PRO  | C-N-CA  | 7.35  | 127.39      | 119.90   |
| 16  | DC    | 776  | ASN  | N-CA-C  | -7.34 | 103.46      | 113.30   |
| 107 | BE    | 310  | LYS  | CA-C-N  | 7.33  | 127.04      | 119.56   |
| 107 | BE    | 310  | LYS  | C-N-CA  | 7.33  | 127.04      | 119.56   |
| 23  | DT    | 154  | GLN  | CA-C-N  | -7.32 | 111.64      | 122.41   |
| 23  | DT    | 154  | GLN  | C-N-CA  | -7.32 | 111.64      | 122.41   |
| 103 | BA    | 208  | ALA  | CA-C-N  | -7.31 | 114.27      | 121.65   |
| 103 | BA    | 208  | ALA  | C-N-CA  | -7.31 | 114.27      | 121.65   |
| 51  | Cm    | 43   | THR  | N-CA-C  | -7.29 | 104.19      | 113.23   |
| 92  | Ag    | 22   | ALA  | CA-C-N  | 7.29  | 126.92      | 119.56   |
| 92  | Ag    | 22   | ALA  | C-N-CA  | 7.29  | 126.92      | 119.56   |
| 79  | AP    | 39   | ASN  | N-CA-C  | 7.28  | 122.34      | 113.17   |
| 15  | DB    | 510  | ASN  | N-CA-C  | 7.28  | 121.01      | 112.72   |
| 106 | BD    | 284  | PRO  | N-CA-CB | 7.27  | 110.20      | 103.15   |
| 26  | DX    | 128  | GLY  | N-CA-C  | 7.26  | 127.15      | 112.34   |
| 106 | BD    | 409  | PRO  | N-CA-CB | 7.25  | 110.47      | 103.51   |
| 6   | DN    | 225  | GLY  | CA-C-N  | 7.23  | 127.40      | 120.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | DN    | 225  | GLY  | C-N-CA      | 7.23  | 127.40      | 120.31   |
| 56  | Cv    | 1123 | GLN  | CA-C-N      | 7.22  | 127.55      | 119.32   |
| 56  | Cv    | 1123 | GLN  | C-N-CA      | 7.22  | 127.55      | 119.32   |
| 1   | DA    | 1314 | GLY  | N-CA-C      | 7.16  | 126.94      | 112.34   |
| 74  | AF    | 316  | LYS  | N-CA-C      | -7.14 | 104.57      | 113.28   |
| 16  | DC    | 598  | ASP  | CA-C-N      | 7.11  | 127.43      | 119.32   |
| 16  | DC    | 598  | ASP  | C-N-CA      | 7.11  | 127.43      | 119.32   |
| 120 | BR    | 30   | GLY  | CA-C-N      | 7.09  | 126.70      | 119.19   |
| 120 | BR    | 30   | GLY  | C-N-CA      | 7.09  | 126.70      | 119.19   |
| 74  | AF    | 73   | SER  | N-CA-C      | -7.08 | 101.77      | 108.07   |
| 24  | DV    | 122  | ILE  | CA-C-N      | 7.08  | 127.11      | 119.89   |
| 24  | DV    | 122  | ILE  | C-N-CA      | 7.08  | 127.11      | 119.89   |
| 108 | BF    | 395  | ASN  | CA-C-N      | 7.07  | 127.22      | 119.87   |
| 108 | BF    | 395  | ASN  | C-N-CA      | 7.07  | 127.22      | 119.87   |
| 48  | Ci    | 151  | GLY  | N-CA-C      | -7.05 | 103.53      | 115.80   |
| 103 | BA    | 174  | ARG  | CA-C-N      | 7.02  | 126.65      | 119.56   |
| 103 | BA    | 174  | ARG  | C-N-CA      | 7.02  | 126.65      | 119.56   |
| 51  | Cm    | 32   | LYS  | CA-C-N      | 7.01  | 128.60      | 119.84   |
| 51  | Cm    | 32   | LYS  | C-N-CA      | 7.01  | 128.60      | 119.84   |
| 23  | DT    | 154  | GLN  | N-CA-C      | -7.00 | 99.91       | 110.28   |
| 119 | BQ    | 95   | GLY  | N-CA-C      | -7.00 | 101.33      | 110.29   |
| 4   | DL    | 229  | THR  | CA-C-N      | 7.00  | 126.48      | 118.85   |
| 4   | DL    | 229  | THR  | C-N-CA      | 7.00  | 126.48      | 118.85   |
| 56  | Cv    | 545  | THR  | CA-C-N      | 6.96  | 128.55      | 119.84   |
| 56  | Cv    | 545  | THR  | C-N-CA      | 6.96  | 128.55      | 119.84   |
| 31  | CH    | 16   | VAL  | CA-C-N      | -6.93 | 113.25      | 120.38   |
| 31  | CH    | 16   | VAL  | C-N-CA      | -6.93 | 113.25      | 120.38   |
| 15  | DB    | 908  | GLN  | CA-C-N      | 6.92  | 127.50      | 119.47   |
| 15  | DB    | 908  | GLN  | C-N-CA      | 6.92  | 127.50      | 119.47   |
| 33  | CJ    | 424  | HIS  | CE1-NE2-CD2 | -6.90 | 102.10      | 109.00   |
| 93  | Aj    | 255  | ARG  | CA-C-N      | -6.90 | 111.22      | 119.84   |
| 93  | Aj    | 255  | ARG  | C-N-CA      | -6.90 | 111.22      | 119.84   |
| 27  | DY    | 34   | ASP  | CA-C-N      | 6.88  | 127.16      | 119.32   |
| 27  | DY    | 34   | ASP  | C-N-CA      | 6.88  | 127.16      | 119.32   |
| 33  | CJ    | 800  | LEU  | CA-C-N      | -6.87 | 111.91      | 119.19   |
| 33  | CJ    | 800  | LEU  | C-N-CA      | -6.87 | 111.91      | 119.19   |
| 96  | Ap    | 244  | PRO  | CA-C-N      | 6.86  | 128.42      | 119.84   |
| 96  | Ap    | 244  | PRO  | C-N-CA      | 6.86  | 128.42      | 119.84   |
| 16  | DC    | 164  | SER  | CA-C-N      | 6.85  | 128.40      | 119.84   |
| 16  | DC    | 164  | SER  | C-N-CA      | 6.85  | 128.40      | 119.84   |
| 41  | CS    | 55   | ARG  | N-CA-C      | -6.84 | 99.81       | 110.14   |
| 55  | Cr    | 31   | PRO  | N-CA-CB     | 6.84  | 110.43      | 103.25   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 106 | BD    | 370  | PRO  | N-CA-CB | 6.83  | 110.76      | 103.52   |
| 19  | DG    | 560  | GLU  | CA-C-N  | 6.82  | 128.37      | 119.84   |
| 19  | DG    | 560  | GLU  | C-N-CA  | 6.82  | 128.37      | 119.84   |
| 33  | CJ    | 52   | PHE  | CA-C-N  | 6.79  | 127.20      | 119.93   |
| 33  | CJ    | 52   | PHE  | C-N-CA  | 6.79  | 127.20      | 119.93   |
| 27  | DY    | 161  | ARG  | N-CA-C  | 6.78  | 118.75      | 111.36   |
| 106 | BD    | 319  | PRO  | N-CA-CB | 6.77  | 110.32      | 102.33   |
| 106 | BD    | 176  | PRO  | N-CA-CB | 6.76  | 110.35      | 103.25   |
| 103 | BA    | 277  | ILE  | N-CA-C  | -6.75 | 100.87      | 109.58   |
| 47  | Cg    | 17   | PRO  | CA-C-N  | 6.74  | 128.26      | 119.84   |
| 47  | Cg    | 17   | PRO  | C-N-CA  | 6.74  | 128.26      | 119.84   |
| 94  | Al    | 50   | MET  | CA-C-N  | 6.72  | 127.30      | 120.38   |
| 94  | Al    | 50   | MET  | C-N-CA  | 6.72  | 127.30      | 120.38   |
| 74  | AF    | 36   | ALA  | CA-C-N  | -6.71 | 113.03      | 120.14   |
| 74  | AF    | 36   | ALA  | C-N-CA  | -6.71 | 113.03      | 120.14   |
| 56  | Cv    | 213  | GLY  | N-CA-C  | -6.70 | 101.71      | 110.29   |
| 15  | DB    | 440  | GLY  | N-CA-C  | 6.70  | 122.57      | 113.99   |
| 94  | Al    | 107  | PRO  | N-CA-CB | 6.68  | 110.27      | 103.25   |
| 106 | BD    | 162  | PRO  | N-CA-CB | 6.67  | 110.26      | 103.25   |
| 106 | BD    | 133  | PRO  | N-CA-CB | 6.67  | 110.26      | 103.25   |
| 126 | BX    | 151  | VAL  | CA-C-N  | -6.67 | 113.65      | 120.85   |
| 126 | BX    | 151  | VAL  | C-N-CA  | -6.67 | 113.65      | 120.85   |
| 16  | DC    | 600  | ASP  | N-CA-C  | 6.65  | 121.14      | 112.89   |
| 95  | Ao    | 54   | GLN  | N-CA-C  | 6.63  | 121.23      | 112.35   |
| 106 | BD    | 463  | PRO  | N-CA-CB | 6.63  | 109.87      | 103.51   |
| 2   | DD    | 355  | SER  | CA-C-N  | 6.62  | 126.31      | 119.82   |
| 2   | DD    | 355  | SER  | C-N-CA  | 6.62  | 126.31      | 119.82   |
| 65  | A1    | 189  | LEU  | CA-C-N  | -6.62 | 113.16      | 119.85   |
| 65  | A1    | 189  | LEU  | C-N-CA  | -6.62 | 113.16      | 119.85   |
| 4   | DL    | 295  | GLY  | CA-C-N  | 6.62  | 126.20      | 119.19   |
| 4   | DL    | 295  | GLY  | C-N-CA  | 6.62  | 126.20      | 119.19   |
| 15  | DB    | 1166 | VAL  | N-CA-C  | 6.61  | 118.20      | 111.00   |
| 125 | BW    | 187  | ASP  | N-CA-C  | 6.59  | 118.87      | 108.79   |
| 56  | Cv    | 440  | GLY  | CA-C-N  | -6.57 | 113.04      | 119.87   |
| 56  | Cv    | 440  | GLY  | C-N-CA  | -6.57 | 113.04      | 119.87   |
| 134 | Bf    | 79   | GLU  | CA-C-N  | 6.55  | 126.48      | 119.28   |
| 134 | Bf    | 79   | GLU  | C-N-CA  | 6.55  | 126.48      | 119.28   |
| 26  | DX    | 164  | THR  | N-CA-C  | 6.55  | 120.73      | 112.87   |
| 39  | CQ    | 166  | GLU  | CA-C-N  | -6.55 | 114.04      | 120.52   |
| 39  | CQ    | 166  | GLU  | C-N-CA  | -6.55 | 114.04      | 120.52   |
| 96  | Ap    | 86   | CYS  | CA-C-N  | -6.51 | 111.70      | 119.84   |
| 96  | Ap    | 86   | CYS  | C-N-CA  | -6.51 | 111.70      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 43  | CZ    | 296  | PRO  | N-CA-CB | 6.50  | 110.08      | 103.25   |
| 114 | BL    | 69   | MET  | CA-C-N  | 6.50  | 126.43      | 119.28   |
| 114 | BL    | 69   | MET  | C-N-CA  | 6.50  | 126.43      | 119.28   |
| 15  | DB    | 1079 | TRP  | N-CA-C  | 6.50  | 118.36      | 111.28   |
| 86  | AX    | 78   | ARG  | CA-C-N  | -6.50 | 111.72      | 119.84   |
| 86  | AX    | 78   | ARG  | C-N-CA  | -6.50 | 111.72      | 119.84   |
| 77  | AK    | 66   | PRO  | N-CA-C  | 6.49  | 118.62      | 110.70   |
| 103 | BA    | 807  | THR  | CA-C-N  | 6.49  | 125.99      | 119.24   |
| 103 | BA    | 807  | THR  | C-N-CA  | 6.49  | 125.99      | 119.24   |
| 106 | BD    | 435  | PRO  | N-CA-CB | 6.49  | 110.71      | 103.44   |
| 37  | CO    | 320  | ASP  | CA-C-N  | 6.48  | 126.17      | 119.82   |
| 37  | CO    | 320  | ASP  | C-N-CA  | 6.48  | 126.17      | 119.82   |
| 91  | Af    | 172  | GLY  | N-CA-C  | -6.48 | 99.72       | 110.80   |
| 94  | Al    | 159  | MET  | CA-C-N  | 6.48  | 126.17      | 119.82   |
| 94  | Al    | 159  | MET  | C-N-CA  | 6.48  | 126.17      | 119.82   |
| 47  | Cg    | 365  | ASP  | N-CA-C  | 6.46  | 121.22      | 112.88   |
| 88  | Ab    | 456  | ALA  | N-CA-C  | 6.46  | 117.09      | 108.38   |
| 75  | AI    | 88   | THR  | CA-C-N  | 6.45  | 126.14      | 119.82   |
| 75  | AI    | 88   | THR  | C-N-CA  | 6.45  | 126.14      | 119.82   |
| 106 | BD    | 153  | PRO  | N-CA-CB | 6.45  | 110.02      | 103.25   |
| 94  | Al    | 134  | ILE  | CA-C-N  | 6.41  | 126.03      | 119.56   |
| 94  | Al    | 134  | ILE  | C-N-CA  | 6.41  | 126.03      | 119.56   |
| 106 | BD    | 277  | PRO  | N-CA-CB | 6.39  | 110.07      | 103.23   |
| 103 | BA    | 780  | TYR  | N-CA-C  | 6.38  | 119.99      | 112.72   |
| 125 | BW    | 65   | ASN  | N-CA-C  | 6.38  | 120.16      | 112.38   |
| 119 | BQ    | 227  | LEU  | N-CA-C  | 6.37  | 121.22      | 113.38   |
| 1   | DA    | 224  | VAL  | N-CA-C  | 6.37  | 121.05      | 113.22   |
| 1   | DA    | 1592 | GLY  | N-CA-C  | -6.36 | 107.42      | 115.31   |
| 109 | BG    | 279  | ASN  | CA-C-N  | 6.35  | 127.78      | 119.84   |
| 109 | BG    | 279  | ASN  | C-N-CA  | 6.35  | 127.78      | 119.84   |
| 1   | DA    | 1484 | PRO  | N-CA-CB | 6.35  | 109.91      | 103.25   |
| 84  | AV    | 211  | VAL  | CB-CA-C | -6.35 | 104.58      | 112.45   |
| 76  | AJ    | 123  | PRO  | N-CA-CB | 6.32  | 110.22      | 103.52   |
| 75  | AI    | 211  | GLU  | N-CA-C  | -6.32 | 105.21      | 113.17   |
| 47  | Cg    | 102  | PRO  | CA-C-N  | 6.31  | 126.52      | 119.32   |
| 47  | Cg    | 102  | PRO  | C-N-CA  | 6.31  | 126.52      | 119.32   |
| 75  | AI    | 71   | TYR  | CA-C-N  | -6.31 | 111.97      | 118.85   |
| 75  | AI    | 71   | TYR  | C-N-CA  | -6.31 | 111.97      | 118.85   |
| 75  | AI    | 97   | ARG  | CA-C-N  | 6.30  | 126.21      | 119.85   |
| 75  | AI    | 97   | ARG  | C-N-CA  | 6.30  | 126.21      | 119.85   |
| 106 | BD    | 483  | PRO  | N-CA-CB | 6.30  | 110.19      | 103.39   |
| 18  | DF    | 59   | GLY  | CA-C-N  | 6.29  | 127.70      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | DF    | 59   | GLY  | C-N-CA  | 6.29  | 127.70      | 119.84   |
| 90  | Ae    | 71   | HIS  | CA-C-N  | -6.28 | 111.99      | 119.84   |
| 90  | Ae    | 71   | HIS  | C-N-CA  | -6.28 | 111.99      | 119.84   |
| 16  | DC    | 1143 | VAL  | CA-C-N  | 6.27  | 127.68      | 119.84   |
| 16  | DC    | 1143 | VAL  | C-N-CA  | 6.27  | 127.68      | 119.84   |
| 24  | DV    | 42   | PHE  | N-CA-C  | -6.26 | 101.84      | 110.35   |
| 33  | CJ    | 58   | GLY  | CA-C-N  | 6.26  | 125.95      | 119.82   |
| 33  | CJ    | 58   | GLY  | C-N-CA  | 6.26  | 125.95      | 119.82   |
| 17  | DE    | 432  | GLU  | N-CA-C  | 6.26  | 119.06      | 110.24   |
| 5   | DM    | 122  | LYS  | CA-C-N  | -6.25 | 112.56      | 119.19   |
| 5   | DM    | 122  | LYS  | C-N-CA  | -6.25 | 112.56      | 119.19   |
| 77  | AK    | 66   | PRO  | CA-C-N  | -6.25 | 112.03      | 119.84   |
| 77  | AK    | 66   | PRO  | C-N-CA  | -6.25 | 112.03      | 119.84   |
| 119 | BQ    | 178  | SER  | N-CA-C  | 6.23  | 121.03      | 113.17   |
| 15  | DB    | 1127 | MET  | CA-C-N  | 6.23  | 125.80      | 119.19   |
| 15  | DB    | 1127 | MET  | C-N-CA  | 6.23  | 125.80      | 119.19   |
| 90  | Ae    | 57   | GLY  | N-CA-C  | 6.23  | 120.60      | 112.25   |
| 3   | DI    | 66   | ARG  | N-CA-C  | 6.23  | 118.88      | 111.71   |
| 85  | AW    | 103  | GLY  | N-CA-C  | -6.23 | 105.92      | 114.64   |
| 87  | AY    | 153  | ILE  | CA-C-N  | 6.21  | 126.57      | 119.92   |
| 87  | AY    | 153  | ILE  | C-N-CA  | 6.21  | 126.57      | 119.92   |
| 35  | CL    | 79   | SER  | CA-C-N  | 6.19  | 126.15      | 120.21   |
| 35  | CL    | 79   | SER  | C-N-CA  | 6.19  | 126.15      | 120.21   |
| 25  | DW    | 51   | GLY  | CA-C-N  | 6.18  | 125.59      | 118.85   |
| 25  | DW    | 51   | GLY  | C-N-CA  | 6.18  | 125.59      | 118.85   |
| 33  | CJ    | 703  | ALA  | N-CA-C  | 6.18  | 118.81      | 111.33   |
| 79  | AP    | 164  | ASN  | N-CA-C  | 6.17  | 119.31      | 110.24   |
| 38  | CP    | 182  | ARG  | CA-C-N  | 6.17  | 126.19      | 119.90   |
| 38  | CP    | 182  | ARG  | C-N-CA  | 6.17  | 126.19      | 119.90   |
| 4   | DL    | 132  | ASN  | CA-C-N  | -6.16 | 115.43      | 121.65   |
| 4   | DL    | 132  | ASN  | C-N-CA  | -6.16 | 115.43      | 121.65   |
| 8   | DP    | 207  | TYR  | C-N-CD  | 6.15  | 134.13      | 120.60   |
| 73  | AE    | 357  | LEU  | CA-C-N  | 6.14  | 126.11      | 120.21   |
| 73  | AE    | 357  | LEU  | C-N-CA  | 6.14  | 126.11      | 120.21   |
| 1   | DA    | 1457 | HIS  | CA-C-N  | 6.14  | 125.76      | 119.56   |
| 1   | DA    | 1457 | HIS  | C-N-CA  | 6.14  | 125.76      | 119.56   |
| 21  | DJ    | 35   | PRO  | CA-C-O  | -6.14 | 116.77      | 121.31   |
| 106 | BD    | 357  | PRO  | N-CA-CB | 6.13  | 109.69      | 103.25   |
| 33  | CJ    | 240  | GLY  | N-CA-C  | 6.12  | 121.27      | 110.80   |
| 36  | CN    | 108  | VAL  | CA-C-N  | 6.12  | 125.52      | 118.85   |
| 36  | CN    | 108  | VAL  | C-N-CA  | 6.12  | 125.52      | 118.85   |
| 56  | Cv    | 402  | ALA  | CA-C-N  | 6.12  | 125.33      | 118.97   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 56  | Cv    | 402  | ALA  | C-N-CA  | 6.12  | 125.33      | 118.97   |
| 88  | Ab    | 151  | LEU  | CA-C-N  | -6.10 | 112.73      | 119.19   |
| 88  | Ab    | 151  | LEU  | C-N-CA  | -6.10 | 112.73      | 119.19   |
| 33  | CJ    | 454  | THR  | CA-C-N  | -6.09 | 112.22      | 119.84   |
| 33  | CJ    | 454  | THR  | C-N-CA  | -6.09 | 112.22      | 119.84   |
| 41  | CS    | 59   | LYS  | CA-C-N  | -6.09 | 114.38      | 122.85   |
| 41  | CS    | 59   | LYS  | C-N-CA  | -6.09 | 114.38      | 122.85   |
| 39  | CQ    | 68   | SER  | N-CA-C  | -6.09 | 105.50      | 113.17   |
| 16  | DC    | 845  | ALA  | N-CA-C  | -6.07 | 97.86       | 110.80   |
| 56  | Cv    | 59   | ILE  | N-CA-C  | 6.07  | 118.00      | 112.29   |
| 55  | Cr    | 29   | PRO  | N-CA-CB | 6.05  | 109.61      | 103.25   |
| 1   | DA    | 1134 | ILE  | N-CA-C  | 6.05  | 114.65      | 109.02   |
| 44  | Ca    | 340  | GLY  | N-CA-C  | -6.04 | 102.15      | 111.64   |
| 71  | A8    | 78   | GLY  | CA-C-N  | 6.04  | 126.60      | 120.38   |
| 71  | A8    | 78   | GLY  | C-N-CA  | 6.04  | 126.60      | 120.38   |
| 18  | DF    | 192  | LEU  | CA-C-N  | 6.04  | 125.74      | 119.82   |
| 18  | DF    | 192  | LEU  | C-N-CA  | 6.04  | 125.74      | 119.82   |
| 92  | Ag    | 31   | THR  | N-CA-C  | 6.04  | 118.77      | 111.40   |
| 97  | At    | 108  | ILE  | N-CA-C  | 6.04  | 116.67      | 110.82   |
| 29  | CE    | 256  | LEU  | CB-CA-C | -6.03 | 109.03      | 117.23   |
| 112 | BJ    | 279  | GLY  | N-CA-C  | -6.03 | 106.20      | 114.64   |
| 17  | DE    | 71   | LEU  | N-CA-C  | -6.03 | 97.96       | 110.80   |
| 106 | BD    | 477  | PRO  | N-CA-CB | 6.03  | 110.19      | 103.44   |
| 78  | AN    | 101  | VAL  | N-CA-C  | 6.01  | 113.50      | 107.55   |
| 33  | CJ    | 398  | PHE  | N-CA-C  | 6.01  | 118.92      | 108.76   |
| 15  | DB    | 735  | VAL  | N-CA-C  | 6.01  | 116.65      | 110.82   |
| 7   | DO    | 239  | LYS  | CA-C-N  | 6.00  | 125.62      | 119.56   |
| 7   | DO    | 239  | LYS  | C-N-CA  | 6.00  | 125.62      | 119.56   |
| 20  | DH    | 135  | ARG  | N-CA-C  | -6.00 | 106.29      | 113.97   |
| 17  | DE    | 479  | PRO  | CA-C-N  | -5.99 | 113.17      | 122.16   |
| 17  | DE    | 479  | PRO  | C-N-CA  | -5.99 | 113.17      | 122.16   |
| 79  | AP    | 346  | HIS  | N-CA-C  | -5.99 | 102.21      | 110.35   |
| 84  | AV    | 128  | ARG  | N-CA-C  | -5.98 | 100.18      | 109.87   |
| 105 | BC    | 204  | TYR  | CA-C-N  | -5.97 | 112.37      | 119.84   |
| 105 | BC    | 204  | TYR  | C-N-CA  | -5.97 | 112.37      | 119.84   |
| 50  | Ck    | 368  | HIS  | CA-C-N  | 5.96  | 125.67      | 119.05   |
| 50  | Ck    | 368  | HIS  | C-N-CA  | 5.96  | 125.67      | 119.05   |
| 16  | DC    | 1119 | GLN  | CA-C-N  | 5.96  | 125.93      | 120.03   |
| 16  | DC    | 1119 | GLN  | C-N-CA  | 5.96  | 125.93      | 120.03   |
| 130 | Bb    | 72   | VAL  | CA-C-N  | -5.96 | 112.39      | 119.84   |
| 130 | Bb    | 72   | VAL  | C-N-CA  | -5.96 | 112.39      | 119.84   |
| 106 | BD    | 243  | PRO  | N-CA-CB | 5.94  | 109.49      | 103.25   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 74  | AF    | 126 | TYR  | N-CA-C  | 5.94  | 117.96      | 110.24   |
| 51  | Cm    | 34  | THR  | N-CA-C  | 5.93  | 117.62      | 111.03   |
| 33  | CJ    | 584 | GLU  | N-CA-C  | 5.93  | 118.25      | 111.02   |
| 128 | BZ    | 82  | LEU  | N-CA-C  | 5.93  | 116.38      | 108.38   |
| 44  | Ca    | 31  | GLU  | CA-C-N  | 5.91  | 126.47      | 120.38   |
| 44  | Ca    | 31  | GLU  | C-N-CA  | 5.91  | 126.47      | 120.38   |
| 33  | CJ    | 429 | CYS  | N-CA-C  | 5.91  | 117.83      | 108.79   |
| 92  | Ag    | 167 | THR  | N-CA-C  | 5.90  | 120.61      | 113.17   |
| 47  | Cg    | 149 | GLY  | CA-C-N  | 5.90  | 126.72      | 120.11   |
| 47  | Cg    | 149 | GLY  | C-N-CA  | 5.90  | 126.72      | 120.11   |
| 116 | BN    | 37  | ASN  | N-CA-C  | -5.89 | 105.41      | 113.30   |
| 33  | CJ    | 461 | HIS  | N-CA-C  | 5.88  | 119.77      | 112.59   |
| 33  | CJ    | 26  | GLY  | CA-C-N  | 5.88  | 127.19      | 119.84   |
| 33  | CJ    | 26  | GLY  | C-N-CA  | 5.88  | 127.19      | 119.84   |
| 44  | Ca    | 168 | TYR  | CA-C-N  | 5.87  | 125.57      | 119.05   |
| 44  | Ca    | 168 | TYR  | C-N-CA  | 5.87  | 125.57      | 119.05   |
| 49  | Cj    | 38  | MET  | CA-C-N  | 5.87  | 125.41      | 119.19   |
| 49  | Cj    | 38  | MET  | C-N-CA  | 5.87  | 125.41      | 119.19   |
| 18  | DF    | 569 | GLN  | CA-C-N  | 5.87  | 127.17      | 119.84   |
| 18  | DF    | 569 | GLN  | C-N-CA  | 5.87  | 127.17      | 119.84   |
| 119 | BQ    | 179 | GLY  | N-CA-C  | 5.87  | 122.00      | 111.03   |
| 74  | AF    | 56  | HIS  | CA-C-N  | 5.86  | 125.56      | 119.82   |
| 74  | AF    | 56  | HIS  | C-N-CA  | 5.86  | 125.56      | 119.82   |
| 33  | CJ    | 405 | LEU  | CA-C-N  | 5.86  | 125.96      | 119.87   |
| 33  | CJ    | 405 | LEU  | C-N-CA  | 5.86  | 125.96      | 119.87   |
| 47  | Cg    | 464 | VAL  | N-CA-C  | 5.86  | 118.63      | 112.83   |
| 2   | DD    | 469 | GLY  | N-CA-C  | -5.84 | 102.47      | 111.64   |
| 15  | DB    | 382 | GLY  | CA-C-O  | -5.84 | 118.43      | 122.22   |
| 96  | Ap    | 57  | LYS  | CA-C-N  | -5.83 | 114.55      | 121.90   |
| 96  | Ap    | 57  | LYS  | C-N-CA  | -5.83 | 114.55      | 121.90   |
| 98  | Av    | 136 | TRP  | CA-C-N  | 5.82  | 125.20      | 118.85   |
| 98  | Av    | 136 | TRP  | C-N-CA  | 5.82  | 125.20      | 118.85   |
| 15  | DB    | 471 | TYR  | N-CA-C  | -5.82 | 101.00      | 110.20   |
| 134 | Bf    | 94  | ARG  | CA-C-N  | 5.81  | 126.10      | 119.83   |
| 134 | Bf    | 94  | ARG  | C-N-CA  | 5.81  | 126.10      | 119.83   |
| 93  | Aj    | 106 | ASP  | CA-C-N  | 5.81  | 125.67      | 119.28   |
| 93  | Aj    | 106 | ASP  | C-N-CA  | 5.81  | 125.67      | 119.28   |
| 93  | Aj    | 137 | VAL  | N-CA-C  | -5.81 | 100.63      | 108.06   |
| 122 | BT    | 105 | VAL  | CB-CA-C | -5.80 | 104.56      | 111.81   |
| 16  | DC    | 242 | HIS  | N-CA-C  | -5.80 | 100.60      | 109.65   |
| 52  | Cn    | 157 | TYR  | CA-C-N  | -5.80 | 112.59      | 119.84   |
| 52  | Cn    | 157 | TYR  | C-N-CA  | -5.80 | 112.59      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | DK    | 241 | VAL  | CB-CA-C | -5.80 | 104.46      | 111.88   |
| 10  | DR    | 92  | LEU  | CA-C-N  | 5.79  | 125.81      | 119.90   |
| 10  | DR    | 92  | LEU  | C-N-CA  | 5.79  | 125.81      | 119.90   |
| 125 | BW    | 27  | TYR  | CA-C-N  | 5.79  | 125.46      | 119.56   |
| 125 | BW    | 27  | TYR  | C-N-CA  | 5.79  | 125.46      | 119.56   |
| 115 | BM    | 68  | ARG  | N-CA-C  | -5.79 | 101.34      | 109.96   |
| 18  | DF    | 128 | HIS  | N-CA-C  | 5.79  | 120.49      | 112.45   |
| 41  | CS    | 112 | THR  | N-CA-C  | 5.78  | 117.26      | 111.07   |
| 55  | Cr    | 115 | PRO  | CA-C-N  | 5.78  | 125.15      | 118.85   |
| 55  | Cr    | 115 | PRO  | C-N-CA  | 5.78  | 125.15      | 118.85   |
| 5   | DM    | 2   | GLU  | N-CA-C  | 5.77  | 117.44      | 111.03   |
| 41  | CS    | 68  | ALA  | CA-C-N  | -5.76 | 113.09      | 119.19   |
| 41  | CS    | 68  | ALA  | C-N-CA  | -5.76 | 113.09      | 119.19   |
| 94  | Al    | 154 | HIS  | CA-C-N  | 5.76  | 125.37      | 119.56   |
| 94  | Al    | 154 | HIS  | C-N-CA  | 5.76  | 125.37      | 119.56   |
| 104 | BB    | 261 | VAL  | N-CA-C  | -5.75 | 106.14      | 113.22   |
| 31  | CH    | 125 | LYS  | CA-C-N  | 5.75  | 126.20      | 119.99   |
| 31  | CH    | 125 | LYS  | C-N-CA  | 5.75  | 126.20      | 119.99   |
| 128 | BZ    | 66  | GLN  | N-CA-C  | 5.74  | 120.40      | 113.17   |
| 33  | CJ    | 353 | ASP  | CA-C-N  | 5.73  | 125.35      | 119.56   |
| 33  | CJ    | 353 | ASP  | C-N-CA  | 5.73  | 125.35      | 119.56   |
| 105 | BC    | 236 | THR  | CA-C-N  | 5.72  | 125.43      | 119.82   |
| 105 | BC    | 236 | THR  | C-N-CA  | 5.72  | 125.43      | 119.82   |
| 79  | AP    | 347 | LEU  | CA-C-N  | -5.71 | 114.01      | 122.41   |
| 79  | AP    | 347 | LEU  | C-N-CA  | -5.71 | 114.01      | 122.41   |
| 22  | DK    | 241 | VAL  | N-CA-C  | 5.71  | 116.36      | 110.36   |
| 84  | AV    | 93  | VAL  | N-CA-C  | 5.71  | 115.90      | 110.53   |
| 21  | DJ    | 16  | ASN  | CA-C-N  | 5.71  | 125.38      | 119.56   |
| 21  | DJ    | 16  | ASN  | C-N-CA  | 5.71  | 125.38      | 119.56   |
| 92  | Ag    | 168 | CYS  | N-CA-C  | 5.71  | 120.24      | 113.28   |
| 85  | AW    | 72  | THR  | N-CA-C  | 5.71  | 122.95      | 110.80   |
| 26  | DX    | 102 | MET  | N-CA-C  | 5.70  | 120.37      | 112.45   |
| 1   | DA    | 949 | ARG  | CA-C-N  | 5.70  | 125.40      | 119.82   |
| 1   | DA    | 949 | ARG  | C-N-CA  | 5.70  | 125.40      | 119.82   |
| 107 | BE    | 79  | VAL  | CA-C-N  | 5.70  | 125.63      | 119.76   |
| 107 | BE    | 79  | VAL  | C-N-CA  | 5.70  | 125.63      | 119.76   |
| 119 | BQ    | 20  | VAL  | CA-C-N  | 5.70  | 126.08      | 119.47   |
| 119 | BQ    | 20  | VAL  | C-N-CA  | 5.70  | 126.08      | 119.47   |
| 6   | DN    | 130 | ASN  | CA-C-N  | 5.69  | 125.66      | 120.03   |
| 6   | DN    | 130 | ASN  | C-N-CA  | 5.69  | 125.66      | 120.03   |
| 16  | DC    | 88  | LEU  | N-CA-C  | 5.69  | 119.20      | 112.72   |
| 36  | CN    | 93  | ASP  | N-CA-C  | 5.68  | 118.25      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 77  | AK    | 64   | THR  | N-CA-C  | -5.68 | 106.20      | 113.02   |
| 129 | Ba    | 59   | ASP  | CA-C-N  | -5.68 | 116.35      | 122.59   |
| 129 | Ba    | 59   | ASP  | C-N-CA  | -5.68 | 116.35      | 122.59   |
| 33  | CJ    | 210  | TRP  | N-CA-C  | 5.67  | 117.47      | 108.79   |
| 19  | DG    | 261  | ARG  | CA-C-N  | 5.67  | 125.52      | 119.28   |
| 19  | DG    | 261  | ARG  | C-N-CA  | 5.67  | 125.52      | 119.28   |
| 33  | CJ    | 544  | THR  | N-CA-C  | 5.66  | 116.38      | 108.00   |
| 20  | DH    | 452  | ARG  | CA-C-N  | 5.64  | 125.66      | 119.90   |
| 20  | DH    | 452  | ARG  | C-N-CA  | 5.64  | 125.66      | 119.90   |
| 71  | A8    | 67   | MET  | N-CA-C  | 5.64  | 118.25      | 110.35   |
| 44  | Ca    | 524  | VAL  | CA-C-N  | 5.64  | 125.65      | 119.90   |
| 44  | Ca    | 524  | VAL  | C-N-CA  | 5.64  | 125.65      | 119.90   |
| 93  | Aj    | 228  | VAL  | CA-C-N  | 5.64  | 126.12      | 120.14   |
| 93  | Aj    | 228  | VAL  | C-N-CA  | 5.64  | 126.12      | 120.14   |
| 15  | DB    | 622  | ALA  | N-CA-C  | 5.64  | 117.57      | 110.24   |
| 80  | AQ    | 148  | ILE  | CA-C-N  | 5.64  | 125.31      | 119.56   |
| 80  | AQ    | 148  | ILE  | C-N-CA  | 5.64  | 125.31      | 119.56   |
| 1   | DA    | 732  | ALA  | CB-CA-C | -5.63 | 110.09      | 116.63   |
| 20  | DH    | 272  | HIS  | N-CA-C  | 5.63  | 119.46      | 112.59   |
| 75  | AI    | 178  | ILE  | CA-C-N  | 5.63  | 125.91      | 119.83   |
| 75  | AI    | 178  | ILE  | C-N-CA  | 5.63  | 125.91      | 119.83   |
| 80  | AQ    | 33   | ASP  | CA-C-N  | 5.62  | 125.24      | 119.56   |
| 80  | AQ    | 33   | ASP  | C-N-CA  | 5.62  | 125.24      | 119.56   |
| 120 | BR    | 29   | LEU  | N-CA-C  | 5.62  | 117.10      | 110.97   |
| 16  | DC    | 965  | ASN  | N-CA-C  | 5.62  | 118.25      | 111.40   |
| 118 | BP    | 144  | PHE  | N-CA-C  | 5.62  | 120.06      | 108.71   |
| 81  | AR    | 55   | LEU  | CA-C-N  | 5.62  | 125.63      | 119.90   |
| 81  | AR    | 55   | LEU  | C-N-CA  | 5.62  | 125.63      | 119.90   |
| 48  | Ci    | 84   | LEU  | N-CA-C  | 5.61  | 116.96      | 109.83   |
| 16  | DC    | 1074 | TYR  | N-CA-C  | 5.61  | 118.13      | 110.55   |
| 15  | DB    | 1023 | ARG  | CA-C-N  | 5.61  | 125.56      | 119.78   |
| 15  | DB    | 1023 | ARG  | C-N-CA  | 5.61  | 125.56      | 119.78   |
| 26  | DX    | 115  | ARG  | CA-C-N  | -5.61 | 113.24      | 119.19   |
| 26  | DX    | 115  | ARG  | C-N-CA  | -5.61 | 113.24      | 119.19   |
| 28  | CC    | 67   | ASN  | N-CA-C  | 5.61  | 120.24      | 113.17   |
| 65  | A1    | 148  | LEU  | CA-C-N  | -5.61 | 113.67      | 122.65   |
| 65  | A1    | 148  | LEU  | C-N-CA  | -5.61 | 113.67      | 122.65   |
| 65  | A1    | 22   | ALA  | CA-C-N  | 5.61  | 125.13      | 119.19   |
| 65  | A1    | 22   | ALA  | C-N-CA  | 5.61  | 125.13      | 119.19   |
| 107 | BE    | 39   | GLY  | CA-C-N  | 5.60  | 125.27      | 119.56   |
| 107 | BE    | 39   | GLY  | C-N-CA  | 5.60  | 125.27      | 119.56   |
| 111 | BI    | 216  | MET  | N-CA-C  | -5.60 | 98.87       | 110.80   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 77  | AK    | 137  | GLY  | CA-C-N  | 5.60  | 125.61      | 119.90   |
| 77  | AK    | 137  | GLY  | C-N-CA  | 5.60  | 125.61      | 119.90   |
| 38  | CP    | 65   | GLY  | N-CA-C  | 5.59  | 119.16      | 110.88   |
| 92  | Ag    | 111  | GLY  | N-CA-C  | -5.59 | 104.31      | 110.96   |
| 108 | BF    | 319  | LYS  | N-CA-C  | -5.58 | 105.10      | 111.07   |
| 16  | DC    | 774  | ASP  | CA-C-N  | -5.58 | 114.52      | 122.77   |
| 16  | DC    | 774  | ASP  | C-N-CA  | -5.58 | 114.52      | 122.77   |
| 20  | DH    | 148  | ASP  | CA-C-N  | 5.58  | 125.42      | 119.28   |
| 20  | DH    | 148  | ASP  | C-N-CA  | 5.58  | 125.42      | 119.28   |
| 5   | DM    | 284  | ARG  | CA-C-N  | -5.57 | 113.52      | 119.98   |
| 5   | DM    | 284  | ARG  | C-N-CA  | -5.57 | 113.52      | 119.98   |
| 69  | A5    | 69   | TRP  | N-CA-C  | 5.57  | 116.71      | 108.86   |
| 1   | DA    | 883  | ASN  | CA-C-N  | 5.57  | 125.18      | 119.56   |
| 1   | DA    | 883  | ASN  | C-N-CA  | 5.57  | 125.18      | 119.56   |
| 103 | BA    | 424  | GLY  | CA-C-N  | 5.56  | 125.22      | 119.05   |
| 103 | BA    | 424  | GLY  | C-N-CA  | 5.56  | 125.22      | 119.05   |
| 95  | Ao    | 78   | GLY  | CA-C-N  | 5.56  | 125.18      | 119.56   |
| 95  | Ao    | 78   | GLY  | C-N-CA  | 5.56  | 125.18      | 119.56   |
| 18  | DF    | 247  | LEU  | N-CA-C  | -5.56 | 105.54      | 112.93   |
| 40  | CR    | 80   | LEU  | N-CA-C  | 5.55  | 117.77      | 111.11   |
| 79  | AP    | 37   | SER  | N-CA-C  | -5.53 | 102.71      | 110.35   |
| 21  | DJ    | 37   | GLY  | N-CA-C  | -5.53 | 104.16      | 112.89   |
| 54  | Cq    | 146  | PRO  | CA-C-N  | 5.53  | 126.07      | 120.38   |
| 54  | Cq    | 146  | PRO  | C-N-CA  | 5.53  | 126.07      | 120.38   |
| 116 | BN    | 71   | GLN  | CA-C-N  | -5.53 | 114.28      | 120.14   |
| 116 | BN    | 71   | GLN  | C-N-CA  | -5.53 | 114.28      | 120.14   |
| 111 | BI    | 85   | THR  | CA-C-N  | -5.52 | 114.28      | 119.85   |
| 111 | BI    | 85   | THR  | C-N-CA  | -5.52 | 114.28      | 119.85   |
| 20  | DH    | 307  | ARG  | N-CA-C  | -5.50 | 101.90      | 110.10   |
| 83  | AU    | 120  | PRO  | O-C-N   | 5.50  | 123.73      | 121.15   |
| 56  | Cv    | 1084 | GLU  | CA-C-N  | 5.50  | 124.96      | 119.24   |
| 56  | Cv    | 1084 | GLU  | C-N-CA  | 5.50  | 124.96      | 119.24   |
| 2   | DD    | 255  | VAL  | N-CA-C  | 5.49  | 120.75      | 108.88   |
| 94  | Al    | 208  | VAL  | CB-CA-C | -5.49 | 104.94      | 111.97   |
| 18  | DF    | 242  | VAL  | CB-CA-C | -5.48 | 106.82      | 114.00   |
| 40  | CR    | 71   | PHE  | CA-C-N  | 5.48  | 125.30      | 119.28   |
| 40  | CR    | 71   | PHE  | C-N-CA  | 5.48  | 125.30      | 119.28   |
| 115 | BM    | 241  | MET  | CA-C-N  | 5.47  | 125.48      | 119.90   |
| 115 | BM    | 241  | MET  | C-N-CA  | 5.47  | 125.48      | 119.90   |
| 12  | DU    | 205  | ALA  | CA-C-N  | -5.47 | 113.00      | 119.84   |
| 12  | DU    | 205  | ALA  | C-N-CA  | -5.47 | 113.00      | 119.84   |
| 56  | Cv    | 1021 | SER  | N-CA-C  | -5.47 | 105.23      | 111.14   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 51  | Cm    | 65   | GLY  | N-CA-C  | -5.47 | 107.70      | 115.30   |
| 2   | DD    | 752  | PHE  | CA-C-N  | 5.46  | 126.67      | 119.84   |
| 2   | DD    | 752  | PHE  | C-N-CA  | 5.46  | 126.67      | 119.84   |
| 33  | CJ    | 544  | THR  | CB-CA-C | -5.46 | 108.69      | 116.34   |
| 5   | DM    | 208  | HIS  | N-CA-C  | 5.46  | 120.05      | 113.17   |
| 41  | CS    | 129  | ASN  | N-CA-C  | -5.46 | 106.67      | 113.55   |
| 15  | DB    | 891  | GLN  | CB-CA-C | -5.45 | 109.81      | 117.23   |
| 26  | DX    | 130  | GLN  | N-CA-C  | 5.45  | 117.98      | 111.71   |
| 113 | BK    | 114  | HIS  | CA-C-N  | -5.45 | 113.03      | 119.84   |
| 113 | BK    | 114  | HIS  | C-N-CA  | -5.45 | 113.03      | 119.84   |
| 17  | DE    | 447  | ARG  | CA-C-N  | 5.43  | 125.41      | 120.03   |
| 17  | DE    | 447  | ARG  | C-N-CA  | 5.43  | 125.41      | 120.03   |
| 111 | BI    | 234  | SER  | N-CA-C  | 5.43  | 116.92      | 110.19   |
| 105 | BC    | 344  | PHE  | N-CA-C  | 5.43  | 118.69      | 111.75   |
| 1   | DA    | 1260 | VAL  | CA-C-N  | 5.42  | 126.62      | 119.84   |
| 1   | DA    | 1260 | VAL  | C-N-CA  | 5.42  | 126.62      | 119.84   |
| 1   | DA    | 1526 | GLY  | CA-C-N  | 5.42  | 125.04      | 119.56   |
| 1   | DA    | 1526 | GLY  | C-N-CA  | 5.42  | 125.04      | 119.56   |
| 104 | BB    | 190  | LEU  | N-CA-C  | 5.42  | 116.88      | 109.18   |
| 112 | BJ    | 194  | SER  | CA-C-N  | 5.42  | 125.88      | 120.14   |
| 112 | BJ    | 194  | SER  | C-N-CA  | 5.42  | 125.88      | 120.14   |
| 1   | DA    | 952  | ASN  | N-CA-C  | 5.42  | 118.35      | 111.69   |
| 74  | AF    | 205  | LYS  | CA-C-N  | 5.42  | 125.49      | 119.32   |
| 74  | AF    | 205  | LYS  | C-N-CA  | 5.42  | 125.49      | 119.32   |
| 119 | BQ    | 67   | GLY  | N-CA-C  | -5.42 | 107.56      | 115.63   |
| 128 | BZ    | 30   | CYS  | CA-C-N  | 5.41  | 124.60      | 118.97   |
| 128 | BZ    | 30   | CYS  | C-N-CA  | 5.41  | 124.60      | 118.97   |
| 120 | BR    | 76   | LYS  | CA-C-N  | -5.41 | 113.69      | 122.34   |
| 120 | BR    | 76   | LYS  | C-N-CA  | -5.41 | 113.69      | 122.34   |
| 2   | DD    | 713  | GLY  | CA-C-N  | 5.40  | 125.02      | 119.56   |
| 2   | DD    | 713  | GLY  | C-N-CA  | 5.40  | 125.02      | 119.56   |
| 20  | DH    | 345  | VAL  | CB-CA-C | -5.40 | 104.17      | 112.05   |
| 39  | CQ    | 156  | TYR  | N-CA-C  | 5.40  | 119.97      | 113.17   |
| 122 | BT    | 176  | GLY  | N-CA-C  | 5.40  | 119.11      | 112.14   |
| 16  | DC    | 462  | THR  | N-CA-C  | -5.40 | 106.70      | 113.72   |
| 88  | Ab    | 115  | PRO  | CA-C-N  | 5.40  | 125.40      | 119.90   |
| 88  | Ab    | 115  | PRO  | C-N-CA  | 5.40  | 125.40      | 119.90   |
| 53  | Cp    | 53   | VAL  | CA-C-N  | 5.39  | 124.73      | 118.85   |
| 53  | Cp    | 53   | VAL  | C-N-CA  | 5.39  | 124.73      | 118.85   |
| 79  | AP    | 347  | LEU  | N-CA-C  | -5.39 | 103.58      | 110.53   |
| 107 | BE    | 37   | PHE  | CA-C-N  | 5.39  | 125.70      | 119.93   |
| 107 | BE    | 37   | PHE  | C-N-CA  | 5.39  | 125.70      | 119.93   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | DT    | 210  | GLY  | CA-C-N  | 5.38  | 125.20      | 119.28   |
| 23  | DT    | 210  | GLY  | C-N-CA  | 5.38  | 125.20      | 119.28   |
| 20  | DH    | 41   | LYS  | N-CA-C  | -5.38 | 105.33      | 111.14   |
| 4   | DL    | 209  | ARG  | CA-C-N  | 5.38  | 125.45      | 119.32   |
| 4   | DL    | 209  | ARG  | C-N-CA  | 5.38  | 125.45      | 119.32   |
| 15  | DB    | 472  | GLY  | CA-C-N  | -5.38 | 118.09      | 123.04   |
| 15  | DB    | 472  | GLY  | C-N-CA  | -5.38 | 118.09      | 123.04   |
| 1   | DA    | 254  | PHE  | CA-C-N  | -5.38 | 115.01      | 123.13   |
| 1   | DA    | 254  | PHE  | C-N-CA  | -5.38 | 115.01      | 123.13   |
| 44  | Ca    | 438  | SER  | N-CA-C  | 5.37  | 115.38      | 108.34   |
| 3   | DI    | 64   | GLU  | N-CA-C  | 5.37  | 116.99      | 111.03   |
| 2   | DD    | 683  | ASP  | N-CA-C  | 5.36  | 118.28      | 111.69   |
| 4   | DL    | 276  | HIS  | N-CA-C  | 5.35  | 119.80      | 113.16   |
| 1   | DA    | 108  | TYR  | N-CA-C  | 5.35  | 116.97      | 111.03   |
| 15  | DB    | 626  | LEU  | N-CA-C  | -5.35 | 100.46      | 109.07   |
| 110 | BH    | 155  | PHE  | N-CA-C  | 5.34  | 119.95      | 113.38   |
| 16  | DC    | 245  | GLY  | N-CA-C  | 5.34  | 120.69      | 110.86   |
| 107 | BE    | 93   | ASP  | CA-C-N  | 5.34  | 125.41      | 119.32   |
| 107 | BE    | 93   | ASP  | C-N-CA  | 5.34  | 125.41      | 119.32   |
| 87  | AY    | 110  | ILE  | N-CA-C  | 5.33  | 117.23      | 111.58   |
| 88  | Ab    | 469  | ASP  | CA-C-N  | 5.33  | 124.94      | 119.56   |
| 88  | Ab    | 469  | ASP  | C-N-CA  | 5.33  | 124.94      | 119.56   |
| 15  | DB    | 946  | PRO  | CA-C-N  | -5.32 | 115.34      | 122.42   |
| 15  | DB    | 946  | PRO  | C-N-CA  | -5.32 | 115.34      | 122.42   |
| 79  | AP    | 48   | TRP  | N-CA-C  | -5.32 | 106.79      | 113.28   |
| 1   | DA    | 1250 | ARG  | CB-CA-C | -5.32 | 109.99      | 117.23   |
| 4   | DL    | 21   | VAL  | CA-C-N  | 5.32  | 125.32      | 119.90   |
| 4   | DL    | 21   | VAL  | C-N-CA  | 5.32  | 125.32      | 119.90   |
| 33  | CJ    | 485  | GLU  | N-CA-C  | 5.31  | 116.76      | 110.97   |
| 67  | A3    | 58   | PRO  | N-CA-C  | -5.31 | 102.24      | 111.32   |
| 33  | CJ    | 304  | ARG  | N-CA-C  | -5.31 | 105.16      | 111.69   |
| 112 | BJ    | 204  | ARG  | N-CA-C  | 5.31  | 119.24      | 112.87   |
| 33  | CJ    | 88   | ARG  | CA-C-N  | 5.29  | 125.27      | 120.03   |
| 33  | CJ    | 88   | ARG  | C-N-CA  | 5.29  | 125.27      | 120.03   |
| 36  | CN    | 38   | ASP  | N-CA-C  | 5.29  | 120.39      | 113.30   |
| 107 | BE    | 57   | PHE  | CA-C-N  | 5.29  | 124.95      | 119.56   |
| 107 | BE    | 57   | PHE  | C-N-CA  | 5.29  | 124.95      | 119.56   |
| 38  | CP    | 185  | ALA  | N-CA-C  | 5.29  | 120.75      | 113.77   |
| 65  | A1    | 145  | GLY  | CA-C-N  | 5.29  | 126.45      | 119.84   |
| 65  | A1    | 145  | GLY  | C-N-CA  | 5.29  | 126.45      | 119.84   |
| 10  | DR    | 188  | LYS  | N-CA-C  | -5.28 | 105.04      | 112.12   |
| 53  | Cp    | 48   | PRO  | O-C-N   | 5.27  | 123.63      | 121.15   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | DH    | 81   | LYS  | CB-CA-C    | -5.27 | 110.06      | 117.23   |
| 33  | CJ    | 205  | VAL  | N-CA-C     | 5.27  | 115.93      | 110.82   |
| 15  | DB    | 1043 | THR  | CA-C-N     | 5.26  | 125.18      | 119.76   |
| 15  | DB    | 1043 | THR  | C-N-CA     | 5.26  | 125.18      | 119.76   |
| 21  | DJ    | 156  | LYS  | CA-C-N     | 5.26  | 123.50      | 119.66   |
| 21  | DJ    | 156  | LYS  | C-N-CA     | 5.26  | 123.50      | 119.66   |
| 104 | BB    | 114  | ALA  | CA-C-N     | 5.26  | 124.87      | 119.56   |
| 104 | BB    | 114  | ALA  | C-N-CA     | 5.26  | 124.87      | 119.56   |
| 70  | A6    | 44   | ALA  | CA-C-N     | -5.26 | 114.68      | 122.41   |
| 70  | A6    | 44   | ALA  | C-N-CA     | -5.26 | 114.68      | 122.41   |
| 33  | CJ    | 196  | ALA  | N-CA-C     | 5.25  | 116.70      | 110.97   |
| 130 | Bb    | 70   | ASN  | N-CA-C     | 5.25  | 121.42      | 109.81   |
| 1   | DA    | 323  | HIS  | ND1-CG-CD2 | -5.25 | 100.85      | 106.10   |
| 1   | DA    | 1004 | GLY  | N-CA-C     | -5.25 | 106.47      | 115.08   |
| 6   | DN    | 276  | GLN  | N-CA-C     | 5.25  | 115.99      | 108.74   |
| 38  | CP    | 169  | ASN  | N-CA-C     | 5.24  | 117.94      | 110.24   |
| 107 | BE    | 271  | ASP  | CA-C-N     | 5.24  | 125.30      | 119.32   |
| 107 | BE    | 271  | ASP  | C-N-CA     | 5.24  | 125.30      | 119.32   |
| 106 | BD    | 450  | PRO  | N-CA-CB    | 5.23  | 108.75      | 103.25   |
| 12  | DU    | 124  | SER  | CA-C-N     | 5.23  | 125.31      | 119.87   |
| 12  | DU    | 124  | SER  | C-N-CA     | 5.23  | 125.31      | 119.87   |
| 5   | DM    | 164  | ILE  | N-CA-C     | 5.23  | 113.59      | 107.89   |
| 52  | Cn    | 234  | GLY  | N-CA-C     | 5.23  | 118.97      | 112.64   |
| 107 | BE    | 181  | THR  | CA-C-N     | -5.23 | 113.65      | 119.19   |
| 107 | BE    | 181  | THR  | C-N-CA     | -5.23 | 113.65      | 119.19   |
| 95  | Ao    | 71   | GLY  | N-CA-C     | -5.23 | 103.67      | 112.77   |
| 104 | BB    | 415  | ASP  | N-CA-C     | 5.23  | 117.38      | 111.11   |
| 33  | CJ    | 357  | SER  | N-CA-C     | 5.22  | 116.78      | 108.79   |
| 79  | AP    | 271  | TYR  | CA-C-N     | 5.22  | 124.83      | 119.56   |
| 79  | AP    | 271  | TYR  | C-N-CA     | 5.22  | 124.83      | 119.56   |
| 75  | AI    | 10   | ALA  | CA-C-N     | -5.22 | 114.54      | 119.76   |
| 75  | AI    | 10   | ALA  | C-N-CA     | -5.22 | 114.54      | 119.76   |
| 55  | Cr    | 83   | VAL  | CB-CA-C    | -5.22 | 108.75      | 113.70   |
| 54  | Cq    | 227  | ILE  | N-CA-C     | 5.21  | 115.43      | 110.42   |
| 55  | Cr    | 170  | ALA  | CB-CA-C    | -5.21 | 110.54      | 116.54   |
| 17  | DE    | 239  | TYR  | CA-C-N     | 5.21  | 125.21      | 120.21   |
| 17  | DE    | 239  | TYR  | C-N-CA     | 5.21  | 125.21      | 120.21   |
| 19  | DG    | 496  | ARG  | N-CA-C     | 5.21  | 117.45      | 109.95   |
| 113 | BK    | 287  | PRO  | CA-C-N     | 5.21  | 124.72      | 119.19   |
| 113 | BK    | 287  | PRO  | C-N-CA     | 5.21  | 124.72      | 119.19   |
| 1   | DA    | 1088 | ALA  | N-CA-C     | -5.21 | 103.73      | 110.19   |
| 41  | CS    | 61   | THR  | N-CA-C     | -5.21 | 105.67      | 112.23   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 80  | AQ    | 79   | PHE  | N-CA-C  | 5.21  | 117.11      | 109.24   |
| 95  | Ao    | 98   | GLY  | N-CA-C  | -5.20 | 106.49      | 112.73   |
| 33  | CJ    | 158  | THR  | N-CA-C  | 5.20  | 117.63      | 110.35   |
| 44  | Ca    | 254  | ARG  | N-CA-C  | 5.20  | 117.69      | 111.71   |
| 29  | CE    | 255  | ASN  | N-CA-C  | 5.20  | 118.88      | 111.92   |
| 33  | CJ    | 768  | ASP  | N-CA-C  | 5.20  | 116.88      | 109.14   |
| 33  | CJ    | 346  | PRO  | N-CA-C  | 5.19  | 122.19      | 113.78   |
| 41  | CS    | 65   | ASN  | CA-C-N  | 5.19  | 125.48      | 119.93   |
| 41  | CS    | 65   | ASN  | C-N-CA  | 5.19  | 125.48      | 119.93   |
| 74  | AF    | 90   | LEU  | CA-C-N  | 5.19  | 124.85      | 119.56   |
| 74  | AF    | 90   | LEU  | C-N-CA  | 5.19  | 124.85      | 119.56   |
| 78  | AN    | 94   | VAL  | N-CA-C  | 5.19  | 116.93      | 109.51   |
| 103 | BA    | 313  | GLY  | N-CA-C  | -5.19 | 100.89      | 113.18   |
| 56  | Cv    | 1116 | GLU  | N-CA-C  | 5.18  | 119.75      | 113.38   |
| 74  | AF    | 371  | LEU  | CA-C-N  | 5.18  | 123.44      | 119.66   |
| 74  | AF    | 371  | LEU  | C-N-CA  | 5.18  | 123.44      | 119.66   |
| 3   | DI    | 331  | VAL  | N-CA-C  | 5.18  | 115.29      | 110.42   |
| 47  | Cg    | 88   | PHE  | CA-C-N  | -5.18 | 117.09      | 122.89   |
| 47  | Cg    | 88   | PHE  | C-N-CA  | -5.18 | 117.09      | 122.89   |
| 74  | AF    | 371  | LEU  | N-CA-C  | 5.18  | 115.56      | 109.60   |
| 106 | BD    | 140  | PRO  | N-CA-CB | 5.18  | 108.69      | 103.25   |
| 1   | DA    | 947  | GLY  | CA-C-N  | 5.17  | 124.94      | 119.76   |
| 1   | DA    | 947  | GLY  | C-N-CA  | 5.17  | 124.94      | 119.76   |
| 96  | Ap    | 137  | SER  | CA-C-N  | 5.17  | 124.89      | 119.82   |
| 96  | Ap    | 137  | SER  | C-N-CA  | 5.17  | 124.89      | 119.82   |
| 44  | Ca    | 599  | ILE  | N-CA-C  | 5.17  | 120.06      | 108.88   |
| 13  | DZ    | 40   | ILE  | CA-C-N  | 5.17  | 124.78      | 119.56   |
| 13  | DZ    | 40   | ILE  | C-N-CA  | 5.17  | 124.78      | 119.56   |
| 18  | DF    | 3    | VAL  | N-CA-C  | 5.17  | 115.30      | 107.80   |
| 33  | CJ    | 56   | ILE  | N-CA-C  | 5.16  | 115.27      | 110.42   |
| 24  | DV    | 109  | ILE  | CA-C-N  | 5.16  | 125.16      | 119.90   |
| 24  | DV    | 109  | ILE  | C-N-CA  | 5.16  | 125.16      | 119.90   |
| 20  | DH    | 370  | VAL  | N-CA-C  | 5.16  | 115.59      | 110.23   |
| 79  | AP    | 323  | PRO  | CA-C-N  | 5.16  | 124.66      | 119.19   |
| 79  | AP    | 323  | PRO  | C-N-CA  | 5.16  | 124.66      | 119.19   |
| 103 | BA    | 277  | ILE  | CA-C-N  | -5.15 | 115.69      | 122.85   |
| 103 | BA    | 277  | ILE  | C-N-CA  | -5.15 | 115.69      | 122.85   |
| 134 | Bf    | 99   | ILE  | N-CA-C  | -5.15 | 98.62       | 109.34   |
| 47  | Cg    | 369  | GLY  | N-CA-C  | -5.15 | 103.81      | 112.77   |
| 122 | BT    | 76   | GLY  | N-CA-C  | -5.14 | 108.13      | 115.64   |
| 1   | DA    | 890  | VAL  | CA-C-N  | 5.13  | 125.29      | 119.90   |
| 1   | DA    | 890  | VAL  | C-N-CA  | 5.13  | 125.29      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 88  | Ab    | 292  | VAL  | N-CA-C | 5.13  | 115.97      | 108.58   |
| 33  | CJ    | 156  | PRO  | CA-C-N | 5.13  | 126.25      | 119.84   |
| 33  | CJ    | 156  | PRO  | C-N-CA | 5.13  | 126.25      | 119.84   |
| 8   | DP    | 85   | GLY  | N-CA-C | 5.12  | 122.79      | 112.34   |
| 112 | BJ    | 246  | ILE  | N-CA-C | 5.12  | 115.65      | 108.17   |
| 16  | DC    | 755  | ASP  | N-CA-C | 5.12  | 116.76      | 108.26   |
| 6   | DN    | 40   | ASP  | CA-C-N | -5.11 | 113.45      | 119.84   |
| 6   | DN    | 40   | ASP  | C-N-CA | -5.11 | 113.45      | 119.84   |
| 120 | BR    | 70   | TYR  | N-CA-C | 5.11  | 117.73      | 108.69   |
| 25  | DW    | 157  | ASN  | CA-C-N | 5.10  | 125.14      | 119.32   |
| 25  | DW    | 157  | ASN  | C-N-CA | 5.10  | 125.14      | 119.32   |
| 48  | Ci    | 108  | PRO  | CA-C-N | -5.10 | 115.86      | 123.11   |
| 48  | Ci    | 108  | PRO  | C-N-CA | -5.10 | 115.86      | 123.11   |
| 1   | DA    | 149  | GLY  | N-CA-C | 5.09  | 120.75      | 114.69   |
| 29  | CE    | 210  | GLY  | CA-C-N | 5.09  | 124.85      | 119.76   |
| 29  | CE    | 210  | GLY  | C-N-CA | 5.09  | 124.85      | 119.76   |
| 23  | DT    | 223  | LEU  | CA-C-N | -5.09 | 113.48      | 119.84   |
| 23  | DT    | 223  | LEU  | C-N-CA | -5.09 | 113.48      | 119.84   |
| 26  | DX    | 39   | GLY  | N-CA-C | -5.09 | 104.81      | 111.37   |
| 66  | A2    | 434  | CYS  | CA-C-N | 5.09  | 124.70      | 119.56   |
| 66  | A2    | 434  | CYS  | C-N-CA | 5.09  | 124.70      | 119.56   |
| 56  | Cv    | 995  | VAL  | N-CA-C | 5.08  | 119.91      | 109.34   |
| 7   | DO    | 116  | ALA  | N-CA-C | -5.07 | 106.60      | 112.89   |
| 50  | Ck    | 659  | GLY  | N-CA-C | -5.07 | 101.99      | 112.34   |
| 33  | CJ    | 373  | PHE  | N-CA-C | 5.07  | 116.78      | 109.07   |
| 18  | DF    | 194  | THR  | N-CA-C | 5.06  | 118.23      | 111.75   |
| 116 | BN    | 116  | ILE  | N-CA-C | -5.06 | 98.81       | 109.34   |
| 119 | BQ    | 97   | ILE  | N-CA-C | 5.06  | 115.21      | 110.30   |
| 1   | DA    | 1181 | THR  | N-CA-C | 5.06  | 117.18      | 111.11   |
| 15  | DB    | 1082 | LYS  | N-CA-C | 5.06  | 117.06      | 110.43   |
| 87  | AY    | 97   | TYR  | N-CA-C | 5.06  | 118.48      | 112.72   |
| 18  | DF    | 302  | VAL  | N-CA-C | 5.05  | 115.72      | 110.82   |
| 1   | DA    | 1311 | SER  | N-CA-C | 5.04  | 119.58      | 113.38   |
| 119 | BQ    | 176  | VAL  | N-CA-C | 5.04  | 115.27      | 110.53   |
| 6   | DN    | 269  | LEU  | N-CA-C | -5.04 | 106.91      | 113.16   |
| 1   | DA    | 774  | GLY  | N-CA-C | 5.04  | 121.77      | 114.67   |
| 94  | Al    | 123  | PRO  | O-C-N  | 5.04  | 123.52      | 121.15   |
| 98  | Av    | 100  | PRO  | O-C-N  | 5.03  | 123.62      | 121.31   |
| 95  | Ao    | 133  | ILE  | CA-C-N | 5.03  | 125.03      | 119.90   |
| 95  | Ao    | 133  | ILE  | C-N-CA | 5.03  | 125.03      | 119.90   |
| 18  | DF    | 242  | VAL  | N-CA-C | 5.03  | 118.38      | 112.35   |
| 67  | A3    | 146  | PRO  | CA-C-N | 5.03  | 124.64      | 119.56   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 67  | A3    | 146 | PRO  | C-N-CA | 5.03 | 124.64      | 119.56   |
| 88  | Ab    | 258 | ASP  | N-CA-C | 5.03 | 119.10      | 112.92   |
| 15  | DB    | 436 | GLU  | N-CA-C | 5.03 | 116.45      | 111.07   |
| 66  | A2    | 470 | ASP  | N-CA-C | 5.02 | 119.49      | 113.17   |
| 103 | BA    | 357 | MET  | CA-C-N | 5.02 | 124.63      | 119.56   |
| 103 | BA    | 357 | MET  | C-N-CA | 5.02 | 124.63      | 119.56   |
| 94  | Al    | 147 | PRO  | N-CA-C | 5.01 | 120.64      | 113.47   |
| 88  | Ab    | 282 | SER  | N-CA-C | 5.01 | 116.61      | 109.14   |
| 84  | AV    | 200 | THR  | CA-C-N | 5.01 | 124.50      | 119.19   |
| 84  | AV    | 200 | THR  | C-N-CA | 5.01 | 124.50      | 119.19   |
| 6   | DN    | 209 | ARG  | CA-C-N | 5.00 | 125.27      | 119.47   |
| 6   | DN    | 209 | ARG  | C-N-CA | 5.00 | 125.27      | 119.47   |

There are no chirality outliers.

All (75) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 66  | A2    | 133 | GLY  | Peptide |
| 66  | A2    | 293 | PHE  | Peptide |
| 67  | A3    | 57  | GLY  | Peptide |
| 71  | A8    | 90  | GLY  | Peptide |
| 71  | A8    | 91  | LYS  | Peptide |
| 73  | AE    | 359 | ALA  | Peptide |
| 74  | AF    | 314 | TYR  | Peptide |
| 74  | AF    | 318 | ALA  | Peptide |
| 74  | AF    | 325 | GLY  | Peptide |
| 81  | AR    | 140 | ASN  | Peptide |
| 81  | AR    | 166 | LYS  | Peptide |
| 81  | AR    | 235 | TRP  | Peptide |
| 83  | AU    | 25  | ARG  | Peptide |
| 84  | AV    | 128 | ARG  | Peptide |
| 85  | AW    | 71  | ILE  | Peptide |
| 87  | AY    | 107 | SER  | Peptide |
| 87  | AY    | 243 | ASP  | Peptide |
| 88  | Ab    | 288 | GLY  | Peptide |
| 98  | Av    | 231 | ILE  | Peptide |
| 104 | BB    | 259 | GLU  | Peptide |
| 105 | BC    | 400 | GLU  | Peptide |
| 107 | BE    | 383 | SER  | Peptide |
| 107 | BE    | 42  | GLY  | Peptide |
| 108 | BF    | 336 | GLY  | Peptide |
| 109 | BG    | 165 | GLU  | Peptide |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 110        | BH           | 229        | ALA         | Peptide      |
| 113        | BK           | 311        | GLU         | Peptide      |
| 113        | BK           | 324        | LYS         | Peptide      |
| 115        | BM           | 134        | ALA         | Peptide      |
| 115        | BM           | 76         | TRP         | Peptide      |
| 116        | BN           | 114        | ASP         | Peptide      |
| 116        | BN           | 36         | GLU         | Peptide      |
| 116        | BN           | 37         | ASN         | Peptide      |
| 117        | BO           | 75         | PHE         | Peptide      |
| 118        | BP           | 144        | PHE         | Peptide      |
| 118        | BP           | 59         | GLN         | Peptide      |
| 120        | BR           | 173        | GLY         | Peptide      |
| 120        | BR           | 174        | ALA         | Peptide      |
| 130        | Bb           | 70         | ASN         | Peptide      |
| 130        | Bb           | 73         | PRO         | Peptide      |
| 134        | Bf           | 92         | HIS         | Peptide      |
| 134        | Bf           | 98         | TYR         | Peptide      |
| 136        | Bh           | 60         | VAL         | Peptide      |
| 136        | Bh           | 88         | LYS         | Peptide      |
| 31         | CH           | 92         | PRO         | Peptide      |
| 33         | CJ           | 100        | ARG         | Peptide      |
| 44         | Ca           | 599        | ILE         | Peptide      |
| 47         | Cg           | 50         | PRO         | Peptide      |
| 48         | Ci           | 150        | SER         | Peptide      |
| 49         | Cj           | 53         | ASN         | Peptide      |
| 50         | Ck           | 230        | LEU         | Peptide      |
| 56         | Cv           | 545        | THR         | Peptide      |
| 56         | Cv           | 943        | LEU         | Peptide      |
| 1          | DA           | 166        | TYR         | Peptide      |
| 15         | DB           | 383        | ARG         | Sidechain    |
| 15         | DB           | 586        | ARG         | Sidechain    |
| 16         | DC           | 497        | PRO         | Peptide      |
| 16         | DC           | 775        | ALA         | Peptide      |
| 2          | DD           | 248        | ASP         | Peptide      |
| 2          | DD           | 255        | VAL         | Peptide      |
| 19         | DG           | 184        | ALA         | Peptide      |
| 19         | DG           | 592        | THR         | Peptide      |
| 21         | DJ           | 35         | PRO         | Peptide      |
| 4          | DL           | 269        | MET         | Peptide      |
| 4          | DL           | 270        | THR         | Peptide      |
| 6          | DN           | 142        | ARG         | Peptide      |
| 6          | DN           | 292        | TYR         | Peptide      |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 7   | DO    | 124 | CYS  | Peptide |
| 7   | DO    | 251 | ASN  | Peptide |
| 10  | DR    | 23  | VAL  | Peptide |
| 23  | DT    | 43  | ASP  | Peptide |
| 26  | DX    | 127 | MET  | Peptide |
| 140 | UD    | 47  | UNK  | Peptide |
| 142 | UN    | 3   | UNK  | Peptide |
| 147 | UU    | 7   | UNK  | 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   | DA    | 12482 | 0        | 12152    | 366     | 0            |
| 2   | DD    | 6523  | 0        | 6307     | 216     | 0            |
| 3   | DI    | 3182  | 0        | 3153     | 80      | 0            |
| 4   | DL    | 2287  | 0        | 2273     | 186     | 0            |
| 5   | DM    | 2430  | 0        | 2427     | 81      | 0            |
| 6   | DN    | 2091  | 0        | 2076     | 121     | 0            |
| 7   | DO    | 1804  | 0        | 1752     | 49      | 0            |
| 8   | DP    | 1760  | 0        | 1723     | 76      | 0            |
| 9   | DQ    | 2061  | 0        | 2041     | 85      | 0            |
| 10  | DR    | 2025  | 0        | 2029     | 105     | 0            |
| 11  | DS    | 1904  | 0        | 1855     | 55      | 0            |
| 12  | DU    | 1754  | 0        | 1687     | 84      | 0            |
| 13  | DZ    | 697   | 0        | 644      | 27      | 0            |
| 14  | Da    | 501   | 0        | 473      | 23      | 0            |
| 15  | DB    | 9148  | 0        | 8834     | 247     | 0            |
| 16  | DC    | 8748  | 0        | 8532     | 189     | 0            |
| 17  | DE    | 4831  | 0        | 4789     | 116     | 0            |
| 18  | DF    | 4747  | 0        | 4723     | 151     | 0            |
| 19  | DG    | 4575  | 0        | 4490     | 181     | 0            |
| 20  | DH    | 4578  | 0        | 4520     | 132     | 0            |
| 21  | DJ    | 2572  | 0        | 2495     | 81      | 0            |
| 22  | DK    | 2007  | 0        | 1998     | 51      | 0            |
| 23  | DT    | 2058  | 0        | 1928     | 55      | 0            |
| 24  | DV    | 1346  | 0        | 1335     | 43      | 0            |
| 25  | DW    | 1359  | 0        | 1342     | 72      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26  | DX    | 1196  | 0        | 1189     | 39      | 0            |
| 27  | DY    | 1293  | 0        | 1287     | 43      | 0            |
| 28  | CC    | 646   | 0        | 679      | 20      | 0            |
| 29  | CE    | 3399  | 0        | 3376     | 152     | 0            |
| 30  | CF    | 1292  | 0        | 1261     | 33      | 0            |
| 31  | CH    | 2228  | 0        | 2204     | 68      | 0            |
| 32  | CI    | 3386  | 0        | 3373     | 158     | 0            |
| 33  | CJ    | 6516  | 0        | 6259     | 220     | 0            |
| 34  | CK    | 2418  | 0        | 2360     | 115     | 0            |
| 35  | CL    | 733   | 0        | 738      | 38      | 0            |
| 36  | CN    | 1322  | 0        | 1304     | 47      | 0            |
| 37  | CO    | 3003  | 0        | 2995     | 116     | 0            |
| 38  | CP    | 1489  | 0        | 1510     | 57      | 0            |
| 39  | CQ    | 1584  | 0        | 1601     | 48      | 0            |
| 40  | CR    | 2567  | 0        | 2503     | 222     | 0            |
| 41  | CS    | 1175  | 0        | 1191     | 44      | 0            |
| 42  | CU    | 1538  | 0        | 1539     | 48      | 0            |
| 43  | CZ    | 1212  | 0        | 1178     | 29      | 0            |
| 44  | Ca    | 5004  | 0        | 4776     | 190     | 0            |
| 45  | Cb    | 2056  | 0        | 2031     | 93      | 0            |
| 46  | Cd    | 2389  | 0        | 2228     | 108     | 0            |
| 47  | Cg    | 3904  | 0        | 3785     | 100     | 0            |
| 48  | Ci    | 1348  | 0        | 1306     | 56      | 0            |
| 49  | Cj    | 1792  | 0        | 1744     | 58      | 0            |
| 50  | Ck    | 5596  | 0        | 5613     | 147     | 0            |
| 51  | Cm    | 1577  | 0        | 1505     | 100     | 0            |
| 52  | Cn    | 912   | 0        | 969      | 38      | 0            |
| 53  | Cp    | 1483  | 0        | 1438     | 54      | 0            |
| 54  | Cq    | 2005  | 0        | 1916     | 66      | 0            |
| 55  | Cr    | 1999  | 0        | 2007     | 62      | 0            |
| 56  | Cv    | 8557  | 0        | 8252     | 266     | 0            |
| 57  | CA    | 13122 | 0        | 6562     | 283     | 0            |
| 58  | UO    | 30    | 0        | 33       | 0       | 0            |
| 59  | UP    | 42    | 0        | 44       | 0       | 0            |
| 59  | UW    | 42    | 0        | 44       | 3       | 0            |
| 60  | UQ    | 192   | 0        | 194      | 2       | 0            |
| 61  | UR    | 48    | 0        | 50       | 6       | 0            |
| 61  | UV    | 48    | 0        | 50       | 0       | 0            |
| 61  | UX    | 48    | 0        | 50       | 5       | 0            |
| 62  | US    | 324   | 0        | 326      | 9       | 0            |
| 63  | UT    | 264   | 0        | 267      | 10      | 0            |
| 64  | A0    | 1269  | 0        | 1285     | 48      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 65  | A1    | 1788  | 0        | 1814     | 73      | 0            |
| 66  | A2    | 3638  | 0        | 3601     | 106     | 0            |
| 67  | A3    | 1215  | 0        | 1272     | 44      | 0            |
| 68  | A4    | 1387  | 0        | 1406     | 71      | 0            |
| 69  | A5    | 483   | 0        | 494      | 33      | 0            |
| 70  | A6    | 568   | 0        | 590      | 16      | 0            |
| 71  | A8    | 1203  | 0        | 1225     | 69      | 0            |
| 72  | A9    | 459   | 0        | 430      | 17      | 0            |
| 73  | AE    | 2390  | 0        | 2279     | 100     | 0            |
| 74  | AF    | 3597  | 0        | 3509     | 114     | 0            |
| 75  | AI    | 1790  | 0        | 1765     | 75      | 0            |
| 76  | AJ    | 965   | 0        | 906      | 55      | 0            |
| 77  | AK    | 2676  | 0        | 2685     | 104     | 0            |
| 78  | AN    | 1508  | 0        | 1487     | 73      | 0            |
| 79  | AP    | 2904  | 0        | 2847     | 120     | 0            |
| 80  | AQ    | 1020  | 0        | 1011     | 23      | 0            |
| 81  | AR    | 1912  | 0        | 1858     | 72      | 0            |
| 82  | AT    | 287   | 0        | 291      | 5       | 0            |
| 83  | AU    | 1423  | 0        | 1447     | 35      | 0            |
| 84  | AV    | 1424  | 0        | 1456     | 43      | 0            |
| 85  | AW    | 2235  | 0        | 2270     | 89      | 0            |
| 86  | AX    | 1416  | 0        | 1396     | 53      | 0            |
| 87  | AY    | 2712  | 0        | 2605     | 91      | 0            |
| 88  | Ab    | 3545  | 0        | 3343     | 110     | 0            |
| 89  | Ad    | 2122  | 0        | 2031     | 115     | 0            |
| 90  | Ae    | 927   | 0        | 911      | 25      | 0            |
| 91  | Af    | 1013  | 0        | 999      | 41      | 0            |
| 92  | Ag    | 2193  | 0        | 2127     | 78      | 0            |
| 93  | Aj    | 2246  | 0        | 2149     | 88      | 0            |
| 94  | Al    | 1618  | 0        | 1615     | 51      | 0            |
| 95  | Ao    | 1475  | 0        | 1437     | 52      | 0            |
| 96  | Ap    | 2143  | 0        | 2124     | 109     | 0            |
| 97  | At    | 1100  | 0        | 1085     | 49      | 0            |
| 98  | Av    | 1792  | 0        | 1782     | 78      | 0            |
| 99  | AB    | 280   | 0        | 279      | 3       | 0            |
| 100 | AC    | 140   | 0        | 139      | 3       | 0            |
| 100 | AD    | 140   | 0        | 139      | 0       | 0            |
| 101 | AG    | 135   | 0        | 134      | 1       | 0            |
| 102 | AA    | 12491 | 0        | 6245     | 319     | 0            |
| 103 | BA    | 5384  | 0        | 5427     | 163     | 0            |
| 104 | BB    | 3050  | 0        | 2897     | 107     | 0            |
| 105 | BC    | 3821  | 0        | 3778     | 141     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 106 | BD    | 2063  | 0        | 967      | 24      | 0            |
| 107 | BE    | 3105  | 0        | 3030     | 105     | 0            |
| 108 | BF    | 2838  | 0        | 2819     | 87      | 0            |
| 109 | BG    | 2503  | 0        | 2476     | 87      | 0            |
| 110 | BH    | 1729  | 0        | 1691     | 57      | 0            |
| 111 | BI    | 2609  | 0        | 2543     | 85      | 0            |
| 112 | BJ    | 1339  | 0        | 1307     | 43      | 0            |
| 113 | BK    | 1998  | 0        | 1867     | 50      | 0            |
| 114 | BL    | 1887  | 0        | 1831     | 55      | 0            |
| 115 | BM    | 2015  | 0        | 1937     | 74      | 0            |
| 116 | BN    | 1746  | 0        | 1663     | 72      | 0            |
| 117 | BO    | 1146  | 0        | 1183     | 47      | 0            |
| 118 | BP    | 1550  | 0        | 1519     | 52      | 0            |
| 119 | BQ    | 1675  | 0        | 1619     | 42      | 0            |
| 120 | BR    | 1650  | 0        | 1632     | 67      | 0            |
| 121 | BS    | 784   | 0        | 773      | 32      | 0            |
| 122 | BT    | 1389  | 0        | 1357     | 38      | 0            |
| 123 | BU    | 694   | 0        | 697      | 26      | 0            |
| 124 | BV    | 1307  | 0        | 1295     | 44      | 0            |
| 125 | BW    | 1557  | 0        | 1517     | 49      | 0            |
| 126 | BX    | 867   | 0        | 812      | 35      | 0            |
| 127 | BY    | 877   | 0        | 826      | 31      | 0            |
| 128 | BZ    | 1390  | 0        | 1343     | 35      | 0            |
| 129 | Ba    | 1224  | 0        | 1169     | 48      | 0            |
| 130 | Bb    | 770   | 0        | 773      | 26      | 0            |
| 131 | Bc    | 781   | 0        | 752      | 30      | 0            |
| 132 | Bd    | 1113  | 0        | 1094     | 64      | 0            |
| 133 | Be    | 822   | 0        | 794      | 27      | 0            |
| 134 | Bf    | 434   | 0        | 402      | 34      | 0            |
| 135 | Bg    | 656   | 0        | 649      | 32      | 0            |
| 136 | Bh    | 730   | 0        | 708      | 44      | 0            |
| 137 | UA    | 276   | 0        | 280      | 16      | 0            |
| 138 | UB    | 240   | 0        | 242      | 8       | 0            |
| 139 | UC    | 72    | 0        | 75       | 12      | 0            |
| 139 | UH    | 72    | 0        | 75       | 2       | 0            |
| 140 | UD    | 1062  | 0        | 1075     | 58      | 0            |
| 141 | UE    | 132   | 0        | 134      | 14      | 0            |
| 142 | UF    | 144   | 0        | 146      | 6       | 0            |
| 142 | UG    | 144   | 0        | 146      | 3       | 0            |
| 142 | UN    | 144   | 0        | 147      | 7       | 0            |
| 143 | UI    | 102   | 0        | 105      | 9       | 0            |
| 144 | UK    | 60    | 0        | 62       | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 145 | UL    | 90     | 0        | 93       | 7       | 0            |
| 146 | UM    | 36     | 0        | 38       | 6       | 0            |
| 147 | UU    | 66     | 0        | 68       | 5       | 0            |
| 148 | A5    | 1      | 0        | 0        | 1       | 0            |
| 148 | A9    | 1      | 0        | 0        | 0       | 0            |
| 148 | BX    | 2      | 0        | 0        | 0       | 0            |
| 148 | Be    | 1      | 0        | 0        | 0       | 0            |
| 148 | Bh    | 1      | 0        | 0        | 0       | 0            |
| 148 | Cr    | 1      | 0        | 0        | 0       | 0            |
| 148 | DA    | 1      | 0        | 0        | 0       | 0            |
| 148 | DS    | 2      | 0        | 0        | 0       | 0            |
| 149 | CA    | 30     | 0        | 57       | 3       | 0            |
| 149 | DL    | 10     | 0        | 19       | 0       | 0            |
| 150 | DJ    | 29     | 0        | 11       | 5       | 0            |
| 151 | AA    | 7      | 0        | 0        | 0       | 0            |
| 151 | CA    | 34     | 0        | 0        | 0       | 0            |
| 151 | CO    | 1      | 0        | 0        | 0       | 0            |
| 151 | CQ    | 1      | 0        | 0        | 0       | 0            |
| 151 | Ca    | 1      | 0        | 0        | 0       | 0            |
| 151 | Cg    | 1      | 0        | 0        | 0       | 0            |
| 151 | Cv    | 1      | 0        | 0        | 0       | 0            |
| 152 | Cg    | 32     | 0        | 12       | 7       | 0            |
| 153 | CA    | 14     | 0        | 26       | 1       | 0            |
| 154 | Av    | 44     | 0        | 26       | 4       | 0            |
| 155 | UB    | 1      | 0        | 0        | 0       | 0            |
| 156 | Cg    | 3      | 0        | 0        | 1       | 0            |
| All | All   | 311240 | 0        | 291767   | 8297    | 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 14.

All (8297) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:CR:308:MET:HE3  | 57:CA:388:U:C4'   | 1.24                     | 1.57              |
| 40:CR:308:MET:CE   | 57:CA:388:U:H4'   | 1.12                     | 1.57              |
| 33:CJ:36:MET:HE1   | 51:Cm:52:THR:CG2  | 1.11                     | 1.56              |
| 19:DG:111:ARG:HH12 | 45:Cb:197:PRO:CG  | 1.19                     | 1.54              |
| 4:DL:74:ARG:HH22   | 29:CE:110:LEU:CD1 | 1.21                     | 1.51              |
| 33:CJ:484:HIS:CD2  | 33:CJ:495:ARG:NH1 | 1.87                     | 1.42              |
| 19:DG:111:ARG:HH12 | 45:Cb:197:PRO:CB  | 1.31                     | 1.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:36:MET:CE    | 51:Cm:52:THR:HB    | 1.50                     | 1.40              |
| 40:CR:308:MET:CE   | 57:CA:388:U:C4'    | 1.82                     | 1.40              |
| 1:DA:1002:PRO:C    | 4:DL:78:ALA:HB1    | 1.46                     | 1.39              |
| 33:CJ:36:MET:HE1   | 51:Cm:52:THR:CB    | 1.50                     | 1.38              |
| 33:CJ:544:THR:HG21 | 33:CJ:552:ILE:N    | 1.36                     | 1.38              |
| 33:CJ:544:THR:CG2  | 33:CJ:552:ILE:HG12 | 1.53                     | 1.38              |
| 4:DL:74:ARG:NH2    | 29:CE:110:LEU:HD12 | 1.10                     | 1.38              |
| 1:DA:1278:THR:HG23 | 54:Cq:152:GLU:CD   | 0.93                     | 1.35              |
| 33:CJ:484:HIS:HD2  | 33:CJ:495:ARG:NH1  | 1.17                     | 1.34              |
| 19:DG:64:ARG:HH21  | 40:CR:249:GLN:NE2  | 1.22                     | 1.33              |
| 19:DG:111:ARG:NH1  | 45:Cb:197:PRO:HG2  | 1.40                     | 1.33              |
| 25:DW:127:PHE:N    | 40:CR:287:MET:HE1  | 1.43                     | 1.33              |
| 4:DL:63:ASP:OD2    | 51:Cm:21:GLN:HG2   | 1.28                     | 1.32              |
| 1:DA:1186:CYS:SG   | 1:DA:1193:HIS:NE2  | 2.03                     | 1.32              |
| 33:CJ:36:MET:CE    | 51:Cm:52:THR:CB    | 2.05                     | 1.32              |
| 1:DA:1002:PRO:O    | 4:DL:78:ALA:HB1    | 1.21                     | 1.32              |
| 1:DA:1280:GLU:OE1  | 54:Cq:151:ARG:NH1  | 1.62                     | 1.31              |
| 33:CJ:484:HIS:CD2  | 33:CJ:495:ARG:HH12 | 1.48                     | 1.30              |
| 10:DR:128:PRO:CD   | 10:DR:133:LEU:O    | 1.77                     | 1.30              |
| 33:CJ:36:MET:CE    | 51:Cm:52:THR:CG2   | 2.08                     | 1.29              |
| 4:DL:74:ARG:NH2    | 29:CE:110:LEU:CD1  | 1.80                     | 1.28              |
| 1:DA:1016:MET:SD   | 4:DL:74:ARG:HB3    | 1.74                     | 1.26              |
| 38:CP:23:ALA:HB2   | 38:CP:51:HIS:CG    | 1.68                     | 1.26              |
| 4:DL:117:ASP:O     | 4:DL:121:ILE:HG13  | 1.35                     | 1.25              |
| 19:DG:57:GLU:OE2   | 32:CI:245:ARG:NH2  | 1.70                     | 1.24              |
| 19:DG:111:ARG:NH1  | 45:Cb:197:PRO:CG   | 1.93                     | 1.24              |
| 106:BD:109:CYS:CB  | 106:BD:343:LEU:CB  | 2.17                     | 1.23              |
| 1:DA:1186:CYS:SG   | 1:DA:1193:HIS:CE1  | 2.31                     | 1.22              |
| 33:CJ:544:THR:HG22 | 33:CJ:552:ILE:CG1  | 1.68                     | 1.22              |
| 19:DG:64:ARG:NH2   | 40:CR:249:GLN:HE22 | 1.38                     | 1.21              |
| 25:DW:126:ARG:C    | 40:CR:287:MET:HE1  | 1.64                     | 1.21              |
| 19:DG:111:ARG:NH1  | 45:Cb:197:PRO:CB   | 2.01                     | 1.19              |
| 6:DN:75:VAL:HG11   | 6:DN:110:ALA:CB    | 1.73                     | 1.18              |
| 4:DL:63:ASP:CG     | 51:Cm:21:GLN:HG2   | 1.67                     | 1.18              |
| 1:DA:1278:THR:CB   | 54:Cq:152:GLU:OE1  | 1.92                     | 1.17              |
| 4:DL:68:LEU:O      | 29:CE:112:THR:HG21 | 1.44                     | 1.17              |
| 40:CR:8:ILE:CG2    | 56:Cv:909:LEU:HD23 | 1.72                     | 1.17              |
| 32:CI:241:ARG:HG3  | 33:CJ:56:ILE:O     | 1.41                     | 1.17              |
| 40:CR:316:GLY:O    | 46:Cd:279:ARG:HD2  | 1.38                     | 1.17              |
| 4:DL:63:ASP:OD2    | 51:Cm:21:GLN:CG    | 1.93                     | 1.16              |
| 4:DL:114:SER:HA    | 4:DL:254:ARG:CZ    | 1.75                     | 1.16              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Cm:137:SER:OG   | 57:CA:394:A:C2     | 1.98                     | 1.16              |
| 106:BD:205:GLU:H   | 106:BD:451:ALA:HB1 | 1.00                     | 1.15              |
| 25:DW:127:PHE:HA   | 40:CR:287:MET:HE3  | 1.27                     | 1.15              |
| 1:DA:1186:CYS:HG   | 1:DA:1193:HIS:CE1  | 1.63                     | 1.15              |
| 34:CK:14:PRO:HD3   | 40:CR:300:TYR:CD2  | 1.80                     | 1.15              |
| 1:DA:1002:PRO:O    | 4:DL:78:ALA:CB     | 1.94                     | 1.15              |
| 5:DM:64:THR:HG23   | 5:DM:69:PHE:O      | 1.43                     | 1.15              |
| 40:CR:316:GLY:O    | 46:Cd:279:ARG:CD   | 1.93                     | 1.14              |
| 15:DB:1154:LYS:HD3 | 89:Ad:150:ARG:CD   | 1.78                     | 1.13              |
| 10:DR:128:PRO:HD2  | 10:DR:133:LEU:O    | 1.34                     | 1.12              |
| 40:CR:8:ILE:HG21   | 56:Cv:909:LEU:CD2  | 1.80                     | 1.12              |
| 40:CR:308:MET:HE1  | 57:CA:388:U:C4'    | 1.75                     | 1.12              |
| 40:CR:316:GLY:C    | 46:Cd:279:ARG:HB3  | 1.54                     | 1.12              |
| 1:DA:1278:THR:HG21 | 54:Cq:152:GLU:OE1  | 1.42                     | 1.11              |
| 6:DN:113:ALA:HB3   | 6:DN:133:PHE:CE1   | 1.85                     | 1.11              |
| 1:DA:1016:MET:SD   | 4:DL:74:ARG:CB     | 2.39                     | 1.11              |
| 38:CP:23:ALA:CB    | 38:CP:51:HIS:CG    | 2.32                     | 1.11              |
| 18:DF:426:LEU:HB3  | 20:DH:200:THR:HG21 | 1.13                     | 1.10              |
| 106:BD:346:LYS:CB  | 106:BD:364:CYS:HA  | 1.81                     | 1.10              |
| 25:DW:127:PHE:HA   | 40:CR:287:MET:CE   | 1.81                     | 1.10              |
| 34:CK:14:PRO:CD    | 40:CR:300:TYR:CD2  | 2.35                     | 1.10              |
| 4:DL:114:SER:HA    | 4:DL:254:ARG:NH2   | 1.67                     | 1.09              |
| 34:CK:14:PRO:HG3   | 40:CR:300:TYR:CD2  | 1.88                     | 1.09              |
| 19:DG:68:TYR:HE2   | 40:CR:250:GLN:NE2  | 1.51                     | 1.08              |
| 40:CR:320:VAL:O    | 46:Cd:278:ALA:N    | 1.86                     | 1.08              |
| 4:DL:271:PRO:O     | 4:DL:274:THR:HG23  | 1.51                     | 1.08              |
| 15:DB:635:MET:HG3  | 50:Ck:373:ARG:HH11 | 1.16                     | 1.07              |
| 15:DB:423:THR:HG23 | 22:DK:138:ALA:O    | 1.52                     | 1.07              |
| 32:CI:409:PRO:HG3  | 40:CR:253:PHE:CE2  | 1.88                     | 1.07              |
| 19:DG:68:TYR:CE2   | 40:CR:250:GLN:NE2  | 2.22                     | 1.06              |
| 1:DA:1186:CYS:HA   | 1:DA:1193:HIS:ND1  | 1.70                     | 1.06              |
| 40:CR:315:LEU:HB2  | 46:Cd:279:ARG:HH21 | 1.15                     | 1.06              |
| 4:DL:117:ASP:O     | 4:DL:121:ILE:CG1   | 2.04                     | 1.05              |
| 15:DB:1154:LYS:HD3 | 89:Ad:150:ARG:HD3  | 1.07                     | 1.05              |
| 33:CJ:36:MET:CE    | 51:Cm:52:THR:HG22  | 1.78                     | 1.05              |
| 106:BD:270:ALA:HB1 | 106:BD:406:ALA:HB1 | 1.36                     | 1.05              |
| 27:DY:69:HIS:O     | 40:CR:265:ARG:NH1  | 1.87                     | 1.05              |
| 12:DU:191:SER:HB3  | 12:DU:192:PRO:HD2  | 1.31                     | 1.05              |
| 106:BD:204:ALA:H   | 106:BD:451:ALA:HB3 | 1.15                     | 1.05              |
| 9:DQ:250:ARG:CD    | 9:DQ:252:LYS:HE3   | 1.87                     | 1.05              |
| 15:DB:423:THR:CG2  | 22:DK:138:ALA:O    | 2.04                     | 1.05              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:CP:23:ALA:HB2   | 38:CP:51:HIS:CD2    | 1.92                     | 1.05              |
| 10:DR:18:LYS:NZ    | 57:CA:165:A:OP1     | 1.91                     | 1.04              |
| 21:DJ:308:ARG:HH11 | 21:DJ:308:ARG:HG3   | 1.21                     | 1.04              |
| 37:CO:151:LYS:NZ   | 37:CO:179:ASP:OD2   | 1.89                     | 1.04              |
| 25:DW:58:ARG:HG2   | 25:DW:58:ARG:HH11   | 1.21                     | 1.04              |
| 32:CI:409:PRO:CG   | 40:CR:253:PHE:HE2   | 1.70                     | 1.04              |
| 25:DW:126:ARG:C    | 40:CR:287:MET:CE    | 2.31                     | 1.03              |
| 1:DA:1012:THR:O    | 4:DL:77:LEU:HD21    | 1.58                     | 1.03              |
| 9:DQ:250:ARG:HD3   | 9:DQ:252:LYS:HE3    | 1.39                     | 1.02              |
| 18:DF:426:LEU:O    | 20:DH:200:THR:HG22  | 1.57                     | 1.02              |
| 47:Cg:109:PHE:HA   | 152:Cg:501:GTP:HN21 | 1.22                     | 1.02              |
| 34:CK:14:PRO:HD3   | 40:CR:300:TYR:HD2   | 1.22                     | 1.01              |
| 25:DW:127:PHE:CA   | 40:CR:287:MET:CE    | 2.38                     | 1.01              |
| 33:CJ:36:MET:HE2   | 51:Cm:52:THR:HB     | 1.05                     | 1.01              |
| 106:BD:203:ASP:CB  | 106:BD:451:ALA:HB2  | 1.90                     | 1.01              |
| 34:CK:104:MET:HE1  | 45:Cb:100:ARG:NH1   | 1.74                     | 1.01              |
| 40:CR:316:GLY:C    | 46:Cd:279:ARG:CB    | 2.29                     | 1.01              |
| 32:CI:409:PRO:HG3  | 40:CR:253:PHE:HE2   | 1.20                     | 1.00              |
| 1:DA:1278:THR:HG23 | 54:Cq:152:GLU:CG    | 1.92                     | 1.00              |
| 57:CA:564:U:H3     | 57:CA:570:A:H61     | 1.05                     | 1.00              |
| 1:DA:1058:ARG:NH1  | 54:Cq:253:ARG:HH12  | 1.57                     | 1.00              |
| 6:DN:73:VAL:HG11   | 6:DN:112:ILE:CD1    | 1.92                     | 0.99              |
| 40:CR:315:LEU:HB2  | 46:Cd:279:ARG:NH2   | 1.71                     | 0.99              |
| 43:CZ:254:ILE:HG21 | 43:CZ:318:LEU:HD21  | 1.44                     | 0.99              |
| 18:DF:426:LEU:HB3  | 20:DH:200:THR:CG2   | 1.92                     | 0.99              |
| 5:DM:65:THR:HG22   | 5:DM:69:PHE:HB3     | 1.43                     | 0.99              |
| 33:CJ:484:HIS:HD2  | 33:CJ:495:ARG:HH11  | 1.05                     | 0.98              |
| 4:DL:116:ASN:ND2   | 4:DL:120:PHE:CZ     | 2.21                     | 0.98              |
| 40:CR:320:VAL:C    | 46:Cd:277:VAL:HB    | 1.89                     | 0.98              |
| 9:DQ:250:ARG:NE    | 9:DQ:252:LYS:HE3    | 1.78                     | 0.98              |
| 6:DN:75:VAL:HG11   | 6:DN:110:ALA:HB3    | 1.42                     | 0.98              |
| 39:CQ:56:ARG:HG2   | 39:CQ:56:ARG:HH11   | 1.29                     | 0.98              |
| 51:Cm:137:SER:CB   | 57:CA:394:A:C2      | 2.46                     | 0.98              |
| 97:At:136:ARG:HH11 | 97:At:136:ARG:HB3   | 1.29                     | 0.97              |
| 34:CK:14:PRO:CG    | 40:CR:300:TYR:CD2   | 2.46                     | 0.97              |
| 40:CR:314:THR:C    | 46:Cd:279:ARG:HG3   | 1.83                     | 0.97              |
| 33:CJ:544:THR:CG2  | 33:CJ:552:ILE:N     | 2.27                     | 0.97              |
| 27:DY:148:ARG:NH1  | 57:CA:517:U:OP2     | 1.97                     | 0.97              |
| 33:CJ:36:MET:HE1   | 51:Cm:52:THR:HG22   | 0.99                     | 0.96              |
| 15:DB:511:ARG:HH11 | 15:DB:511:ARG:HG3   | 1.29                     | 0.96              |
| 34:CK:14:PRO:HG3   | 40:CR:300:TYR:CE2   | 2.00                     | 0.96              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 106:BD:205:GLU:N    | 106:BD:451:ALA:HB1  | 1.80                     | 0.96              |
| 114:BL:264:LEU:HD21 | 114:BL:287:ARG:HH12 | 1.24                     | 0.96              |
| 4:DL:114:SER:HB2    | 4:DL:254:ARG:NE     | 1.80                     | 0.96              |
| 6:DN:75:VAL:CG1     | 6:DN:110:ALA:HB3    | 1.95                     | 0.96              |
| 106:BD:204:ALA:N    | 106:BD:451:ALA:CB   | 2.29                     | 0.96              |
| 4:DL:63:ASP:OD2     | 51:Cm:21:GLN:CD     | 2.08                     | 0.96              |
| 4:DL:110:TYR:CD2    | 32:CI:235:SER:O     | 2.18                     | 0.96              |
| 1:DA:1003:PHE:CD1   | 4:DL:78:ALA:HA      | 2.01                     | 0.96              |
| 18:DF:426:LEU:O     | 20:DH:200:THR:CG2   | 2.14                     | 0.96              |
| 1:DA:90:MET:O       | 2:DD:123:ARG:NH1    | 1.98                     | 0.96              |
| 40:CR:314:THR:O     | 46:Cd:279:ARG:HG3   | 1.62                     | 0.96              |
| 33:CJ:544:THR:HG21  | 33:CJ:551:ARG:C     | 1.90                     | 0.96              |
| 25:DW:127:PHE:N     | 40:CR:287:MET:CE    | 2.29                     | 0.95              |
| 1:DA:1186:CYS:HA    | 1:DA:1193:HIS:CE1   | 2.00                     | 0.95              |
| 4:DL:114:SER:CB     | 4:DL:254:ARG:NE     | 2.29                     | 0.95              |
| 102:AA:57:A:O2'     | 61:UX:2:UNK:HG1     | 1.65                     | 0.95              |
| 40:CR:310:PHE:CZ    | 57:CA:588:U:O4      | 2.19                     | 0.95              |
| 56:Cv:590:THR:O     | 56:Cv:787:LYS:NZ    | 1.99                     | 0.95              |
| 51:Cm:117:ARG:HH12  | 51:Cm:121:ALA:HB2   | 1.31                     | 0.95              |
| 2:DD:647:ARG:NH2    | 10:DR:230:ARG:HH11  | 1.64                     | 0.95              |
| 15:DB:1007:GLU:OE2  | 32:CI:256:LYS:N     | 2.00                     | 0.95              |
| 19:DG:196:ARG:NH1   | 19:DG:211:TYR:OH    | 1.98                     | 0.95              |
| 89:Ad:269:ARG:HH12  | 118:BP:64:PRO:HG3   | 1.29                     | 0.95              |
| 18:DF:216:LYS:NZ    | 33:CJ:472:SER:O     | 2.00                     | 0.94              |
| 4:DL:116:ASN:O      | 4:DL:120:PHE:CD2    | 2.20                     | 0.94              |
| 19:DG:300:ASP:OD2   | 32:CI:59:ARG:NH1    | 2.01                     | 0.94              |
| 6:DN:75:VAL:HG11    | 6:DN:110:ALA:HB2    | 1.50                     | 0.94              |
| 29:CE:345:ASP:O     | 29:CE:348:TYR:O     | 1.82                     | 0.94              |
| 40:CR:306:LYS:NZ    | 57:CA:389:A:H3'     | 1.83                     | 0.94              |
| 40:CR:316:GLY:O     | 46:Cd:279:ARG:CB    | 2.15                     | 0.94              |
| 106:BD:204:ALA:H    | 106:BD:451:ALA:CB   | 1.81                     | 0.94              |
| 10:DR:128:PRO:HD3   | 10:DR:133:LEU:O     | 1.65                     | 0.93              |
| 33:CJ:36:MET:HE1    | 51:Cm:52:THR:HG21   | 1.49                     | 0.93              |
| 3:DI:340:ARG:HH12   | 3:DI:342:ARG:NH1    | 1.66                     | 0.93              |
| 32:CI:293:ARG:NH2   | 32:CI:407:ARG:HH12  | 1.66                     | 0.93              |
| 38:CP:23:ALA:HB1    | 38:CP:51:HIS:HB2    | 1.49                     | 0.93              |
| 104:BB:87:LEU:HD11  | 104:BB:109:GLU:HG2  | 1.51                     | 0.93              |
| 29:CE:308:ARG:HA    | 29:CE:311:LYS:NZ    | 1.84                     | 0.93              |
| 53:Cp:52:TYR:O      | 53:Cp:62:ARG:NH1    | 2.02                     | 0.92              |
| 6:DN:75:VAL:CG1     | 6:DN:110:ALA:CB     | 2.47                     | 0.92              |
| 18:DF:426:LEU:CB    | 20:DH:200:THR:HG21  | 1.99                     | 0.92              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:1280:GLU:CD   | 54:Cq:151:ARG:HH11 | 1.76                     | 0.92              |
| 6:DN:74:HIS:O      | 6:DN:109:ASN:ND2   | 2.03                     | 0.92              |
| 1:DA:1058:ARG:HH11 | 54:Cq:253:ARG:HH12 | 0.94                     | 0.92              |
| 32:CI:106:LEU:HD21 | 34:CK:107:GLN:HG3  | 1.52                     | 0.92              |
| 18:DF:57:ARG:HG2   | 18:DF:57:ARG:HH11  | 1.34                     | 0.92              |
| 19:DG:68:TYR:OH    | 40:CR:249:GLN:OE1  | 1.86                     | 0.92              |
| 1:DA:1278:THR:CG2  | 54:Cq:152:GLU:OE1  | 0.62                     | 0.91              |
| 1:DA:1505:ASP:HB2  | 5:DM:163:THR:HG23  | 1.50                     | 0.91              |
| 1:DA:1186:CYS:HG   | 1:DA:1193:HIS:HE2  | 0.94                     | 0.91              |
| 15:DB:1154:LYS:CD  | 89:Ad:150:ARG:HD3  | 1.97                     | 0.91              |
| 25:DW:104:VAL:HG21 | 40:CR:279:LYS:HG3  | 1.53                     | 0.91              |
| 6:DN:73:VAL:HG11   | 6:DN:112:ILE:HD11  | 1.50                     | 0.91              |
| 87:AY:64:HIS:HD2   | 87:AY:66:ARG:H     | 1.16                     | 0.91              |
| 1:DA:225:GLY:HA3   | 1:DA:233:ARG:HH11  | 1.35                     | 0.91              |
| 33:CJ:698:HIS:HB3  | 36:CN:65:LYS:HZ1   | 1.34                     | 0.91              |
| 90:Ae:75:ARG:HH12  | 90:Ae:135:THR:HG22 | 1.36                     | 0.91              |
| 78:AN:65:ILE:HD11  | 78:AN:156:ALA:HB2  | 1.51                     | 0.91              |
| 4:DL:92:ILE:CG2    | 32:CI:248:PHE:HA   | 2.01                     | 0.91              |
| 17:DE:144:PRO:HG2  | 17:DE:147:MET:HG3  | 1.52                     | 0.90              |
| 52:Cn:236:LYS:H    | 52:Cn:245:LYS:HZ3  | 1.17                     | 0.90              |
| 1:DA:1186:CYS:HG   | 1:DA:1193:HIS:CD2  | 1.88                     | 0.90              |
| 4:DL:74:ARG:NH2    | 29:CE:110:LEU:HD11 | 1.87                     | 0.90              |
| 4:DL:117:ASP:HB3   | 4:DL:121:ILE:HD11  | 1.52                     | 0.90              |
| 93:Aj:62:HIS:HA    | 109:BG:144:TRP:HE1 | 1.36                     | 0.90              |
| 51:Cm:196:GLY:O    | 51:Cm:200:VAL:HG22 | 1.71                     | 0.90              |
| 96:Ap:123:LYS:NZ   | 146:UM:5:UNK:O     | 2.05                     | 0.90              |
| 102:AA:836:A:HO2'  | 131:Bc:10:ASP:N    | 1.69                     | 0.90              |
| 26:DX:50:ARG:NH1   | 41:CS:145:LYS:O    | 2.04                     | 0.90              |
| 40:CR:308:MET:CE   | 57:CA:388:U:O4'    | 2.19                     | 0.89              |
| 96:Ap:124:PRO:HD2  | 142:UN:7:UNK:HB1   | 1.52                     | 0.89              |
| 71:A8:172:LYS:NZ   | 79:AP:259:HIS:HD2  | 1.71                     | 0.89              |
| 1:DA:1280:GLU:CD   | 54:Cq:151:ARG:NH1  | 2.30                     | 0.89              |
| 4:DL:116:ASN:O     | 4:DL:120:PHE:HD2   | 1.56                     | 0.89              |
| 44:Ca:299:ARG:HH11 | 44:Ca:299:ARG:HG3  | 1.37                     | 0.89              |
| 108:BF:60:LEU:HA   | 108:BF:63:ARG:HD2  | 1.55                     | 0.89              |
| 78:AN:30:ASN:O     | 78:AN:39:ARG:NH1   | 2.05                     | 0.89              |
| 4:DL:116:ASN:ND2   | 4:DL:120:PHE:HZ    | 1.70                     | 0.89              |
| 77:AK:285:ARG:HH11 | 77:AK:307:ARG:HH21 | 1.21                     | 0.89              |
| 4:DL:114:SER:HA    | 4:DL:254:ARG:NE    | 1.87                     | 0.88              |
| 89:Ad:42:MET:HE1   | 132:Bd:103:GLY:HA2 | 1.56                     | 0.88              |
| 37:CO:411:ARG:HH11 | 37:CO:424:LYS:HD2  | 1.35                     | 0.88              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 47:Cg:341:LYS:NZ    | 50:Ck:811:GLU:OE2   | 2.06                     | 0.88              |
| 18:DF:589:GLN:HE21  | 20:DH:191:HIS:N     | 1.71                     | 0.88              |
| 27:DY:69:HIS:C      | 40:CR:265:ARG:HH12  | 1.82                     | 0.88              |
| 105:BC:266:PRO:HG3  | 105:BC:490:LEU:HD11 | 1.55                     | 0.88              |
| 106:BD:204:ALA:N    | 106:BD:451:ALA:HB3  | 1.85                     | 0.88              |
| 15:DB:1154:LYS:NZ   | 89:Ad:150:ARG:NE    | 2.21                     | 0.88              |
| 109:BG:192:ARG:HH12 | 109:BG:253:ARG:HD2  | 1.37                     | 0.88              |
| 18:DF:188:ARG:NH1   | 150:DJ:401:UTP:O2G  | 2.07                     | 0.88              |
| 38:CP:23:ALA:HB1    | 38:CP:51:HIS:CB     | 2.04                     | 0.88              |
| 25:DW:127:PHE:CA    | 40:CR:287:MET:HE1   | 2.00                     | 0.87              |
| 30:CF:129:ASN:HB3   | 40:CR:125:ASN:HD22  | 1.39                     | 0.87              |
| 6:DN:113:ALA:HB3    | 6:DN:133:PHE:HE1    | 1.34                     | 0.87              |
| 66:A2:387:TRP:O     | 86:AX:108:LYS:NZ    | 2.07                     | 0.87              |
| 85:AW:112:LEU:HD13  | 114:BL:156:LEU:HD22 | 1.57                     | 0.87              |
| 86:AX:156:THR:HG22  | 86:AX:158:ARG:H     | 1.36                     | 0.87              |
| 10:DR:128:PRO:HG3   | 10:DR:133:LEU:CB    | 2.03                     | 0.87              |
| 108:BF:60:LEU:HD22  | 108:BF:63:ARG:NH1   | 1.90                     | 0.87              |
| 109:BG:130:CYS:HA   | 109:BG:160:MET:HE1  | 1.55                     | 0.87              |
| 81:AR:211:ARG:NH1   | 107:BE:440:ILE:O    | 2.07                     | 0.87              |
| 2:DD:607:GLN:O      | 10:DR:227:ARG:NH2   | 2.07                     | 0.86              |
| 6:DN:293:PRO:C      | 29:CE:118:ARG:HH21  | 1.83                     | 0.86              |
| 19:DG:64:ARG:NH2    | 40:CR:249:GLN:NE2   | 2.06                     | 0.86              |
| 110:BH:71:LYS:HZ2   | 139:UC:4:UNK:HG1    | 1.39                     | 0.86              |
| 4:DL:71:GLU:OE2     | 44:Ca:243:THR:HA    | 1.74                     | 0.86              |
| 18:DF:383:ASP:HB3   | 18:DF:468:MET:HE1   | 1.57                     | 0.86              |
| 22:DK:254:GLU:HG3   | 22:DK:261:SER:HB3   | 1.56                     | 0.86              |
| 19:DG:472:ARG:HG2   | 19:DG:472:ARG:HH11  | 1.40                     | 0.86              |
| 79:AP:163:ARG:HG2   | 79:AP:163:ARG:HH11  | 1.40                     | 0.86              |
| 40:CR:8:ILE:HG21    | 56:Cv:909:LEU:HD23  | 0.88                     | 0.86              |
| 40:CR:317:ILE:C     | 46:Cd:283:GLU:OE2   | 2.19                     | 0.86              |
| 37:CO:87:THR:HG23   | 37:CO:88:PRO:HD3    | 1.55                     | 0.86              |
| 44:Ca:536:ARG:NH1   | 44:Ca:539:GLN:OE1   | 2.09                     | 0.85              |
| 68:A4:20:ARG:HH11   | 68:A4:20:ARG:HB2    | 1.40                     | 0.85              |
| 1:DA:1002:PRO:C     | 4:DL:78:ALA:CB      | 2.43                     | 0.85              |
| 11:DS:201:HIS:HD2   | 11:DS:203:ASP:H     | 1.25                     | 0.85              |
| 19:DG:111:ARG:NH1   | 45:Cb:197:PRO:HB2   | 1.90                     | 0.85              |
| 106:BD:346:LYS:CB   | 106:BD:364:CYS:CA   | 2.54                     | 0.85              |
| 19:DG:111:ARG:HH11  | 45:Cb:197:PRO:HG2   | 1.36                     | 0.85              |
| 51:Cm:137:SER:OG    | 57:CA:394:A:N3      | 1.98                     | 0.85              |
| 84:AV:100:GLN:HE22  | 102:AA:466:G:H21    | 1.23                     | 0.85              |
| 4:DL:110:TYR:CE2    | 32:CI:235:SER:O     | 2.29                     | 0.85              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 116:BN:128:ARG:HH21 | 136:Bh:34:ARG:HH11 | 1.22                     | 0.85              |
| 10:DR:79:LEU:O      | 12:DU:139:LYS:NZ   | 2.10                     | 0.85              |
| 33:CJ:792:HIS:HD2   | 33:CJ:795:LYS:H    | 1.22                     | 0.85              |
| 4:DL:68:LEU:O       | 29:CE:112:THR:CG2  | 2.25                     | 0.84              |
| 4:DL:271:PRO:O      | 4:DL:274:THR:CG2   | 2.24                     | 0.84              |
| 15:DB:539:GLN:HG3   | 15:DB:585:MET:HE2  | 1.59                     | 0.84              |
| 25:DW:99:HIS:CE1    | 40:CR:270:TYR:OH   | 2.29                     | 0.84              |
| 25:DW:101:LEU:HB3   | 40:CR:275:GLY:O    | 1.76                     | 0.84              |
| 50:Ck:129:THR:HG22  | 50:Ck:131:ASN:H    | 1.41                     | 0.84              |
| 15:DB:78:ARG:HH11   | 15:DB:78:ARG:HG3   | 1.41                     | 0.84              |
| 1:DA:1186:CYS:CA    | 1:DA:1193:HIS:CE1  | 2.61                     | 0.84              |
| 51:Cm:88:SER:HB2    | 57:CA:394:A:H5''   | 1.60                     | 0.84              |
| 114:BL:193:ARG:NH1  | 114:BL:301:TRP:O   | 2.09                     | 0.84              |
| 19:DG:111:ARG:HH22  | 45:Cb:197:PRO:HB3  | 1.43                     | 0.84              |
| 31:CH:68:GLN:NE2    | 57:CA:4:A:N1       | 2.25                     | 0.84              |
| 8:DP:195:THR:O      | 8:DP:211:GLU:HG2   | 1.76                     | 0.84              |
| 123:BU:139:ARG:HH11 | 135:Bg:35:LEU:HD21 | 1.43                     | 0.84              |
| 40:CR:319:LYS:NZ    | 46:Cd:281:MET:O    | 2.10                     | 0.84              |
| 83:AU:131:GLU:HG2   | 97:At:91:ARG:HH12  | 1.42                     | 0.84              |
| 40:CR:306:LYS:HZ2   | 57:CA:389:A:H3'    | 1.37                     | 0.83              |
| 25:DW:113:PRO:HG2   | 40:CR:289:THR:HG23 | 1.60                     | 0.83              |
| 5:DM:65:THR:CG2     | 5:DM:69:PHE:HB3    | 2.09                     | 0.83              |
| 12:DU:113:GLN:O     | 12:DU:117:LEU:HG   | 1.78                     | 0.83              |
| 12:DU:189:LYS:NZ    | 12:DU:190:ARG:HB2  | 1.93                     | 0.83              |
| 31:CH:16:VAL:HB     | 31:CH:17:PRO:HD2   | 1.60                     | 0.83              |
| 40:CR:320:VAL:HB    | 46:Cd:281:MET:HE2  | 1.61                     | 0.83              |
| 3:DI:88:GLN:NE2     | 3:DI:92:GLU:OE2    | 2.11                     | 0.83              |
| 92:Ag:89:THR:HG22   | 92:Ag:91:ASN:H     | 1.40                     | 0.83              |
| 8:DP:139:ARG:NH1    | 8:DP:176:PRO:O     | 2.12                     | 0.83              |
| 16:DC:155:VAL:HG13  | 16:DC:168:PHE:HE1  | 1.42                     | 0.83              |
| 25:DW:104:VAL:CG2   | 40:CR:279:LYS:HG3  | 2.08                     | 0.83              |
| 88:Ab:84:ASN:HD22   | 88:Ab:140:ARG:HH11 | 1.23                     | 0.83              |
| 28:CC:44:LEU:HD13   | 28:CC:52:ILE:HG12  | 1.61                     | 0.83              |
| 96:Ap:39:LYS:NZ     | 102:AA:1111:A:N7   | 2.26                     | 0.83              |
| 120:BR:40:ARG:CZ    | 120:BR:95:ARG:HH12 | 1.91                     | 0.83              |
| 11:DS:168:LYS:NZ    | 53:Cp:34:GLU:OE2   | 2.12                     | 0.83              |
| 130:Bb:45:LYS:O     | 130:Bb:49:LYS:NZ   | 2.11                     | 0.83              |
| 74:AF:457:MET:HG2   | 79:AP:275:MET:HE2  | 1.61                     | 0.82              |
| 1:DA:1058:ARG:HH11  | 54:Cq:253:ARG:NH1  | 1.75                     | 0.82              |
| 41:CS:164:TYR:HB3   | 41:CS:170:LEU:HD13 | 1.58                     | 0.82              |
| 81:AR:264:ALA:O     | 113:BK:131:ARG:NH2 | 2.11                     | 0.82              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 117:BO:77:ALA:HA    | 121:BS:32:ARG:HH11  | 1.43                     | 0.82              |
| 23:DT:14:THR:HG21   | 57:CA:438:U:O2      | 1.79                     | 0.82              |
| 34:CK:42:PHE:CD1    | 40:CR:252:GLN:O     | 2.33                     | 0.82              |
| 98:Av:174:ASN:HB2   | 105:BC:486:ASN:HD21 | 1.42                     | 0.82              |
| 110:BH:71:LYS:NZ    | 139:UC:4:UNK:HG1    | 1.93                     | 0.82              |
| 1:DA:74:LYS:NZ      | 57:CA:71:U:OP1      | 2.12                     | 0.82              |
| 20:DH:80:ARG:HG2    | 20:DH:85:LEU:HG     | 1.60                     | 0.82              |
| 52:Cn:171:MET:HE2   | 57:CA:555:A:H4'     | 1.62                     | 0.82              |
| 32:CI:241:ARG:CG    | 33:CJ:56:ILE:O      | 2.25                     | 0.82              |
| 15:DB:285:MET:HE1   | 50:Ck:37:ILE:HD11   | 1.62                     | 0.82              |
| 1:DA:695:MET:HE2    | 1:DA:713:PHE:HB3    | 1.61                     | 0.81              |
| 1:DA:90:MET:HE1     | 2:DD:122:GLN:HE22   | 1.45                     | 0.81              |
| 22:DK:238:ILE:HG21  | 22:DK:260:VAL:HG22  | 1.61                     | 0.81              |
| 55:Cr:172:ARG:HH21  | 55:Cr:176:LEU:HD23  | 1.44                     | 0.81              |
| 4:DL:110:TYR:HD2    | 32:CI:235:SER:O     | 1.63                     | 0.81              |
| 89:Ad:101:LYS:HD3   | 89:Ad:109:LEU:HD11  | 1.61                     | 0.81              |
| 125:BW:56:ASN:H     | 125:BW:65:ASN:HD21  | 1.28                     | 0.81              |
| 30:CF:136:ALA:HB3   | 34:CK:171:GLN:HB3   | 1.63                     | 0.81              |
| 40:CR:308:MET:HE3   | 57:CA:388:U:C3'     | 2.11                     | 0.81              |
| 40:CR:317:ILE:HA    | 46:Cd:283:GLU:OE2   | 1.81                     | 0.81              |
| 4:DL:181:ARG:HH11   | 4:DL:181:ARG:HG3    | 1.44                     | 0.81              |
| 32:CI:106:LEU:HD11  | 34:CK:107:GLN:HE21  | 1.46                     | 0.81              |
| 77:AK:54:ARG:NH1    | 102:AA:402:A:OP2    | 2.13                     | 0.81              |
| 89:Ad:269:ARG:NH1   | 118:BP:64:PRO:HG3   | 1.95                     | 0.81              |
| 4:DL:92:ILE:HG21    | 32:CI:248:PHE:HA    | 1.62                     | 0.81              |
| 4:DL:114:SER:HB2    | 4:DL:254:ARG:CD     | 2.10                     | 0.81              |
| 10:DR:128:PRO:CG    | 10:DR:133:LEU:H     | 1.94                     | 0.81              |
| 38:CP:130:GLN:O     | 44:Ca:432:ARG:NH1   | 2.14                     | 0.81              |
| 15:DB:1000:ARG:NH2  | 32:CI:262:ASP:OD2   | 2.13                     | 0.81              |
| 55:Cr:125:GLN:HE21  | 55:Cr:162:PRO:HD2   | 1.44                     | 0.81              |
| 98:Av:29:MET:HB2    | 98:Av:44:ASN:HD21   | 1.44                     | 0.81              |
| 136:Bh:46:VAL:HG23  | 140:UD:11:UNK:HG2   | 1.62                     | 0.81              |
| 1:DA:1014:TYR:HE1   | 4:DL:67:ASN:C       | 1.86                     | 0.80              |
| 2:DD:129:ARG:HA     | 39:CQ:88:PRO:HB3    | 1.63                     | 0.80              |
| 5:DM:27:GLN:HE22    | 56:Cv:1013:ARG:H    | 1.29                     | 0.80              |
| 15:DB:635:MET:HG3   | 50:Ck:373:ARG:NH1   | 1.95                     | 0.80              |
| 109:BG:172:THR:HG21 | 109:BG:324:TRP:HE1  | 1.45                     | 0.80              |
| 4:DL:109:VAL:HG11   | 32:CI:234:PHE:CE2   | 2.16                     | 0.80              |
| 138:UB:2:UNK:HB2    | 138:UB:4:UNK:HG3    | 1.63                     | 0.80              |
| 18:DF:38:GLY:H      | 18:DF:41:ASN:HD22   | 1.29                     | 0.80              |
| 18:DF:425:ILE:HD13  | 20:DH:196:LEU:HD11  | 1.62                     | 0.80              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:DA:1465:ASP:HA    | 1:DA:1605:ARG:HH12  | 1.46                     | 0.80              |
| 19:DG:476:GLN:HE22  | 19:DG:560:GLU:H     | 1.29                     | 0.80              |
| 56:Cv:67:THR:HG22   | 56:Cv:69:GLN:H      | 1.46                     | 0.80              |
| 32:CI:241:ARG:HB2   | 33:CJ:55:SER:O      | 1.82                     | 0.80              |
| 38:CP:22:GLY:HA3    | 57:CA:164:G:O6      | 1.82                     | 0.80              |
| 38:CP:23:ALA:HB2    | 38:CP:51:HIS:ND1    | 1.96                     | 0.80              |
| 56:Cv:283:ASP:HB3   | 56:Cv:398:ARG:HD2   | 1.64                     | 0.80              |
| 1:DA:1058:ARG:NH1   | 54:Cq:253:ARG:NH1   | 2.30                     | 0.80              |
| 6:DN:235:ASN:ND2    | 29:CE:18:LYS:O      | 2.13                     | 0.80              |
| 16:DC:844:ALA:HB1   | 17:DE:68:PRO:HB3    | 1.64                     | 0.80              |
| 97:At:38:GLU:OE2    | 120:BR:127:ARG:NH2  | 2.15                     | 0.80              |
| 20:DH:192:PHE:O     | 20:DH:196:LEU:HB2   | 1.81                     | 0.80              |
| 29:CE:220:ASP:HB2   | 56:Cv:44:ARG:HH12   | 1.46                     | 0.80              |
| 75:AI:70:ARG:HH11   | 75:AI:70:ARG:HB2    | 1.46                     | 0.80              |
| 22:DK:252:ILE:HG22  | 22:DK:260:VAL:HG13  | 1.64                     | 0.80              |
| 4:DL:114:SER:HB2    | 4:DL:254:ARG:HE     | 1.47                     | 0.80              |
| 105:BC:60:LEU:H     | 105:BC:292:ASN:HD21 | 1.27                     | 0.80              |
| 108:BF:28:ARG:HG2   | 59:UW:1:UNK:H2      | 1.47                     | 0.80              |
| 4:DL:114:SER:CA     | 4:DL:254:ARG:NE     | 2.46                     | 0.79              |
| 4:DL:116:ASN:C      | 4:DL:120:PHE:HD2    | 1.86                     | 0.79              |
| 11:DS:54:ASN:HB3    | 11:DS:87:ARG:HG2    | 1.63                     | 0.79              |
| 21:DJ:31:HIS:HD2    | 21:DJ:33:ASN:H      | 1.29                     | 0.79              |
| 8:DP:195:THR:HG23   | 8:DP:211:GLU:HB3    | 1.63                     | 0.79              |
| 21:DJ:308:ARG:HG3   | 21:DJ:308:ARG:NH1   | 1.95                     | 0.79              |
| 51:Cm:137:SER:OG    | 57:CA:394:A:H2      | 1.59                     | 0.79              |
| 2:DD:647:ARG:NH2    | 10:DR:230:ARG:NH1   | 2.30                     | 0.79              |
| 9:DQ:23:ARG:HD3     | 37:CO:397:MET:HE1   | 1.62                     | 0.79              |
| 29:CE:71:ILE:HG23   | 29:CE:320:GLY:HA2   | 1.64                     | 0.79              |
| 44:Ca:367:ASN:HA    | 56:Cv:954:ARG:HH22  | 1.47                     | 0.79              |
| 88:Ab:273:ARG:O     | 115:BM:96:ARG:NH1   | 2.15                     | 0.79              |
| 1:DA:1278:THR:HG22  | 54:Cq:152:GLU:OE1   | 0.97                     | 0.79              |
| 6:DN:235:ASN:HD21   | 29:CE:18:LYS:H      | 1.28                     | 0.79              |
| 19:DG:40:ALA:O      | 32:CI:252:ARG:NH1   | 2.14                     | 0.79              |
| 92:Ag:50:ARG:HB3    | 92:Ag:50:ARG:HH11   | 1.45                     | 0.79              |
| 17:DE:431:SER:O     | 17:DE:532:TYR:HB2   | 1.83                     | 0.79              |
| 25:DW:58:ARG:HG2    | 25:DW:58:ARG:NH1    | 1.91                     | 0.79              |
| 32:CI:115:LEU:HD21  | 34:CK:82:MET:HE1    | 1.65                     | 0.79              |
| 42:CU:52:GLU:HB2    | 46:Cd:250:LEU:HD11  | 1.64                     | 0.79              |
| 87:AY:264:VAL:HG21  | 128:BZ:126:SER:HB3  | 1.61                     | 0.79              |
| 123:BU:135:ARG:HH22 | 123:BU:139:ARG:HH21 | 1.31                     | 0.79              |
| 12:DU:191:SER:HB3   | 12:DU:192:PRO:CD    | 2.12                     | 0.79              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:DB:92:HIS:HD2    | 15:DB:94:ASP:H      | 1.28                     | 0.79              |
| 4:DL:71:GLU:OE2     | 44:Ca:243:THR:HG23  | 1.82                     | 0.79              |
| 32:CI:409:PRO:CG    | 40:CR:253:PHE:CE2   | 2.57                     | 0.79              |
| 37:CO:313:THR:OG1   | 39:CQ:166:GLU:OE1   | 2.00                     | 0.79              |
| 110:BH:160:THR:HG1  | 110:BH:168:THR:HG1  | 1.26                     | 0.79              |
| 4:DL:106:PHE:CE1    | 32:CI:239:PHE:HZ    | 2.01                     | 0.79              |
| 15:DB:236:ASP:HA    | 17:DE:587:MET:HE1   | 1.64                     | 0.79              |
| 18:DF:426:LEU:H     | 20:DH:200:THR:HG23  | 1.47                     | 0.79              |
| 24:DV:30:ASP:OD1    | 48:CI:59:ARG:NH2    | 2.14                     | 0.79              |
| 102:AA:158:A:H4'    | 102:AA:159:U:H5'    | 1.65                     | 0.79              |
| 5:DM:168:LYS:NZ     | 29:CE:342:GLY:O     | 2.16                     | 0.78              |
| 16:DC:119:THR:HG23  | 16:DC:132:SER:HB2   | 1.64                     | 0.78              |
| 104:BB:212:HIS:HB3  | 123:BU:111:LEU:HD22 | 1.65                     | 0.78              |
| 19:DG:563:PHE:HA    | 19:DG:623:MET:HE1   | 1.65                     | 0.78              |
| 47:Cg:270:MET:HG2   | 47:Cg:338:GLY:HA3   | 1.63                     | 0.78              |
| 51:Cm:210:ARG:NH2   | 57:CA:358:U:OP2     | 2.16                     | 0.78              |
| 2:DD:605:ARG:NH1    | 2:DD:642:ASP:OD2    | 2.16                     | 0.78              |
| 5:DM:26:ARG:HH22    | 44:Ca:266:GLU:HG3   | 1.47                     | 0.78              |
| 16:DC:155:VAL:HG13  | 16:DC:168:PHE:CE1   | 2.19                     | 0.78              |
| 33:CJ:639:ARG:HH21  | 33:CJ:646:THR:HG22  | 1.48                     | 0.78              |
| 69:A5:49:LEU:HB2    | 87:AY:3:ALA:HB3     | 1.66                     | 0.78              |
| 75:AI:71:TYR:OH     | 98:Av:105:LEU:O     | 2.01                     | 0.78              |
| 2:DD:537:ARG:HA     | 10:DR:218:TRP:HZ3   | 1.48                     | 0.78              |
| 15:DB:511:ARG:HH11  | 15:DB:511:ARG:CG    | 1.96                     | 0.78              |
| 25:DW:104:VAL:HB    | 40:CR:279:LYS:CG    | 2.14                     | 0.78              |
| 29:CE:308:ARG:O     | 29:CE:311:LYS:NZ    | 2.17                     | 0.78              |
| 64:A0:94:ILE:HG23   | 120:BR:17:LEU:HD12  | 1.65                     | 0.78              |
| 79:AP:257:MET:HE3   | 125:BW:11:ARG:HH12  | 1.47                     | 0.78              |
| 34:CK:104:MET:HE1   | 45:Cb:100:ARG:HH11  | 1.46                     | 0.78              |
| 56:Cv:702:ILE:HG21  | 56:Cv:761:MET:HB2   | 1.64                     | 0.78              |
| 103:BA:327:ARG:HD3  | 103:BA:365:ASP:OD2  | 1.84                     | 0.78              |
| 1:DA:615:ALA:HB1    | 1:DA:628:LEU:HD12   | 1.66                     | 0.78              |
| 1:DA:1016:MET:SD    | 4:DL:74:ARG:HB2     | 2.23                     | 0.78              |
| 15:DB:964:ARG:NH1   | 15:DB:1005:ILE:HD13 | 1.98                     | 0.78              |
| 1:DA:286:VAL:HG11   | 1:DA:370:GLN:HB3    | 1.65                     | 0.78              |
| 4:DL:109:VAL:HG11   | 32:CI:234:PHE:HE2   | 1.48                     | 0.78              |
| 12:DU:171:ASP:HA    | 12:DU:174:ARG:HH12  | 1.47                     | 0.78              |
| 16:DC:1152:PRO:HG2  | 16:DC:1160:GLN:HE22 | 1.48                     | 0.78              |
| 104:BB:87:LEU:HA    | 104:BB:90:LYS:HZ3   | 1.48                     | 0.78              |
| 107:BE:300:ARG:HH11 | 107:BE:323:TRP:HZ3  | 1.32                     | 0.78              |
| 2:DD:746:PRO:HD3    | 31:CH:77:VAL:HG12   | 1.65                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:CE:400:LEU:HD13  | 29:CE:406:THR:O     | 1.84                     | 0.78              |
| 81:AR:73:MET:HE2    | 81:AR:93:LEU:HG     | 1.65                     | 0.78              |
| 1:DA:1440:ILE:HD11  | 1:DA:1562:GLN:HB3   | 1.66                     | 0.78              |
| 6:DN:142:ARG:HH12   | 31:CH:18:PRO:HB2    | 1.49                     | 0.78              |
| 18:DF:589:GLN:CB    | 20:DH:192:PHE:CE1   | 2.67                     | 0.78              |
| 81:AR:148:ARG:HH11  | 102:AA:1163:A:H62   | 1.28                     | 0.78              |
| 105:BC:109:THR:HG22 | 105:BC:222:LYS:HG3  | 1.63                     | 0.78              |
| 78:AN:20:LYS:NZ     | 102:AA:837:A:OP2    | 2.16                     | 0.77              |
| 117:BO:86:THR:HG22  | 117:BO:88:ARG:H     | 1.47                     | 0.77              |
| 123:BU:174:TYR:HB3  | 123:BU:178:VAL:HG21 | 1.64                     | 0.77              |
| 4:DL:106:PHE:CZ     | 32:CI:237:ARG:HG2   | 2.18                     | 0.77              |
| 16:DC:240:VAL:HG23  | 16:DC:251:TRP:HZ3   | 1.49                     | 0.77              |
| 29:CE:149:MET:HE2   | 29:CE:161:GLN:HB3   | 1.65                     | 0.77              |
| 34:CK:158:ARG:NH2   | 56:Cv:617:ASP:OD2   | 2.18                     | 0.77              |
| 81:AR:194:GLU:HA    | 81:AR:197:LYS:HE3   | 1.66                     | 0.77              |
| 92:Ag:50:ARG:HB3    | 92:Ag:50:ARG:NH1    | 1.99                     | 0.77              |
| 10:DR:128:PRO:HG3   | 10:DR:133:LEU:HB3   | 1.67                     | 0.77              |
| 34:CK:14:PRO:CG     | 40:CR:300:TYR:CE2   | 2.66                     | 0.77              |
| 105:BC:276:ALA:HB2  | 105:BC:505:ARG:HE   | 1.48                     | 0.77              |
| 75:AI:19:ASP:OD2    | 75:AI:45:ARG:NH2    | 2.18                     | 0.77              |
| 15:DB:423:THR:HG21  | 22:DK:138:ALA:O     | 1.84                     | 0.77              |
| 30:CF:71:MET:HG3    | 30:CF:76:MET:HE3    | 1.66                     | 0.77              |
| 84:AV:122:ARG:NH1   | 91:Af:102:PRO:HA    | 1.98                     | 0.77              |
| 94:Al:64:ARG:HH21   | 94:Al:75:ARG:HD3    | 1.50                     | 0.77              |
| 95:Ao:229:LYS:HZ1   | 102:AA:387:A:H3'    | 1.49                     | 0.77              |
| 1:DA:212:ARG:HA     | 11:DS:134:GLN:HE22  | 1.48                     | 0.77              |
| 37:CO:70:HIS:HB3    | 37:CO:71:PRO:HD2    | 1.67                     | 0.77              |
| 29:CE:42:ARG:HH11   | 29:CE:105:GLN:NE2   | 1.83                     | 0.77              |
| 32:CI:326:ASN:ND2   | 32:CI:330:ASN:O     | 2.17                     | 0.77              |
| 76:AJ:83:PHE:HD2    | 96:Ap:205:ARG:HH11  | 1.32                     | 0.77              |
| 111:BI:290:LEU:HD23 | 111:BI:293:THR:HG21 | 1.67                     | 0.77              |
| 2:DD:736:TYR:HB3    | 31:CH:84:PRO:HG3    | 1.67                     | 0.77              |
| 8:DP:203:ASP:HB3    | 8:DP:205:LEU:HG     | 1.67                     | 0.77              |
| 64:A0:108:GLN:HG2   | 115:BM:84:ASP:HB3   | 1.66                     | 0.77              |
| 71:A8:111:ARG:HG2   | 71:A8:111:ARG:HH11  | 1.50                     | 0.77              |
| 10:DR:100:ARG:HH12  | 10:DR:122:ALA:HB1   | 1.50                     | 0.76              |
| 40:CR:24:ASN:HD22   | 56:Cv:144:PHE:HA    | 1.50                     | 0.76              |
| 70:A6:41:ARG:NH2    | 70:A6:91:PHE:O      | 2.17                     | 0.76              |
| 23:DT:9:GLN:O       | 57:CA:438:U:N3      | 2.17                     | 0.76              |
| 43:CZ:305:HIS:HD2   | 43:CZ:307:LYS:HB2   | 1.51                     | 0.76              |
| 68:A4:140:GLU:HB3   | 68:A4:161:LYS:HB3   | 1.66                     | 0.76              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 104:BB:422:MET:HB3  | 104:BB:427:PHE:HE1  | 1.47                     | 0.76              |
| 2:DD:272:LYS:NZ     | 39:CQ:84:ILE:O      | 2.16                     | 0.76              |
| 29:CE:231:ARG:NH1   | 57:CA:16:U:O4       | 2.18                     | 0.76              |
| 78:AN:89:LYS:HZ3    | 96:Ap:62:LYS:HZ1    | 1.33                     | 0.76              |
| 94:Al:85:LEU:HB3    | 94:Al:87:LEU:HD23   | 1.66                     | 0.76              |
| 96:Ap:123:LYS:HZ3   | 146:UM:5:UNK:C      | 1.95                     | 0.76              |
| 1:DA:59:HIS:HD2     | 1:DA:86:TYR:H       | 1.32                     | 0.76              |
| 1:DA:916:ASP:HB2    | 6:DN:11:ARG:HA      | 1.68                     | 0.76              |
| 1:DA:1278:THR:CG2   | 54:Cq:152:GLU:CD    | 1.81                     | 0.76              |
| 3:DI:88:GLN:CD      | 3:DI:92:GLU:OE2     | 2.29                     | 0.76              |
| 4:DL:67:ASN:HD22    | 29:CE:125:PRO:HB3   | 1.50                     | 0.76              |
| 19:DG:390:GLY:O     | 19:DG:497:ARG:NH2   | 2.19                     | 0.76              |
| 25:DW:37:MET:HG2    | 57:CA:519:U:H2'     | 1.66                     | 0.76              |
| 51:Cm:117:ARG:NH1   | 51:Cm:121:ALA:HB2   | 2.00                     | 0.76              |
| 79:AP:310:HIS:HD2   | 79:AP:312:ALA:H     | 1.34                     | 0.76              |
| 88:Ab:162:VAL:HG23  | 88:Ab:406:ALA:HB2   | 1.66                     | 0.76              |
| 115:BM:121:GLU:HA   | 115:BM:205:GLN:HE22 | 1.49                     | 0.76              |
| 18:DF:373:ASP:N     | 18:DF:373:ASP:OD1   | 2.19                     | 0.76              |
| 47:Cg:109:PHE:HA    | 152:Cg:501:GTP:N2   | 1.99                     | 0.76              |
| 93:Aj:56:VAL:HB     | 93:Aj:170:LEU:HB3   | 1.66                     | 0.76              |
| 4:DL:114:SER:CA     | 4:DL:254:ARG:CZ     | 2.61                     | 0.76              |
| 10:DR:255:PRO:O     | 10:DR:268:HIS:ND1   | 2.11                     | 0.76              |
| 42:CU:185:ARG:NH1   | 42:CU:189:ARG:O     | 2.19                     | 0.76              |
| 87:AY:254:LYS:HZ2   | 87:AY:255:ARG:HH12  | 1.34                     | 0.76              |
| 137:UA:39:UNK:HG2   | 137:UA:40:UNK:HG2   | 1.66                     | 0.76              |
| 108:BF:209:ILE:HD11 | 108:BF:239:VAL:HG11 | 1.67                     | 0.76              |
| 37:CO:411:ARG:NH1   | 37:CO:424:LYS:HD2   | 2.01                     | 0.76              |
| 80:AQ:92:VAL:HB     | 80:AQ:110:HIS:HB3   | 1.68                     | 0.76              |
| 3:DI:27:THR:H       | 3:DI:30:GLN:HE21    | 1.35                     | 0.75              |
| 25:DW:104:VAL:CB    | 40:CR:279:LYS:HG3   | 2.16                     | 0.75              |
| 36:CN:104:THR:HG21  | 41:CS:48:ARG:HH22   | 1.51                     | 0.75              |
| 65:A1:114:LEU:HA    | 65:A1:163:ARG:HE    | 1.51                     | 0.75              |
| 81:AR:61:ARG:H      | 81:AR:65:HIS:HD2    | 1.32                     | 0.75              |
| 111:BI:250:SER:OG   | 111:BI:254:ARG:NH2  | 2.19                     | 0.75              |
| 8:DP:128:LEU:HD22   | 8:DP:161:VAL:HG21   | 1.69                     | 0.75              |
| 9:DQ:215:PRO:HA     | 9:DQ:218:ARG:NH1    | 2.01                     | 0.75              |
| 74:AF:77:PRO:HG2    | 108:BF:360:THR:HG21 | 1.67                     | 0.75              |
| 79:AP:257:MET:HE3   | 125:BW:11:ARG:NH1   | 2.01                     | 0.75              |
| 122:BT:61:ARG:NH1   | 129:Ba:138:GLU:OE2  | 2.18                     | 0.75              |
| 126:BX:69:ARG:HH11  | 126:BX:71:MET:HE2   | 1.51                     | 0.75              |
| 1:DA:74:LYS:O       | 38:CP:59:ARG:NH2    | 2.19                     | 0.75              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 109:BG:336:LYS:HG2  | 109:BG:340:GLN:HE22 | 1.51                     | 0.75              |
| 4:DL:242:ARG:NH2    | 51:Cm:38:ASP:OD2    | 2.19                     | 0.75              |
| 16:DC:441:VAL:HG11  | 16:DC:496:LYS:HD3   | 1.69                     | 0.75              |
| 40:CR:8:ILE:CG2     | 56:Cv:909:LEU:CD2   | 2.53                     | 0.75              |
| 40:CR:320:VAL:O     | 46:Cd:277:VAL:HB    | 1.86                     | 0.75              |
| 93:Aj:62:HIS:HA     | 109:BG:144:TRP:NE1  | 2.01                     | 0.75              |
| 25:DW:102:MET:HE1   | 40:CR:271:MET:HE1   | 1.69                     | 0.75              |
| 29:CE:102:GLU:HG3   | 45:Cb:56:ARG:NH2    | 2.00                     | 0.75              |
| 37:CO:127:THR:HG22  | 37:CO:131:LYS:NZ    | 2.00                     | 0.75              |
| 48:Ci:101:LEU:HD13  | 50:Ck:697:MET:HE1   | 1.68                     | 0.75              |
| 75:AI:15:PRO:O      | 129:Ba:104:ARG:NH2  | 2.19                     | 0.75              |
| 85:AW:193:LYS:NZ    | 107:BE:390:SER:OG   | 2.15                     | 0.75              |
| 87:AY:279:ARG:HH12  | 128:BZ:174:SER:HB2  | 1.51                     | 0.75              |
| 1:DA:446:ARG:NH1    | 1:DA:503:SER:OG     | 2.18                     | 0.75              |
| 1:DA:1187:ASP:O     | 1:DA:1188:GLU:O     | 2.04                     | 0.75              |
| 15:DB:1053:ALA:HB2  | 20:DH:345:VAL:HG13  | 1.68                     | 0.75              |
| 18:DF:548:ARG:NE    | 18:DF:574:GLU:OE2   | 2.20                     | 0.75              |
| 21:DJ:308:ARG:HH11  | 21:DJ:308:ARG:CG    | 1.96                     | 0.75              |
| 32:CI:175:ARG:NH1   | 32:CI:179:CYS:SG    | 2.59                     | 0.75              |
| 55:Cr:275:TYR:HD1   | 55:Cr:280:ARG:NH1   | 1.85                     | 0.75              |
| 56:Cv:293:LEU:HD11  | 56:Cv:407:MET:HB2   | 1.69                     | 0.75              |
| 69:A5:69:TRP:CE2    | 69:A5:79:LYS:HB2    | 2.21                     | 0.75              |
| 79:AP:45:ARG:H      | 79:AP:45:ARG:HD2    | 1.51                     | 0.75              |
| 87:AY:194:ARG:HG2   | 87:AY:201:MET:HG2   | 1.68                     | 0.75              |
| 93:Aj:221:SER:OG    | 93:Aj:225:GLN:NE2   | 2.20                     | 0.75              |
| 56:Cv:304:THR:HG22  | 56:Cv:306:TYR:H     | 1.51                     | 0.75              |
| 79:AP:113:ILE:HG22  | 79:AP:114:LYS:HG3   | 1.68                     | 0.75              |
| 111:BI:147:TYR:HD2  | 111:BI:170:MET:HG2  | 1.50                     | 0.75              |
| 15:DB:1068:GLY:HA2  | 50:Ck:660:PRO:HG3   | 1.66                     | 0.75              |
| 40:CR:317:ILE:CA    | 46:Cd:283:GLU:OE2   | 2.35                     | 0.75              |
| 67:A3:170:ARG:NH2   | 94:Al:187:LYS:O     | 2.20                     | 0.75              |
| 79:AP:374:LEU:HD11  | 105:BC:497:GLU:HA   | 1.69                     | 0.75              |
| 88:Ab:170:GLY:HA3   | 88:Ab:202:MET:HE3   | 1.68                     | 0.75              |
| 98:Av:54:THR:N      | 98:Av:57:GLU:OE2    | 2.19                     | 0.75              |
| 33:CJ:544:THR:HG21  | 33:CJ:552:ILE:CA    | 2.16                     | 0.74              |
| 37:CO:128:ARG:NH2   | 37:CO:209:GLU:OE1   | 2.20                     | 0.74              |
| 19:DG:547:MET:HE1   | 19:DG:561:PRO:HB3   | 1.68                     | 0.74              |
| 52:Cn:236:LYS:N     | 52:Cn:245:LYS:HZ3   | 1.85                     | 0.74              |
| 102:AA:1164:A:H5"   | 103:BA:767:ARG:HH12 | 1.51                     | 0.74              |
| 114:BL:264:LEU:HD21 | 114:BL:287:ARG:NH1  | 1.98                     | 0.74              |
| 1:DA:1014:TYR:CE1   | 4:DL:67:ASN:C       | 2.66                     | 0.74              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:DD:213:CYS:HB3    | 2:DD:297:ARG:HH12   | 1.52                     | 0.74              |
| 66:A2:219:THR:CG2   | 122:BT:112:ARG:HH12 | 2.01                     | 0.74              |
| 88:Ab:419:GLN:HE21  | 105:BC:73:ARG:HH11  | 1.33                     | 0.74              |
| 120:BR:115:SER:HB3  | 120:BR:197:LYS:HE2  | 1.70                     | 0.74              |
| 121:BS:43:PRO:O     | 121:BS:113:ARG:NH2  | 2.19                     | 0.74              |
| 1:DA:990:VAL:HG11   | 1:DA:1185:ARG:HG3   | 1.70                     | 0.74              |
| 25:DW:113:PRO:HG2   | 40:CR:289:THR:CG2   | 2.18                     | 0.74              |
| 78:AN:28:LEU:HG     | 131:Bc:18:ARG:HH22  | 1.52                     | 0.74              |
| 110:BH:160:THR:HG22 | 110:BH:245:ASN:HB3  | 1.69                     | 0.74              |
| 130:Bb:46:LEU:HB3   | 130:Bb:47:ARG:NH1   | 2.02                     | 0.74              |
| 1:DA:1181:THR:OG1   | 1:DA:1182:ARG:NH1   | 2.20                     | 0.74              |
| 40:CR:317:ILE:HA    | 46:Cd:283:GLU:CD    | 2.11                     | 0.74              |
| 112:BJ:222:PRO:O    | 112:BJ:227:ARG:NH1  | 2.18                     | 0.74              |
| 20:DH:269:ARG:NH1   | 33:CJ:288:GLN:OE1   | 2.19                     | 0.74              |
| 34:CK:14:PRO:HG3    | 40:CR:300:TYR:CG    | 2.21                     | 0.74              |
| 81:AR:167:ASN:HD21  | 81:AR:170:MET:HG2   | 1.53                     | 0.74              |
| 1:DA:235:THR:HG23   | 1:DA:281:MET:HE2    | 1.70                     | 0.74              |
| 14:Da:35:ALA:HB2    | 14:Da:42:ARG:HD2    | 1.70                     | 0.74              |
| 40:CR:134:ARG:HH21  | 40:CR:185:PHE:HB3   | 1.53                     | 0.74              |
| 90:Ae:57:GLY:HA3    | 90:Ae:62:GLY:HA2    | 1.70                     | 0.74              |
| 124:BV:30:LYS:HZ3   | 124:BV:32:VAL:HA    | 1.50                     | 0.74              |
| 134:Bf:44:ARG:HD3   | 141:UE:6:UNK:HG3    | 1.69                     | 0.74              |
| 1:DA:1312:TRP:CZ2   | 1:DA:1314:GLY:HA2   | 2.23                     | 0.74              |
| 3:DI:340:ARG:HH12   | 3:DI:342:ARG:HH11   | 1.33                     | 0.74              |
| 19:DG:111:ARG:NH2   | 45:Cb:197:PRO:HB3   | 2.02                     | 0.74              |
| 29:CE:311:LYS:H     | 29:CE:311:LYS:HD2   | 1.53                     | 0.74              |
| 34:CK:201:ARG:NH1   | 42:CU:79:TYR:OH     | 2.21                     | 0.74              |
| 35:CL:78:MET:HE3    | 35:CL:105:ARG:HH21  | 1.51                     | 0.74              |
| 85:AW:158:ARG:HH11  | 85:AW:242:LEU:HD13  | 1.50                     | 0.74              |
| 93:Aj:191:THR:HG21  | 93:Aj:205:ARG:HE    | 1.53                     | 0.74              |
| 109:BG:61:PRO:HB3   | 109:BG:132:ARG:HH21 | 1.53                     | 0.74              |
| 1:DA:1486:ALA:O     | 1:DA:1488:GLN:NE2   | 2.20                     | 0.74              |
| 34:CK:262:ARG:NH1   | 34:CK:269:MET:SD    | 2.61                     | 0.74              |
| 50:Ck:331:ARG:NH2   | 50:Ck:595:ASP:OD1   | 2.21                     | 0.74              |
| 68:A4:42:VAL:HG13   | 68:A4:44:ARG:NH1    | 2.03                     | 0.74              |
| 76:AJ:14:ARG:NH2    | 96:Ap:226:ASP:OD2   | 2.19                     | 0.74              |
| 118:BP:121:ARG:HG2  | 118:BP:121:ARG:HH11 | 1.53                     | 0.74              |
| 4:DL:114:SER:CB     | 4:DL:254:ARG:CD     | 2.66                     | 0.73              |
| 5:DM:45:ARG:HH11    | 5:DM:45:ARG:HG3     | 1.52                     | 0.73              |
| 15:DB:1154:LYS:HZ2  | 89:Ad:150:ARG:NE    | 1.86                     | 0.73              |
| 27:DY:36:GLU:OE2    | 27:DY:40:ARG:NH1    | 2.21                     | 0.73              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:DU:86:ILE:HD11   | 12:DU:99:GLN:HB2    | 1.70                     | 0.73              |
| 21:DJ:192:THR:HG21  | 21:DJ:222:GLU:HG2   | 1.69                     | 0.73              |
| 25:DW:121:HIS:HD2   | 25:DW:123:ALA:H     | 1.34                     | 0.73              |
| 34:CK:215:ARG:NH2   | 57:CA:298:U:O2'     | 2.20                     | 0.73              |
| 70:A6:37:MET:HE1    | 102:AA:954:U:H5''   | 1.70                     | 0.73              |
| 78:AN:54:LEU:HG     | 78:AN:91:VAL:HG11   | 1.70                     | 0.73              |
| 102:AA:442:A:N7     | 115:BM:271:ARG:NH1  | 2.35                     | 0.73              |
| 110:BH:66:GLU:HG3   | 139:UC:11:UNK:HG1   | 1.68                     | 0.73              |
| 5:DM:64:THR:CG2     | 5:DM:69:PHE:O       | 2.32                     | 0.73              |
| 30:CF:50:ARG:HD3    | 42:CU:35:ILE:HD11   | 1.68                     | 0.73              |
| 121:BS:48:GLY:HA2   | 121:BS:72:THR:HG23  | 1.70                     | 0.73              |
| 51:Cm:137:SER:HA    | 57:CA:394:A:H2      | 1.52                     | 0.73              |
| 76:AJ:83:PHE:HB3    | 96:Ap:205:ARG:NH1   | 2.03                     | 0.73              |
| 107:BE:11:TYR:O     | 107:BE:13:ARG:NH1   | 2.21                     | 0.73              |
| 8:DP:208:PRO:HD2    | 8:DP:211:GLU:HB2    | 1.70                     | 0.73              |
| 38:CP:96:ILE:HD11   | 44:Ca:470:ARG:CZ    | 2.18                     | 0.73              |
| 1:DA:1003:PHE:CD1   | 4:DL:78:ALA:CA      | 2.71                     | 0.73              |
| 2:DD:637:ARG:NH1    | 38:CP:153:ARG:HD2   | 2.04                     | 0.73              |
| 2:DD:647:ARG:HH22   | 10:DR:230:ARG:HH11  | 1.36                     | 0.73              |
| 33:CJ:793:HIS:CD2   | 33:CJ:794:GLU:HG2   | 2.24                     | 0.73              |
| 51:Cm:164:HIS:HB3   | 57:CA:611:U:H5''    | 1.70                     | 0.73              |
| 107:BE:147:SER:HB2  | 107:BE:257:ASP:OD2  | 1.88                     | 0.73              |
| 1:DA:1012:THR:C     | 4:DL:77:LEU:HD21    | 2.14                     | 0.73              |
| 15:DB:490:ARG:HB2   | 15:DB:962:MET:HE1   | 1.71                     | 0.73              |
| 78:AN:82:HIS:HD2    | 78:AN:157:TRP:HE1   | 1.37                     | 0.73              |
| 92:Ag:72:LYS:NZ     | 102:AA:491:A:OP2    | 2.18                     | 0.73              |
| 93:Aj:63:PRO:HD3    | 109:BG:144:TRP:NE1  | 2.03                     | 0.73              |
| 95:Ao:226:ARG:HE    | 102:AA:448:A:H2'    | 1.54                     | 0.73              |
| 103:BA:296:ARG:HH11 | 103:BA:296:ARG:HG3  | 1.53                     | 0.73              |
| 114:BL:281:SER:N    | 114:BL:284:ARG:HH12 | 1.87                     | 0.73              |
| 6:DN:74:HIS:O       | 6:DN:109:ASN:CG     | 2.31                     | 0.73              |
| 15:DB:455:ARG:NH1   | 15:DB:461:GLN:O     | 2.22                     | 0.73              |
| 32:CI:307:VAL:HG22  | 32:CI:322:LEU:HD22  | 1.71                     | 0.73              |
| 40:CR:319:LYS:NZ    | 46:Cd:283:GLU:O     | 2.21                     | 0.73              |
| 68:A4:109:ARG:NH1   | 132:Bd:130:GLU:O    | 2.21                     | 0.73              |
| 75:AI:48:ARG:HH11   | 75:AI:48:ARG:CG     | 2.01                     | 0.73              |
| 11:DS:114:LYS:NZ    | 57:CA:206:A:OP1     | 2.16                     | 0.73              |
| 77:AK:234:GLU:HA    | 77:AK:241:ARG:HH12  | 1.52                     | 0.73              |
| 97:At:136:ARG:HB3   | 97:At:136:ARG:NH1   | 2.04                     | 0.73              |
| 111:BI:197:ASP:HA   | 111:BI:200:GLU:HB3  | 1.71                     | 0.73              |
| 3:DI:340:ARG:NH1    | 3:DI:342:ARG:HD2    | 2.04                     | 0.72              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 17:DE:182:ASP:OD1   | 17:DE:543:ARG:NH2  | 2.21                     | 0.72              |
| 39:CQ:16:THR:HG21   | 53:Cp:18:SER:HA    | 1.70                     | 0.72              |
| 39:CQ:56:ARG:HG2    | 39:CQ:56:ARG:NH1   | 2.01                     | 0.72              |
| 50:Ck:617:VAL:HG21  | 50:Ck:638:ARG:HD2  | 1.70                     | 0.72              |
| 78:AN:170:ASN:OD1   | 84:AV:223:LYS:NZ   | 2.22                     | 0.72              |
| 102:AA:289:U:H4'    | 102:AA:290:A:H5'   | 1.68                     | 0.72              |
| 128:BZ:150:CYS:SG   | 128:BZ:151:ILE:N   | 2.62                     | 0.72              |
| 133:Be:21:ARG:HG2   | 133:Be:21:ARG:HH11 | 1.53                     | 0.72              |
| 134:Bf:44:ARG:HH11  | 141:UE:6:UNK:HA    | 1.53                     | 0.72              |
| 6:DN:16:ASP:HB3     | 6:DN:175:LYS:HE2   | 1.70                     | 0.72              |
| 19:DG:366:ASP:HA    | 19:DG:370:ARG:HH12 | 1.54                     | 0.72              |
| 43:CZ:234:ILE:HG12  | 43:CZ:240:VAL:HG21 | 1.71                     | 0.72              |
| 50:Ck:832:THR:HG22  | 50:Ck:834:MET:H    | 1.54                     | 0.72              |
| 54:Cq:177:THR:OG1   | 55:Cr:64:ARG:NH1   | 2.22                     | 0.72              |
| 98:Av:166:TYR:CE1   | 118:BP:212:PRO:HB3 | 2.23                     | 0.72              |
| 1:DA:1090:GLY:O     | 1:DA:1384:ARG:NH2  | 2.22                     | 0.72              |
| 9:DQ:103:CYS:HA     | 9:DQ:106:MET:HE3   | 1.72                     | 0.72              |
| 12:DU:46:THR:HG22   | 12:DU:48:PHE:H     | 1.53                     | 0.72              |
| 19:DG:50:LEU:HD22   | 32:CI:249:GLU:OE1  | 1.89                     | 0.72              |
| 21:DJ:209:ARG:NH2   | 150:DJ:401:UTP:O2B | 2.22                     | 0.72              |
| 55:Cr:282:GLU:HG3   | 55:Cr:285:ARG:HH21 | 1.54                     | 0.72              |
| 3:DI:233:ARG:NH2    | 3:DI:272:CYS:O     | 2.22                     | 0.72              |
| 9:DQ:122:ILE:HG23   | 9:DQ:130:LEU:HD12  | 1.71                     | 0.72              |
| 25:DW:126:ARG:O     | 40:CR:287:MET:CE   | 2.37                     | 0.72              |
| 102:AA:301:A:OP1    | 108:BF:262:ARG:NH2 | 2.20                     | 0.72              |
| 30:CF:149:PHE:HA    | 56:Cv:627:LEU:HD11 | 1.72                     | 0.72              |
| 47:Cg:289:ASN:HD21  | 47:Cg:358:THR:H    | 1.34                     | 0.72              |
| 105:BC:260:LEU:HD13 | 118:BP:92:VAL:HG11 | 1.71                     | 0.72              |
| 116:BN:10:GLN:H     | 116:BN:14:HIS:HD2  | 1.36                     | 0.72              |
| 2:DD:637:ARG:HH11   | 38:CP:153:ARG:NH1  | 1.87                     | 0.72              |
| 4:DL:114:SER:HB2    | 4:DL:254:ARG:HD2   | 1.69                     | 0.72              |
| 65:A1:46:CYS:SG     | 143:UI:13:UNK:HG1  | 2.29                     | 0.72              |
| 73:AE:319:LYS:HA    | 73:AE:371:LEU:HD21 | 1.71                     | 0.72              |
| 93:Aj:63:PRO:HD3    | 109:BG:144:TRP:HE1 | 1.55                     | 0.72              |
| 96:Ap:142:GLU:N     | 96:Ap:142:GLU:OE1  | 2.22                     | 0.72              |
| 16:DC:172:SER:HB2   | 16:DC:511:ARG:NH1  | 2.05                     | 0.72              |
| 26:DX:50:ARG:NH2    | 41:CS:122:PHE:O    | 2.22                     | 0.72              |
| 79:AP:227:PRO:HD3   | 94:Al:118:ALA:HB2  | 1.70                     | 0.72              |
| 85:AW:84:ARG:HH12   | 108:BF:383:MET:HE2 | 1.54                     | 0.72              |
| 106:BD:205:GLU:H    | 106:BD:451:ALA:CB  | 1.92                     | 0.72              |
| 130:Bb:46:LEU:HB3   | 130:Bb:47:ARG:HH12 | 1.55                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:339:ARG:HH22  | 57:CA:85:U:H1'     | 1.55                     | 0.72              |
| 9:DQ:250:ARG:HD3   | 9:DQ:252:LYS:CE    | 2.19                     | 0.72              |
| 24:DV:31:HIS:H     | 24:DV:83:GLN:HE22  | 1.37                     | 0.72              |
| 77:AK:234:GLU:HA   | 77:AK:241:ARG:NH1  | 2.03                     | 0.72              |
| 90:Ae:75:ARG:NH1   | 90:Ae:135:THR:O    | 2.22                     | 0.72              |
| 127:BY:79:GLU:HA   | 127:BY:82:ARG:HH22 | 1.53                     | 0.72              |
| 136:Bh:2:ALA:N     | 136:Bh:47:SER:HG   | 1.87                     | 0.72              |
| 19:DG:57:GLU:OE2   | 32:CI:245:ARG:CZ   | 2.38                     | 0.72              |
| 27:DY:37:ARG:HH21  | 27:DY:106:GLN:HE22 | 1.36                     | 0.72              |
| 76:AJ:78:THR:HG22  | 76:AJ:80:ARG:H     | 1.54                     | 0.72              |
| 76:AJ:103:ARG:HH12 | 100:AC:75:ALA:HB2  | 1.55                     | 0.72              |
| 120:BR:25:THR:HG23 | 120:BR:69:CYS:HA   | 1.71                     | 0.72              |
| 2:DD:340:ARG:NH1   | 12:DU:58:HIS:HB3   | 2.05                     | 0.71              |
| 15:DB:358:ASN:HB3  | 20:DH:542:LEU:HD21 | 1.72                     | 0.71              |
| 20:DH:19:THR:HG22  | 20:DH:21:LEU:H     | 1.53                     | 0.71              |
| 20:DH:85:LEU:H     | 20:DH:85:LEU:HD12  | 1.53                     | 0.71              |
| 34:CK:214:LYS:HB3  | 34:CK:214:LYS:NZ   | 2.05                     | 0.71              |
| 78:AN:89:LYS:NZ    | 96:Ap:62:LYS:NZ    | 2.38                     | 0.71              |
| 114:BL:173:GLY:O   | 114:BL:256:ARG:NH1 | 2.23                     | 0.71              |
| 6:DN:288:PHE:O     | 29:CE:118:ARG:NH1  | 2.23                     | 0.71              |
| 18:DF:589:GLN:HB2  | 20:DH:192:PHE:CD1  | 2.24                     | 0.71              |
| 1:DA:502:LYS:NZ    | 1:DA:502:LYS:HB3   | 2.04                     | 0.71              |
| 10:DR:128:PRO:HG3  | 10:DR:133:LEU:CA   | 2.20                     | 0.71              |
| 15:DB:876:LEU:HD12 | 15:DB:877:PRO:HD2  | 1.72                     | 0.71              |
| 15:DB:1154:LYS:HZ3 | 89:Ad:150:ARG:NE   | 1.87                     | 0.71              |
| 19:DG:83:MET:HE3   | 19:DG:105:LEU:HD23 | 1.72                     | 0.71              |
| 23:DT:164:GLY:O    | 23:DT:168:GLU:HB2  | 1.90                     | 0.71              |
| 56:Cv:255:PHE:HB3  | 56:Cv:292:LYS:HG3  | 1.71                     | 0.71              |
| 84:AV:73:LEU:HG    | 84:AV:122:ARG:HG2  | 1.71                     | 0.71              |
| 104:BB:181:ARG:NH1 | 104:BB:221:TYR:HD2 | 1.88                     | 0.71              |
| 131:Bc:34:GLN:NE2  | 131:Bc:38:ASN:OD1  | 2.23                     | 0.71              |
| 81:AR:73:MET:HE1   | 81:AR:89:ARG:HB3   | 1.73                     | 0.71              |
| 133:Be:77:ASP:OD1  | 133:Be:77:ASP:N    | 2.22                     | 0.71              |
| 6:DN:12:MET:HE3    | 6:DN:171:LEU:HD13  | 1.72                     | 0.71              |
| 15:DB:472:GLY:HA3  | 50:Ck:93:THR:O     | 1.91                     | 0.71              |
| 29:CE:60:TYR:HB3   | 29:CE:85:ASN:HD21  | 1.54                     | 0.71              |
| 68:A4:85:GLN:NE2   | 68:A4:93:ARG:HH12  | 1.86                     | 0.71              |
| 95:Ao:229:LYS:NZ   | 102:AA:387:A:H3'   | 2.05                     | 0.71              |
| 4:DL:71:GLU:OE2    | 44:Ca:244:PRO:HD2  | 1.91                     | 0.71              |
| 17:DE:467:MET:HE1  | 17:DE:486:ILE:HD13 | 1.72                     | 0.71              |
| 19:DG:12:ASN:O     | 33:CJ:415:ARG:NH2  | 2.23                     | 0.71              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 19:DG:22:GLN:HG2   | 50:Ck:102:PRO:HD3   | 1.71                     | 0.71              |
| 45:Cb:221:VAL:HG21 | 55:Cr:303:LEU:HD11  | 1.70                     | 0.71              |
| 56:Cv:1006:GLU:OE2 | 56:Cv:1008:ARG:NH1  | 2.22                     | 0.71              |
| 2:DD:734:ARG:NH2   | 3:DI:164:GLU:OE2    | 2.24                     | 0.71              |
| 12:DU:170:ARG:O    | 12:DU:174:ARG:NH1   | 2.24                     | 0.71              |
| 12:DU:171:ASP:HA   | 12:DU:174:ARG:NH1   | 2.06                     | 0.71              |
| 68:A4:20:ARG:HB2   | 68:A4:20:ARG:NH1    | 2.05                     | 0.71              |
| 75:AI:80:GLU:HG2   | 75:AI:95:ARG:HD2    | 1.73                     | 0.71              |
| 96:Ap:166:PRO:HB3  | 141:UE:9:UNK:HG1    | 1.72                     | 0.71              |
| 135:Bg:92:LYS:HZ2  | 135:Bg:96:ARG:HD2   | 1.56                     | 0.71              |
| 87:AY:254:LYS:NZ   | 87:AY:255:ARG:HH12  | 1.87                     | 0.71              |
| 1:DA:985:LYS:HE3   | 1:DA:1205:THR:HG21  | 1.72                     | 0.71              |
| 1:DA:985:LYS:NZ    | 1:DA:985:LYS:HB3    | 2.06                     | 0.71              |
| 74:AF:140:GLU:H    | 74:AF:225:MET:HE3   | 1.55                     | 0.71              |
| 94:Al:15:THR:HG21  | 94:Al:26:MET:HG2    | 1.71                     | 0.71              |
| 110:BH:106:GLU:HA  | 110:BH:249:ARG:NH1  | 2.06                     | 0.71              |
| 15:DB:110:ARG:NH2  | 15:DB:309:SER:O     | 2.24                     | 0.71              |
| 15:DB:1164:ASP:HB3 | 25:DW:11:ALA:HB2    | 1.73                     | 0.71              |
| 18:DF:53:ARG:HG2   | 18:DF:53:ARG:HH11   | 1.55                     | 0.71              |
| 19:DG:68:TYR:OH    | 40:CR:250:GLN:NE2   | 2.24                     | 0.71              |
| 48:Ci:145:ASN:HD21 | 48:Ci:152:ASN:HD21  | 1.36                     | 0.71              |
| 68:A4:76:PRO:HA    | 93:Aj:81:ARG:HB3    | 1.72                     | 0.71              |
| 75:AI:158:THR:HG22 | 75:AI:159:PRO:HD2   | 1.73                     | 0.71              |
| 77:AK:133:ARG:NH1  | 77:AK:134:ARG:HH21  | 1.89                     | 0.71              |
| 117:BO:215:LEU:HA  | 117:BO:219:ARG:HH11 | 1.54                     | 0.71              |
| 15:DB:801:LEU:HB2  | 15:DB:805:GLU:HB2   | 1.72                     | 0.70              |
| 16:DC:115:ASP:OD1  | 16:DC:116:TYR:N     | 2.24                     | 0.70              |
| 29:CE:308:ARG:CA   | 29:CE:311:LYS:NZ    | 2.54                     | 0.70              |
| 33:CJ:463:MET:HE1  | 48:Ci:85:PRO:HB2    | 1.72                     | 0.70              |
| 57:CA:309:A:O2'    | 57:CA:350:U:O2'     | 2.05                     | 0.70              |
| 74:AF:423:PRO:HG3  | 125:BW:84:MET:HE3   | 1.71                     | 0.70              |
| 32:CI:90:GLU:H     | 34:CK:114:MET:HE3   | 1.57                     | 0.70              |
| 45:Cb:19:PRO:HD2   | 51:Cm:156:THR:HG21  | 1.71                     | 0.70              |
| 64:A0:71:ARG:NH1   | 94:Al:45:ILE:HD11   | 2.06                     | 0.70              |
| 81:AR:134:ARG:NH2  | 123:BU:166:GLN:O    | 2.20                     | 0.70              |
| 91:Af:58:ARG:NH1   | 102:AA:381:U:OP1    | 2.24                     | 0.70              |
| 105:BC:116:ARG:HG3 | 105:BC:140:LEU:HB3  | 1.72                     | 0.70              |
| 129:Ba:89:PRO:HG2  | 129:Ba:92:TYR:HD2   | 1.56                     | 0.70              |
| 10:DR:266:TRP:CG   | 49:Cj:210:PRO:HA    | 2.26                     | 0.70              |
| 40:CR:308:MET:HE1  | 57:CA:388:U:O4'     | 1.84                     | 0.70              |
| 2:DD:340:ARG:HH11  | 12:DU:58:HIS:HB3    | 1.56                     | 0.70              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 15:DB:303:PRO:O     | 17:DE:489:ARG:NH2   | 2.25                     | 0.70              |
| 116:BN:173:SER:HB2  | 116:BN:177:ARG:HH12 | 1.57                     | 0.70              |
| 4:DL:118:ASP:O      | 4:DL:159:GLN:NE2    | 2.24                     | 0.70              |
| 18:DF:576:SER:HB2   | 50:Ck:118:ASP:OD1   | 1.90                     | 0.70              |
| 56:Cv:626:VAL:HB    | 56:Cv:628:LYS:NZ    | 2.05                     | 0.70              |
| 70:A6:94:LYS:HZ1    | 79:AP:345:TRP:HZ3   | 1.36                     | 0.70              |
| 85:AW:82:TRP:CD1    | 85:AW:95:ARG:HG3    | 2.27                     | 0.70              |
| 1:DA:1052:ALA:HB1   | 32:CI:202:LEU:HD21  | 1.71                     | 0.70              |
| 4:DL:25:PRO:O       | 23:DT:202:LYS:NZ    | 2.24                     | 0.70              |
| 4:DL:117:ASP:C      | 4:DL:121:ILE:HG13   | 2.15                     | 0.70              |
| 18:DF:29:ARG:H      | 21:DJ:314:GLN:HE22  | 1.36                     | 0.70              |
| 25:DW:104:VAL:CB    | 40:CR:279:LYS:CG    | 2.68                     | 0.70              |
| 32:CI:409:PRO:CB    | 40:CR:253:PHE:HE2   | 2.04                     | 0.70              |
| 1:DA:577:ASP:OD1    | 1:DA:578:LYS:N      | 2.23                     | 0.70              |
| 10:DR:126:LEU:CD1   | 10:DR:137:CYS:SG    | 2.80                     | 0.70              |
| 37:CO:90:MET:HB3    | 37:CO:91:PRO:HD2    | 1.73                     | 0.70              |
| 67:A3:171:ARG:HG2   | 67:A3:171:ARG:HH11  | 1.56                     | 0.70              |
| 88:Ab:98:PRO:HB2    | 105:BC:208:ARG:HD3  | 1.73                     | 0.70              |
| 111:BI:190:ARG:HH12 | 111:BI:230:GLU:HB3  | 1.57                     | 0.70              |
| 18:DF:589:GLN:NE2   | 20:DH:191:HIS:N     | 2.38                     | 0.70              |
| 31:CH:154:ASP:O     | 31:CH:158:ARG:HG2   | 1.92                     | 0.70              |
| 37:CO:127:THR:HG22  | 37:CO:131:LYS:HZ2   | 1.55                     | 0.70              |
| 67:A3:180:ARG:NH2   | 94:Al:178:GLU:OE1   | 2.25                     | 0.70              |
| 79:AP:25:MET:HG3    | 95:Ao:82:GLU:HG3    | 1.73                     | 0.70              |
| 9:DQ:46:ARG:NH1     | 12:DU:121:GLU:OE2   | 2.24                     | 0.70              |
| 57:CA:84:U:H4'      | 57:CA:85:U:OP1      | 1.92                     | 0.70              |
| 68:A4:61:ARG:HH21   | 89:Ad:49:ARG:HH11   | 1.37                     | 0.70              |
| 78:AN:149:ARG:NH1   | 102:AA:836:A:H62    | 1.90                     | 0.70              |
| 79:AP:332:THR:HG22  | 79:AP:334:GLU:H     | 1.55                     | 0.70              |
| 95:Ao:76:LYS:HA     | 95:Ao:81:ARG:HD2    | 1.74                     | 0.70              |
| 117:BO:134:PRO:HG3  | 121:BS:26:ARG:NH1   | 2.07                     | 0.70              |
| 33:CJ:293:ASP:HB2   | 33:CJ:296:LEU:H     | 1.57                     | 0.70              |
| 41:CS:48:ARG:HG3    | 41:CS:48:ARG:HH11   | 1.56                     | 0.70              |
| 98:Av:48:ALA:HB2    | 102:AA:50:A:H4'     | 1.73                     | 0.70              |
| 105:BC:461:ASP:OD1  | 105:BC:461:ASP:N    | 2.25                     | 0.70              |
| 2:DD:52:LYS:NZ      | 57:CA:138:U:O4      | 2.25                     | 0.69              |
| 2:DD:149:SER:O      | 2:DD:153:THR:OG1    | 2.10                     | 0.69              |
| 2:DD:414:ARG:NH1    | 2:DD:568:GLU:OE1    | 2.25                     | 0.69              |
| 4:DL:164:ARG:HH22   | 45:Cb:64:ASN:HD21   | 1.40                     | 0.69              |
| 16:DC:327:GLU:OE2   | 16:DC:410:ARG:HD2   | 1.91                     | 0.69              |
| 18:DF:499:THR:HG22  | 20:DH:272:HIS:NE2   | 2.06                     | 0.69              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 27:DY:37:ARG:NH2   | 27:DY:106:GLN:HE22  | 1.90                     | 0.69              |
| 41:CS:106:TYR:HD2  | 41:CS:140:MET:HE1   | 1.57                     | 0.69              |
| 56:Cv:292:LYS:NZ   | 56:Cv:511:HIS:O     | 2.24                     | 0.69              |
| 78:AN:46:LEU:HB2   | 78:AN:171:PRO:HB2   | 1.74                     | 0.69              |
| 105:BC:157:TYR:OH  | 105:BC:271:GLU:OE2  | 2.08                     | 0.69              |
| 2:DD:527:THR:HB    | 10:DR:223:GLN:HG3   | 1.74                     | 0.69              |
| 7:DO:178:ARG:NH2   | 46:Cd:136:GLU:OE2   | 2.24                     | 0.69              |
| 9:DQ:254:SER:N     | 9:DQ:255:PRO:HD2    | 2.06                     | 0.69              |
| 10:DR:126:LEU:HD12 | 10:DR:137:CYS:SG    | 2.32                     | 0.69              |
| 16:DC:574:GLN:HE21 | 16:DC:807:VAL:H     | 1.38                     | 0.69              |
| 16:DC:699:VAL:HB   | 16:DC:702:LEU:HD12  | 1.73                     | 0.69              |
| 25:DW:89:ILE:HD13  | 27:DY:48:LEU:HD22   | 1.73                     | 0.69              |
| 42:CU:16:HIS:HD2   | 42:CU:18:LYS:H      | 1.40                     | 0.69              |
| 75:AI:112:ARG:HD2  | 127:BY:145:TRP:CD2  | 2.26                     | 0.69              |
| 77:AK:315:LEU:HD12 | 77:AK:316:PRO:HD2   | 1.74                     | 0.69              |
| 109:BG:192:ARG:NH1 | 109:BG:253:ARG:HD2  | 2.07                     | 0.69              |
| 110:BH:257:ASP:OD1 | 110:BH:257:ASP:N    | 2.22                     | 0.69              |
| 123:BU:136:ASP:HB2 | 135:Bg:37:LEU:HD21  | 1.74                     | 0.69              |
| 1:DA:1183:SER:HB3  | 1:DA:1186:CYS:HB2   | 1.72                     | 0.69              |
| 67:A3:61:ARG:HG2   | 67:A3:61:ARG:HH11   | 1.56                     | 0.69              |
| 6:DN:29:ARG:HH11   | 6:DN:29:ARG:HG3     | 1.56                     | 0.69              |
| 11:DS:182:TYR:OH   | 11:DS:189:ARG:NH2   | 2.25                     | 0.69              |
| 16:DC:240:VAL:HG23 | 16:DC:251:TRP:CZ3   | 2.27                     | 0.69              |
| 21:DJ:242:LEU:HB3  | 21:DJ:294:MET:HE2   | 1.74                     | 0.69              |
| 25:DW:104:VAL:HB   | 40:CR:279:LYS:HG2   | 1.74                     | 0.69              |
| 30:CF:44:ILE:HD11  | 30:CF:63:ARG:HH12   | 1.58                     | 0.69              |
| 37:CO:93:ARG:HH21  | 57:CA:358:U:H3      | 1.40                     | 0.69              |
| 66:A2:142:LYS:HG3  | 66:A2:325:TYR:HE1   | 1.57                     | 0.69              |
| 6:DN:293:PRO:HB3   | 29:CE:109:LYS:NZ    | 2.08                     | 0.69              |
| 13:DZ:44:PHE:CZ    | 29:CE:24:GLY:HA3    | 2.27                     | 0.69              |
| 38:CP:26:ALA:HB2   | 57:CA:77:A:O4'      | 1.92                     | 0.69              |
| 51:Cm:27:ASN:HD22  | 51:Cm:32:LYS:HG3    | 1.57                     | 0.69              |
| 73:AE:239:LYS:HD3  | 131:Bc:97:GLN:HB2   | 1.74                     | 0.69              |
| 85:AW:100:GLU:HB3  | 114:BL:238:GLN:HE22 | 1.57                     | 0.69              |
| 93:Aj:100:ASP:OD1  | 132:Bd:119:GLN:NE2  | 2.24                     | 0.69              |
| 2:DD:339:ARG:NH2   | 57:CA:85:U:H1'      | 2.07                     | 0.69              |
| 11:DS:225:GLU:HB3  | 11:DS:229:ARG:HH12  | 1.56                     | 0.69              |
| 34:CK:156:LYS:HB2  | 34:CK:156:LYS:NZ    | 2.07                     | 0.69              |
| 64:A0:61:LEU:HD11  | 64:A0:65:ARG:HD3    | 1.75                     | 0.69              |
| 78:AN:35:GLN:O     | 103:BA:710:LYS:NZ   | 2.23                     | 0.69              |
| 78:AN:89:LYS:NZ    | 96:Ap:62:LYS:HZ1    | 1.89                     | 0.69              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 38:CP:23:ALA:HB1    | 38:CP:51:HIS:CG     | 2.21                     | 0.69              |
| 44:Ca:76:GLN:HA     | 44:Ca:79:MET:HE2    | 1.75                     | 0.69              |
| 56:Cv:594:LEU:HD23  | 56:Cv:600:GLY:HA2   | 1.73                     | 0.69              |
| 71:A8:172:LYS:HZ1   | 79:AP:259:HIS:HD2   | 1.39                     | 0.69              |
| 4:DL:106:PHE:CE1    | 32:CI:239:PHE:CZ    | 2.81                     | 0.69              |
| 8:DP:10:ALA:N       | 57:CA:55:U:O4       | 2.25                     | 0.69              |
| 20:DH:193:VAL:N     | 20:DH:194:PRO:HD2   | 2.07                     | 0.69              |
| 22:DK:119:ARG:NH2   | 22:DK:151:ASN:OD1   | 2.26                     | 0.69              |
| 53:Cp:53:VAL:HG11   | 53:Cp:59:PHE:HD1    | 1.56                     | 0.69              |
| 57:CA:232:G:N1      | 57:CA:248:A:OP1     | 2.25                     | 0.69              |
| 73:AE:233:LEU:HD22  | 73:AE:362:THR:HG21  | 1.75                     | 0.69              |
| 89:Ad:160:PRO:HG2   | 132:Bd:69:LEU:HD11  | 1.75                     | 0.69              |
| 4:DL:114:SER:CB     | 4:DL:254:ARG:HD2    | 2.23                     | 0.69              |
| 9:DQ:215:PRO:HA     | 9:DQ:218:ARG:HH12   | 1.57                     | 0.69              |
| 73:AE:111:PHE:HB3   | 73:AE:114:LEU:HD13  | 1.74                     | 0.69              |
| 73:AE:131:ASN:HB3   | 73:AE:134:TYR:HB3   | 1.75                     | 0.69              |
| 102:AA:383:A:HI1'   | 142:UF:8:UNK:HG1    | 1.75                     | 0.69              |
| 106:BD:270:ALA:CB   | 106:BD:406:ALA:HB1  | 2.19                     | 0.69              |
| 117:BO:143:ARG:HA   | 117:BO:152:ARG:HH12 | 1.58                     | 0.69              |
| 131:Bc:34:GLN:HA    | 131:Bc:37:ARG:NH1   | 2.08                     | 0.69              |
| 4:DL:67:ASN:ND2     | 29:CE:125:PRO:HB3   | 2.07                     | 0.69              |
| 77:AK:64:THR:HG23   | 77:AK:79:ALA:HB3    | 1.75                     | 0.69              |
| 114:BL:177:LEU:HD21 | 114:BL:291:LEU:HD11 | 1.75                     | 0.69              |
| 1:DA:1002:PRO:O     | 4:DL:78:ALA:C       | 2.36                     | 0.68              |
| 74:AF:137:MET:HE3   | 74:AF:224:ARG:HH12  | 1.57                     | 0.68              |
| 121:BS:85:ASP:OD1   | 121:BS:86:GLU:N     | 2.25                     | 0.68              |
| 3:DI:367:SER:H      | 3:DI:370:GLN:HE21   | 1.38                     | 0.68              |
| 22:DK:254:GLU:CG    | 22:DK:261:SER:HB3   | 2.22                     | 0.68              |
| 24:DV:123:PRO:O     | 24:DV:144:ARG:NH2   | 2.26                     | 0.68              |
| 31:CH:132:ASP:N     | 31:CH:132:ASP:OD1   | 2.25                     | 0.68              |
| 66:A2:270:ASN:HD22  | 66:A2:272:LEU:H     | 1.41                     | 0.68              |
| 68:A4:29:HIS:HD2    | 68:A4:32:LEU:HD23   | 1.58                     | 0.68              |
| 74:AF:56:HIS:HD2    | 74:AF:58:LEU:H      | 1.40                     | 0.68              |
| 78:AN:71:PRO:HB3    | 83:AU:69:ALA:HB2    | 1.74                     | 0.68              |
| 87:AY:195:ASN:HB3   | 87:AY:198:THR:HB    | 1.76                     | 0.68              |
| 109:BG:180:LEU:H    | 109:BG:287:HIS:HE1  | 1.41                     | 0.68              |
| 8:DP:183:ASP:HB3    | 8:DP:186:HIS:CD2    | 2.29                     | 0.68              |
| 13:DZ:20:ARG:HH11   | 13:DZ:20:ARG:HG3    | 1.59                     | 0.68              |
| 15:DB:550:LEU:HD13  | 15:DB:877:PRO:HB3   | 1.73                     | 0.68              |
| 16:DC:340:PHE:HB3   | 16:DC:364:MET:HE1   | 1.74                     | 0.68              |
| 40:CR:112:GLY:H     | 40:CR:149:PRO:HB2   | 1.56                     | 0.68              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 86:AX:187:ARG:NH1  | 102:AA:535:U:O2'    | 2.26                     | 0.68              |
| 92:Ag:170:GLN:HE22 | 92:Ag:227:PRO:HG2   | 1.58                     | 0.68              |
| 97:At:34:ARG:NE    | 120:BR:127:ARG:HH12 | 1.91                     | 0.68              |
| 34:CK:78:ASP:HB2   | 45:Cb:178:ARG:NH1   | 2.08                     | 0.68              |
| 37:CO:411:ARG:HH21 | 57:CA:68:A:H5'      | 1.57                     | 0.68              |
| 10:DR:249:GLU:HG3  | 10:DR:265:MET:HG2   | 1.75                     | 0.68              |
| 15:DB:231:ASP:OD1  | 15:DB:232:ARG:N     | 2.27                     | 0.68              |
| 19:DG:111:ARG:HH12 | 45:Cb:197:PRO:HB3   | 1.49                     | 0.68              |
| 24:DV:70:LYS:HD3   | 57:CA:513:U:H5'     | 1.74                     | 0.68              |
| 47:Cg:301:HIS:HD2  | 47:Cg:303:ASP:H     | 1.40                     | 0.68              |
| 65:A1:142:LYS:HB3  | 65:A1:142:LYS:HZ2   | 1.58                     | 0.68              |
| 76:AJ:83:PHE:HB3   | 96:Ap:205:ARG:HH12  | 1.56                     | 0.68              |
| 77:AK:28:GLU:OE2   | 77:AK:30:LEU:HB2    | 1.94                     | 0.68              |
| 85:AW:109:ASN:HD22 | 85:AW:112:LEU:HG    | 1.58                     | 0.68              |
| 93:Aj:264:VAL:HG13 | 93:Aj:268:GLU:HG2   | 1.75                     | 0.68              |
| 116:BN:97:ARG:HH11 | 136:Bh:87:CYS:HB3   | 1.57                     | 0.68              |
| 1:DA:1558:ASN:HA   | 1:DA:1596:VAL:HG21  | 1.75                     | 0.68              |
| 5:DM:51:VAL:HA     | 56:Cv:987:SER:HB3   | 1.75                     | 0.68              |
| 6:DN:75:VAL:CG1    | 6:DN:110:ALA:HB2    | 2.20                     | 0.68              |
| 10:DR:128:PRO:HG2  | 10:DR:133:LEU:H     | 1.57                     | 0.68              |
| 12:DU:189:LYS:HZ2  | 12:DU:190:ARG:HB2   | 1.58                     | 0.68              |
| 15:DB:478:ILE:HG22 | 50:Ck:46:ILE:HD11   | 1.74                     | 0.68              |
| 41:CS:31:LEU:HD12  | 41:CS:39:GLY:HA2    | 1.74                     | 0.68              |
| 10:DR:96:PHE:HE1   | 10:DR:128:PRO:HD3   | 1.59                     | 0.68              |
| 20:DH:14:TYR:OH    | 48:Ci:140:ASN:OD1   | 2.10                     | 0.68              |
| 51:Cm:118:GLU:N    | 51:Cm:118:GLU:OE1   | 2.27                     | 0.68              |
| 57:CA:73:U:H4'     | 57:CA:74:G:H5'      | 1.76                     | 0.68              |
| 81:AR:66:ARG:NH2   | 102:AA:798:U:OP1    | 2.23                     | 0.68              |
| 81:AR:94:ARG:HH21  | 103:BA:775:PRO:HB2  | 1.57                     | 0.68              |
| 88:Ab:122:HIS:HA   | 88:Ab:125:LEU:HD13  | 1.76                     | 0.68              |
| 116:BN:173:SER:HB2 | 116:BN:177:ARG:NH1  | 2.09                     | 0.68              |
| 127:BY:93:GLU:OE1  | 127:BY:93:GLU:N     | 2.27                     | 0.68              |
| 9:DQ:14:ARG:HH11   | 9:DQ:14:ARG:HB2     | 1.59                     | 0.68              |
| 18:DF:548:ARG:HD2  | 50:Ck:116:THR:HG22  | 1.75                     | 0.68              |
| 39:CQ:193:ARG:HH12 | 52:Cn:194:PRO:HD3   | 1.59                     | 0.68              |
| 44:Ca:522:GLU:HG2  | 44:Ca:588:LYS:HE3   | 1.75                     | 0.68              |
| 71:A8:166:ALA:HB3  | 102:AA:72:A:H61     | 1.58                     | 0.68              |
| 74:AF:455:TRP:HD1  | 79:AP:275:MET:HE3   | 1.59                     | 0.68              |
| 97:At:94:THR:OG1   | 97:At:96:GLU:OE1    | 2.12                     | 0.68              |
| 8:DP:183:ASP:HB3   | 8:DP:186:HIS:HD2    | 1.57                     | 0.68              |
| 19:DG:625:VAL:HG11 | 32:Cl:35:GLY:HA3    | 1.76                     | 0.68              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 79:AP:314:GLY:HA2  | 105:BC:469:THR:HG21 | 1.76                     | 0.68              |
| 9:DQ:254:SER:N     | 9:DQ:255:PRO:CD     | 2.57                     | 0.68              |
| 16:DC:77:ASP:H     | 16:DC:81:HIS:HD2    | 1.42                     | 0.68              |
| 17:DE:65:ILE:HD11  | 17:DE:83:LEU:HD23   | 1.76                     | 0.68              |
| 51:Cm:137:SER:HA   | 57:CA:394:A:C2      | 2.29                     | 0.68              |
| 51:Cm:137:SER:CA   | 57:CA:394:A:H2      | 2.06                     | 0.68              |
| 51:Cm:210:ARG:HG2  | 57:CA:288:U:H5''    | 1.75                     | 0.68              |
| 88:Ab:283:ASN:H    | 88:Ab:351:GLN:HE22  | 1.42                     | 0.68              |
| 89:Ad:55:ARG:HH11  | 89:Ad:55:ARG:HG2    | 1.59                     | 0.68              |
| 94:Al:177:GLU:OE2  | 94:Al:191:VAL:HG22  | 1.94                     | 0.68              |
| 103:BA:162:ARG:HG2 | 103:BA:162:ARG:HH11 | 1.58                     | 0.68              |
| 107:BE:290:ALA:HB2 | 107:BE:385:LEU:HD11 | 1.74                     | 0.68              |
| 10:DR:51:LEU:HD22  | 10:DR:84:LEU:HD21   | 1.76                     | 0.67              |
| 20:DH:421:THR:O    | 33:CJ:16:ARG:NH2    | 2.28                     | 0.67              |
| 33:CJ:544:THR:HG21 | 33:CJ:552:ILE:H     | 1.50                     | 0.67              |
| 33:CJ:544:THR:HG22 | 33:CJ:552:ILE:HG12  | 0.73                     | 0.67              |
| 33:CJ:712:THR:HG23 | 33:CJ:714:THR:H     | 1.58                     | 0.67              |
| 103:BA:591:THR:HA  | 103:BA:631:LYS:HG2  | 1.76                     | 0.67              |
| 8:DP:20:MET:HE1    | 8:DP:29:TRP:HB2     | 1.76                     | 0.67              |
| 27:DY:33:ALA:CB    | 27:DY:62:GLN:HG2    | 2.24                     | 0.67              |
| 57:CA:564:U:H3     | 57:CA:570:A:N6      | 1.87                     | 0.67              |
| 68:A4:149:LEU:HD11 | 93:Aj:26:PRO:HG2    | 1.76                     | 0.67              |
| 102:AA:1172:A:N6   | 103:BA:783:THR:O    | 2.27                     | 0.67              |
| 118:BP:58:ILE:HD11 | 132:Bd:7:ARG:HD3    | 1.75                     | 0.67              |
| 1:DA:1416:VAL:HG11 | 1:DA:1442:VAL:HG13  | 1.75                     | 0.67              |
| 40:CR:308:MET:HE1  | 57:CA:388:U:C5'     | 2.23                     | 0.67              |
| 86:AX:191:ARG:NH1  | 102:AA:532:U:O3'    | 2.27                     | 0.67              |
| 96:Ap:170:HIS:ND1  | 96:Ap:284:ASP:OD2   | 2.28                     | 0.67              |
| 105:BC:412:ALA:HA  | 105:BC:417:LEU:HB2  | 1.74                     | 0.67              |
| 7:DO:94:ILE:HG23   | 7:DO:99:LEU:HB2     | 1.75                     | 0.67              |
| 16:DC:349:ASP:O    | 16:DC:353:LEU:N     | 2.28                     | 0.67              |
| 20:DH:35:TYR:OH    | 21:DJ:46:ARG:NH2    | 2.27                     | 0.67              |
| 20:DH:253:SER:HA   | 20:DH:258:MET:HE1   | 1.77                     | 0.67              |
| 44:Ca:461:LEU:HD22 | 44:Ca:488:MET:HE2   | 1.76                     | 0.67              |
| 104:BB:445:TRP:HE3 | 104:BB:448:ARG:HE   | 1.40                     | 0.67              |
| 1:DA:420:ASN:ND2   | 1:DA:491:VAL:O      | 2.26                     | 0.67              |
| 92:Ag:190:GLN:HE22 | 100:AC:73:ALA:HB1   | 1.58                     | 0.67              |
| 4:DL:114:SER:HA    | 4:DL:254:ARG:HH21   | 1.58                     | 0.67              |
| 25:DW:168:MET:HE2  | 47:Cg:16:ARG:HH12   | 1.60                     | 0.67              |
| 55:Cr:125:GLN:HE22 | 55:Cr:161:ARG:HG3   | 1.58                     | 0.67              |
| 64:A0:168:PHE:HB2  | 64:A0:176:LEU:HD13  | 1.77                     | 0.67              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:A2:275:LEU:HD22  | 113:BK:328:LEU:HD13 | 1.76                     | 0.67              |
| 96:Ap:149:GLU:HB3   | 111:BI:220:THR:HG21 | 1.77                     | 0.67              |
| 21:DJ:31:HIS:CD2    | 21:DJ:33:ASN:H      | 2.13                     | 0.67              |
| 51:Cm:210:ARG:O     | 57:CA:357:A:N6      | 2.26                     | 0.67              |
| 87:AY:180:PRO:HG3   | 87:AY:214:MET:HE1   | 1.75                     | 0.67              |
| 116:BN:113:ARG:NH2  | 116:BN:118:ASN:OD1  | 2.28                     | 0.67              |
| 4:DL:109:VAL:CG1    | 32:CI:234:PHE:HE2   | 2.07                     | 0.67              |
| 7:DO:122:LEU:O      | 7:DO:163:ARG:NH1    | 2.28                     | 0.67              |
| 8:DP:199:LEU:HD12   | 8:DP:206:TYR:CZ     | 2.30                     | 0.67              |
| 16:DC:305:ARG:HH12  | 16:DC:359:GLU:CD    | 2.02                     | 0.67              |
| 34:CK:42:PHE:CE1    | 40:CR:252:GLN:O     | 2.47                     | 0.67              |
| 47:Cg:38:PRO:O      | 47:Cg:57:THR:OG1    | 2.13                     | 0.67              |
| 98:Av:34:GLN:HB3    | 98:Av:36:MET:HE2    | 1.77                     | 0.67              |
| 120:BR:84:ASN:HD21  | 120:BR:86:GLU:HG2   | 1.60                     | 0.67              |
| 1:DA:463:VAL:HG11   | 1:DA:840:TYR:HB3    | 1.75                     | 0.67              |
| 40:CR:314:THR:C     | 46:Cd:279:ARG:CG    | 2.66                     | 0.67              |
| 41:CS:161:ARG:NH1   | 41:CS:170:LEU:HD23  | 2.10                     | 0.67              |
| 104:BB:196:TRP:HZ2  | 104:BB:213:LEU:HD23 | 1.60                     | 0.67              |
| 126:BX:126:LEU:HD13 | 126:BX:131:PHE:HB3  | 1.77                     | 0.67              |
| 2:DD:173:GLN:OE1    | 12:DU:65:TRP:NE1    | 2.28                     | 0.67              |
| 2:DD:449:LEU:HD23   | 2:DD:452:LEU:HD11   | 1.75                     | 0.67              |
| 6:DN:114:GLY:HA3    | 6:DN:130:ASN:OD1    | 1.95                     | 0.67              |
| 12:DU:107:LYS:NZ    | 12:DU:107:LYS:HB3   | 2.10                     | 0.67              |
| 15:DB:189:VAL:HG13  | 17:DE:471:ARG:HG2   | 1.75                     | 0.67              |
| 23:DT:176:ASP:OD1   | 23:DT:176:ASP:N     | 2.25                     | 0.67              |
| 26:DX:89:ARG:HH11   | 26:DX:89:ARG:CG     | 2.08                     | 0.67              |
| 72:A9:72:CYS:HB3    | 72:A9:74:TYR:H      | 1.60                     | 0.67              |
| 79:AP:182:TRP:HE3   | 94:Al:119:VAL:HG11  | 1.57                     | 0.67              |
| 116:BN:128:ARG:HH21 | 136:Bh:34:ARG:NH1   | 1.92                     | 0.67              |
| 1:DA:1134:ILE:HG12  | 54:Cq:70:ALA:HA     | 1.76                     | 0.66              |
| 5:DM:76:ASN:ND2     | 56:Cv:971:LEU:H     | 1.93                     | 0.66              |
| 16:DC:862:PRO:HG2   | 16:DC:865:CYS:HB2   | 1.77                     | 0.66              |
| 19:DG:192:MET:HG3   | 19:DG:214:TYR:CE2   | 2.30                     | 0.66              |
| 29:CE:15:TRP:HA     | 29:CE:18:LYS:HE2    | 1.78                     | 0.66              |
| 66:A2:61:LEU:HD21   | 66:A2:83:ARG:HB3    | 1.77                     | 0.66              |
| 75:Al:54:ARG:NH2    | 122:BT:68:ASN:OD1   | 2.27                     | 0.66              |
| 98:Av:57:GLU:HA     | 98:Av:60:ARG:HG2    | 1.78                     | 0.66              |
| 102:AA:528:A:O2'    | 102:AA:529:U:OP1    | 2.13                     | 0.66              |
| 109:BG:179:PRO:HG3  | 109:BG:225:PRO:HG2  | 1.77                     | 0.66              |
| 112:BJ:198:ALA:HA   | 112:BJ:201:ARG:NH1  | 2.09                     | 0.66              |
| 124:BV:64:LYS:NZ    | 124:BV:66:VAL:HG12  | 2.10                     | 0.66              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 19:DG:111:ARG:CZ   | 45:Cb:197:PRO:CB    | 2.72                     | 0.66              |
| 40:CR:320:VAL:O    | 46:Cd:281:MET:SD    | 2.45                     | 0.66              |
| 117:BO:78:ARG:HH12 | 121:BS:104:ARG:NH1  | 1.94                     | 0.66              |
| 18:DF:288:MET:HE3  | 20:DH:363:PRO:HG3   | 1.77                     | 0.66              |
| 18:DF:425:ILE:HG21 | 20:DH:196:LEU:HD11  | 1.77                     | 0.66              |
| 29:CE:42:ARG:HH11  | 29:CE:42:ARG:HG3    | 1.59                     | 0.66              |
| 34:CK:283:GLY:H    | 34:CK:311:THR:HG23  | 1.60                     | 0.66              |
| 53:Cp:135:THR:HG21 | 53:Cp:139:SER:H     | 1.59                     | 0.66              |
| 84:AV:137:THR:HB   | 84:AV:177:GLU:HG3   | 1.77                     | 0.66              |
| 87:AY:271:TYR:CZ   | 87:AY:275:GLU:HG3   | 2.29                     | 0.66              |
| 102:AA:80:U:H4'    | 102:AA:81:A:H5'     | 1.77                     | 0.66              |
| 102:AA:536:A:N1    | 135:Bg:89:ARG:HB2   | 2.11                     | 0.66              |
| 116:BN:10:GLN:H    | 116:BN:14:HIS:CD2   | 2.11                     | 0.66              |
| 129:Ba:150:ASP:HA  | 129:Ba:152:ARG:NH1  | 2.10                     | 0.66              |
| 136:Bh:42:ARG:HB2  | 140:UD:24:UNK:HG1   | 1.76                     | 0.66              |
| 2:DD:264:LEU:HD12  | 2:DD:272:LYS:HE3    | 1.77                     | 0.66              |
| 6:DN:73:VAL:HG21   | 6:DN:132:TYR:CE1    | 2.31                     | 0.66              |
| 19:DG:77:CYS:O     | 19:DG:108:ARG:NH1   | 2.29                     | 0.66              |
| 35:CL:72:PHE:HB2   | 35:CL:119:PHE:HE1   | 1.60                     | 0.66              |
| 47:Cg:289:ASN:ND2  | 47:Cg:358:THR:H     | 1.93                     | 0.66              |
| 66:A2:345:ILE:HG13 | 66:A2:348:ALA:HB3   | 1.77                     | 0.66              |
| 69:A5:60:CYS:SG    | 148:A5:100:ZN:ZN    | 1.84                     | 0.66              |
| 85:AW:274:THR:HB   | 107:BE:318:ARG:HH22 | 1.59                     | 0.66              |
| 116:BN:215:TRP:NE1 | 123:BU:164:ARG:HE   | 1.92                     | 0.66              |
| 1:DA:70:ARG:NH2    | 57:CA:73:U:OP2      | 2.29                     | 0.66              |
| 6:DN:222:LEU:HD11  | 44:Ca:301:ILE:HD11  | 1.78                     | 0.66              |
| 11:DS:49:VAL:HB    | 44:Ca:600:PRO:HG3   | 1.78                     | 0.66              |
| 15:DB:549:LEU:HD23 | 15:DB:554:GLU:HG2   | 1.78                     | 0.66              |
| 31:CH:229:GLU:HG2  | 31:CH:276:ARG:HD3   | 1.78                     | 0.66              |
| 44:Ca:474:ARG:NH1  | 44:Ca:478:GLY:O     | 2.28                     | 0.66              |
| 45:Cb:56:ARG:HH11  | 45:Cb:57:MET:CE     | 2.09                     | 0.66              |
| 68:A4:107:HIS:HB2  | 89:Ad:148:ARG:HA    | 1.76                     | 0.66              |
| 78:AN:89:LYS:HZ3   | 96:Ap:62:LYS:NZ     | 1.91                     | 0.66              |
| 92:Ag:77:MET:HB2   | 108:BF:347:ASN:HD21 | 1.59                     | 0.66              |
| 3:DI:340:ARG:NH1   | 3:DI:342:ARG:NH1    | 2.43                     | 0.66              |
| 11:DS:57:LEU:HD11  | 11:DS:83:LEU:HD23   | 1.77                     | 0.66              |
| 19:DG:190:GLU:HG3  | 34:CK:54:LEU:HD13   | 1.77                     | 0.66              |
| 23:DT:183:LEU:HB2  | 23:DT:219:GLN:HE22  | 1.61                     | 0.66              |
| 29:CE:22:ARG:HH21  | 29:CE:240:ASP:HB3   | 1.61                     | 0.66              |
| 33:CJ:376:SER:HB2  | 57:CA:452:A:O2'     | 1.95                     | 0.66              |
| 46:Cd:137:ARG:HG2  | 46:Cd:137:ARG:HH11  | 1.59                     | 0.66              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 51:Cm:137:SER:CB    | 57:CA:394:A:H2      | 1.99                     | 0.66              |
| 69:A5:70:CYS:HB2    | 69:A5:75:CYS:SG     | 2.36                     | 0.66              |
| 88:Ab:366:LYS:NZ    | 88:Ab:425:ARG:O     | 2.25                     | 0.66              |
| 88:Ab:492:ARG:HG3   | 119:BQ:215:LEU:HD11 | 1.78                     | 0.66              |
| 124:BV:108:TYR:HA   | 124:BV:111:LYS:NZ   | 2.11                     | 0.66              |
| 8:DP:64:MET:HE1     | 8:DP:68:PRO:HG3     | 1.78                     | 0.66              |
| 23:DT:93:MET:HE1    | 23:DT:102:TRP:NE1   | 2.10                     | 0.66              |
| 33:CJ:548:ASP:OD2   | 33:CJ:553:ARG:NH2   | 2.29                     | 0.66              |
| 77:AK:285:ARG:NH1   | 77:AK:307:ARG:HH21  | 1.91                     | 0.66              |
| 78:AN:59:ALA:HA     | 78:AN:137:GLU:HG3   | 1.76                     | 0.66              |
| 79:AP:222:GLY:N     | 102:AA:172:U:OP2    | 2.20                     | 0.66              |
| 103:BA:324:GLU:HA   | 103:BA:327:ARG:HB2  | 1.78                     | 0.66              |
| 116:BN:128:ARG:NH2  | 136:Bh:34:ARG:HH11  | 1.93                     | 0.66              |
| 2:DD:637:ARG:NH1    | 38:CP:153:ARG:HH11  | 1.94                     | 0.66              |
| 8:DP:199:LEU:HD12   | 8:DP:206:TYR:CE2    | 2.30                     | 0.66              |
| 33:CJ:231:GLU:HG3   | 33:CJ:434:ILE:HD12  | 1.77                     | 0.66              |
| 35:CL:137:ARG:NH2   | 57:CA:265:U:O2      | 2.28                     | 0.66              |
| 88:Ab:84:ASN:HD22   | 88:Ab:140:ARG:HD2   | 1.60                     | 0.66              |
| 91:Af:148:ALA:N     | 103:BA:710:LYS:O    | 2.28                     | 0.66              |
| 93:Aj:53:ARG:HD2    | 93:Aj:174:LEU:HB2   | 1.78                     | 0.66              |
| 97:At:34:ARG:CZ     | 120:BR:127:ARG:NH1  | 2.59                     | 0.66              |
| 108:BF:198:LEU:HD22 | 108:BF:209:ILE:HG22 | 1.77                     | 0.66              |
| 6:DN:237:ARG:NH2    | 44:Ca:350:GLU:OE2   | 2.29                     | 0.66              |
| 40:CR:308:MET:CE    | 57:CA:388:U:C5'     | 2.71                     | 0.66              |
| 85:AW:149:ILE:HD11  | 85:AW:230:LEU:HD13  | 1.78                     | 0.66              |
| 98:Av:232:LYS:H     | 98:Av:232:LYS:HD3   | 1.61                     | 0.66              |
| 114:BL:172:ILE:O    | 114:BL:256:ARG:NH1  | 2.25                     | 0.66              |
| 1:DA:319:ARG:HG2    | 1:DA:319:ARG:HH11   | 1.61                     | 0.66              |
| 3:DI:349:THR:HG23   | 3:DI:350:TYR:HD1    | 1.60                     | 0.66              |
| 8:DP:206:TYR:HE1    | 8:DP:215:LEU:HD13   | 1.61                     | 0.66              |
| 15:DB:881:ARG:HG2   | 15:DB:881:ARG:HH11  | 1.60                     | 0.66              |
| 29:CE:81:LYS:NZ     | 56:Cv:512:MET:O     | 2.26                     | 0.66              |
| 48:Ci:60:SER:HB2    | 48:Ci:69:THR:HG22   | 1.78                     | 0.66              |
| 76:AJ:67:GLN:HA     | 96:Ap:208:ILE:HD12  | 1.77                     | 0.66              |
| 76:AJ:82:ILE:HD11   | 115:BM:275:PHE:CD1  | 2.31                     | 0.66              |
| 81:AR:242:HIS:HD2   | 81:AR:244:SER:H     | 1.43                     | 0.66              |
| 84:AV:122:ARG:HH12  | 91:Af:102:PRO:HA    | 1.58                     | 0.66              |
| 94:Al:71:ASN:HA     | 94:Al:119:VAL:HG13  | 1.78                     | 0.66              |
| 105:BC:75:MET:HB2   | 105:BC:78:LYS:HB2   | 1.78                     | 0.66              |
| 4:DL:68:LEU:C       | 29:CE:112:THR:HG21  | 2.21                     | 0.65              |
| 47:Cg:82:ASN:OD1    | 47:Cg:107:ARG:NH1   | 2.28                     | 0.65              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:Cq:195:VAL:HG23  | 54:Cq:196:HIS:HD2   | 1.61                     | 0.65              |
| 89:Ad:66:ARG:HG2    | 109:BG:268:ARG:HH21 | 1.60                     | 0.65              |
| 1:DA:1179:GLN:HE22  | 54:Cq:147:PRO:HA    | 1.61                     | 0.65              |
| 3:DI:45:LEU:HD13    | 3:DI:158:ARG:HB2    | 1.77                     | 0.65              |
| 17:DE:210:MET:HG3   | 17:DE:426:PHE:HZ    | 1.62                     | 0.65              |
| 31:CH:172:VAL:HG22  | 31:CH:173:PRO:HD2   | 1.77                     | 0.65              |
| 33:CJ:541:LEU:O     | 33:CJ:544:THR:CG2   | 2.44                     | 0.65              |
| 50:Ck:682:ASN:HD22  | 50:Ck:682:ASN:H     | 1.42                     | 0.65              |
| 74:AF:145:SER:OG    | 79:AP:97:LEU:O      | 2.10                     | 0.65              |
| 90:Ae:115:ASN:HB3   | 90:Ae:118:VAL:HG22  | 1.78                     | 0.65              |
| 102:AA:3:U:H5'      | 103:BA:754:ARG:HH12 | 1.61                     | 0.65              |
| 117:BO:101:GLN:HG2  | 117:BO:117:LEU:HD23 | 1.76                     | 0.65              |
| 128:BZ:2:ARG:HH11   | 128:BZ:28:ARG:NE    | 1.95                     | 0.65              |
| 3:DI:88:GLN:O       | 3:DI:92:GLU:HG3     | 1.95                     | 0.65              |
| 40:CR:184:LYS:HB2   | 40:CR:184:LYS:NZ    | 2.11                     | 0.65              |
| 65:A1:71:GLN:HG2    | 129:Ba:98:TRP:CD2   | 2.31                     | 0.65              |
| 88:Ab:192:VAL:HG21  | 88:Ab:199:ASN:HD21  | 1.61                     | 0.65              |
| 95:Ao:230:ARG:NH1   | 95:Ao:242:ASP:HA    | 2.11                     | 0.65              |
| 97:At:19:LEU:HD12   | 147:UU:1:UNK:H2     | 1.61                     | 0.65              |
| 109:BG:74:ARG:HG2   | 109:BG:74:ARG:HH11  | 1.60                     | 0.65              |
| 1:DA:568:SER:OG     | 6:DN:144:ARG:NH1    | 2.29                     | 0.65              |
| 10:DR:128:PRO:HG3   | 10:DR:133:LEU:N     | 2.11                     | 0.65              |
| 16:DC:349:ASP:HB2   | 16:DC:352:GLU:HB2   | 1.78                     | 0.65              |
| 19:DG:236:VAL:HG13  | 19:DG:258:VAL:HG21  | 1.78                     | 0.65              |
| 71:A8:162:ARG:HH22  | 102:AA:72:A:H5''    | 1.61                     | 0.65              |
| 79:AP:324:PRO:O     | 98:Av:147:ASN:ND2   | 2.30                     | 0.65              |
| 86:AX:85:VAL:O      | 129:Ba:28:ARG:NH1   | 2.29                     | 0.65              |
| 92:Ag:202:ARG:NH1   | 92:Ag:202:ARG:HB3   | 2.11                     | 0.65              |
| 96:Ap:294:LYS:NZ    | 102:AA:429:A:N3     | 2.44                     | 0.65              |
| 97:At:34:ARG:CZ     | 120:BR:127:ARG:HH12 | 2.09                     | 0.65              |
| 102:AA:283:A:O2'    | 102:AA:285:A:OP2    | 2.13                     | 0.65              |
| 108:BF:43:LEU:HD13  | 108:BF:252:MET:HG3  | 1.78                     | 0.65              |
| 6:DN:291:PRO:O      | 29:CE:114:TYR:OH    | 2.10                     | 0.65              |
| 39:CQ:198:LEU:O     | 39:CQ:199:ASN:ND2   | 2.30                     | 0.65              |
| 64:A0:66:PRO:HG3    | 64:A0:72:MET:HB2    | 1.77                     | 0.65              |
| 88:Ab:83:GLU:N      | 88:Ab:83:GLU:OE1    | 2.30                     | 0.65              |
| 88:Ab:490:TRP:CD1   | 94:Al:81:GLU:HG2    | 2.31                     | 0.65              |
| 92:Ag:19:SER:HB3    | 108:BF:371:GLU:OE2  | 1.96                     | 0.65              |
| 105:BC:337:VAL:HG11 | 105:BC:359:GLU:HG2  | 1.79                     | 0.65              |
| 119:BQ:53:ILE:HG23  | 119:BQ:54:VAL:HG23  | 1.78                     | 0.65              |
| 4:DL:117:ASP:OD1    | 4:DL:220:ARG:NH2    | 2.29                     | 0.65              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 41:CS:148:MET:HE2  | 41:CS:150:LEU:HB3   | 1.78                     | 0.65              |
| 56:Cv:969:ASP:OD1  | 56:Cv:969:ASP:N     | 2.28                     | 0.65              |
| 68:A4:14:PRO:O     | 118:BP:103:ARG:NH2  | 2.30                     | 0.65              |
| 1:DA:225:GLY:HA3   | 1:DA:233:ARG:NH1    | 2.10                     | 0.65              |
| 1:DA:1113:LEU:HB3  | 1:DA:1145:THR:HG21  | 1.78                     | 0.65              |
| 6:DN:57:ARG:NH2    | 6:DN:70:GLU:OE2     | 2.30                     | 0.65              |
| 8:DP:13:ARG:NH1    | 57:CA:55:U:OP1      | 2.28                     | 0.65              |
| 24:DV:31:HIS:CD2   | 24:DV:82:VAL:HG11   | 2.32                     | 0.65              |
| 45:Cb:289:LYS:NZ   | 55:Cr:177:LEU:O     | 2.19                     | 0.65              |
| 102:AA:380:G:C6    | 147:UU:5:UNK:HG3    | 2.31                     | 0.65              |
| 102:AA:561:U:P     | 126:BX:154:ARG:HH22 | 2.18                     | 0.65              |
| 113:BK:384:ARG:HG2 | 113:BK:385:PRO:HD2  | 1.78                     | 0.65              |
| 124:BV:108:TYR:HA  | 124:BV:111:LYS:HZ3  | 1.61                     | 0.65              |
| 1:DA:1662:ARG:HH22 | 29:CE:402:ARG:HH12  | 1.45                     | 0.65              |
| 52:Cn:178:LYS:HE3  | 52:Cn:182:PHE:HE2   | 1.62                     | 0.65              |
| 56:Cv:286:THR:HG21 | 56:Cv:402:ALA:HB1   | 1.78                     | 0.65              |
| 64:A0:41:THR:HG23  | 115:BM:79:ALA:HB2   | 1.78                     | 0.65              |
| 84:AV:128:ARG:O    | 84:AV:130:LEU:N     | 2.29                     | 0.65              |
| 85:AW:142:TRP:CD1  | 85:AW:205:PRO:HA    | 2.31                     | 0.65              |
| 6:DN:57:ARG:HG3    | 6:DN:66:GLY:HA3     | 1.78                     | 0.65              |
| 9:DQ:217:GLN:HB3   | 9:DQ:221:LEU:HD12   | 1.78                     | 0.65              |
| 21:DJ:113:ASP:HB3  | 21:DJ:116:THR:HB    | 1.79                     | 0.65              |
| 33:CJ:698:HIS:CB   | 36:CN:65:LYS:HZ1    | 2.07                     | 0.65              |
| 38:CP:23:ALA:HB2   | 38:CP:51:HIS:CE1    | 2.32                     | 0.65              |
| 40:CR:310:PHE:HZ   | 57:CA:588:U:O4      | 1.75                     | 0.65              |
| 47:Cg:276:GLU:O    | 47:Cg:350:ASN:ND2   | 2.30                     | 0.65              |
| 64:A0:139:GLU:OE2  | 115:BM:212:ARG:NH1  | 2.30                     | 0.65              |
| 71:A8:147:ILE:HD12 | 79:AP:165:ARG:HH12  | 1.61                     | 0.65              |
| 114:BL:105:SER:HA  | 114:BL:179:ASP:OD2  | 1.96                     | 0.65              |
| 116:BN:168:SER:HA  | 116:BN:172:SER:HB3  | 1.79                     | 0.65              |
| 132:Bd:10:ALA:HB2  | 132:Bd:79:ALA:HB2   | 1.77                     | 0.65              |
| 136:Bh:47:SER:HB3  | 136:Bh:67:THR:HG21  | 1.77                     | 0.65              |
| 6:DN:29:ARG:HG3    | 6:DN:29:ARG:NH1     | 2.12                     | 0.65              |
| 8:DP:189:TYR:CG    | 8:DP:197:TYR:HB3    | 2.31                     | 0.65              |
| 23:DT:16:HIS:HA    | 23:DT:28:GLU:OE2    | 1.97                     | 0.65              |
| 74:AF:120:LEU:HD22 | 74:AF:255:LEU:HD11  | 1.79                     | 0.65              |
| 81:AR:49:GLY:HA3   | 81:AR:54:LYS:HD2    | 1.79                     | 0.65              |
| 88:Ab:292:VAL:HG11 | 88:Ab:320:ILE:HB    | 1.79                     | 0.65              |
| 124:BV:64:LYS:HZ2  | 124:BV:66:VAL:HG12  | 1.62                     | 0.65              |
| 132:Bd:16:HIS:HA   | 132:Bd:19:MET:HE2   | 1.79                     | 0.65              |
| 12:DU:147:LEU:CD2  | 12:DU:152:ILE:HD12  | 2.26                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:511:ARG:HG3  | 15:DB:511:ARG:NH1  | 2.06                     | 0.64              |
| 16:DC:87:MET:HE3   | 16:DC:90:GLY:HA2   | 1.78                     | 0.64              |
| 22:DK:36:ARG:NH1   | 22:DK:106:SER:HB3  | 2.12                     | 0.64              |
| 29:CE:42:ARG:HG3   | 29:CE:105:GLN:HE22 | 1.62                     | 0.64              |
| 34:CK:26:ARG:HB2   | 57:CA:460:U:H5     | 1.63                     | 0.64              |
| 44:Ca:521:GLN:HG2  | 44:Ca:564:ARG:HH22 | 1.61                     | 0.64              |
| 77:AK:244:ARG:NH1  | 77:AK:314:ARG:NH1  | 2.45                     | 0.64              |
| 119:BQ:152:ASP:OD1 | 119:BQ:152:ASP:N   | 2.29                     | 0.64              |
| 8:DP:90:LEU:HD13   | 8:DP:127:ASP:HB3   | 1.78                     | 0.64              |
| 15:DB:276:VAL:O    | 15:DB:486:HIS:HE1  | 1.80                     | 0.64              |
| 20:DH:504:ARG:NH1  | 22:DK:287:ILE:HG23 | 2.12                     | 0.64              |
| 32:CI:89:ARG:HD2   | 34:CK:114:MET:HE2  | 1.80                     | 0.64              |
| 66:A2:181:VAL:HG21 | 66:A2:320:GLY:HA3  | 1.79                     | 0.64              |
| 87:AY:148:VAL:HG22 | 87:AY:167:GLU:HG3  | 1.80                     | 0.64              |
| 109:BG:47:TRP:HA   | 109:BG:50:ARG:HH21 | 1.62                     | 0.64              |
| 1:DA:195:MET:HE3   | 1:DA:198:ARG:HH11  | 1.62                     | 0.64              |
| 6:DN:224:ARG:HB3   | 6:DN:224:ARG:HH11  | 1.61                     | 0.64              |
| 7:DO:86:ARG:NH2    | 7:DO:126:PRO:HG2   | 2.13                     | 0.64              |
| 12:DU:207:ARG:HD3  | 57:CA:161:G:O6     | 1.98                     | 0.64              |
| 33:CJ:436:ARG:NH2  | 50:Ck:671:PRO:HB2  | 2.12                     | 0.64              |
| 50:Ck:644:HIS:HD2  | 50:Ck:669:ASN:H    | 1.46                     | 0.64              |
| 53:Cp:162:LEU:HD12 | 53:Cp:163:PRO:HD2  | 1.79                     | 0.64              |
| 53:Cp:163:PRO:HG2  | 53:Cp:165:TYR:HE1  | 1.62                     | 0.64              |
| 81:AR:153:ARG:NH2  | 102:AA:515:U:O4    | 2.30                     | 0.64              |
| 105:BC:176:GLU:HG2 | 105:BC:185:ARG:HD2 | 1.80                     | 0.64              |
| 116:BN:51:ILE:HG22 | 123:BU:182:GLU:OE2 | 1.97                     | 0.64              |
| 11:DS:108:ASN:OD1  | 11:DS:108:ASN:N    | 2.30                     | 0.64              |
| 56:Cv:692:LYS:HD3  | 56:Cv:732:LEU:HD22 | 1.80                     | 0.64              |
| 85:AW:212:ILE:HG12 | 85:AW:222:TRP:CZ3  | 2.33                     | 0.64              |
| 120:BR:40:ARG:NH1  | 120:BR:95:ARG:HH12 | 1.94                     | 0.64              |
| 136:Bh:7:PHE:HE1   | 136:Bh:42:ARG:HB3  | 1.62                     | 0.64              |
| 2:DD:777:GLY:O     | 44:Ca:332:ARG:NH2  | 2.27                     | 0.64              |
| 4:DL:116:ASN:C     | 4:DL:120:PHE:CD2   | 2.69                     | 0.64              |
| 8:DP:199:LEU:HD21  | 8:DP:204:ASN:HA    | 1.79                     | 0.64              |
| 8:DP:200:SER:HB3   | 8:DP:203:ASP:HB2   | 1.80                     | 0.64              |
| 10:DR:67:LYS:HA    | 10:DR:67:LYS:NZ    | 2.11                     | 0.64              |
| 33:CJ:544:THR:CG2  | 33:CJ:552:ILE:CG1  | 2.45                     | 0.64              |
| 41:CS:100:VAL:HG21 | 41:CS:104:GLN:NE2  | 2.11                     | 0.64              |
| 46:Cd:194:VAL:HG12 | 46:Cd:195:GLU:HG3  | 1.78                     | 0.64              |
| 69:A5:42:LEU:HD22  | 103:BA:226:LYS:HA  | 1.78                     | 0.64              |
| 71:A8:172:LYS:HZ2  | 79:AP:259:HIS:HD2  | 1.46                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 79:AP:322:LYS:HG2   | 79:AP:323:PRO:HD2   | 1.79                     | 0.64              |
| 85:AW:207:PRO:HB3   | 107:BE:42:GLY:HA3   | 1.79                     | 0.64              |
| 88:Ab:84:ASN:ND2    | 88:Ab:140:ARG:HD2   | 2.13                     | 0.64              |
| 96:Ap:237:LEU:HB3   | 96:Ap:275:ARG:HH21  | 1.62                     | 0.64              |
| 107:BE:73:THR:HG23  | 107:BE:74:TYR:H     | 1.63                     | 0.64              |
| 113:BK:87:LEU:HD23  | 113:BK:140:LEU:HD13 | 1.78                     | 0.64              |
| 3:DI:313:ARG:HH11   | 3:DI:407:LEU:C      | 2.06                     | 0.64              |
| 9:DQ:171:GLU:OE2    | 39:CQ:172:ARG:NH1   | 2.31                     | 0.64              |
| 15:DB:885:PHE:HE2   | 15:DB:929:MET:HE2   | 1.63                     | 0.64              |
| 16:DC:871:GLN:HG3   | 17:DE:67:ASN:HD21   | 1.62                     | 0.64              |
| 16:DC:952:GLU:H     | 16:DC:952:GLU:CD    | 2.06                     | 0.64              |
| 18:DF:426:LEU:N     | 20:DH:200:THR:HG23  | 2.13                     | 0.64              |
| 33:CJ:27:PRO:CB     | 51:Cm:28:GLN:HE22   | 2.11                     | 0.64              |
| 49:Cj:138:ASP:OD1   | 49:Cj:138:ASP:N     | 2.31                     | 0.64              |
| 51:Cm:171:ALA:HB1   | 56:Cv:54:ASN:HB3    | 1.78                     | 0.64              |
| 65:A1:113:VAL:HG11  | 65:A1:160:ILE:HG23  | 1.80                     | 0.64              |
| 76:AJ:72:GLU:OE1    | 76:AJ:89:ARG:NH2    | 2.30                     | 0.64              |
| 91:Af:147:VAL:HG11  | 103:BA:674:LEU:HD11 | 1.79                     | 0.64              |
| 111:BI:97:CYS:HB3   | 111:BI:135:HIS:CE1  | 2.33                     | 0.64              |
| 18:DF:27:ARG:NH1    | 57:CA:435:G:O2'     | 2.31                     | 0.64              |
| 18:DF:57:ARG:HG2    | 18:DF:57:ARG:NH1    | 2.06                     | 0.64              |
| 39:CQ:57:HIS:O      | 57:CA:97:U:O2'      | 2.16                     | 0.64              |
| 86:AX:191:ARG:HD3   | 86:AX:193:ARG:HH21  | 1.62                     | 0.64              |
| 105:BC:497:GLU:OE1  | 105:BC:497:GLU:N    | 2.28                     | 0.64              |
| 106:BD:388:LYS:O    | 106:BD:389:VAL:CB   | 2.46                     | 0.64              |
| 108:BF:213:LEU:HD11 | 108:BF:236:ALA:HB2  | 1.77                     | 0.64              |
| 110:BH:261:GLU:HA   | 110:BH:264:SER:HB2  | 1.80                     | 0.64              |
| 116:BN:23:GLY:N     | 116:BN:191:ARG:HH12 | 1.96                     | 0.64              |
| 127:BY:85:TRP:HB2   | 139:UC:8:UNK:HG1    | 1.78                     | 0.64              |
| 1:DA:150:ILE:HG12   | 1:DA:151:PRO:HD2    | 1.80                     | 0.64              |
| 2:DD:357:TRP:O      | 2:DD:626:ARG:NH2    | 2.31                     | 0.64              |
| 4:DL:85:PHE:N       | 32:CI:270:PHE:HZ    | 1.96                     | 0.64              |
| 18:DF:262:PHE:O     | 21:DJ:90:ARG:NH2    | 2.30                     | 0.64              |
| 19:DG:50:LEU:HD12   | 32:CI:245:ARG:NH1   | 2.12                     | 0.64              |
| 19:DG:401:CYS:N     | 19:DG:454:ASP:OD2   | 2.30                     | 0.64              |
| 21:DJ:132:ARG:NH1   | 21:DJ:171:LYS:O     | 2.31                     | 0.64              |
| 25:DW:87:ASN:HD21   | 25:DW:158:PRO:HB3   | 1.63                     | 0.64              |
| 46:Cd:139:SER:O     | 46:Cd:143:GLN:HG2   | 1.97                     | 0.64              |
| 56:Cv:1042:ARG:HH21 | 56:Cv:1046:ASN:HB2  | 1.63                     | 0.64              |
| 78:AN:103:ILE:HD11  | 78:AN:118:LEU:HD23  | 1.80                     | 0.64              |
| 84:AV:56:ALA:N      | 84:AV:58:GLY:H      | 1.95                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 102:AA:518:A:OP2    | 102:AA:567:G:N2     | 2.30                     | 0.64              |
| 103:BA:296:ARG:NH2  | 103:BA:309:THR:HG21 | 2.12                     | 0.64              |
| 103:BA:791:PHE:HE2  | 103:BA:796:LEU:HG   | 1.63                     | 0.64              |
| 115:BM:120:GLN:OE1  | 115:BM:139:GLN:NE2  | 2.27                     | 0.64              |
| 117:BO:188:ALA:HB2  | 117:BO:213:ALA:HB1  | 1.80                     | 0.64              |
| 133:Be:70:HIS:HD2   | 133:Be:72:HIS:H     | 1.44                     | 0.64              |
| 6:DN:118:LEU:HD22   | 6:DN:129:LEU:HD11   | 1.79                     | 0.64              |
| 10:DR:93:PRO:HB2    | 10:DR:96:PHE:HD2    | 1.63                     | 0.64              |
| 16:DC:381:LEU:O     | 16:DC:385:THR:OG1   | 2.05                     | 0.64              |
| 19:DG:472:ARG:HH11  | 19:DG:472:ARG:CG    | 2.11                     | 0.64              |
| 32:CI:89:ARG:NH1    | 34:CK:117:GLU:OE2   | 2.30                     | 0.64              |
| 33:CJ:541:LEU:HA    | 33:CJ:552:ILE:HG13  | 1.80                     | 0.64              |
| 34:CK:188:TYR:HA    | 34:CK:192:MET:HE3   | 1.80                     | 0.64              |
| 79:AP:163:ARG:HG2   | 79:AP:163:ARG:NH1   | 2.06                     | 0.64              |
| 81:AR:154:ARG:HD2   | 107:BE:400:GLY:O    | 1.98                     | 0.64              |
| 107:BE:375:PRO:HG2  | 107:BE:378:LEU:HB2  | 1.79                     | 0.64              |
| 117:BO:78:ARG:NH1   | 121:BS:104:ARG:HH12 | 1.96                     | 0.64              |
| 1:DA:151:PRO:HG3    | 2:DD:280:LEU:HD21   | 1.80                     | 0.64              |
| 2:DD:312:GLN:HE22   | 2:DD:440:ARG:NH1    | 1.96                     | 0.64              |
| 15:DB:1030:ARG:HH11 | 15:DB:1030:ARG:CG   | 2.09                     | 0.64              |
| 68:A4:52:THR:O      | 68:A4:56:GLN:NE2    | 2.31                     | 0.64              |
| 112:BJ:320:ARG:NH1  | 112:BJ:324:MET:HE3  | 2.13                     | 0.64              |
| 2:DD:626:ARG:HD3    | 2:DD:627:TYR:CZ     | 2.33                     | 0.63              |
| 7:DO:186:MET:HE1    | 46:Cd:132:PHE:HD2   | 1.62                     | 0.63              |
| 10:DR:100:ARG:HH12  | 10:DR:122:ALA:CB    | 2.11                     | 0.63              |
| 11:DS:225:GLU:HB3   | 11:DS:229:ARG:NH1   | 2.13                     | 0.63              |
| 21:DJ:232:ARG:HD3   | 57:CA:427:U:H3'     | 1.78                     | 0.63              |
| 25:DW:127:PHE:CA    | 40:CR:287:MET:HE3   | 2.09                     | 0.63              |
| 34:CK:315:LEU:O     | 56:Cv:175:ARG:NH1   | 2.31                     | 0.63              |
| 68:A4:50:ARG:HD3    | 98:Av:188:GLU:OE2   | 1.98                     | 0.63              |
| 81:AR:226:ARG:HG2   | 81:AR:246:VAL:HG21  | 1.78                     | 0.63              |
| 87:AY:193:VAL:HG22  | 113:BK:326:VAL:HG22 | 1.80                     | 0.63              |
| 104:BB:83:ASN:O     | 104:BB:87:LEU:HB2   | 1.97                     | 0.63              |
| 113:BK:322:ASP:OD1  | 113:BK:323:VAL:N    | 2.30                     | 0.63              |
| 12:DU:147:LEU:HD22  | 12:DU:152:ILE:HD12  | 1.80                     | 0.63              |
| 16:DC:635:MET:O     | 16:DC:652:ARG:NH2   | 2.30                     | 0.63              |
| 33:CJ:713:PRO:HB3   | 57:CA:507:A:C2      | 2.33                     | 0.63              |
| 39:CQ:105:LYS:H     | 39:CQ:137:LEU:HD21  | 1.62                     | 0.63              |
| 54:Cq:64:VAL:HG11   | 54:Cq:77:PHE:CD2    | 2.33                     | 0.63              |
| 66:A2:126:PRO:O     | 128:BZ:84:GLN:NE2   | 2.32                     | 0.63              |
| 83:AU:75:THR:HG21   | 91:Af:77:VAL:HG13   | 1.80                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 99:AB:40:ALA:HB3   | 101:AG:72:ALA:HA   | 1.80                     | 0.63              |
| 102:AA:579:U:O4    | 102:AA:580:A:N6    | 2.31                     | 0.63              |
| 103:BA:799:ASP:OD1 | 103:BA:801:ARG:NH1 | 2.31                     | 0.63              |
| 114:BL:281:SER:OG  | 114:BL:284:ARG:NH1 | 2.32                     | 0.63              |
| 118:BP:60:HIS:HD1  | 118:BP:60:HIS:H    | 1.44                     | 0.63              |
| 120:BR:66:GLY:HA2  | 120:BR:82:GLU:HA   | 1.79                     | 0.63              |
| 1:DA:112:GLN:HG2   | 1:DA:131:ASP:CG    | 2.24                     | 0.63              |
| 2:DD:247:VAL:HG12  | 2:DD:250:LYS:HZ2   | 1.62                     | 0.63              |
| 4:DL:63:ASP:CG     | 51:Cm:21:GLN:CG    | 2.55                     | 0.63              |
| 15:DB:1065:ASP:OD2 | 33:CJ:437:ARG:NH2  | 2.31                     | 0.63              |
| 18:DF:358:MET:HG2  | 18:DF:368:ILE:HB   | 1.79                     | 0.63              |
| 19:DG:324:LEU:HD23 | 19:DG:361:SER:HB2  | 1.79                     | 0.63              |
| 19:DG:628:LEU:O    | 47:Cg:124:LYS:NZ   | 2.30                     | 0.63              |
| 33:CJ:541:LEU:HD13 | 33:CJ:551:ARG:HE   | 1.63                     | 0.63              |
| 76:AJ:94:LEU:O     | 76:AJ:98:THR:OG1   | 2.16                     | 0.63              |
| 87:AY:233:PRO:HG2  | 87:AY:236:ASP:OD2  | 1.97                     | 0.63              |
| 4:DL:176:ARG:HE    | 45:Cb:79:PRO:HA    | 1.63                     | 0.63              |
| 10:DR:128:PRO:CD   | 10:DR:133:LEU:C    | 2.69                     | 0.63              |
| 27:DY:69:HIS:C     | 40:CR:265:ARG:NH1  | 2.51                     | 0.63              |
| 33:CJ:460:HIS:O    | 33:CJ:465:SER:OG   | 2.15                     | 0.63              |
| 40:CR:167:ARG:NH1  | 57:CA:317:U:O4     | 2.31                     | 0.63              |
| 40:CR:317:ILE:HA   | 46:Cd:283:GLU:OE1  | 1.98                     | 0.63              |
| 45:Cb:303:GLU:C    | 55:Cr:105:ARG:HH12 | 2.06                     | 0.63              |
| 83:AU:200:GLU:OE2  | 108:BF:154:LYS:HD3 | 1.98                     | 0.63              |
| 107:BE:306:GLN:HG3 | 107:BE:307:PRO:HD3 | 1.81                     | 0.63              |
| 116:BN:193:PHE:HE2 | 140:UD:222:UNK:HG1 | 1.63                     | 0.63              |
| 119:BQ:219:PRO:HG2 | 119:BQ:224:LEU:HG  | 1.80                     | 0.63              |
| 122:BT:32:THR:OG1  | 122:BT:33:ASN:N    | 2.31                     | 0.63              |
| 4:DL:92:ILE:HG23   | 32:CI:248:PHE:CA   | 2.28                     | 0.63              |
| 15:DB:139:LEU:HD11 | 15:DB:219:GLU:HG2  | 1.79                     | 0.63              |
| 15:DB:1133:PRO:HA  | 15:DB:1137:MET:HB2 | 1.80                     | 0.63              |
| 18:DF:589:GLN:HB3  | 20:DH:192:PHE:CE1  | 2.33                     | 0.63              |
| 19:DG:244:GLU:HG2  | 19:DG:251:ARG:HG3  | 1.80                     | 0.63              |
| 50:Ck:188:LEU:HD11 | 50:Ck:224:LYS:HB3  | 1.81                     | 0.63              |
| 55:Cr:22:LEU:HD22  | 55:Cr:90:ILE:HD13  | 1.80                     | 0.63              |
| 71:A8:147:ILE:HD12 | 79:AP:165:ARG:NH1  | 2.13                     | 0.63              |
| 74:AF:137:MET:HE3  | 74:AF:224:ARG:NH1  | 2.13                     | 0.63              |
| 77:AK:230:GLN:HG3  | 77:AK:319:GLU:OE2  | 1.98                     | 0.63              |
| 117:BO:77:ALA:HA   | 121:BS:32:ARG:NH1  | 2.12                     | 0.63              |
| 17:DE:246:ILE:HG13 | 17:DE:423:PHE:CG   | 2.34                     | 0.63              |
| 20:DH:28:ASN:HD21  | 21:DJ:42:HIS:CE1   | 2.16                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 31:CH:106:THR:HG23 | 56:Cv:107:LEU:HD11  | 1.79                     | 0.63              |
| 45:Cb:12:PRO:HG2   | 45:Cb:15:MET:CG     | 2.28                     | 0.63              |
| 49:Cj:124:GLY:O    | 49:Cj:207:LYS:NZ    | 2.24                     | 0.63              |
| 50:Ck:167:PHE:HE2  | 50:Ck:235:GLY:HA2   | 1.63                     | 0.63              |
| 56:Cv:1042:ARG:NH2 | 56:Cv:1046:ASN:HB2  | 2.13                     | 0.63              |
| 65:A1:142:LYS:HB3  | 65:A1:142:LYS:NZ    | 2.14                     | 0.63              |
| 66:A2:426:LEU:O    | 87:AY:166:ARG:NH2   | 2.29                     | 0.63              |
| 74:AF:182:MET:HB3  | 74:AF:184:MET:HG3   | 1.80                     | 0.63              |
| 76:AJ:82:ILE:HD11  | 115:BM:275:PHE:HD1  | 1.63                     | 0.63              |
| 88:Ab:280:MET:HB3  | 88:Ab:328:VAL:HB    | 1.80                     | 0.63              |
| 92:Ag:131:GLN:O    | 92:Ag:134:ARG:HD2   | 1.99                     | 0.63              |
| 98:Av:74:GLN:OE1   | 98:Av:74:GLN:N      | 2.28                     | 0.63              |
| 10:DR:269:TRP:H    | 49:Cj:126:TYR:HB2   | 1.64                     | 0.63              |
| 12:DU:142:ASP:HB2  | 12:DU:145:LYS:HG2   | 1.79                     | 0.63              |
| 26:DX:164:THR:HG22 | 26:DX:167:HIS:HB2   | 1.80                     | 0.63              |
| 30:CF:129:ASN:HB3  | 40:CR:125:ASN:ND2   | 2.12                     | 0.63              |
| 68:A4:21:PRO:HG3   | 105:BC:211:TRP:CD1  | 2.34                     | 0.63              |
| 71:A8:172:LYS:NZ   | 79:AP:259:HIS:CD2   | 2.61                     | 0.63              |
| 79:AP:12:ARG:HH21  | 97:At:33:LYS:HD2    | 1.63                     | 0.63              |
| 93:Aj:36:VAL:HG22  | 93:Aj:196:ARG:HE    | 1.64                     | 0.63              |
| 103:BA:134:MET:HB2 | 117:BO:145:LEU:HD13 | 1.81                     | 0.63              |
| 104:BB:392:TYR:HD2 | 104:BB:393:LEU:HD12 | 1.64                     | 0.63              |
| 109:BG:53:GLY:HA3  | 109:BG:56:ARG:NH1   | 2.14                     | 0.63              |
| 118:BP:38:LEU:HD23 | 118:BP:38:LEU:H     | 1.64                     | 0.63              |
| 125:BW:56:ASN:H    | 125:BW:65:ASN:ND2   | 1.97                     | 0.63              |
| 17:DE:147:MET:HE1  | 17:DE:567:HIS:CD2   | 2.34                     | 0.63              |
| 18:DF:57:ARG:HH11  | 18:DF:57:ARG:CG     | 2.08                     | 0.63              |
| 24:DV:107:ILE:HG12 | 33:CJ:754:VAL:HG22  | 1.80                     | 0.63              |
| 35:CL:122:GLU:HG3  | 57:CA:266:A:H4'     | 1.81                     | 0.63              |
| 86:AX:66:ARG:HH11  | 61:UX:8:UNK:HG1     | 1.62                     | 0.63              |
| 88:Ab:115:PRO:O    | 88:Ab:201:TRP:NE1   | 2.32                     | 0.63              |
| 89:Ad:56:LYS:HE3   | 93:Aj:78:ARG:NH1    | 2.14                     | 0.63              |
| 95:Ao:127:SER:HB3  | 119:BQ:188:ARG:HH22 | 1.63                     | 0.63              |
| 103:BA:791:PHE:CE2 | 103:BA:796:LEU:HG   | 2.34                     | 0.63              |
| 1:DA:1013:SER:O    | 4:DL:68:LEU:HD21    | 1.89                     | 0.63              |
| 2:DD:431:LEU:HD11  | 2:DD:469:GLY:HA3    | 1.81                     | 0.63              |
| 11:DS:33:LEU:HG    | 11:DS:35:TYR:HB2    | 1.81                     | 0.63              |
| 18:DF:5:GLY:HA3    | 48:Ci:159:SER:HB3   | 1.81                     | 0.63              |
| 19:DG:192:MET:HG3  | 19:DG:214:TYR:HE2   | 1.64                     | 0.63              |
| 33:CJ:275:ILE:HD13 | 33:CJ:412:PHE:HB2   | 1.81                     | 0.63              |
| 38:CP:23:ALA:CB    | 38:CP:51:HIS:CD2    | 2.73                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 50:Ck:568:LEU:HD12  | 50:Ck:569:GLY:H     | 1.64                     | 0.63              |
| 74:AF:165:GLU:HB2   | 74:AF:203:PRO:HG3   | 1.80                     | 0.63              |
| 90:Ae:75:ARG:NH1    | 90:Ae:135:THR:HG22  | 2.11                     | 0.63              |
| 91:Af:105:GLU:H     | 91:Af:105:GLU:CD    | 2.07                     | 0.63              |
| 3:DI:296:ASN:HA     | 3:DI:334:ILE:HD11   | 1.81                     | 0.62              |
| 4:DL:117:ASP:O      | 4:DL:121:ILE:CB     | 2.47                     | 0.62              |
| 9:DQ:31:PRO:HG2     | 57:CA:85:U:H4'      | 1.81                     | 0.62              |
| 15:DB:214:ARG:NE    | 17:DE:539:ARG:HH12  | 1.96                     | 0.62              |
| 15:DB:560:THR:HG23  | 18:DF:548:ARG:NH1   | 2.14                     | 0.62              |
| 21:DJ:71:MET:HE1    | 21:DJ:75:PHE:HB2    | 1.80                     | 0.62              |
| 27:DY:39:VAL:HG21   | 47:Cg:461:GLN:HG2   | 1.81                     | 0.62              |
| 30:CF:2:VAL:HG13    | 30:CF:37:ARG:HD2    | 1.81                     | 0.62              |
| 40:CR:308:MET:HE2   | 57:CA:388:U:H4'     | 1.61                     | 0.62              |
| 56:Cv:531:MET:HE3   | 56:Cv:531:MET:H     | 1.63                     | 0.62              |
| 57:CA:518:G:H4'     | 57:CA:519:U:H5''    | 1.80                     | 0.62              |
| 130:Bb:79:HIS:HD2   | 130:Bb:81:HIS:HB2   | 1.63                     | 0.62              |
| 2:DD:247:VAL:HG12   | 2:DD:250:LYS:NZ     | 2.13                     | 0.62              |
| 5:DM:10:ARG:HH12    | 29:CE:325:LEU:HB2   | 1.62                     | 0.62              |
| 5:DM:45:ARG:HG3     | 5:DM:45:ARG:NH1     | 2.11                     | 0.62              |
| 19:DG:206:LEU:N     | 19:DG:234:GLU:OE2   | 2.31                     | 0.62              |
| 19:DG:624:ARG:HG2   | 24:DV:183:LEU:HD12  | 1.81                     | 0.62              |
| 29:CE:308:ARG:C     | 29:CE:311:LYS:NZ    | 2.57                     | 0.62              |
| 66:A2:25:LYS:HB3    | 66:A2:25:LYS:HZ3    | 1.64                     | 0.62              |
| 74:AF:214:MET:HE2   | 74:AF:219:TRP:HE3   | 1.63                     | 0.62              |
| 115:BM:223:THR:HG22 | 115:BM:224:THR:H    | 1.64                     | 0.62              |
| 16:DC:46:ARG:HH11   | 16:DC:475:LEU:HB3   | 1.64                     | 0.62              |
| 51:Cm:202:THR:HG23  | 57:CA:338:U:H3      | 1.64                     | 0.62              |
| 56:Cv:681:HIS:NE2   | 56:Cv:695:SER:OG    | 2.33                     | 0.62              |
| 73:AE:315:ARG:NH2   | 82:AT:36:GLU:OE1    | 2.32                     | 0.62              |
| 76:AJ:53:TYR:OH     | 76:AJ:55:ARG:NH2    | 2.31                     | 0.62              |
| 85:AW:275:ALA:HB2   | 107:BE:243:THR:HG21 | 1.81                     | 0.62              |
| 88:Ab:88:THR:HG22   | 88:Ab:208:ASN:HA    | 1.80                     | 0.62              |
| 105:BC:237:PRO:HA   | 105:BC:240:LYS:HD2  | 1.81                     | 0.62              |
| 6:DN:73:VAL:CG1     | 6:DN:112:ILE:CD1    | 2.74                     | 0.62              |
| 15:DB:1154:LYS:HZ2  | 89:Ad:150:ARG:HE    | 1.46                     | 0.62              |
| 18:DF:6:VAL:HG11    | 36:CN:10:MET:HE2    | 1.81                     | 0.62              |
| 33:CJ:374:TRP:CZ3   | 36:CN:106:GLU:HB3   | 2.35                     | 0.62              |
| 40:CR:316:GLY:O     | 46:Cd:279:ARG:HB2   | 1.97                     | 0.62              |
| 41:CS:48:ARG:HG3    | 41:CS:48:ARG:NH1    | 2.14                     | 0.62              |
| 42:CU:77:ARG:HH11   | 56:Cv:175:ARG:HH22  | 1.45                     | 0.62              |
| 56:Cv:408:THR:HG21  | 56:Cv:422:SER:HA    | 1.80                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:A2:102:ASP:OD1   | 87:AY:255:ARG:NH2   | 2.30                     | 0.62              |
| 73:AE:166:PRO:HG3   | 73:AE:190:MET:HG2   | 1.81                     | 0.62              |
| 81:AR:172:ASP:OD1   | 81:AR:173:ASN:N     | 2.31                     | 0.62              |
| 102:AA:527:U:O2'    | 102:AA:548:A:N6     | 2.22                     | 0.62              |
| 117:BO:78:ARG:NH1   | 121:BS:104:ARG:NH1  | 2.46                     | 0.62              |
| 1:DA:466:VAL:HG11   | 56:Cv:1067:LEU:HD22 | 1.81                     | 0.62              |
| 10:DR:127:VAL:HG22  | 10:DR:134:LEU:CD2   | 2.29                     | 0.62              |
| 13:DZ:39:ASN:ND2    | 57:CA:225:A:OP1     | 2.26                     | 0.62              |
| 15:DB:1154:LYS:HZ3  | 89:Ad:150:ARG:CZ    | 2.12                     | 0.62              |
| 16:DC:119:THR:HG21  | 16:DC:136:TRP:HE1   | 1.65                     | 0.62              |
| 29:CE:308:ARG:HA    | 29:CE:311:LYS:HZ2   | 1.61                     | 0.62              |
| 43:CZ:282:ALA:HB1   | 43:CZ:321:MET:HG3   | 1.79                     | 0.62              |
| 56:Cv:204:ILE:HD12  | 56:Cv:209:VAL:HG11  | 1.82                     | 0.62              |
| 95:Ao:155:GLU:O     | 115:BM:229:TYR:OH   | 2.14                     | 0.62              |
| 140:UD:65:UNK:HB1   | 140:UD:67:UNK:HG2   | 1.82                     | 0.62              |
| 6:DN:10:PHE:HE1     | 6:DN:12:MET:HE2     | 1.61                     | 0.62              |
| 8:DP:70:TRP:CD2     | 12:DU:182:GLU:HG2   | 2.35                     | 0.62              |
| 9:DQ:105:PRO:HG2    | 9:DQ:221:LEU:HD21   | 1.81                     | 0.62              |
| 17:DE:229:ARG:NH1   | 17:DE:255:PHE:CE1   | 2.68                     | 0.62              |
| 45:Cb:301:THR:HG22  | 55:Cr:180:TRP:HH2   | 1.65                     | 0.62              |
| 74:AF:65:ASN:HD22   | 125:BW:174:ILE:HD11 | 1.64                     | 0.62              |
| 89:Ad:221:GLN:HE22  | 132:Bd:47:ARG:HE    | 1.48                     | 0.62              |
| 105:BC:325:ALA:HB1  | 105:BC:336:LEU:HD11 | 1.82                     | 0.62              |
| 108:BF:161:PRO:O    | 108:BF:167:ARG:NH1  | 2.32                     | 0.62              |
| 120:BR:134:LYS:HE3  | 120:BR:138:GLN:HE21 | 1.64                     | 0.62              |
| 123:BU:139:ARG:HH11 | 135:Bg:35:LEU:CD2   | 2.10                     | 0.62              |
| 4:DL:65:PRO:HG2     | 29:CE:133:ARG:NH2   | 2.14                     | 0.62              |
| 11:DS:166:THR:HG21  | 11:DS:194:GLU:HG3   | 1.82                     | 0.62              |
| 12:DU:147:LEU:HD22  | 12:DU:152:ILE:CD1   | 2.30                     | 0.62              |
| 18:DF:589:GLN:OE1   | 20:DH:192:PHE:CZ    | 2.53                     | 0.62              |
| 20:DH:253:SER:HB2   | 20:DH:287:GLY:HA3   | 1.81                     | 0.62              |
| 29:CE:400:LEU:O     | 29:CE:404:GLY:N     | 2.32                     | 0.62              |
| 34:CK:71:SER:O      | 34:CK:73:GLN:NE2    | 2.33                     | 0.62              |
| 54:Cq:195:VAL:HG23  | 54:Cq:196:HIS:CD2   | 2.35                     | 0.62              |
| 67:A3:70:CYS:HB2    | 67:A3:90:LEU:HD13   | 1.82                     | 0.62              |
| 89:Ad:200:ILE:HD13  | 132:Bd:54:MET:HG3   | 1.80                     | 0.62              |
| 103:BA:190:THR:HB   | 103:BA:194:ARG:HE   | 1.65                     | 0.62              |
| 107:BE:25:HIS:CD2   | 107:BE:27:THR:H     | 2.17                     | 0.62              |
| 137:UA:13:UNK:HA    | 137:UA:16:UNK:HG3   | 1.80                     | 0.62              |
| 1:DA:385:ARG:HH11   | 6:DN:195:TYR:HD1    | 1.45                     | 0.62              |
| 6:DN:77:LEU:N       | 6:DN:78:PRO:HD2     | 2.14                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:975:LYS:HG2  | 19:DG:92:GLN:HE22  | 1.64                     | 0.62              |
| 17:DE:604:ASP:OD1  | 17:DE:717:ARG:NH2  | 2.30                     | 0.62              |
| 18:DF:589:GLN:HB2  | 20:DH:192:PHE:CE1  | 2.35                     | 0.62              |
| 27:DY:33:ALA:HB2   | 27:DY:62:GLN:HG2   | 1.82                     | 0.62              |
| 39:CQ:174:ARG:HH21 | 39:CQ:183:PRO:HD3  | 1.65                     | 0.62              |
| 57:CA:449:G:O2'    | 57:CA:475:A:N6     | 2.29                     | 0.62              |
| 71:A8:175:ASP:OD1  | 71:A8:175:ASP:N    | 2.28                     | 0.62              |
| 94:AI:26:MET:HG3   | 94:AI:27:PRO:HD2   | 1.82                     | 0.62              |
| 125:BW:98:LYS:NZ   | 138:UB:18:UNK:O    | 2.23                     | 0.62              |
| 1:DA:1014:TYR:HE1  | 4:DL:67:ASN:O      | 1.82                     | 0.62              |
| 2:DD:28:MET:HE1    | 31:CH:236:MET:HB3  | 1.82                     | 0.62              |
| 2:DD:637:ARG:NH1   | 38:CP:153:ARG:NH1  | 2.48                     | 0.62              |
| 4:DL:92:ILE:HG23   | 32:CI:248:PHE:HB2  | 1.82                     | 0.62              |
| 15:DB:893:ILE:HG12 | 50:Ck:312:VAL:HB   | 1.80                     | 0.62              |
| 15:DB:1154:LYS:NZ  | 89:Ad:150:ARG:CZ   | 2.63                     | 0.62              |
| 33:CJ:753:ASN:ND2  | 48:CI:16:GLY:O     | 2.32                     | 0.62              |
| 34:CK:205:TYR:HD2  | 34:CK:221:THR:HG23 | 1.65                     | 0.62              |
| 45:Cb:101:LYS:NZ   | 45:Cb:101:LYS:HB3  | 2.15                     | 0.62              |
| 48:CI:33:LEU:HD11  | 50:Ck:785:PRO:HB3  | 1.81                     | 0.62              |
| 54:Cq:99:THR:HG23  | 54:Cq:101:LEU:H    | 1.64                     | 0.62              |
| 65:A1:122:MET:HE2  | 65:A1:127:MET:HG2  | 1.82                     | 0.62              |
| 75:AI:124:GLU:H    | 75:AI:124:GLU:CD   | 2.08                     | 0.62              |
| 85:AW:28:GLN:HG2   | 85:AW:29:ARG:H     | 1.64                     | 0.62              |
| 95:Ao:224:LYS:O    | 120:BR:156:ARG:NH2 | 2.33                     | 0.62              |
| 96:Ap:37:ASN:HB2   | 111:BI:27:LEU:HD12 | 1.82                     | 0.62              |
| 7:DO:114:GLY:O     | 7:DO:116:ALA:N     | 2.33                     | 0.62              |
| 15:DB:1133:PRO:O   | 26:DX:115:ARG:NH1  | 2.32                     | 0.62              |
| 21:DJ:22:MET:HG2   | 28:CC:67:ASN:HB2   | 1.81                     | 0.62              |
| 24:DV:100:LYS:HG3  | 33:CJ:773:GLU:HB3  | 1.82                     | 0.62              |
| 40:CR:261:ILE:HG13 | 40:CR:262:SER:H    | 1.65                     | 0.62              |
| 57:CA:35:U:H3'     | 57:CA:36:U:H5''    | 1.81                     | 0.62              |
| 67:A3:60:ARG:NH1   | 97:At:53:SER:O     | 2.33                     | 0.62              |
| 74:AF:421:ASP:HB3  | 98:Av:131:LEU:HD22 | 1.81                     | 0.62              |
| 76:AJ:60:GLU:HA    | 76:AJ:66:GLU:OE2   | 2.00                     | 0.62              |
| 76:AJ:73:ARG:NH1   | 76:AJ:83:PHE:HE1   | 1.98                     | 0.62              |
| 88:Ab:419:GLN:NE2  | 105:BC:73:ARG:HH11 | 1.96                     | 0.62              |
| 102:AA:387:A:O2'   | 102:AA:388:U:O5'   | 2.17                     | 0.62              |
| 102:AA:484:U:H1'   | 102:AA:485:A:H5'   | 1.81                     | 0.62              |
| 108:BF:362:HIS:HD2 | 125:BW:177:VAL:H   | 1.46                     | 0.62              |
| 119:BQ:28:ASN:HB3  | 119:BQ:49:LEU:O    | 2.00                     | 0.62              |
| 2:DD:417:THR:HG22  | 2:DD:419:ALA:H     | 1.65                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:DQ:79:LEU:HB3     | 9:DQ:83:ASN:ND2     | 2.15                     | 0.61              |
| 17:DE:451:THR:HB    | 17:DE:501:HIS:HD2   | 1.65                     | 0.61              |
| 17:DE:610:LEU:HD22  | 17:DE:615:LEU:HD13  | 1.82                     | 0.61              |
| 19:DG:215:LEU:HD22  | 19:DG:224:LEU:HD12  | 1.81                     | 0.61              |
| 34:CK:42:PHE:CG     | 40:CR:252:GLN:O     | 2.52                     | 0.61              |
| 56:Cv:292:LYS:O     | 56:Cv:405:PRO:HG2   | 1.99                     | 0.61              |
| 67:A3:161:ARG:HG2   | 67:A3:161:ARG:HH11  | 1.64                     | 0.61              |
| 75:AI:152:ARG:NH1   | 112:BJ:292:ARG:O    | 2.33                     | 0.61              |
| 116:BN:125:THR:HG22 | 116:BN:127:GLU:H    | 1.64                     | 0.61              |
| 1:DA:653:LYS:HB2    | 1:DA:726:GLU:HB2    | 1.81                     | 0.61              |
| 9:DQ:142:PHE:HE2    | 9:DQ:246:VAL:HG11   | 1.64                     | 0.61              |
| 20:DH:474:ASP:OD1   | 20:DH:474:ASP:N     | 2.34                     | 0.61              |
| 24:DV:42:PHE:CD2    | 24:DV:43:ASN:HB3    | 2.35                     | 0.61              |
| 31:CH:253:TYR:CE2   | 31:CH:280:MET:HE3   | 2.35                     | 0.61              |
| 33:CJ:37:ASN:CB     | 51:Cm:50:ARG:HB3    | 2.30                     | 0.61              |
| 56:Cv:813:ARG:HG2   | 56:Cv:926:ILE:HD13  | 1.81                     | 0.61              |
| 66:A2:376:ARG:HD2   | 66:A2:380:ARG:NH1   | 2.15                     | 0.61              |
| 89:Ad:230:LEU:HD22  | 89:Ad:260:MET:HE1   | 1.81                     | 0.61              |
| 118:BP:74:GLU:OE1   | 118:BP:74:GLU:N     | 2.27                     | 0.61              |
| 4:DL:139:ARG:NH2    | 4:DL:203:ARG:HH12   | 1.98                     | 0.61              |
| 9:DQ:41:GLN:HE21    | 12:DU:123:GLN:H     | 1.47                     | 0.61              |
| 15:DB:1107:THR:O    | 36:CN:70:LYS:HE3    | 2.00                     | 0.61              |
| 51:Cm:137:SER:CA    | 57:CA:394:A:C2      | 2.81                     | 0.61              |
| 54:Cq:181:HIS:ND1   | 54:Cq:201:GLU:OE2   | 2.33                     | 0.61              |
| 64:A0:108:GLN:O     | 64:A0:112:ARG:HG2   | 2.00                     | 0.61              |
| 78:AN:56:ARG:NH1    | 78:AN:182:LYS:O     | 2.33                     | 0.61              |
| 85:AW:168:LEU:HD21  | 107:BE:399:LYS:HE3  | 1.83                     | 0.61              |
| 91:Af:162:ARG:HB2   | 91:Af:168:GLN:HE22  | 1.64                     | 0.61              |
| 108:BF:163:ASN:HA   | 108:BF:197:MET:HE2  | 1.81                     | 0.61              |
| 123:BU:121:HIS:CG   | 135:Bg:102:LEU:HD21 | 2.34                     | 0.61              |
| 129:Ba:58:MET:HE1   | 129:Ba:65:GLU:HG2   | 1.81                     | 0.61              |
| 4:DL:74:ARG:HH21    | 29:CE:110:LEU:HD12  | 1.50                     | 0.61              |
| 8:DP:111:THR:HG22   | 8:DP:113:ASP:H      | 1.65                     | 0.61              |
| 18:DF:121:LEU:HD22  | 18:DF:154:ASN:HA    | 1.83                     | 0.61              |
| 20:DH:17:ILE:HD13   | 21:DJ:12:TYR:HE1    | 1.65                     | 0.61              |
| 77:AK:229:ARG:HA    | 77:AK:232:GLU:HB3   | 1.82                     | 0.61              |
| 104:BB:419:VAL:HA   | 104:BB:427:PHE:CZ   | 2.35                     | 0.61              |
| 108:BF:171:ARG:NH2  | 108:BF:190:ASN:OD1  | 2.30                     | 0.61              |
| 4:DL:181:ARG:NH2    | 56:Cv:494:THR:O     | 2.33                     | 0.61              |
| 5:DM:227:LEU:HB2    | 56:Cv:1008:ARG:HD3  | 1.83                     | 0.61              |
| 5:DM:293:ARG:HE     | 54:Cq:59:ARG:HB2    | 1.63                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:DP:195:THR:OG1    | 8:DP:211:GLU:HG3    | 1.98                     | 0.61              |
| 9:DQ:120:MET:HB2    | 9:DQ:196:LEU:HD23   | 1.81                     | 0.61              |
| 14:Da:53:ARG:NH1    | 57:CA:333:U:OP2     | 2.33                     | 0.61              |
| 15:DB:964:ARG:HH12  | 15:DB:1005:ILE:HD13 | 1.65                     | 0.61              |
| 21:DJ:261:PHE:O     | 21:DJ:305:ARG:NH2   | 2.28                     | 0.61              |
| 31:CH:107:ARG:HH12  | 31:CH:133:ARG:CZ    | 2.13                     | 0.61              |
| 33:CJ:281:VAL:HB    | 50:Ck:103:GLU:OE2   | 1.99                     | 0.61              |
| 50:Ck:728:GLN:HE22  | 50:Ck:731:ARG:HH11  | 1.47                     | 0.61              |
| 77:AK:48:ARG:NH1    | 96:Ap:213:PRO:HA    | 2.15                     | 0.61              |
| 106:BD:143:PRO:CB   | 110:BH:174:LEU:HD12 | 2.31                     | 0.61              |
| 111:BI:46:LEU:HD21  | 111:BI:49:PRO:HG2   | 1.81                     | 0.61              |
| 128:BZ:2:ARG:HH11   | 128:BZ:28:ARG:HE    | 1.48                     | 0.61              |
| 134:Bf:99:ILE:O     | 134:Bf:102:LYS:N    | 2.33                     | 0.61              |
| 8:DP:195:THR:C      | 8:DP:211:GLU:HG2    | 2.26                     | 0.61              |
| 16:DC:1055:ARG:HH11 | 16:DC:1055:ARG:HA   | 1.65                     | 0.61              |
| 17:DE:570:GLU:HA    | 17:DE:573:GLN:HB2   | 1.80                     | 0.61              |
| 17:DE:649:TYR:CG    | 17:DE:721:ASP:HB2   | 2.36                     | 0.61              |
| 29:CE:308:ARG:CA    | 29:CE:311:LYS:HZ2   | 2.13                     | 0.61              |
| 34:CK:314:PRO:HB3   | 42:CU:15:TYR:CZ     | 2.35                     | 0.61              |
| 43:CZ:236:ARG:O     | 43:CZ:237:ARG:HB3   | 2.01                     | 0.61              |
| 47:Cg:316:THR:HG23  | 47:Cg:318:ILE:HG13  | 1.80                     | 0.61              |
| 83:AU:81:ARG:HG3    | 95:Ao:61:ARG:HG3    | 1.81                     | 0.61              |
| 107:BE:53:THR:O     | 135:Bg:69:ARG:NH2   | 2.33                     | 0.61              |
| 109:BG:149:THR:HG21 | 109:BG:154:ALA:N    | 2.15                     | 0.61              |
| 2:DD:541:ARG:HD2    | 10:DR:215:ARG:NH1   | 2.16                     | 0.61              |
| 33:CJ:385:LEU:HD11  | 41:CS:45:ARG:HD3    | 1.82                     | 0.61              |
| 47:Cg:84:GLU:OE1    | 47:Cg:84:GLU:N      | 2.33                     | 0.61              |
| 48:Ci:69:THR:HG23   | 48:Ci:71:TYR:H      | 1.64                     | 0.61              |
| 65:A1:110:TYR:CG    | 75:AI:150:PRO:HA    | 2.36                     | 0.61              |
| 81:AR:211:ARG:NH2   | 123:BU:147:GLU:OE2  | 2.34                     | 0.61              |
| 88:Ab:172:TYR:CD1   | 88:Ab:202:MET:HE2   | 2.36                     | 0.61              |
| 88:Ab:257:PRO:O     | 115:BM:96:ARG:NH2   | 2.34                     | 0.61              |
| 89:Ad:228:GLN:O     | 89:Ad:231:ILE:HG13  | 2.00                     | 0.61              |
| 102:AA:3:U:H5'      | 103:BA:754:ARG:NH1  | 2.15                     | 0.61              |
| 134:Bf:104:ASN:HB2  | 134:Bf:111:SER:HB2  | 1.81                     | 0.61              |
| 1:DA:649:LEU:HD12   | 1:DA:729:ARG:HH11   | 1.65                     | 0.61              |
| 2:DD:149:SER:HB2    | 2:DD:152:ALA:HB3    | 1.83                     | 0.61              |
| 2:DD:647:ARG:HG3    | 2:DD:647:ARG:HH11   | 1.66                     | 0.61              |
| 6:DN:217:MET:HE3    | 44:Ca:267:LEU:HD23  | 1.83                     | 0.61              |
| 9:DQ:134:ILE:HG21   | 9:DQ:248:LEU:HD22   | 1.82                     | 0.61              |
| 10:DR:63:ILE:HG22   | 10:DR:64:ILE:HG13   | 1.82                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:DR:128:PRO:HG3   | 10:DR:133:LEU:H     | 1.66                     | 0.61              |
| 15:DB:233:ASP:N     | 15:DB:233:ASP:OD1   | 2.33                     | 0.61              |
| 16:DC:200:VAL:HG13  | 16:DC:205:GLN:HB2   | 1.82                     | 0.61              |
| 16:DC:1143:VAL:HG12 | 16:DC:1144:PRO:HD2  | 1.83                     | 0.61              |
| 23:DT:87:ARG:HD3    | 23:DT:139:HIS:CE1   | 2.36                     | 0.61              |
| 29:CE:209:GLU:OE2   | 44:Ca:347:ARG:NH1   | 2.34                     | 0.61              |
| 44:Ca:507:MET:HE3   | 44:Ca:557:PHE:HB3   | 1.81                     | 0.61              |
| 71:A8:119:ARG:HD3   | 102:AA:340:U:OP2    | 2.01                     | 0.61              |
| 78:AN:125:ASP:HB3   | 78:AN:128:MET:HB2   | 1.83                     | 0.61              |
| 102:AA:948:A:H5'    | 127:BY:165:ARG:HH22 | 1.65                     | 0.61              |
| 1:DA:1029:LYS:HZ1   | 5:DM:254:HIS:CE1    | 2.18                     | 0.61              |
| 1:DA:1583:LEU:O     | 1:DA:1587:LEU:HG    | 2.01                     | 0.61              |
| 17:DE:543:ARG:HG2   | 17:DE:543:ARG:HH11  | 1.65                     | 0.61              |
| 18:DF:425:ILE:HD13  | 20:DH:196:LEU:CD1   | 2.29                     | 0.61              |
| 22:DK:238:ILE:HG21  | 22:DK:260:VAL:CG2   | 2.31                     | 0.61              |
| 40:CR:25:GLU:HB3    | 56:Cv:143:THR:HG21  | 1.83                     | 0.61              |
| 47:Cg:158:LEU:HD22  | 47:Cg:401:ILE:HD11  | 1.82                     | 0.61              |
| 73:AE:50:ARG:NH2    | 111:BI:40:GLN:O     | 2.34                     | 0.61              |
| 147:UU:5:UNK:HA     | 147:UU:11:UNK:HG1   | 1.83                     | 0.61              |
| 2:DD:799:ASP:OD1    | 2:DD:799:ASP:N      | 2.34                     | 0.61              |
| 4:DL:116:ASN:HB2    | 4:DL:216:GLU:OE1    | 2.01                     | 0.61              |
| 9:DQ:142:PHE:HE1    | 9:DQ:180:ALA:HB1    | 1.66                     | 0.61              |
| 12:DU:189:LYS:HZ1   | 12:DU:190:ARG:HB2   | 1.66                     | 0.61              |
| 15:DB:78:ARG:HG3    | 15:DB:78:ARG:NH1    | 2.15                     | 0.61              |
| 23:DT:33:HIS:CD2    | 23:DT:35:LYS:HD2    | 2.36                     | 0.61              |
| 36:CN:54:PRO:HB3    | 36:CN:60:VAL:HG13   | 1.83                     | 0.61              |
| 36:CN:108:VAL:HG21  | 36:CN:118:MET:HG3   | 1.83                     | 0.61              |
| 40:CR:295:LYS:HE3   | 40:CR:298:ASN:HB3   | 1.83                     | 0.61              |
| 48:CI:109:ASN:HB2   | 48:CI:112:ASN:HD22  | 1.65                     | 0.61              |
| 52:Cn:179:ARG:HD2   | 52:Cn:183:ARG:NH1   | 2.16                     | 0.61              |
| 73:AE:172:LYS:HB3   | 73:AE:186:TYR:HB2   | 1.83                     | 0.61              |
| 76:AJ:80:ARG:HH11   | 76:AJ:80:ARG:HG3    | 1.66                     | 0.61              |
| 104:BB:347:LYS:HD3  | 104:BB:422:MET:HG2  | 1.81                     | 0.61              |
| 1:DA:617:PRO:HG2    | 1:DA:746:GLN:NE2    | 2.16                     | 0.60              |
| 6:DN:62:ARG:NH2     | 44:Ca:390:GLN:OE1   | 2.33                     | 0.60              |
| 6:DN:142:ARG:CZ     | 31:CH:19:LEU:HD12   | 2.31                     | 0.60              |
| 15:DB:488:ASN:OD1   | 15:DB:493:ARG:NH1   | 2.34                     | 0.60              |
| 15:DB:785:ASN:ND2   | 50:Ck:154:SER:OG    | 2.32                     | 0.60              |
| 16:DC:413:LEU:HD21  | 16:DC:422:VAL:HG21  | 1.82                     | 0.60              |
| 19:DG:346:ARG:HH21  | 19:DG:497:ARG:HD3   | 1.66                     | 0.60              |
| 35:CL:59:MET:HG3    | 35:CL:62:LEU:HD12   | 1.83                     | 0.60              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 40:CR:184:LYS:HB2   | 40:CR:184:LYS:HZ2   | 1.66                     | 0.60              |
| 71:A8:61:TYR:OH     | 102:AA:61:A:OP2     | 2.14                     | 0.60              |
| 72:A9:85:CYS:SG     | 72:A9:97:ARG:HG2    | 2.40                     | 0.60              |
| 77:AK:24:ASN:HB2    | 124:BV:103:THR:HG22 | 1.82                     | 0.60              |
| 79:AP:46:ASN:OD1    | 79:AP:46:ASN:N      | 2.34                     | 0.60              |
| 95:Ao:236:ARG:NH1   | 124:BV:155:MET:HE1  | 2.15                     | 0.60              |
| 108:BF:202:THR:HG22 | 108:BF:203:ARG:HG3  | 1.83                     | 0.60              |
| 108:BF:383:MET:O    | 108:BF:388:ARG:NH2  | 2.34                     | 0.60              |
| 111:BI:178:ASN:O    | 111:BI:181:SER:OG   | 2.19                     | 0.60              |
| 8:DP:132:LEU:HD21   | 8:DP:154:PHE:HE1    | 1.65                     | 0.60              |
| 14:Da:14:TYR:OH     | 39:CQ:40:ARG:NH2    | 2.34                     | 0.60              |
| 17:DE:317:GLU:HG2   | 17:DE:318:PRO:HD2   | 1.83                     | 0.60              |
| 18:DF:170:ARG:O     | 48:CI:104:ARG:NH2   | 2.34                     | 0.60              |
| 19:DG:336:MET:HE2   | 19:DG:336:MET:HA    | 1.81                     | 0.60              |
| 23:DT:104:PRO:HG2   | 23:DT:107:GLU:HG3   | 1.82                     | 0.60              |
| 32:CI:62:GLU:OE2    | 34:CK:48:ARG:NH1    | 2.34                     | 0.60              |
| 48:CI:133:TYR:CE2   | 48:CI:137:LYS:HE3   | 2.36                     | 0.60              |
| 86:AX:145:ARG:HG2   | 86:AX:162:GLN:HB2   | 1.82                     | 0.60              |
| 95:Ao:104:LYS:HG3   | 97:At:144:VAL:HG11  | 1.82                     | 0.60              |
| 102:AA:574:A:H61    | 102:AA:1167:A:N6    | 1.99                     | 0.60              |
| 116:BN:207:ASN:HB3  | 136:Bh:28:ARG:HH11  | 1.66                     | 0.60              |
| 1:DA:80:PRO:HD3     | 57:CA:154:G:N2      | 2.16                     | 0.60              |
| 2:DD:11:ARG:NH2     | 52:Cn:157:TYR:O     | 2.34                     | 0.60              |
| 6:DN:209:ARG:HD3    | 6:DN:211:TRP:CZ2    | 2.36                     | 0.60              |
| 25:DW:63:THR:HG22   | 25:DW:65:ASP:H      | 1.66                     | 0.60              |
| 33:CJ:441:HIS:HD2   | 50:Ck:768:SER:HB2   | 1.66                     | 0.60              |
| 40:CR:306:LYS:HZ3   | 57:CA:389:A:H3'     | 1.64                     | 0.60              |
| 44:Ca:43:VAL:HG21   | 56:Cv:1129:ASN:HB3  | 1.83                     | 0.60              |
| 49:Cj:132:LEU:HD21  | 49:Cj:135:ILE:HG13  | 1.83                     | 0.60              |
| 66:A2:182:LEU:HD11  | 75:AI:53:LYS:HE3    | 1.84                     | 0.60              |
| 73:AE:102:ASP:OD2   | 96:Ap:115:VAL:HG11  | 2.00                     | 0.60              |
| 107:BE:12:GLN:HG3   | 107:BE:28:LEU:HD22  | 1.82                     | 0.60              |
| 140:UD:216:UNK:HA   | 140:UD:219:UNK:HG3  | 1.84                     | 0.60              |
| 10:DR:252:ALA:HA    | 10:DR:262:ARG:HG3   | 1.82                     | 0.60              |
| 32:CI:132:GLY:HA3   | 40:CR:225:LEU:HD13  | 1.83                     | 0.60              |
| 35:CL:129:LEU:HD12  | 35:CL:130:PRO:HD2   | 1.82                     | 0.60              |
| 56:Cv:147:HIS:HD2   | 56:Cv:149:ASP:H     | 1.49                     | 0.60              |
| 71:A8:150:GLY:HA3   | 102:AA:59:U:O2      | 2.01                     | 0.60              |
| 74:AF:167:ARG:NH2   | 86:AX:69:GLU:OE1    | 2.29                     | 0.60              |
| 77:AK:62:ALA:HB2    | 77:AK:86:PHE:HD2    | 1.65                     | 0.60              |
| 85:AW:91:VAL:HG11   | 108:BF:388:ARG:HD3  | 1.83                     | 0.60              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 102:AA:439:C:H1'    | 124:BV:160:MET:HE2  | 1.84                     | 0.60              |
| 108:BF:134:ASP:HB3  | 108:BF:149:TYR:OH   | 2.01                     | 0.60              |
| 2:DD:242:LEU:HG     | 2:DD:246:GLU:HG2    | 1.84                     | 0.60              |
| 15:DB:776:THR:HG22  | 15:DB:783:VAL:HG22  | 1.83                     | 0.60              |
| 17:DE:697:THR:HG23  | 22:DK:59:TRP:HH2    | 1.66                     | 0.60              |
| 40:CR:137:THR:HG23  | 40:CR:139:THR:H     | 1.65                     | 0.60              |
| 42:CU:13:MET:HE3    | 57:CA:314:A:H5''    | 1.83                     | 0.60              |
| 75:AI:35:ARG:NH1    | 102:AA:49:A:OP1     | 2.34                     | 0.60              |
| 76:AJ:57:ILE:HB     | 92:Ag:197:LEU:HD13  | 1.83                     | 0.60              |
| 78:AN:41:GLY:O      | 78:AN:70:ARG:NH2    | 2.34                     | 0.60              |
| 108:BF:286:VAL:HG11 | 108:BF:316:MET:HE1  | 1.82                     | 0.60              |
| 6:DN:75:VAL:O       | 6:DN:75:VAL:HG13    | 2.01                     | 0.60              |
| 9:DQ:250:ARG:CZ     | 9:DQ:252:LYS:HE3    | 2.31                     | 0.60              |
| 16:DC:119:THR:HG21  | 16:DC:136:TRP:NE1   | 2.17                     | 0.60              |
| 17:DE:195:ILE:HG23  | 17:DE:198:CYS:SG    | 2.42                     | 0.60              |
| 17:DE:319:ASN:N     | 17:DE:319:ASN:OD1   | 2.34                     | 0.60              |
| 19:DG:335:GLU:OE2   | 32:CI:17:ARG:NH2    | 2.33                     | 0.60              |
| 34:CK:180:ASP:HA    | 46:Cd:182:GLN:HE21  | 1.66                     | 0.60              |
| 40:CR:316:GLY:O     | 46:Cd:279:ARG:CG    | 2.45                     | 0.60              |
| 71:A8:89:GLY:N      | 71:A8:111:ARG:NH1   | 2.49                     | 0.60              |
| 75:AI:70:ARG:HB2    | 75:AI:70:ARG:NH1    | 2.15                     | 0.60              |
| 76:AJ:58:ASN:HA     | 96:Ap:222:PHE:HD1   | 1.67                     | 0.60              |
| 84:AV:235:LEU:HD21  | 91:Af:100:THR:HG21  | 1.82                     | 0.60              |
| 87:AY:82:ARG:HH11   | 87:AY:82:ARG:HB2    | 1.67                     | 0.60              |
| 95:Ao:25:ASN:HD22   | 95:Ao:26:TYR:H      | 1.48                     | 0.60              |
| 95:Ao:224:LYS:NZ    | 95:Ao:224:LYS:HB3   | 2.17                     | 0.60              |
| 102:AA:329:U:C4     | 119:BQ:217:THR:HG22 | 2.37                     | 0.60              |
| 103:BA:520:LEU:HB2  | 103:BA:570:SER:HB2  | 1.82                     | 0.60              |
| 109:BG:106:ASP:OD1  | 109:BG:106:ASP:N    | 2.34                     | 0.60              |
| 117:BO:215:LEU:HD23 | 117:BO:219:ARG:NH1  | 2.17                     | 0.60              |
| 126:BX:69:ARG:NH1   | 126:BX:71:MET:HE2   | 2.17                     | 0.60              |
| 1:DA:1186:CYS:CB    | 1:DA:1193:HIS:CE1   | 2.84                     | 0.60              |
| 6:DN:223:GLN:HB2    | 44:Ca:256:GLU:CD    | 2.26                     | 0.60              |
| 12:DU:73:ARG:NH1    | 12:DU:73:ARG:O      | 2.34                     | 0.60              |
| 18:DF:125:TYR:H     | 18:DF:175:GLN:HE22  | 1.48                     | 0.60              |
| 29:CE:83:MET:HE1    | 29:CE:307:ILE:HD11  | 1.83                     | 0.60              |
| 34:CK:14:PRO:CD     | 40:CR:300:TYR:CE2   | 2.84                     | 0.60              |
| 45:Cb:175:ILE:HG23  | 45:Cb:179:GLU:HB2   | 1.82                     | 0.60              |
| 56:Cv:95:ARG:HH11   | 56:Cv:95:ARG:HG3    | 1.66                     | 0.60              |
| 56:Cv:440:GLY:HA2   | 56:Cv:443:VAL:HG22  | 1.83                     | 0.60              |
| 57:CA:38:U:H4'      | 57:CA:39:U:OP2      | 2.01                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:A8:74:PHE:HD1   | 71:A8:87:ALA:HB2   | 1.64                     | 0.60              |
| 76:AJ:83:PHE:HD2   | 96:Ap:205:ARG:HD3  | 1.66                     | 0.60              |
| 88:Ab:358:ALA:HA   | 88:Ab:392:MET:HE1  | 1.83                     | 0.60              |
| 116:BN:140:SER:HB3 | 140:UD:207:UNK:HG2 | 1.84                     | 0.60              |
| 132:Bd:21:CYS:SG   | 132:Bd:75:SER:HB3  | 2.42                     | 0.60              |
| 1:DA:195:MET:HE3   | 1:DA:198:ARG:NH1   | 2.16                     | 0.60              |
| 4:DL:241:GLU:OE1   | 4:DL:242:ARG:N     | 2.35                     | 0.60              |
| 9:DQ:171:GLU:HG2   | 37:CO:319:MET:HE2  | 1.84                     | 0.60              |
| 13:DZ:11:LYS:H     | 44:Ca:91:ASP:HA    | 1.66                     | 0.60              |
| 26:DX:89:ARG:HG3   | 26:DX:89:ARG:NH1   | 2.16                     | 0.60              |
| 57:CA:360:C:H2'    | 57:CA:361:A:H5'    | 1.84                     | 0.60              |
| 63:UT:19:UNK:HA    | 63:UT:24:UNK:HB1   | 1.82                     | 0.60              |
| 78:AN:121:MET:HG2  | 78:AN:129:LEU:HG   | 1.82                     | 0.60              |
| 89:Ad:82:PHE:HZ    | 132:Bd:14:MET:HE2  | 1.67                     | 0.60              |
| 102:AA:566:A:H61   | 135:Bg:48:PRO:HA   | 1.66                     | 0.60              |
| 108:BF:188:LEU:HG  | 108:BF:192:GLU:OE2 | 2.02                     | 0.60              |
| 140:UD:205:UNK:HA  | 140:UD:208:UNK:HG3 | 1.82                     | 0.60              |
| 2:DD:352:VAL:HG12  | 2:DD:359:LEU:HD22  | 1.84                     | 0.60              |
| 4:DL:117:ASP:HB3   | 4:DL:121:ILE:CD1   | 2.29                     | 0.60              |
| 15:DB:663:VAL:HG23 | 15:DB:665:ARG:HG3  | 1.83                     | 0.60              |
| 45:Cb:307:TYR:OH   | 55:Cr:97:ASP:OD2   | 2.18                     | 0.60              |
| 75:AI:182:PRO:HG2  | 75:AI:183:ARG:NH1  | 2.16                     | 0.60              |
| 79:AP:79:TRP:CD2   | 79:AP:90:ILE:HD13  | 2.37                     | 0.60              |
| 83:AU:71:ARG:NH2   | 91:Af:61:PRO:O     | 2.35                     | 0.60              |
| 96:Ap:260:MET:HA   | 96:Ap:260:MET:HE2  | 1.83                     | 0.60              |
| 119:BQ:72:SER:OG   | 119:BQ:73:GLN:N    | 2.28                     | 0.60              |
| 125:BW:51:ASP:OD1  | 125:BW:75:ARG:NH2  | 2.34                     | 0.60              |
| 128:BZ:2:ARG:O     | 128:BZ:5:GLU:HG3   | 2.02                     | 0.60              |
| 2:DD:83:THR:O      | 2:DD:87:MET:N      | 2.31                     | 0.60              |
| 7:DO:136:ASP:HA    | 7:DO:139:GLU:HG3   | 1.84                     | 0.60              |
| 15:DB:823:PRO:HD2  | 15:DB:826:LEU:HG   | 1.83                     | 0.60              |
| 26:DX:89:ARG:HH11  | 26:DX:89:ARG:HG3   | 1.66                     | 0.60              |
| 33:CJ:490:ASP:OD1  | 33:CJ:490:ASP:N    | 2.35                     | 0.60              |
| 51:Cm:141:TRP:CE2  | 57:CA:394:A:N6     | 2.70                     | 0.60              |
| 57:CA:350:U:O2'    | 57:CA:351:A:OP2    | 2.14                     | 0.60              |
| 64:A0:106:ASP:HB3  | 115:BM:86:VAL:HG21 | 1.84                     | 0.60              |
| 71:A8:111:ARG:HG2  | 71:A8:111:ARG:NH1  | 2.16                     | 0.60              |
| 85:AW:95:ARG:HD3   | 85:AW:110:TRP:CD2  | 2.37                     | 0.60              |
| 104:BB:79:ARG:HG3  | 104:BB:79:ARG:HH11 | 1.65                     | 0.60              |
| 140:UD:170:UNK:HA  | 140:UD:173:UNK:HB2 | 1.84                     | 0.60              |
| 6:DN:73:VAL:HG11   | 6:DN:112:ILE:HD12  | 1.83                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 16:DC:1157:ALA:HA   | 20:DH:41:LYS:HZ1    | 1.67                     | 0.59              |
| 29:CE:209:GLU:CD    | 44:Ca:347:ARG:HH12  | 2.10                     | 0.59              |
| 31:CH:107:ARG:NH1   | 31:CH:133:ARG:CZ    | 2.65                     | 0.59              |
| 40:CR:109:ASP:HB3   | 40:CR:112:GLY:HA2   | 1.84                     | 0.59              |
| 44:Ca:61:LEU:HB2    | 44:Ca:76:GLN:NE2    | 2.17                     | 0.59              |
| 67:A3:104:GLN:HE21  | 67:A3:104:GLN:H     | 1.50                     | 0.59              |
| 83:AU:10:HIS:N      | 102:AA:296:A:O5'    | 2.35                     | 0.59              |
| 97:At:59:ALA:HB1    | 97:At:62:ARG:HH11   | 1.66                     | 0.59              |
| 1:DA:1399:ASN:HD21  | 1:DA:1502:PHE:H     | 1.50                     | 0.59              |
| 72:A9:76:ARG:HH12   | 72:A9:89:PRO:HG3    | 1.66                     | 0.59              |
| 88:Ab:125:LEU:HD21  | 88:Ab:133:PRO:HB2   | 1.84                     | 0.59              |
| 93:Aj:185:LYS:HD3   | 93:Aj:277:GLN:HA    | 1.84                     | 0.59              |
| 109:BG:39:PHE:HB3   | 109:BG:65:MET:HG3   | 1.83                     | 0.59              |
| 111:BI:272:ARG:HA   | 111:BI:275:MET:HG2  | 1.82                     | 0.59              |
| 126:BX:112:PHE:HD2  | 126:BX:117:PHE:HA   | 1.67                     | 0.59              |
| 4:DL:139:ARG:HH22   | 4:DL:203:ARG:HH12   | 1.48                     | 0.59              |
| 21:DJ:247:ASN:HD22  | 21:DJ:250:VAL:HG23  | 1.68                     | 0.59              |
| 37:CO:75:LEU:HD11   | 52:Cn:230:VAL:HG22  | 1.84                     | 0.59              |
| 66:A2:219:THR:HG22  | 122:BT:112:ARG:HH12 | 1.67                     | 0.59              |
| 68:A4:145:ALA:HA    | 89:Ad:178:GLU:HA    | 1.85                     | 0.59              |
| 85:AW:179:LEU:HD23  | 85:AW:232:LEU:HD21  | 1.85                     | 0.59              |
| 96:Ap:124:PRO:CD    | 142:UN:7:UNK:HB1    | 2.28                     | 0.59              |
| 102:AA:301:A:N7     | 108:BF:266:ASN:ND2  | 2.47                     | 0.59              |
| 102:AA:945:U:H3     | 102:AA:955:G:H22    | 1.49                     | 0.59              |
| 103:BA:569:LEU:HD22 | 103:BA:659:GLU:HB3  | 1.84                     | 0.59              |
| 104:BB:179:LEU:HB3  | 104:BB:247:TYR:CD1  | 2.37                     | 0.59              |
| 110:BH:186:SER:HB3  | 110:BH:224:LEU:HG   | 1.85                     | 0.59              |
| 115:BM:232:LEU:HD13 | 120:BR:172:PRO:HD2  | 1.82                     | 0.59              |
| 119:BQ:52:ASP:OD1   | 119:BQ:53:ILE:N     | 2.34                     | 0.59              |
| 120:BR:74:THR:HB    | 120:BR:76:LYS:NZ    | 2.18                     | 0.59              |
| 1:DA:1236:ILE:HG23  | 1:DA:1298:VAL:HG11  | 1.85                     | 0.59              |
| 8:DP:189:TYR:CD1    | 8:DP:197:TYR:N      | 2.71                     | 0.59              |
| 12:DU:207:ARG:H     | 12:DU:207:ARG:HD2   | 1.67                     | 0.59              |
| 19:DG:118:ASP:OD1   | 50:Ck:406:ARG:NH2   | 2.35                     | 0.59              |
| 37:CO:112:LYS:HB2   | 37:CO:112:LYS:NZ    | 2.17                     | 0.59              |
| 66:A2:186:GLU:HB3   | 75:AI:52:TRP:CZ3    | 2.37                     | 0.59              |
| 74:AF:103:VAL:HG11  | 74:AF:371:LEU:HD11  | 1.85                     | 0.59              |
| 76:AJ:103:ARG:NH1   | 100:AC:75:ALA:HB2   | 2.17                     | 0.59              |
| 85:AW:76:LEU:HD13   | 87:AY:29:MET:HE1    | 1.83                     | 0.59              |
| 86:AX:129:GLU:N     | 86:AX:129:GLU:OE2   | 2.34                     | 0.59              |
| 102:AA:567:G:N3     | 136:Bh:23:ARG:NH1   | 2.50                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 103:BA:301:HIS:HD2  | 103:BA:303:ILE:HG12 | 1.68                     | 0.59              |
| 121:BS:51:ILE:HD11  | 121:BS:70:ILE:O     | 2.02                     | 0.59              |
| 18:DF:93:PRO:HG2    | 41:CS:89:TYR:CD1    | 2.38                     | 0.59              |
| 18:DF:156:ALA:O     | 57:CA:415:U:H3'     | 2.03                     | 0.59              |
| 19:DG:117:VAL:HG13  | 19:DG:145:VAL:HG12  | 1.84                     | 0.59              |
| 34:CK:27:ARG:NH2    | 57:CA:465:U:OP1     | 2.36                     | 0.59              |
| 34:CK:320:MET:H     | 42:CU:81:GLU:HG2    | 1.68                     | 0.59              |
| 50:Ck:638:ARG:HH11  | 50:Ck:638:ARG:HG3   | 1.67                     | 0.59              |
| 52:Cn:236:LYS:H     | 52:Cn:245:LYS:NZ    | 1.97                     | 0.59              |
| 56:Cv:84:GLY:HA2    | 56:Cv:87:GLN:HG3    | 1.84                     | 0.59              |
| 56:Cv:470:PHE:HD1   | 56:Cv:556:PHE:HE2   | 1.50                     | 0.59              |
| 73:AE:78:PRO:HG2    | 73:AE:84:TRP:CD1    | 2.38                     | 0.59              |
| 86:AX:163:ILE:HD11  | 86:AX:172:LEU:HD13  | 1.83                     | 0.59              |
| 107:BE:137:LYS:HB2  | 107:BE:137:LYS:NZ   | 2.17                     | 0.59              |
| 114:BL:73:GLY:HA2   | 114:BL:78:ARG:HH21  | 1.67                     | 0.59              |
| 18:DF:452:VAL:HG12  | 18:DF:453:MET:HE2   | 1.84                     | 0.59              |
| 72:A9:68:LEU:HD23   | 72:A9:77:PHE:HE1    | 1.67                     | 0.59              |
| 77:AK:244:ARG:HH12  | 77:AK:314:ARG:NH1   | 2.00                     | 0.59              |
| 83:AU:103:GLU:HG2   | 84:AV:79:PHE:CZ     | 2.38                     | 0.59              |
| 103:BA:223:LYS:NZ   | 103:BA:232:TYR:CD1  | 2.67                     | 0.59              |
| 119:BQ:132:MET:HE2  | 119:BQ:161:CYS:SG   | 2.43                     | 0.59              |
| 1:DA:112:GLN:HG2    | 1:DA:131:ASP:OD1    | 2.03                     | 0.59              |
| 7:DO:244:ARG:O      | 46:Cd:129:ARG:NH2   | 2.36                     | 0.59              |
| 15:DB:190:HIS:HD2   | 15:DB:192:ILE:H     | 1.49                     | 0.59              |
| 15:DB:1003:LYS:HE2  | 32:CI:254:MET:O     | 2.03                     | 0.59              |
| 33:CJ:698:HIS:HB3   | 36:CN:65:LYS:NZ     | 2.13                     | 0.59              |
| 55:Cr:18:LEU:HD23   | 55:Cr:90:ILE:HG13   | 1.84                     | 0.59              |
| 68:A4:85:GLN:HE22   | 68:A4:93:ARG:HH12   | 1.50                     | 0.59              |
| 89:Ad:36:LYS:NZ     | 93:Aj:97:GLN:OE1    | 2.35                     | 0.59              |
| 96:Ap:287:TRP:HE1   | 141:UE:9:UNK:HG3    | 1.67                     | 0.59              |
| 102:AA:426:A:O2'    | 102:AA:427:U:OP1    | 2.19                     | 0.59              |
| 102:AA:440:U:O5'    | 115:BM:277:LYS:NZ   | 2.35                     | 0.59              |
| 105:BC:505:ARG:HD3  | 105:BC:517:LEU:HD13 | 1.85                     | 0.59              |
| 111:BI:265:THR:HG21 | 111:BI:305:LYS:NZ   | 2.17                     | 0.59              |
| 119:BQ:75:PRO:O     | 119:BQ:97:ILE:HG21  | 2.03                     | 0.59              |
| 1:DA:985:LYS:HB3    | 1:DA:985:LYS:HZ2    | 1.68                     | 0.59              |
| 1:DA:1003:PHE:HA    | 4:DL:78:ALA:O       | 2.03                     | 0.59              |
| 2:DD:339:ARG:HH22   | 57:CA:85:U:C1'      | 2.15                     | 0.59              |
| 4:DL:118:ASP:OD1    | 4:DL:119:MET:N      | 2.36                     | 0.59              |
| 9:DQ:73:HIS:CE1     | 9:DQ:250:ARG:HB2    | 2.38                     | 0.59              |
| 23:DT:223:LEU:N     | 23:DT:229:GLU:OE1   | 2.31                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 31:CH:146:GLU:OE2   | 31:CH:149:TYR:OH    | 2.12                     | 0.59              |
| 32:CI:54:SER:HB3    | 47:Cg:414:ARG:HH22  | 1.67                     | 0.59              |
| 33:CJ:54:MET:HE1    | 33:CJ:59:PRO:HA     | 1.83                     | 0.59              |
| 33:CJ:261:ALA:O     | 33:CJ:265:CYS:HB2   | 2.03                     | 0.59              |
| 40:CR:153:GLU:HG2   | 56:Cv:183:LEU:HD23  | 1.85                     | 0.59              |
| 45:Cb:168:ALA:HB1   | 45:Cb:174:PHE:HD2   | 1.67                     | 0.59              |
| 93:Aj:274:GLU:HG3   | 109:BG:50:ARG:NH1   | 2.18                     | 0.59              |
| 102:AA:948:A:H61    | 118:BP:220:ARG:H    | 1.51                     | 0.59              |
| 109:BG:99:ILE:HD13  | 109:BG:317:VAL:HG11 | 1.85                     | 0.59              |
| 116:BN:104:ARG:HH22 | 136:Bh:79:ALA:HA    | 1.66                     | 0.59              |
| 127:BY:84:ARG:HH21  | 139:UC:8:UNK:HA     | 1.67                     | 0.59              |
| 1:DA:630:ASP:OD2    | 1:DA:694:ARG:NH1    | 2.36                     | 0.59              |
| 2:DD:283:MET:HE1    | 3:DI:69:PRO:HB3     | 1.84                     | 0.59              |
| 9:DQ:41:GLN:NE2     | 12:DU:123:GLN:H     | 2.00                     | 0.59              |
| 11:DS:128:SER:HB3   | 11:DS:197:GLN:NE2   | 2.18                     | 0.59              |
| 16:DC:973:PRO:HB3   | 22:DK:244:LEU:HD21  | 1.84                     | 0.59              |
| 16:DC:1088:PHE:CE1  | 22:DK:241:VAL:HG21  | 2.37                     | 0.59              |
| 20:DH:274:GLU:CD    | 20:DH:274:GLU:H     | 2.10                     | 0.59              |
| 27:DY:74:PRO:HA     | 40:CR:264:HIS:ND1   | 2.17                     | 0.59              |
| 40:CR:89:VAL:HG21   | 54:Cq:112:LYS:HG3   | 1.85                     | 0.59              |
| 73:AE:92:THR:HG21   | 111:BI:228:GLN:HE22 | 1.68                     | 0.59              |
| 73:AE:115:TYR:OH    | 134:Bf:48:TRP:O     | 2.19                     | 0.59              |
| 77:AK:264:LEU:HD21  | 77:AK:295:ARG:HE    | 1.67                     | 0.59              |
| 96:Ap:290:LEU:HD22  | 141:UE:13:UNK:HG2   | 1.84                     | 0.59              |
| 119:BQ:98:LEU:HG    | 119:BQ:99:LEU:HG    | 1.85                     | 0.59              |
| 8:DP:88:THR:HG22    | 8:DP:90:LEU:H       | 1.67                     | 0.59              |
| 15:DB:940:GLN:OE1   | 15:DB:948:ARG:NH1   | 2.35                     | 0.59              |
| 16:DC:1027:THR:HG22 | 16:DC:1027:THR:O    | 2.01                     | 0.59              |
| 18:DF:53:ARG:HG2    | 18:DF:53:ARG:NH1    | 2.15                     | 0.59              |
| 37:CO:70:HIS:HB3    | 37:CO:71:PRO:CD     | 2.33                     | 0.59              |
| 44:Ca:579:VAL:O     | 57:CA:260:U:O2'     | 2.20                     | 0.59              |
| 64:A0:28:LYS:O      | 64:A0:50:ARG:NH2    | 2.36                     | 0.59              |
| 80:AQ:142:LEU:HD23  | 124:BV:167:GLN:HE21 | 1.67                     | 0.59              |
| 83:AU:20:ILE:HG13   | 114:BL:67:ALA:HB2   | 1.83                     | 0.59              |
| 86:AX:197:ARG:NH2   | 102:AA:529:U:O4'    | 2.36                     | 0.59              |
| 87:AY:10:LYS:O      | 87:AY:14:ARG:HG2    | 2.03                     | 0.59              |
| 96:Ap:123:LYS:NZ    | 146:UM:5:UNK:C      | 2.64                     | 0.59              |
| 102:AA:3:U:H3       | 103:BA:223:LYS:HE3  | 1.66                     | 0.59              |
| 104:BB:357:THR:HA   | 104:BB:364:VAL:HG12 | 1.84                     | 0.59              |
| 107:BE:69:GLU:O     | 107:BE:73:THR:HG22  | 2.02                     | 0.59              |
| 111:BI:77:ASN:O     | 111:BI:80:ASP:N     | 2.35                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 128:BZ:118:PRO:HG3  | 128:BZ:141:LYS:HA   | 1.85                     | 0.59              |
| 140:UD:56:UNK:HA    | 140:UD:59:UNK:HG3   | 1.83                     | 0.59              |
| 1:DA:1179:GLN:O     | 1:DA:1182:ARG:NH1   | 2.36                     | 0.58              |
| 2:DD:735:GLY:HA3    | 3:DI:96:CYS:SG      | 2.43                     | 0.58              |
| 4:DL:74:ARG:HH22    | 29:CE:110:LEU:HD12  | 0.45                     | 0.58              |
| 4:DL:92:ILE:CG2     | 32:CI:248:PHE:CA    | 2.77                     | 0.58              |
| 10:DR:100:ARG:NH1   | 10:DR:122:ALA:HB1   | 2.16                     | 0.58              |
| 11:DS:52:ASP:O      | 11:DS:58:ASN:ND2    | 2.35                     | 0.58              |
| 12:DU:83:ARG:CZ     | 12:DU:157:GLN:HG3   | 2.33                     | 0.58              |
| 15:DB:110:ARG:HH21  | 15:DB:116:GLY:HA2   | 1.66                     | 0.58              |
| 16:DC:50:GLU:OE1    | 16:DC:405:ILE:HD11  | 2.02                     | 0.58              |
| 29:CE:188:GLU:OE2   | 51:Cm:29:TYR:OH     | 2.20                     | 0.58              |
| 31:CH:251:VAL:HG11  | 31:CH:280:MET:HE2   | 1.85                     | 0.58              |
| 45:Cb:287:ARG:HH12  | 55:Cr:52:ARG:HH12   | 1.50                     | 0.58              |
| 50:Ck:130:MET:HE3   | 50:Ck:325:LEU:HD23  | 1.84                     | 0.58              |
| 64:A0:119:ALA:O     | 64:A0:123:ARG:HG2   | 2.03                     | 0.58              |
| 73:AE:218:GLY:N     | 102:AA:1110:A:OP1   | 2.26                     | 0.58              |
| 78:AN:149:ARG:HH12  | 102:AA:836:A:H62    | 1.49                     | 0.58              |
| 86:AX:121:PRO:HG3   | 87:AY:259:MET:HE3   | 1.85                     | 0.58              |
| 104:BB:92:ILE:HD11  | 104:BB:129:TRP:CE2  | 2.38                     | 0.58              |
| 136:Bh:2:ALA:N      | 136:Bh:47:SER:OG    | 2.35                     | 0.58              |
| 4:DL:74:ARG:CZ      | 29:CE:110:LEU:CD1   | 2.77                     | 0.58              |
| 18:DF:343:GLU:HB3   | 18:DF:345:LEU:HG    | 1.84                     | 0.58              |
| 18:DF:462:ARG:HH11  | 18:DF:474:GLN:NE2   | 2.01                     | 0.58              |
| 32:CI:409:PRO:HG3   | 40:CR:253:PHE:CZ    | 2.35                     | 0.58              |
| 34:CK:113:ARG:NH2   | 40:CR:192:GLU:OE1   | 2.36                     | 0.58              |
| 42:CU:108:PHE:HZ    | 51:Cm:85:ILE:HG23   | 1.68                     | 0.58              |
| 56:Cv:318:PHE:HE1   | 56:Cv:887:ARG:HB2   | 1.68                     | 0.58              |
| 67:A3:140:ASP:N     | 67:A3:140:ASP:OD1   | 2.34                     | 0.58              |
| 81:AR:78:ILE:HD11   | 81:AR:100:VAL:HG11  | 1.85                     | 0.58              |
| 98:Av:88:VAL:HG11   | 98:Av:138:LEU:HD11  | 1.85                     | 0.58              |
| 108:BF:211:GLU:OE1  | 108:BF:281:ARG:NH1  | 2.33                     | 0.58              |
| 115:BM:232:LEU:HD11 | 120:BR:171:LEU:HD12 | 1.84                     | 0.58              |
| 117:BO:75:PHE:O     | 117:BO:77:ALA:N     | 2.36                     | 0.58              |
| 119:BQ:115:ASP:HB3  | 119:BQ:159:VAL:HG21 | 1.83                     | 0.58              |
| 1:DA:1003:PHE:HD1   | 4:DL:78:ALA:HA      | 1.59                     | 0.58              |
| 4:DL:302:PRO:HD2    | 32:CI:422:ARG:HH21  | 1.67                     | 0.58              |
| 11:DS:150:GLN:HE22  | 11:DS:176:ARG:HH21  | 1.50                     | 0.58              |
| 15:DB:519:PHE:HD2   | 15:DB:522:MET:HE2   | 1.67                     | 0.58              |
| 15:DB:859:GLY:O     | 50:Ck:104:SER:HB2   | 2.02                     | 0.58              |
| 17:DE:732:ASP:OD1   | 17:DE:735:ARG:NH2   | 2.35                     | 0.58              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 29:CE:115:ASN:HD22 | 29:CE:134:GLY:HA2   | 1.68                     | 0.58              |
| 31:CH:259:ASP:HB3  | 31:CH:261:ARG:HD3   | 1.85                     | 0.58              |
| 53:Cp:171:MET:HE2  | 53:Cp:175:ALA:HB1   | 1.85                     | 0.58              |
| 79:AP:175:LEU:HD23 | 79:AP:234:LEU:HD11  | 1.85                     | 0.58              |
| 79:AP:196:THR:H    | 79:AP:199:HIS:HD2   | 1.51                     | 0.58              |
| 83:AU:83:GLU:HG3   | 91:Af:77:VAL:HG23   | 1.85                     | 0.58              |
| 2:DD:181:MET:HE1   | 2:DD:215:TYR:HD1    | 1.68                     | 0.58              |
| 5:DM:76:ASN:HD21   | 56:Cv:971:LEU:H     | 1.51                     | 0.58              |
| 12:DU:94:TRP:CH2   | 12:DU:196:MET:HE1   | 2.38                     | 0.58              |
| 17:DE:184:PHE:O    | 17:DE:536:ARG:NH1   | 2.37                     | 0.58              |
| 21:DJ:223:MET:HE1  | 21:DJ:233:VAL:HG21  | 1.85                     | 0.58              |
| 32:CI:250:ASN:ND2  | 32:CI:276:ASP:OD2   | 2.36                     | 0.58              |
| 33:CJ:661:ARG:O    | 33:CJ:663:PRO:HD3   | 2.03                     | 0.58              |
| 39:CQ:48:ARG:NH2   | 57:CA:375:A:O2'     | 2.36                     | 0.58              |
| 47:Cg:342:MET:HE3  | 47:Cg:351:LYS:HG2   | 1.84                     | 0.58              |
| 50:Ck:135:ASN:ND2  | 50:Ck:137:THR:O     | 2.37                     | 0.58              |
| 74:AF:392:ASP:OD1  | 74:AF:393:CYS:N     | 2.37                     | 0.58              |
| 108:BF:326:ASP:OD1 | 108:BF:327:PHE:N    | 2.37                     | 0.58              |
| 118:BP:145:PRO:HD2 | 118:BP:178:PRO:HD3  | 1.84                     | 0.58              |
| 140:UD:47:UNK:HB1  | 140:UD:147:UNK:HG3  | 1.84                     | 0.58              |
| 2:DD:575:THR:HG22  | 2:DD:577:LYS:HB2    | 1.86                     | 0.58              |
| 13:DZ:13:ALA:H     | 44:Ca:177:GLN:HE22  | 1.51                     | 0.58              |
| 34:CK:320:MET:N    | 42:CU:81:GLU:HG2    | 2.18                     | 0.58              |
| 37:CO:207:TYR:HB3  | 37:CO:226:VAL:HG11  | 1.85                     | 0.58              |
| 48:Ci:34:ARG:NH1   | 48:Ci:43:GLU:OE1    | 2.36                     | 0.58              |
| 66:A2:170:ILE:HD13 | 66:A2:326:ILE:HG23  | 1.86                     | 0.58              |
| 73:AE:73:LEU:HD23  | 73:AE:73:LEU:H      | 1.68                     | 0.58              |
| 74:AF:144:LEU:HD22 | 74:AF:226:MET:HE2   | 1.83                     | 0.58              |
| 76:AJ:58:ASN:HA    | 96:Ap:222:PHE:CD1   | 2.37                     | 0.58              |
| 83:AU:164:SER:O    | 83:AU:169:ARG:NH2   | 2.37                     | 0.58              |
| 85:AW:239:GLU:OE1  | 85:AW:239:GLU:N     | 2.36                     | 0.58              |
| 86:AX:146:LEU:HD21 | 86:AX:151:VAL:HG21  | 1.86                     | 0.58              |
| 89:Ad:221:GLN:NE2  | 132:Bd:47:ARG:HE    | 2.01                     | 0.58              |
| 93:Aj:101:ALA:HB2  | 132:Bd:117:THR:HG21 | 1.84                     | 0.58              |
| 96:Ap:185:VAL:HG13 | 96:Ap:197:GLN:HE22  | 1.67                     | 0.58              |
| 96:Ap:232:ILE:HD12 | 96:Ap:255:LEU:HD23  | 1.86                     | 0.58              |
| 103:BA:296:ARG:HG3 | 103:BA:296:ARG:NH1  | 2.18                     | 0.58              |
| 114:BL:237:ASN:OD1 | 114:BL:237:ASN:N    | 2.34                     | 0.58              |
| 2:DD:156:GLN:HE22  | 46:Cd:67:GLU:HG3    | 1.68                     | 0.58              |
| 16:DC:36:ASP:OD1   | 16:DC:36:ASP:N      | 2.34                     | 0.58              |
| 19:DG:490:ARG:HD3  | 19:DG:571:VAL:HG11  | 1.85                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 19:DG:529:ASP:OD1   | 19:DG:529:ASP:N     | 2.36                     | 0.58              |
| 29:CE:32:TRP:CD1    | 29:CE:33:MET:HG3    | 2.39                     | 0.58              |
| 34:CK:53:ARG:NH2    | 40:CR:234:ALA:HB1   | 2.18                     | 0.58              |
| 34:CK:322:ARG:HH11  | 34:CK:326:LYS:HE2   | 1.69                     | 0.58              |
| 36:CN:158:ARG:NH1   | 36:CN:159:ASN:OD1   | 2.37                     | 0.58              |
| 45:Cb:56:ARG:HH11   | 45:Cb:57:MET:HE1    | 1.69                     | 0.58              |
| 56:Cv:27:LYS:HD2    | 56:Cv:29:LEU:H      | 1.68                     | 0.58              |
| 66:A2:463:ILE:HG13  | 122:BT:42:MET:HE2   | 1.84                     | 0.58              |
| 104:BB:87:LEU:HA    | 104:BB:90:LYS:NZ    | 2.18                     | 0.58              |
| 107:BE:255:TYR:CE1  | 107:BE:288:LEU:HD23 | 2.38                     | 0.58              |
| 111:BI:152:GLN:HE22 | 134:Bf:99:ILE:HA    | 1.68                     | 0.58              |
| 116:BN:205:ASP:OD1  | 116:BN:209:LYS:N    | 2.26                     | 0.58              |
| 119:BQ:226:ILE:HG23 | 119:BQ:227:LEU:HG   | 1.84                     | 0.58              |
| 140:UD:215:UNK:HA   | 140:UD:218:UNK:HG3  | 1.84                     | 0.58              |
| 1:DA:212:ARG:HD2    | 11:DS:134:GLN:NE2   | 2.18                     | 0.58              |
| 1:DA:1181:THR:OG1   | 1:DA:1182:ARG:CZ    | 2.51                     | 0.58              |
| 6:DN:183:ARG:NE     | 6:DN:194:ARG:HH12   | 2.00                     | 0.58              |
| 15:DB:232:ARG:HG2   | 16:DC:953:MET:HE3   | 1.85                     | 0.58              |
| 15:DB:546:ARG:HH21  | 15:DB:550:LEU:HD21  | 1.69                     | 0.58              |
| 44:Ca:570:THR:O     | 57:CA:30:U:O2'      | 2.17                     | 0.58              |
| 66:A2:146:SER:HB3   | 66:A2:348:ALA:O     | 2.03                     | 0.58              |
| 69:A5:79:LYS:O      | 103:BA:785:ARG:NH2  | 2.37                     | 0.58              |
| 70:A6:94:LYS:NZ     | 79:AP:345:TRP:CZ3   | 2.72                     | 0.58              |
| 72:A9:100:TRP:CG    | 72:A9:101:LEU:H     | 2.22                     | 0.58              |
| 74:AF:418:SER:HB2   | 98:Av:78:ARG:HH22   | 1.68                     | 0.58              |
| 81:AR:201:ARG:HG2   | 81:AR:201:ARG:HH11  | 1.67                     | 0.58              |
| 84:AV:59:LEU:HB2    | 84:AV:182:PRO:HG2   | 1.86                     | 0.58              |
| 85:AW:19:ASN:OD1    | 102:AA:294:U:O2'    | 2.22                     | 0.58              |
| 102:AA:534:U:O2'    | 102:AA:535:U:OP1    | 2.20                     | 0.58              |
| 103:BA:615:SER:HB3  | 103:BA:672:GLU:HA   | 1.85                     | 0.58              |
| 104:BB:84:PHE:O     | 104:BB:88:GLU:HB2   | 2.04                     | 0.58              |
| 105:BC:463:ARG:HH11 | 105:BC:463:ARG:HG3  | 1.69                     | 0.58              |
| 112:BJ:240:VAL:HA   | 112:BJ:243:LYS:NZ   | 2.18                     | 0.58              |
| 115:BM:204:LEU:HG   | 115:BM:208:LYS:HE3  | 1.85                     | 0.58              |
| 1:DA:776:GLY:O      | 1:DA:925:SER:HA     | 2.03                     | 0.58              |
| 1:DA:1060:LEU:HD13  | 1:DA:1163:MET:HE1   | 1.86                     | 0.58              |
| 5:DM:271:ARG:NH2    | 54:Cq:21:MET:SD     | 2.76                     | 0.58              |
| 10:DR:149:ALA:HB3   | 10:DR:152:ALA:HB2   | 1.85                     | 0.58              |
| 15:DB:975:LYS:HG2   | 19:DG:92:GLN:NE2    | 2.19                     | 0.58              |
| 16:DC:77:ASP:H      | 16:DC:81:HIS:CD2    | 2.21                     | 0.58              |
| 16:DC:455:TYR:CD1   | 16:DC:485:ILE:HD11  | 2.39                     | 0.58              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 18:DF:188:ARG:HD3  | 150:DJ:401:UTP:H2'  | 1.85                     | 0.58              |
| 19:DG:65:ASN:HD21  | 32:CI:294:ILE:H     | 1.52                     | 0.58              |
| 20:DH:502:GLU:OE2  | 22:DK:301:ARG:HG3   | 2.04                     | 0.58              |
| 23:DT:44:ARG:HB2   | 23:DT:218:MET:HE2   | 1.86                     | 0.58              |
| 23:DT:145:GLU:OE1  | 23:DT:149:TRP:NE1   | 2.36                     | 0.58              |
| 56:Cv:311:LEU:HD21 | 56:Cv:389:LEU:HD23  | 1.85                     | 0.58              |
| 56:Cv:561:SER:HG   | 56:Cv:564:ASP:H     | 1.52                     | 0.58              |
| 77:AK:304:GLU:OE2  | 77:AK:307:ARG:NH1   | 2.37                     | 0.58              |
| 86:AX:88:TYR:CE1   | 129:Ba:21:MET:HG3   | 2.38                     | 0.58              |
| 92:Ag:162:ARG:HE   | 111:BI:280:VAL:HG21 | 1.69                     | 0.58              |
| 94:Al:88:ARG:NH1   | 94:Al:88:ARG:HG2    | 2.19                     | 0.58              |
| 102:AA:524:A:H2'   | 102:AA:525:A:H5'    | 1.86                     | 0.58              |
| 107:BE:236:ARG:HB3 | 107:BE:236:ARG:NH1  | 2.19                     | 0.58              |
| 17:DE:147:MET:HE1  | 17:DE:567:HIS:CG    | 2.39                     | 0.58              |
| 20:DH:421:THR:HG21 | 20:DH:469:ASN:HD21  | 1.67                     | 0.58              |
| 25:DW:104:VAL:HB   | 40:CR:279:LYS:HG3   | 1.83                     | 0.58              |
| 29:CE:280:ARG:HD2  | 31:CH:217:ASN:HD21  | 1.69                     | 0.58              |
| 33:CJ:119:ARG:HG2  | 33:CJ:119:ARG:HH11  | 1.68                     | 0.58              |
| 33:CJ:345:VAL:HG22 | 33:CJ:346:PRO:HD2   | 1.85                     | 0.58              |
| 34:CK:14:PRO:CA    | 40:CR:300:TYR:CE2   | 2.87                     | 0.58              |
| 49:Cj:28:LYS:NZ    | 49:Cj:28:LYS:HB3    | 2.19                     | 0.58              |
| 51:Cm:141:TRP:NE1  | 57:CA:394:A:N6      | 2.51                     | 0.58              |
| 55:Cr:46:GLY:HA3   | 55:Cr:176:LEU:HD11  | 1.86                     | 0.58              |
| 73:AE:316:ILE:HG12 | 73:AE:323:ILE:HG13  | 1.85                     | 0.58              |
| 84:AV:147:ARG:NH1  | 92:Ag:96:PRO:HD3    | 2.19                     | 0.58              |
| 85:AW:131:HIS:NE2  | 87:AY:46:GLU:OE1    | 2.33                     | 0.58              |
| 93:Aj:48:ALA:HB2   | 93:Aj:237:LEU:HD11  | 1.85                     | 0.58              |
| 102:AA:318:A:N6    | 102:AA:343:U:H3     | 2.02                     | 0.58              |
| 117:BO:141:ASP:HB2 | 117:BO:153:ARG:H    | 1.68                     | 0.58              |
| 1:DA:910:HIS:CD2   | 44:Ca:318:ASP:HB2   | 2.39                     | 0.58              |
| 2:DD:700:ASP:HB2   | 2:DD:709:ARG:HD3    | 1.85                     | 0.58              |
| 12:DU:207:ARG:HB2  | 57:CA:160:U:C5      | 2.39                     | 0.58              |
| 21:DJ:27:GLN:HG2   | 28:CC:66:ASN:HD22   | 1.69                     | 0.58              |
| 22:DK:62:PHE:CE1   | 22:DK:102:LYS:HD3   | 2.39                     | 0.58              |
| 34:CK:14:PRO:N     | 40:CR:300:TYR:CE2   | 2.72                     | 0.58              |
| 40:CR:89:VAL:O     | 45:Cb:112:TYR:OH    | 2.22                     | 0.58              |
| 48:Ci:83:ASN:ND2   | 57:CA:507:A:N3      | 2.52                     | 0.58              |
| 71:A8:126:ARG:NH1  | 94:Al:156:ARG:O     | 2.37                     | 0.58              |
| 82:AT:28:ARG:HH11  | 82:AT:28:ARG:HG3    | 1.68                     | 0.58              |
| 84:AV:100:GLN:NE2  | 102:AA:466:G:H21    | 1.98                     | 0.58              |
| 102:AA:48:U:O5'    | 129:Ba:105:ARG:NH2  | 2.37                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 103:BA:582:PHE:HD1  | 103:BA:693:HIS:HB2  | 1.68                     | 0.58              |
| 103:BA:676:LEU:HD11 | 103:BA:694:THR:HG23 | 1.86                     | 0.58              |
| 6:DN:26:ARG:HD2     | 44:Ca:406:MET:O     | 2.04                     | 0.57              |
| 6:DN:123:GLN:HG2    | 6:DN:160:CYS:HB3    | 1.85                     | 0.57              |
| 7:DO:151:GLU:HB2    | 56:Cv:608:ARG:HD3   | 1.86                     | 0.57              |
| 25:DW:114:LEU:O     | 40:CR:294:LYS:NZ    | 2.36                     | 0.57              |
| 33:CJ:730:TRP:CE2   | 33:CJ:731:MET:HG2   | 2.38                     | 0.57              |
| 34:CK:258:LEU:HD13  | 34:CK:275:VAL:HG21  | 1.86                     | 0.57              |
| 37:CO:371:LYS:NZ    | 37:CO:382:GLU:OE2   | 2.32                     | 0.57              |
| 50:Ck:204:LEU:HD11  | 50:Ck:254:ILE:HG22  | 1.86                     | 0.57              |
| 56:Cv:305:ASP:OD1   | 56:Cv:305:ASP:N     | 2.27                     | 0.57              |
| 56:Cv:367:ASP:OD1   | 56:Cv:367:ASP:N     | 2.35                     | 0.57              |
| 67:A3:60:ARG:HG2    | 67:A3:60:ARG:HH11   | 1.69                     | 0.57              |
| 75:AI:44:ASP:OD2    | 75:AI:48:ARG:NH1    | 2.36                     | 0.57              |
| 81:AR:186:PHE:CD2   | 107:BE:424:ASN:HB3  | 2.39                     | 0.57              |
| 89:Ad:99:THR:HG21   | 93:Aj:227:THR:HG21  | 1.86                     | 0.57              |
| 96:Ap:163:VAL:HG23  | 96:Ap:164:VAL:HG23  | 1.86                     | 0.57              |
| 120:BR:46:VAL:HA    | 120:BR:49:LYS:HG2   | 1.86                     | 0.57              |
| 123:BU:139:ARG:HD2  | 135:Bg:35:LEU:HD21  | 1.86                     | 0.57              |
| 1:DA:1016:MET:HG2   | 29:CE:110:LEU:HD11  | 1.84                     | 0.57              |
| 4:DL:266:GLY:HA3    | 34:CK:22:PRO:HD3    | 1.86                     | 0.57              |
| 15:DB:1154:LYS:HD3  | 89:Ad:150:ARG:CG    | 2.34                     | 0.57              |
| 19:DG:394:PRO:O     | 19:DG:451:ARG:NH1   | 2.37                     | 0.57              |
| 32:CI:409:PRO:CA    | 40:CR:253:PHE:CE2   | 2.86                     | 0.57              |
| 49:Cj:50:VAL:HG22   | 57:CA:51:U:H2'      | 1.86                     | 0.57              |
| 66:A2:167:HIS:CD2   | 66:A2:169:GLY:H     | 2.22                     | 0.57              |
| 79:AP:343:GLN:O     | 79:AP:348:ASN:ND2   | 2.37                     | 0.57              |
| 87:AY:285:MET:HE2   | 112:BJ:250:LEU:HD22 | 1.86                     | 0.57              |
| 107:BE:82:GLU:CD    | 107:BE:82:GLU:H     | 2.10                     | 0.57              |
| 112:BJ:192:ARG:HH22 | 137:UA:34:UNK:CB    | 2.17                     | 0.57              |
| 116:BN:14:HIS:O     | 136:Bh:91:ARG:NH2   | 2.37                     | 0.57              |
| 130:Bb:59:ILE:HG23  | 130:Bb:78:LEU:HD23  | 1.86                     | 0.57              |
| 134:Bf:44:ARG:NH1   | 141:UE:6:UNK:HA     | 2.19                     | 0.57              |
| 16:DC:149:ARG:HB3   | 16:DC:155:VAL:HG21  | 1.85                     | 0.57              |
| 16:DC:219:LEU:HD11  | 16:DC:249:LYS:HA    | 1.86                     | 0.57              |
| 17:DE:539:ARG:HG2   | 17:DE:539:ARG:HH11  | 1.69                     | 0.57              |
| 37:CO:124:ILE:HG13  | 37:CO:168:GLU:HG3   | 1.85                     | 0.57              |
| 56:Cv:405:PRO:HB3   | 56:Cv:427:TYR:HE2   | 1.69                     | 0.57              |
| 66:A2:186:GLU:HB3   | 75:AI:52:TRP:CE3    | 2.40                     | 0.57              |
| 78:AN:11:PRO:N      | 102:AA:8:C:H4'      | 2.20                     | 0.57              |
| 88:Ab:256:SER:HB2   | 88:Ab:344:HIS:ND1   | 2.19                     | 0.57              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 102:AA:407:G:N2     | 102:AA:410:U:OP2   | 2.34                     | 0.57              |
| 102:AA:440:U:H4'    | 102:AA:441:A:O5'   | 2.04                     | 0.57              |
| 105:BC:230:MET:SD   | 105:BC:230:MET:N   | 2.71                     | 0.57              |
| 111:BI:263:HIS:HB2  | 111:BI:302:PRO:HB2 | 1.86                     | 0.57              |
| 116:BN:201:LEU:HD12 | 116:BN:202:PRO:HD2 | 1.86                     | 0.57              |
| 120:BR:127:ARG:HB3  | 142:UF:20:UNK:HA   | 1.87                     | 0.57              |
| 121:BS:72:THR:HG22  | 121:BS:74:GLU:H    | 1.70                     | 0.57              |
| 1:DA:602:LEU:HB3    | 1:DA:803:LEU:HB2   | 1.84                     | 0.57              |
| 2:DD:576:MET:HE1    | 2:DD:606:ARG:HB2   | 1.87                     | 0.57              |
| 9:DQ:14:ARG:HB2     | 9:DQ:14:ARG:NH1    | 2.20                     | 0.57              |
| 9:DQ:92:MET:HE1     | 9:DQ:210:VAL:HG11  | 1.85                     | 0.57              |
| 31:CH:113:LYS:O     | 31:CH:120:TYR:OH   | 2.21                     | 0.57              |
| 31:CH:176:ILE:HD13  | 31:CH:179:ARG:HH12 | 1.69                     | 0.57              |
| 34:CK:14:PRO:HG3    | 40:CR:300:TYR:CZ   | 2.39                     | 0.57              |
| 55:Cr:10:ARG:HH12   | 55:Cr:13:ARG:CB    | 2.17                     | 0.57              |
| 66:A2:61:LEU:HD23   | 66:A2:84:LEU:HG    | 1.85                     | 0.57              |
| 71:A8:59:THR:HG23   | 74:AF:318:ALA:HB2  | 1.86                     | 0.57              |
| 71:A8:173:ARG:NH1   | 74:AF:442:GLY:O    | 2.37                     | 0.57              |
| 81:AR:79:ARG:O      | 81:AR:127:LYS:NZ   | 2.38                     | 0.57              |
| 89:Ad:160:PRO:HB2   | 89:Ad:185:LEU:HD11 | 1.86                     | 0.57              |
| 97:At:42:GLU:OE1    | 97:At:45:ARG:NH1   | 2.31                     | 0.57              |
| 103:BA:791:PHE:HE1  | 103:BA:801:ARG:HD3 | 1.69                     | 0.57              |
| 105:BC:60:LEU:H     | 105:BC:292:ASN:ND2 | 2.00                     | 0.57              |
| 109:BG:73:PRO:HB2   | 109:BG:74:ARG:HD3  | 1.86                     | 0.57              |
| 110:BH:165:GLN:O    | 110:BH:241:ARG:NH1 | 2.37                     | 0.57              |
| 113:BK:87:LEU:HD21  | 113:BK:139:VAL:HB  | 1.87                     | 0.57              |
| 1:DA:333:VAL:HG13   | 13:DZ:62:ASP:HB2   | 1.87                     | 0.57              |
| 4:DL:190:ARG:NH1    | 40:CR:71:PHE:CE1   | 2.73                     | 0.57              |
| 6:DN:47:VAL:HG22    | 6:DN:132:TYR:HB2   | 1.86                     | 0.57              |
| 13:DZ:20:ARG:HG3    | 13:DZ:20:ARG:NH1   | 2.19                     | 0.57              |
| 22:DK:2:SER:HA      | 23:DT:133:ASP:OD2  | 2.04                     | 0.57              |
| 23:DT:16:HIS:NE2    | 48:CI:138:ASP:OD1  | 2.37                     | 0.57              |
| 30:CF:133:GLN:NE2   | 46:Cd:178:ASN:O    | 2.37                     | 0.57              |
| 48:CI:107:ILE:HD11  | 48:CI:113:ALA:HB2  | 1.85                     | 0.57              |
| 56:Cv:559:GLN:HG3   | 61:UR:3:UNK:HB1    | 1.87                     | 0.57              |
| 65:A1:50:ASN:HB3    | 102:AA:70:G:H4'    | 1.85                     | 0.57              |
| 67:A3:86:ARG:NH2    | 108:BF:27:THR:O    | 2.37                     | 0.57              |
| 71:A8:168:LEU:HD13  | 79:AP:165:ARG:NH1  | 2.19                     | 0.57              |
| 74:AF:102:ILE:HD11  | 74:AF:132:PRO:HG2  | 1.86                     | 0.57              |
| 77:AK:334:TYR:HD1   | 92:Ag:218:GLU:HA   | 1.69                     | 0.57              |
| 79:AP:116:GLY:H     | 102:AA:321:A:H4'   | 1.67                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 88:Ab:109:PHE:HE1  | 105:BC:243:VAL:HG11 | 1.70                     | 0.57              |
| 93:Aj:268:GLU:OE1  | 93:Aj:268:GLU:N     | 2.34                     | 0.57              |
| 94:Al:201:VAL:HG13 | 94:Al:205:GLY:HA3   | 1.85                     | 0.57              |
| 96:Ap:106:LYS:NZ   | 96:Ap:106:LYS:HB3   | 2.19                     | 0.57              |
| 110:BH:88:GLU:HB3  | 127:BY:150:GLN:HE22 | 1.69                     | 0.57              |
| 4:DL:92:ILE:HG23   | 32:CI:248:PHE:HA    | 1.82                     | 0.57              |
| 20:DH:520:GLY:HA2  | 23:DT:122:MET:HE3   | 1.84                     | 0.57              |
| 32:CI:191:LEU:HD11 | 54:Cq:257:MET:HE3   | 1.87                     | 0.57              |
| 56:Cv:77:TYR:HB2   | 56:Cv:165:GLU:HG3   | 1.86                     | 0.57              |
| 57:CA:110:U:H5'    | 57:CA:111:A:OP2     | 2.05                     | 0.57              |
| 57:CA:310:A:N3     | 57:CA:310:A:H2'     | 2.19                     | 0.57              |
| 73:AE:106:ARG:NH1  | 96:Ap:124:PRO:HG3   | 2.19                     | 0.57              |
| 77:AK:200:SER:HB3  | 124:BV:80:LYS:HD2   | 1.85                     | 0.57              |
| 78:AN:80:GLY:H     | 78:AN:155:LYS:NZ    | 2.02                     | 0.57              |
| 87:AY:194:ARG:HD3  | 87:AY:199:GLY:HA2   | 1.87                     | 0.57              |
| 98:Av:182:LYS:NZ   | 98:Av:182:LYS:HB3   | 2.19                     | 0.57              |
| 102:AA:1096:U:H2'  | 102:AA:1097:A:H8    | 1.69                     | 0.57              |
| 105:BC:285:TYR:OH  | 105:BC:427:LEU:O    | 2.22                     | 0.57              |
| 116:BN:22:ARG:C    | 116:BN:191:ARG:HH12 | 2.12                     | 0.57              |
| 128:BZ:83:ILE:HG21 | 128:BZ:166:ILE:HD11 | 1.86                     | 0.57              |
| 15:DB:514:ARG:HG3  | 15:DB:517:GLU:OE1   | 2.03                     | 0.57              |
| 31:CH:133:ARG:NH2  | 56:Cv:108:HIS:HB2   | 2.19                     | 0.57              |
| 32:CI:439:ARG:NH1  | 57:CA:496:U:O4      | 2.37                     | 0.57              |
| 44:Ca:225:PRO:HG2  | 44:Ca:228:LYS:HB2   | 1.86                     | 0.57              |
| 44:Ca:597:LYS:HB2  | 44:Ca:597:LYS:NZ    | 2.20                     | 0.57              |
| 66:A2:396:GLU:HA   | 66:A2:399:THR:HB    | 1.86                     | 0.57              |
| 69:A5:65:LYS:NZ    | 69:A5:65:LYS:HB3    | 2.19                     | 0.57              |
| 73:AE:234:ASP:OD1  | 73:AE:235:VAL:N     | 2.35                     | 0.57              |
| 79:AP:84:GLN:HE22  | 79:AP:96:ASP:HB3    | 1.69                     | 0.57              |
| 91:Af:164:HIS:CD2  | 91:Af:166:LYS:HE2   | 2.40                     | 0.57              |
| 11:DS:32:PHE:O     | 57:CA:206:A:O2'     | 2.22                     | 0.57              |
| 19:DG:392:ARG:HH11 | 19:DG:392:ARG:HG2   | 1.69                     | 0.57              |
| 21:DJ:192:THR:HG21 | 21:DJ:222:GLU:CG    | 2.33                     | 0.57              |
| 24:DV:179:LEU:HD22 | 47:Cg:117:LEU:HG    | 1.86                     | 0.57              |
| 33:CJ:108:ASP:OD1  | 33:CJ:108:ASP:N     | 2.38                     | 0.57              |
| 34:CK:215:ARG:NH1  | 34:CK:218:ASN:HA    | 2.19                     | 0.57              |
| 34:CK:322:ARG:NH1  | 34:CK:326:LYS:HE2   | 2.19                     | 0.57              |
| 37:CO:399:ILE:HD12 | 37:CO:400:ARG:H     | 1.69                     | 0.57              |
| 41:CS:44:ARG:NH1   | 57:CA:493:U:O2'     | 2.38                     | 0.57              |
| 66:A2:255:ARG:HG2  | 66:A2:255:ARG:NH1   | 2.20                     | 0.57              |
| 73:AE:224:ASP:N    | 73:AE:224:ASP:OD1   | 2.31                     | 0.57              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 75:AI:21:LYS:HD2    | 75:AI:24:MET:HB2   | 1.86                     | 0.57              |
| 88:Ab:155:LEU:HD11  | 88:Ab:347:MET:HE3  | 1.87                     | 0.57              |
| 88:Ab:162:VAL:HG12  | 88:Ab:225:ASP:HA   | 1.86                     | 0.57              |
| 90:Ae:130:TYR:HB3   | 102:AA:540:U:H5    | 1.69                     | 0.57              |
| 107:BE:446:MET:HG2  | 107:BE:447:GLU:HG3 | 1.85                     | 0.57              |
| 134:Bf:44:ARG:NE    | 141:UE:1:UNK:HG2   | 2.20                     | 0.57              |
| 6:DN:288:PHE:HD1    | 6:DN:288:PHE:H     | 1.52                     | 0.57              |
| 19:DG:111:ARG:CZ    | 45:Cb:197:PRO:HB3  | 2.33                     | 0.57              |
| 31:CH:97:ARG:HG2    | 56:Cv:246:ARG:HD2  | 1.85                     | 0.57              |
| 47:Cg:406:GLU:OE2   | 47:Cg:406:GLU:N    | 2.35                     | 0.57              |
| 79:AP:16:PRO:HG2    | 79:AP:19:GLU:OE2   | 2.04                     | 0.57              |
| 88:Ab:175:ARG:HH12  | 105:BC:91:ALA:HB3  | 1.70                     | 0.57              |
| 102:AA:877:A:H62    | 102:AA:893:A:H2    | 1.52                     | 0.57              |
| 103:BA:733:LEU:HD23 | 103:BA:733:LEU:H   | 1.70                     | 0.57              |
| 131:Bc:60:GLU:H     | 131:Bc:60:GLU:CD   | 2.12                     | 0.57              |
| 1:DA:1414:LEU:HD21  | 1:DA:1421:GLU:HG3  | 1.87                     | 0.57              |
| 1:DA:1507:VAL:HB    | 5:DM:175:GLU:HG3   | 1.87                     | 0.57              |
| 10:DR:67:LYS:HA     | 10:DR:67:LYS:HZ3   | 1.67                     | 0.57              |
| 18:DF:187:ASN:HD22  | 18:DF:191:THR:HB   | 1.69                     | 0.57              |
| 19:DG:77:CYS:HB2    | 19:DG:83:MET:HG3   | 1.87                     | 0.57              |
| 40:CR:318:LYS:N     | 46:Cd:283:GLU:OE2  | 2.37                     | 0.57              |
| 44:Ca:62:TRP:CD1    | 44:Ca:79:MET:HE1   | 2.40                     | 0.57              |
| 56:Cv:718:THR:N     | 56:Cv:757:ASP:HB2  | 2.19                     | 0.57              |
| 56:Cv:1012:TRP:CD1  | 56:Cv:1014:ARG:HG3 | 2.40                     | 0.57              |
| 65:A1:206:ILE:HG23  | 87:AY:297:CYS:SG   | 2.45                     | 0.57              |
| 75:AI:32:VAL:HG13   | 75:AI:33:GLY:H     | 1.69                     | 0.57              |
| 79:AP:167:GLU:OE2   | 118:BP:228:HIS:ND1 | 2.38                     | 0.57              |
| 122:BT:42:MET:HE3   | 125:BW:58:PHE:HE1  | 1.70                     | 0.57              |
| 122:BT:94:TYR:HD2   | 125:BW:80:MET:HE1  | 1.69                     | 0.57              |
| 1:DA:562:LYS:HA     | 1:DA:567:ALA:HB3   | 1.86                     | 0.56              |
| 1:DA:912:LEU:HD12   | 44:Ca:276:SER:HB3  | 1.86                     | 0.56              |
| 4:DL:85:PHE:CA      | 32:CI:270:PHE:CZ   | 2.88                     | 0.56              |
| 6:DN:113:ALA:HB3    | 6:DN:133:PHE:CD1   | 2.37                     | 0.56              |
| 9:DQ:79:LEU:HB3     | 9:DQ:83:ASN:HD21   | 1.70                     | 0.56              |
| 17:DE:101:GLU:O     | 17:DE:105:ASN:ND2  | 2.38                     | 0.56              |
| 19:DG:43:ALA:HB3    | 32:CI:249:GLU:CD   | 2.30                     | 0.56              |
| 20:DH:17:ILE:HD13   | 21:DJ:12:TYR:CE1   | 2.39                     | 0.56              |
| 23:DT:109:GLU:CD    | 23:DT:109:GLU:H    | 2.11                     | 0.56              |
| 36:CN:51:LEU:HD23   | 36:CN:55:LEU:HD23  | 1.86                     | 0.56              |
| 40:CR:314:THR:O     | 46:Cd:279:ARG:CG   | 2.45                     | 0.56              |
| 47:Cg:174:LEU:HD23  | 47:Cg:211:PHE:CE1  | 2.40                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 54:Cq:55:PHE:H     | 54:Cq:93:ASN:HD21   | 1.53                     | 0.56              |
| 55:Cr:19:LEU:HD21  | 55:Cr:41:LEU:HD11   | 1.86                     | 0.56              |
| 56:Cv:79:ASP:O     | 56:Cv:83:TRP:HB2    | 2.05                     | 0.56              |
| 56:Cv:626:VAL:HB   | 56:Cv:628:LYS:HZ1   | 1.70                     | 0.56              |
| 71:A8:130:HIS:HE1  | 102:AA:150:A:O3'    | 1.88                     | 0.56              |
| 74:AF:56:HIS:CD2   | 74:AF:58:LEU:H      | 2.23                     | 0.56              |
| 78:AN:60:VAL:HG21  | 78:AN:176:TRP:CE2   | 2.40                     | 0.56              |
| 89:Ad:165:GLU:HB3  | 89:Ad:174:PHE:CD1   | 2.40                     | 0.56              |
| 93:Aj:290:ALA:HA   | 132:Bd:15:PHE:HZ    | 1.69                     | 0.56              |
| 103:BA:174:ARG:O   | 103:BA:179:SER:OG   | 2.22                     | 0.56              |
| 107:BE:332:ASP:HA  | 107:BE:379:ARG:HH12 | 1.70                     | 0.56              |
| 2:DD:156:GLN:NE2   | 46:Cd:70:ARG:HH11   | 2.02                     | 0.56              |
| 2:DD:626:ARG:NH1   | 49:Cj:156:THR:O     | 2.39                     | 0.56              |
| 3:DI:349:THR:HG23  | 3:DI:350:TYR:CD1    | 2.39                     | 0.56              |
| 7:DO:198:ARG:NH1   | 7:DO:256:ARG:NH1    | 2.53                     | 0.56              |
| 9:DQ:34:THR:O      | 10:DR:27:LYS:NZ     | 2.38                     | 0.56              |
| 42:CU:185:ARG:HD2  | 42:CU:187:ASN:O     | 2.05                     | 0.56              |
| 74:AF:282:SER:O    | 74:AF:358:GLN:NE2   | 2.37                     | 0.56              |
| 86:AX:93:ARG:HH11  | 86:AX:207:MET:HE1   | 1.70                     | 0.56              |
| 111:BI:93:TYR:OH   | 111:BI:132:ILE:HA   | 2.05                     | 0.56              |
| 115:BM:96:ARG:HG3  | 115:BM:96:ARG:O     | 2.05                     | 0.56              |
| 118:BP:145:PRO:HD2 | 118:BP:178:PRO:CD   | 2.35                     | 0.56              |
| 120:BR:60:THR:HB   | 120:BR:62:GLU:OE2   | 2.04                     | 0.56              |
| 128:BZ:96:GLN:HE22 | 128:BZ:125:SER:HA   | 1.70                     | 0.56              |
| 132:Bd:38:TYR:HA   | 132:Bd:41:ILE:HD12  | 1.87                     | 0.56              |
| 1:DA:512:GLU:OE1   | 1:DA:512:GLU:N      | 2.33                     | 0.56              |
| 1:DA:904:TRP:CE2   | 44:Ca:399:ASN:HA    | 2.40                     | 0.56              |
| 1:DA:1065:ALA:H    | 1:DA:1161:GLY:HA3   | 1.71                     | 0.56              |
| 2:DD:537:ARG:HA    | 10:DR:218:TRP:CZ3   | 2.36                     | 0.56              |
| 5:DM:21:ARG:HB3    | 5:DM:236:MET:HE2    | 1.86                     | 0.56              |
| 6:DN:160:CYS:HB2   | 6:DN:162:LEU:HB2    | 1.85                     | 0.56              |
| 6:DN:251:PHE:CD2   | 6:DN:273:SER:HB3    | 2.40                     | 0.56              |
| 12:DU:27:ARG:HB3   | 12:DU:27:ARG:HH11   | 1.70                     | 0.56              |
| 15:DB:78:ARG:HH11  | 15:DB:78:ARG:CG     | 2.17                     | 0.56              |
| 16:DC:78:PRO:O     | 16:DC:82:THR:OG1    | 2.23                     | 0.56              |
| 16:DC:116:TYR:CE2  | 17:DE:572:VAL:HG11  | 2.41                     | 0.56              |
| 16:DC:874:THR:HG22 | 16:DC:875:THR:H     | 1.70                     | 0.56              |
| 18:DF:502:ARG:HH21 | 18:DF:575:VAL:HG11  | 1.71                     | 0.56              |
| 19:DG:186:ARG:HG2  | 19:DG:186:ARG:NH1   | 2.21                     | 0.56              |
| 21:DJ:291:ASN:HD22 | 21:DJ:294:MET:H     | 1.52                     | 0.56              |
| 32:CI:32:LYS:O     | 32:CI:37:ARG:NH2    | 2.38                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:Cp:85:PHE:CD2   | 53:Cp:109:VAL:HG13  | 2.40                     | 0.56              |
| 53:Cp:163:PRO:HG2  | 53:Cp:165:TYR:CE1   | 2.40                     | 0.56              |
| 66:A2:96:ARG:HB2   | 113:BK:358:LEU:HD11 | 1.86                     | 0.56              |
| 67:A3:125:GLU:HG3  | 97:At:82:LEU:HD21   | 1.87                     | 0.56              |
| 68:A4:59:GLU:OE2   | 89:Ad:206:THR:HA    | 2.05                     | 0.56              |
| 68:A4:155:ILE:HG23 | 68:A4:157:LYS:HG2   | 1.86                     | 0.56              |
| 73:AE:347:GLY:HA2  | 96:Ap:46:PRO:HB3    | 1.87                     | 0.56              |
| 74:AF:80:GLN:NE2   | 125:BW:162:LYS:HG3  | 2.20                     | 0.56              |
| 80:AQ:51:ILE:HD12  | 80:AQ:155:VAL:HG21  | 1.87                     | 0.56              |
| 81:AR:253:LYS:HG3  | 81:AR:254:GLU:H     | 1.70                     | 0.56              |
| 87:AY:50:LEU:HD13  | 87:AY:62:MET:HE1    | 1.87                     | 0.56              |
| 87:AY:66:ARG:NE    | 102:AA:514:G:OP1    | 2.38                     | 0.56              |
| 89:Ad:92:ARG:NH1   | 93:Aj:284:VAL:HG22  | 2.20                     | 0.56              |
| 90:Ae:133:LYS:NZ   | 90:Ae:133:LYS:HB3   | 2.19                     | 0.56              |
| 93:Aj:273:GLU:HG2  | 109:BG:50:ARG:NH1   | 2.21                     | 0.56              |
| 98:Av:233:THR:HG21 | 132:Bd:104:ARG:HD3  | 1.87                     | 0.56              |
| 102:AA:521:G:O2'   | 102:AA:561:U:O4     | 2.17                     | 0.56              |
| 103:BA:502:HIS:CD2 | 103:BA:641:GLU:HB3  | 2.40                     | 0.56              |
| 103:BA:753:ASP:OD1 | 103:BA:753:ASP:N    | 2.38                     | 0.56              |
| 105:BC:217:PHE:HB3 | 105:BC:219:PHE:CE1  | 2.41                     | 0.56              |
| 114:BL:281:SER:N   | 114:BL:284:ARG:NH1  | 2.52                     | 0.56              |
| 5:DM:217:ALA:O     | 5:DM:221:LYS:NZ     | 2.39                     | 0.56              |
| 8:DP:20:MET:O      | 8:DP:23:LEU:HB2     | 2.06                     | 0.56              |
| 10:DR:101:VAL:HG21 | 10:DR:123:VAL:HG12  | 1.86                     | 0.56              |
| 10:DR:128:PRO:CG   | 10:DR:133:LEU:N     | 2.65                     | 0.56              |
| 18:DF:443:LEU:HD13 | 18:DF:452:VAL:HG11  | 1.87                     | 0.56              |
| 21:DJ:87:PRO:HB3   | 21:DJ:92:LEU:HD12   | 1.87                     | 0.56              |
| 24:DV:31:HIS:CE1   | 24:DV:48:HIS:HE1    | 2.23                     | 0.56              |
| 25:DW:58:ARG:HH11  | 25:DW:58:ARG:CG     | 2.05                     | 0.56              |
| 29:CE:110:LEU:HB2  | 29:CE:113:GLU:HG3   | 1.87                     | 0.56              |
| 34:CK:113:ARG:HG2  | 34:CK:113:ARG:HH11  | 1.70                     | 0.56              |
| 34:CK:231:ASP:HB3  | 34:CK:232:ARG:HD2   | 1.87                     | 0.56              |
| 44:Ca:569:ARG:NH1  | 57:CA:143:U:OP1     | 2.37                     | 0.56              |
| 48:Ci:34:ARG:NH2   | 48:Ci:45:ILE:HG12   | 2.21                     | 0.56              |
| 51:Cm:88:SER:CB    | 57:CA:394:A:H5''    | 2.34                     | 0.56              |
| 51:Cm:193:PHE:HD2  | 51:Cm:197:ALA:HB1   | 1.68                     | 0.56              |
| 54:Cq:150:LEU:HB2  | 54:Cq:252:GLU:HG3   | 1.87                     | 0.56              |
| 56:Cv:62:LEU:O     | 56:Cv:99:VAL:HG22   | 2.04                     | 0.56              |
| 56:Cv:200:ASP:HB2  | 56:Cv:612:THR:HG23  | 1.87                     | 0.56              |
| 77:AK:34:LYS:O     | 77:AK:38:ILE:HG12   | 2.05                     | 0.56              |
| 78:AN:11:PRO:HB2   | 102:AA:815:U:C4     | 2.40                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 80:AQ:38:ASN:HB3    | 80:AQ:116:THR:HG21  | 1.86                     | 0.56              |
| 81:AR:52:ARG:NH1    | 102:AA:1168:U:OP1   | 2.37                     | 0.56              |
| 96:Ap:253:GLN:OE1   | 102:AA:394:U:N3     | 2.38                     | 0.56              |
| 102:AA:440:U:H3'    | 115:BM:277:LYS:NZ   | 2.20                     | 0.56              |
| 103:BA:502:HIS:CG   | 103:BA:641:GLU:HB3  | 2.41                     | 0.56              |
| 108:BF:40:PRO:HG2   | 108:BF:256:LEU:HD21 | 1.87                     | 0.56              |
| 113:BK:290:ASP:O    | 113:BK:307:ARG:N    | 2.38                     | 0.56              |
| 115:BM:218:ARG:HH12 | 120:BR:88:LEU:HD23  | 1.70                     | 0.56              |
| 126:BX:155:ARG:HH11 | 126:BX:158:THR:HG23 | 1.70                     | 0.56              |
| 5:DM:3:VAL:HG21     | 29:CE:318:PRO:HD2   | 1.86                     | 0.56              |
| 10:DR:131:LEU:HD11  | 12:DU:170:ARG:HH21  | 1.71                     | 0.56              |
| 16:DC:305:ARG:NH1   | 16:DC:355:GLU:HG3   | 2.20                     | 0.56              |
| 18:DF:394:GLU:OE2   | 18:DF:476:LEU:HB3   | 2.06                     | 0.56              |
| 20:DH:518:LYS:HG3   | 20:DH:523:ARG:NH1   | 2.20                     | 0.56              |
| 27:DY:111:ARG:NH1   | 27:DY:125:THR:HG23  | 2.20                     | 0.56              |
| 32:CI:409:PRO:HA    | 40:CR:253:PHE:CD2   | 2.41                     | 0.56              |
| 33:CJ:230:PHE:CD2   | 50:Ck:710:ARG:HD2   | 2.41                     | 0.56              |
| 34:CK:203:ASN:OD1   | 34:CK:204:THR:N     | 2.38                     | 0.56              |
| 37:CO:245:ASN:OD1   | 37:CO:245:ASN:N     | 2.38                     | 0.56              |
| 37:CO:332:ARG:NH1   | 37:CO:340:ASP:OD2   | 2.39                     | 0.56              |
| 38:CP:173:LYS:NZ    | 38:CP:181:GLU:OE1   | 2.38                     | 0.56              |
| 42:CU:65:VAL:HG12   | 42:CU:71:ARG:HB3    | 1.87                     | 0.56              |
| 49:Cj:107:ALA:HB2   | 49:Cj:173:MET:HE1   | 1.87                     | 0.56              |
| 50:Ck:724:PHE:O     | 50:Ck:775:ARG:HD3   | 2.05                     | 0.56              |
| 68:A4:86:THR:HB     | 89:Ad:138:PRO:HG3   | 1.86                     | 0.56              |
| 72:A9:105:TRP:H     | 78:AN:100:ARG:NH1   | 2.03                     | 0.56              |
| 74:AF:280:THR:O     | 74:AF:280:THR:OG1   | 2.21                     | 0.56              |
| 82:AT:9:ASN:ND2     | 102:AA:1104:U:OP1   | 2.36                     | 0.56              |
| 98:Av:213:ARG:NH1   | 98:Av:217:MET:HB2   | 2.21                     | 0.56              |
| 102:AA:526:G:N2     | 129:Ba:15:PHE:O     | 2.36                     | 0.56              |
| 104:BB:404:ASP:HA   | 104:BB:407:LYS:NZ   | 2.20                     | 0.56              |
| 105:BC:86:GLN:HE22  | 105:BC:124:ASN:HA   | 1.70                     | 0.56              |
| 110:BH:188:ASP:OD2  | 110:BH:228:VAL:HG13 | 2.05                     | 0.56              |
| 135:Bg:25:ARG:HG2   | 135:Bg:25:ARG:HH11  | 1.70                     | 0.56              |
| 1:DA:1506:ASN:HB2   | 1:DA:1507:VAL:HG13  | 1.87                     | 0.56              |
| 2:DD:108:THR:HB     | 2:DD:707:GLN:HE21   | 1.69                     | 0.56              |
| 6:DN:227:LYS:HE2    | 6:DN:287:ARG:HH22   | 1.70                     | 0.56              |
| 18:DF:502:ARG:HG2   | 18:DF:519:TRP:O     | 2.05                     | 0.56              |
| 19:DG:616:ARG:HG3   | 24:DV:183:LEU:HD11  | 1.88                     | 0.56              |
| 32:CI:183:PRO:HD2   | 40:CR:87:GLU:HG2    | 1.87                     | 0.56              |
| 34:CK:326:LYS:HD2   | 42:CU:83:SER:H      | 1.71                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 45:Cb:276:LYS:NZ   | 55:Cr:292:GLU:HB3   | 2.21                     | 0.56              |
| 50:Ck:275:TRP:CD1  | 50:Ck:314:LEU:HD13  | 2.41                     | 0.56              |
| 64:A0:168:PHE:HZ   | 88:Ab:76:MET:HE3    | 1.71                     | 0.56              |
| 87:AY:64:HIS:CD2   | 87:AY:66:ARG:H      | 2.08                     | 0.56              |
| 90:Ae:127:CYS:SG   | 104:BB:146:TYR:OH   | 2.53                     | 0.56              |
| 95:Ao:226:ARG:HH21 | 102:AA:448:A:H3'    | 1.70                     | 0.56              |
| 96:Ap:83:HIS:CE1   | 134:Bf:84:GLU:HB3   | 2.40                     | 0.56              |
| 98:Av:68:ARG:HG2   | 154:Av:301:NAD:H72N | 1.71                     | 0.56              |
| 119:BQ:25:ASP:OD1  | 119:BQ:26:GLU:N     | 2.38                     | 0.56              |
| 126:BX:67:VAL:HG11 | 136:Bh:70:TRP:HB2   | 1.87                     | 0.56              |
| 128:BZ:68:THR:HG22 | 128:BZ:70:LYS:H     | 1.70                     | 0.56              |
| 130:Bb:47:ARG:HA   | 130:Bb:50:LEU:HG    | 1.86                     | 0.56              |
| 1:DA:649:LEU:CD1   | 1:DA:729:ARG:HH11   | 2.19                     | 0.56              |
| 10:DR:112:ARG:HH11 | 49:Cj:158:THR:HG23  | 1.71                     | 0.56              |
| 19:DG:551:MET:SD   | 19:DG:561:PRO:HD3   | 2.46                     | 0.56              |
| 23:DT:52:ARG:NH1   | 23:DT:213:ASP:OD1   | 2.38                     | 0.56              |
| 26:DX:88:ASP:OD1   | 26:DX:89:ARG:N      | 2.38                     | 0.56              |
| 33:CJ:541:LEU:O    | 33:CJ:544:THR:HG23  | 2.05                     | 0.56              |
| 34:CK:214:LYS:HB3  | 34:CK:214:LYS:HZ2   | 1.68                     | 0.56              |
| 42:CU:69:ARG:NE    | 42:CU:94:GLU:OE2    | 2.39                     | 0.56              |
| 87:AY:4:ARG:HH22   | 102:AA:105:G:H8     | 1.51                     | 0.56              |
| 92:Ag:246:MET:HG2  | 115:BM:253:PRO:HG2  | 1.88                     | 0.56              |
| 125:BW:187:ASP:N   | 125:BW:187:ASP:OD1  | 2.37                     | 0.56              |
| 128:BZ:96:GLN:NE2  | 128:BZ:124:ALA:O    | 2.38                     | 0.56              |
| 1:DA:518:GLU:OE2   | 1:DA:837:ARG:NH2    | 2.39                     | 0.56              |
| 2:DD:654:ARG:HB2   | 46:Cd:48:ASN:HD22   | 1.70                     | 0.56              |
| 3:DI:291:LEU:HD13  | 3:DI:300:LEU:HD23   | 1.86                     | 0.56              |
| 4:DL:110:TYR:HE2   | 32:CI:235:SER:O     | 1.88                     | 0.56              |
| 10:DR:93:PRO:HB2   | 10:DR:96:PHE:CD2    | 2.40                     | 0.56              |
| 18:DF:557:PRO:HB2  | 18:DF:563:SER:HB2   | 1.88                     | 0.56              |
| 19:DG:186:ARG:HG2  | 19:DG:186:ARG:HH11  | 1.71                     | 0.56              |
| 22:DK:225:THR:HG22 | 22:DK:226:LEU:HD13  | 1.88                     | 0.56              |
| 30:CF:112:GLN:HA   | 56:Cv:204:ILE:HG12  | 1.88                     | 0.56              |
| 33:CJ:384:GLU:HG3  | 57:CA:453:A:H4'     | 1.88                     | 0.56              |
| 36:CN:150:HIS:HD2  | 48:CI:67:THR:HG23   | 1.71                     | 0.56              |
| 47:Cg:155:LYS:HB3  | 47:Cg:356:CYS:SG    | 2.45                     | 0.56              |
| 55:Cr:152:VAL:HG12 | 55:Cr:181:PRO:HA    | 1.87                     | 0.56              |
| 75:AI:124:GLU:OE2  | 145:UL:9:UNK:HG2    | 2.05                     | 0.56              |
| 77:AK:38:ILE:HD11  | 124:BV:90:PHE:HE1   | 1.70                     | 0.56              |
| 111:BI:119:GLU:OE2 | 111:BI:234:SER:HB2  | 2.05                     | 0.56              |
| 118:BP:121:ARG:HD3 | 118:BP:122:SER:N    | 2.21                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:193:GLU:N     | 1:DA:193:GLU:OE1   | 2.37                     | 0.56              |
| 4:DL:106:PHE:CE2   | 32:CI:237:ARG:HG2  | 2.41                     | 0.56              |
| 6:DN:165:GLU:HG3   | 6:DN:171:LEU:H     | 1.70                     | 0.56              |
| 11:DS:34:SER:O     | 11:DS:34:SER:OG    | 2.21                     | 0.56              |
| 18:DF:521:THR:HG22 | 18:DF:523:LEU:H    | 1.71                     | 0.56              |
| 19:DG:111:ARG:NH1  | 45:Cb:197:PRO:HB3  | 2.07                     | 0.56              |
| 20:DH:37:SER:O     | 21:DJ:49:ALA:HB1   | 2.06                     | 0.56              |
| 33:CJ:760:MET:HE2  | 33:CJ:762:GLN:HG2  | 1.88                     | 0.56              |
| 34:CK:317:GLY:HA2  | 51:Cm:195:PHE:CD1  | 2.41                     | 0.56              |
| 36:CN:51:LEU:O     | 36:CN:68:GLN:NE2   | 2.38                     | 0.56              |
| 44:Ca:299:ARG:HG3  | 44:Ca:299:ARG:NH1  | 2.10                     | 0.56              |
| 45:Cb:298:ASP:HB3  | 55:Cr:40:HIS:CG    | 2.40                     | 0.56              |
| 65:A1:181:VAL:HG11 | 87:AY:299:MET:HB3  | 1.87                     | 0.56              |
| 66:A2:414:THR:HG21 | 113:BK:373:PRO:HG3 | 1.86                     | 0.56              |
| 69:A5:69:TRP:NE1   | 69:A5:79:LYS:HB2   | 2.20                     | 0.56              |
| 73:AE:364:ILE:HD11 | 131:Bc:84:LEU:HD22 | 1.87                     | 0.56              |
| 75:AI:35:ARG:HD2   | 129:Ba:130:ASP:HA  | 1.88                     | 0.56              |
| 75:AI:94:ILE:O     | 75:AI:97:ARG:NH1   | 2.39                     | 0.56              |
| 79:AP:315:ARG:HB2  | 105:BC:456:ASP:OD2 | 2.06                     | 0.56              |
| 87:AY:25:ASP:HB3   | 87:AY:28:VAL:HG23  | 1.88                     | 0.56              |
| 104:BB:415:ASP:N   | 104:BB:415:ASP:OD1 | 2.37                     | 0.56              |
| 109:BG:330:PRO:HA  | 109:BG:333:PHE:CE2 | 2.40                     | 0.56              |
| 110:BH:85:ASP:OD1  | 139:UC:3:UNK:HG1   | 2.06                     | 0.56              |
| 2:DD:387:GLN:HE22  | 2:DD:453:ASN:H     | 1.53                     | 0.56              |
| 4:DL:85:PHE:HB2    | 32:CI:270:PHE:CZ   | 2.41                     | 0.56              |
| 6:DN:183:ARG:CZ    | 6:DN:194:ARG:NH1   | 2.69                     | 0.56              |
| 25:DW:121:HIS:CD2  | 25:DW:123:ALA:H    | 2.21                     | 0.56              |
| 32:CI:409:PRO:CA   | 40:CR:253:PHE:HE2  | 2.19                     | 0.56              |
| 55:Cr:42:ILE:HD11  | 55:Cr:95:SER:HA    | 1.86                     | 0.56              |
| 56:Cv:559:GLN:NE2  | 61:UR:3:UNK:HG1    | 2.21                     | 0.56              |
| 66:A2:142:LYS:HB3  | 66:A2:354:THR:HG23 | 1.88                     | 0.56              |
| 67:A3:187:LEU:HD21 | 67:A3:191:LYS:HZ1  | 1.70                     | 0.56              |
| 68:A4:13:ALA:H     | 70:A6:77:GLN:HE21  | 1.54                     | 0.56              |
| 77:AK:144:HIS:CD2  | 124:BV:69:LYS:HD3  | 2.41                     | 0.56              |
| 89:Ad:107:HIS:CD2  | 93:Aj:33:ALA:HB2   | 2.41                     | 0.56              |
| 93:Aj:18:GLY:N     | 132:Bd:78:CYS:HB2  | 2.21                     | 0.56              |
| 105:BC:415:LEU:HB2 | 105:BC:417:LEU:HG  | 1.87                     | 0.56              |
| 111:BI:180:GLN:HG3 | 134:Bf:97:VAL:HG13 | 1.87                     | 0.56              |
| 112:BJ:238:LEU:O   | 112:BJ:242:GLN:HG2 | 2.05                     | 0.56              |
| 120:BR:70:TYR:CE2  | 120:BR:72:PRO:HA   | 2.41                     | 0.56              |
| 1:DA:1662:ARG:NH2  | 29:CE:402:ARG:HH12 | 2.04                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 17:DE:597:PHE:O    | 17:DE:601:ILE:HG22  | 2.06                     | 0.55              |
| 31:CH:16:VAL:HB    | 31:CH:17:PRO:CD     | 2.34                     | 0.55              |
| 33:CJ:553:ARG:HG2  | 33:CJ:553:ARG:HH11  | 1.71                     | 0.55              |
| 44:Ca:88:ARG:NH2   | 56:Cv:1110:GLU:OE1  | 2.38                     | 0.55              |
| 45:Cb:303:GLU:HB2  | 55:Cr:105:ARG:NH1   | 2.21                     | 0.55              |
| 47:Cg:109:PHE:CA   | 152:Cg:501:GTP:HN21 | 2.08                     | 0.55              |
| 50:Ck:644:HIS:CD2  | 50:Ck:669:ASN:H     | 2.23                     | 0.55              |
| 56:Cv:77:TYR:N     | 56:Cv:165:GLU:OE2   | 2.37                     | 0.55              |
| 69:A5:26:PRO:HG3   | 102:AA:506:U:O2'    | 2.06                     | 0.55              |
| 79:AP:15:HIS:O     | 79:AP:17:ARG:NH1    | 2.38                     | 0.55              |
| 90:Ae:109:ARG:NH1  | 102:AA:544:G:C2     | 2.74                     | 0.55              |
| 104:BB:82:HIS:CE1  | 104:BB:86:ASN:HD22  | 2.24                     | 0.55              |
| 107:BE:384:HIS:H   | 107:BE:384:HIS:CD2  | 2.24                     | 0.55              |
| 109:BG:184:GLU:OE2 | 109:BG:221:GLU:HA   | 2.06                     | 0.55              |
| 115:BM:76:TRP:O    | 115:BM:80:ARG:NH2   | 2.36                     | 0.55              |
| 122:BT:60:ARG:NH1  | 129:Ba:148:ALA:HB1  | 2.21                     | 0.55              |
| 16:DC:389:GLU:HG3  | 16:DC:496:LYS:NZ    | 2.21                     | 0.55              |
| 18:DF:84:PRO:HG2   | 18:DF:87:GLU:HB2    | 1.88                     | 0.55              |
| 18:DF:589:GLN:CD   | 20:DH:192:PHE:CZ    | 2.84                     | 0.55              |
| 20:DH:504:ARG:HH12 | 22:DK:287:ILE:HG12  | 1.72                     | 0.55              |
| 21:DJ:132:ARG:NH2  | 150:DJ:401:UTP:O1B  | 2.40                     | 0.55              |
| 22:DK:21:SER:HB2   | 22:DK:231:SER:O     | 2.06                     | 0.55              |
| 29:CE:192:GLU:OE2  | 29:CE:195:ARG:NH1   | 2.38                     | 0.55              |
| 35:CL:59:MET:HE2   | 35:CL:123:GLY:HA3   | 1.87                     | 0.55              |
| 50:Ck:113:ASN:O    | 50:Ck:140:ARG:NH2   | 2.38                     | 0.55              |
| 56:Cv:626:VAL:HB   | 56:Cv:628:LYS:HZ2   | 1.70                     | 0.55              |
| 76:AJ:58:ASN:HD21  | 76:AJ:60:GLU:HG2    | 1.70                     | 0.55              |
| 83:AU:179:VAL:HG22 | 108:BF:125:GLU:HB3  | 1.87                     | 0.55              |
| 107:BE:190:ARG:NH1 | 107:BE:191:PHE:HB3  | 2.21                     | 0.55              |
| 5:DM:41:GLU:OE2    | 44:Ca:286:ARG:NH2   | 2.36                     | 0.55              |
| 5:DM:90:LEU:HD12   | 56:Cv:941:ALA:HB2   | 1.88                     | 0.55              |
| 6:DN:142:ARG:HG3   | 31:CH:19:LEU:HD11   | 1.87                     | 0.55              |
| 15:DB:153:HIS:HE1  | 15:DB:173:ARG:CZ    | 2.20                     | 0.55              |
| 16:DC:533:LEU:HD21 | 16:DC:1069:CYS:HA   | 1.87                     | 0.55              |
| 16:DC:594:GLU:HA   | 17:DE:412:GLU:OE2   | 2.06                     | 0.55              |
| 29:CE:397:GLU:OE2  | 29:CE:401:LYS:NZ    | 2.39                     | 0.55              |
| 31:CH:133:ARG:CZ   | 56:Cv:108:HIS:HB2   | 2.36                     | 0.55              |
| 33:CJ:792:HIS:CD2  | 33:CJ:795:LYS:H     | 2.13                     | 0.55              |
| 56:Cv:678:HIS:HD2  | 56:Cv:680:ARG:HD2   | 1.72                     | 0.55              |
| 66:A2:165:GLU:HG2  | 66:A2:167:HIS:CE1   | 2.40                     | 0.55              |
| 73:AE:74:TYR:HD1   | 73:AE:97:ARG:HH11   | 1.51                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 85:AW:99:VAL:HG13   | 114:BL:42:TYR:HB2   | 1.89                     | 0.55              |
| 98:Av:75:LYS:HE3    | 125:BW:80:MET:HG3   | 1.87                     | 0.55              |
| 98:Av:207:ARG:NH2   | 132:Bd:105:MET:SD   | 2.79                     | 0.55              |
| 98:Av:213:ARG:HH11  | 98:Av:217:MET:HB2   | 1.71                     | 0.55              |
| 102:AA:119:A:H5'    | 102:AA:120:A:C8     | 2.41                     | 0.55              |
| 102:AA:423:A:OP2    | 124:BV:138:GLN:NE2  | 2.40                     | 0.55              |
| 111:BI:104:ARG:HH21 | 111:BI:140:PHE:HB3  | 1.71                     | 0.55              |
| 117:BO:224:TYR:OH   | 117:BO:226:GLU:OE1  | 2.23                     | 0.55              |
| 140:UD:73:UNK:HA    | 140:UD:76:UNK:HG3   | 1.88                     | 0.55              |
| 2:DD:94:LYS:HE3     | 2:DD:99:THR:O       | 2.06                     | 0.55              |
| 3:DI:66:ARG:HG3     | 3:DI:178:PHE:CE2    | 2.41                     | 0.55              |
| 15:DB:386:ALA:O     | 15:DB:389:GLN:HG2   | 2.05                     | 0.55              |
| 19:DG:100:ASP:OD2   | 40:CR:244:THR:HG22  | 2.07                     | 0.55              |
| 37:CO:217:ASP:OD1   | 37:CO:220:SER:HB3   | 2.07                     | 0.55              |
| 37:CO:399:ILE:HD12  | 37:CO:400:ARG:N     | 2.22                     | 0.55              |
| 40:CR:312:ASN:O     | 46:Cd:279:ARG:NH1   | 2.39                     | 0.55              |
| 40:CR:319:LYS:HD2   | 46:Cd:283:GLU:O     | 2.06                     | 0.55              |
| 44:Ca:332:ARG:NH1   | 44:Ca:333:ASP:OD1   | 2.40                     | 0.55              |
| 48:CI:24:PRO:O      | 48:CI:25:VAL:HG23   | 2.06                     | 0.55              |
| 51:Cm:85:ILE:HD13   | 51:Cm:87:LEU:HD12   | 1.88                     | 0.55              |
| 54:Cq:181:HIS:HB2   | 54:Cq:201:GLU:HG3   | 1.88                     | 0.55              |
| 55:Cr:143:ARG:HD3   | 55:Cr:187:VAL:HG21  | 1.87                     | 0.55              |
| 70:A6:80:CYS:HA     | 98:Av:184:MET:HE1   | 1.88                     | 0.55              |
| 74:AF:109:MET:HG2   | 74:AF:136:GLY:O     | 2.05                     | 0.55              |
| 93:Aj:271:GLN:O     | 109:BG:50:ARG:NH2   | 2.40                     | 0.55              |
| 104:BB:134:ARG:HA   | 104:BB:137:ARG:NH1  | 2.21                     | 0.55              |
| 105:BC:109:THR:HB   | 105:BC:165:HIS:CE1  | 2.42                     | 0.55              |
| 105:BC:239:ARG:HB3  | 105:BC:239:ARG:NH1  | 2.20                     | 0.55              |
| 117:BO:143:ARG:CA   | 117:BO:152:ARG:HH12 | 2.19                     | 0.55              |
| 128:BZ:18:PRO:HG3   | 128:BZ:184:VAL:HG21 | 1.88                     | 0.55              |
| 1:DA:949:ARG:HD2    | 5:DM:18:HIS:HA      | 1.89                     | 0.55              |
| 2:DD:787:ARG:NH1    | 44:Ca:206:LEU:HD13  | 2.22                     | 0.55              |
| 4:DL:92:ILE:HG23    | 32:CI:248:PHE:CB    | 2.36                     | 0.55              |
| 7:DO:114:GLY:C      | 7:DO:116:ALA:H      | 2.12                     | 0.55              |
| 15:DB:968:VAL:HG13  | 19:DG:42:PRO:HG2    | 1.88                     | 0.55              |
| 18:DF:428:PRO:HB2   | 18:DF:493:MET:HE2   | 1.89                     | 0.55              |
| 37:CO:80:ARG:NH1    | 37:CO:84:GLU:OE2    | 2.39                     | 0.55              |
| 48:CI:101:LEU:HG    | 48:CI:105:ARG:HH11  | 1.71                     | 0.55              |
| 54:Cq:191:VAL:HG12  | 54:Cq:215:PRO:HA    | 1.89                     | 0.55              |
| 56:Cv:955:LEU:HG    | 56:Cv:959:LEU:HD23  | 1.89                     | 0.55              |
| 65:A1:174:GLN:HB2   | 87:AY:295:MET:HE1   | 1.88                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 67:A3:96:THR:HB     | 79:AP:21:ILE:HD11   | 1.87                     | 0.55              |
| 69:A5:78:ILE:HG22   | 85:AW:255:SER:HB3   | 1.89                     | 0.55              |
| 73:AE:163:PHE:HB2   | 73:AE:323:ILE:HG22  | 1.87                     | 0.55              |
| 76:AJ:25:ARG:HB3    | 76:AJ:25:ARG:NH1    | 2.22                     | 0.55              |
| 77:AK:52:ASN:O      | 102:AA:435:A:H4'    | 2.07                     | 0.55              |
| 89:Ad:55:ARG:HG2    | 89:Ad:55:ARG:NH1    | 2.22                     | 0.55              |
| 102:AA:66:C:H42     | 102:AA:944:C:H5'    | 1.70                     | 0.55              |
| 105:BC:318:ASP:O    | 105:BC:320:VAL:N    | 2.37                     | 0.55              |
| 113:BK:321:GLU:OE1  | 113:BK:321:GLU:N    | 2.39                     | 0.55              |
| 138:UB:36:UNK:HA    | 138:UB:39:UNK:HG3   | 1.87                     | 0.55              |
| 1:DA:1384:ARG:HH12  | 1:DA:1628:ARG:HE    | 1.55                     | 0.55              |
| 2:DD:356:PRO:HB2    | 49:Cj:157:THR:CG2   | 2.37                     | 0.55              |
| 3:DI:256:ARG:NH1    | 3:DI:271:TYR:O      | 2.40                     | 0.55              |
| 7:DO:254:ASP:OD1    | 7:DO:254:ASP:N      | 2.38                     | 0.55              |
| 18:DF:371:ASN:HB2   | 18:DF:374:VAL:HG23  | 1.89                     | 0.55              |
| 18:DF:425:ILE:CD1   | 20:DH:196:LEU:HD11  | 2.36                     | 0.55              |
| 20:DH:277:THR:HG22  | 20:DH:278:VAL:H     | 1.71                     | 0.55              |
| 27:DY:15:SER:HG     | 57:CA:518:G:H22     | 1.53                     | 0.55              |
| 40:CR:307:ARG:NH2   | 57:CA:389:A:C8      | 2.67                     | 0.55              |
| 40:CR:318:LYS:H     | 46:Cd:279:ARG:C     | 2.15                     | 0.55              |
| 66:A2:255:ARG:HG2   | 66:A2:255:ARG:HH11  | 1.72                     | 0.55              |
| 88:Ab:484:GLY:N     | 94:Al:204:ASP:OD2   | 2.38                     | 0.55              |
| 98:Av:94:VAL:HG22   | 98:Av:122:LEU:HD21  | 1.89                     | 0.55              |
| 104:BB:134:ARG:HA   | 104:BB:137:ARG:HH12 | 1.70                     | 0.55              |
| 104:BB:404:ASP:HA   | 104:BB:407:LYS:HZ3  | 1.71                     | 0.55              |
| 104:BB:428:LEU:H    | 104:BB:428:LEU:HD12 | 1.71                     | 0.55              |
| 111:BI:105:LEU:O    | 111:BI:108:GLU:HG3  | 2.05                     | 0.55              |
| 116:BN:114:ASP:OD2  | 116:BN:121:LEU:HD22 | 2.07                     | 0.55              |
| 116:BN:219:ARG:NH1  | 116:BN:220:ASP:O    | 2.40                     | 0.55              |
| 117:BO:104:LEU:HD12 | 117:BO:117:LEU:HD21 | 1.89                     | 0.55              |
| 118:BP:54:GLY:H     | 132:Bd:77:HIS:HE1   | 1.55                     | 0.55              |
| 128:BZ:13:ILE:HD11  | 128:BZ:166:ILE:HG22 | 1.87                     | 0.55              |
| 1:DA:59:HIS:CD2     | 1:DA:86:TYR:H       | 2.19                     | 0.55              |
| 1:DA:938:ILE:HD13   | 5:DM:126:MET:HE3    | 1.89                     | 0.55              |
| 1:DA:1301:ASP:OD1   | 1:DA:1302:PHE:N     | 2.40                     | 0.55              |
| 4:DL:246:GLU:CD     | 51:Cm:61:ARG:HH12   | 2.15                     | 0.55              |
| 10:DR:108:GLN:HE22  | 49:Cj:147:TYR:CB    | 2.20                     | 0.55              |
| 12:DU:205:ALA:HB1   | 12:DU:206:PRO:HD2   | 1.88                     | 0.55              |
| 16:DC:326:LYS:HG3   | 16:DC:346:ASP:OD2   | 2.06                     | 0.55              |
| 19:DG:497:ARG:HG2   | 19:DG:497:ARG:HH11  | 1.72                     | 0.55              |
| 29:CE:13:ASN:OD1    | 29:CE:13:ASN:N      | 2.39                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 34:CK:200:ARG:NE    | 34:CK:205:TYR:OH    | 2.38                     | 0.55              |
| 35:CL:97:LEU:HD11   | 62:US:40:UNK:HG3    | 1.89                     | 0.55              |
| 37:CO:71:PRO:HB3    | 52:Cn:192:ASN:HD21  | 1.71                     | 0.55              |
| 43:CZ:265:GLN:HB3   | 43:CZ:308:TYR:CE1   | 2.41                     | 0.55              |
| 50:Ck:728:GLN:HG3   | 50:Ck:784:TRP:CD2   | 2.42                     | 0.55              |
| 52:Cn:141:ARG:HD2   | 57:CA:280:A:N1      | 2.22                     | 0.55              |
| 65:A1:44:ALA:O      | 118:BP:235:ARG:NH1  | 2.38                     | 0.55              |
| 66:A2:275:LEU:HD21  | 113:BK:326:VAL:HG12 | 1.88                     | 0.55              |
| 74:AF:233:GLN:HA    | 79:AP:89:GLN:HE22   | 1.72                     | 0.55              |
| 81:AR:71:ARG:NH1    | 136:Bh:19:ASN:HB2   | 2.21                     | 0.55              |
| 95:Ao:144:PRO:HG3   | 120:BR:133:GLN:HA   | 1.88                     | 0.55              |
| 96:Ap:66:CYS:HB3    | 96:Ap:70:GLU:HB2    | 1.88                     | 0.55              |
| 102:AA:546:A:OP1    | 135:Bg:56:ARG:NH1   | 2.39                     | 0.55              |
| 103:BA:582:PHE:CD1  | 103:BA:693:HIS:HB2  | 2.41                     | 0.55              |
| 105:BC:301:MET:HE1  | 105:BC:421:PHE:CD1  | 2.42                     | 0.55              |
| 105:BC:439:LYS:HG3  | 105:BC:440:ARG:HG3  | 1.87                     | 0.55              |
| 107:BE:137:LYS:HB2  | 107:BE:137:LYS:HZ2  | 1.71                     | 0.55              |
| 110:BH:160:THR:OG1  | 110:BH:168:THR:OG1  | 2.06                     | 0.55              |
| 110:BH:271:PHE:CD1  | 133:Be:8:LYS:NZ     | 2.74                     | 0.55              |
| 5:DM:23:MET:HE3     | 5:DM:28:PHE:HB2     | 1.89                     | 0.55              |
| 6:DN:71:GLU:O       | 6:DN:111:ILE:HG23   | 2.06                     | 0.55              |
| 16:DC:393:THR:HG21  | 16:DC:457:LYS:HE3   | 1.89                     | 0.55              |
| 18:DF:92:MET:HE2    | 41:CS:104:GLN:HE22  | 1.71                     | 0.55              |
| 21:DJ:285:ARG:NH1   | 150:DJ:401:UTP:O1B  | 2.39                     | 0.55              |
| 31:CH:253:TYR:CZ    | 31:CH:280:MET:HE3   | 2.41                     | 0.55              |
| 40:CR:198:THR:HB    | 40:CR:200:SER:H     | 1.72                     | 0.55              |
| 46:Cd:178:ASN:HB2   | 46:Cd:182:GLN:H     | 1.72                     | 0.55              |
| 49:Cj:46:TYR:HA     | 49:Cj:165:PHE:HE2   | 1.72                     | 0.55              |
| 57:CA:134:U:H2'     | 57:CA:135:U:H5''    | 1.89                     | 0.55              |
| 65:A1:113:VAL:HG21  | 65:A1:164:GLN:HG3   | 1.87                     | 0.55              |
| 65:A1:207:ASP:OD2   | 65:A1:210:GLN:HB2   | 2.06                     | 0.55              |
| 77:AK:21:PRO:O      | 77:AK:224:GLN:NE2   | 2.31                     | 0.55              |
| 88:Ab:382:ARG:NH1   | 88:Ab:393:LEU:HD13  | 2.21                     | 0.55              |
| 89:Ad:183:GLU:HG2   | 89:Ad:232:PHE:CD2   | 2.42                     | 0.55              |
| 102:AA:134:U:H2'    | 102:AA:135:G:H5''   | 1.89                     | 0.55              |
| 102:AA:565:U:H5'    | 140:UD:23:UNK:HG3   | 1.89                     | 0.55              |
| 115:BM:274:GLY:H    | 115:BM:279:ASN:HD22 | 1.53                     | 0.55              |
| 120:BR:108:TYR:OH   | 120:BR:164:HIS:HD2  | 1.90                     | 0.55              |
| 125:BW:128:THR:HG22 | 125:BW:129:PRO:HD2  | 1.87                     | 0.55              |
| 130:Bb:66:GLU:OE2   | 130:Bb:106:SER:HB2  | 2.07                     | 0.55              |
| 1:DA:230:PHE:O      | 11:DS:62:ARG:NH2    | 2.39                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:DD:665:GLU:HG3    | 44:Ca:427:TRP:HA    | 1.89                     | 0.55              |
| 4:DL:113:LEU:O      | 4:DL:254:ARG:NH2    | 2.40                     | 0.55              |
| 5:DM:77:PRO:HD3     | 56:Cv:968:LEU:O     | 2.07                     | 0.55              |
| 8:DP:189:TYR:OH     | 8:DP:208:PRO:HD3    | 2.07                     | 0.55              |
| 14:Da:10:ILE:HG23   | 14:Da:22:ARG:HH11   | 1.71                     | 0.55              |
| 16:DC:229:THR:HG22  | 16:DC:232:GLN:H     | 1.72                     | 0.55              |
| 16:DC:243:TYR:O     | 16:DC:248:ARG:HB2   | 2.07                     | 0.55              |
| 34:CK:280:ARG:HA    | 34:CK:308:GLU:O     | 2.06                     | 0.55              |
| 44:Ca:323:LYS:HG3   | 44:Ca:330:TRP:CD2   | 2.42                     | 0.55              |
| 49:Cj:147:TYR:CE1   | 49:Cj:162:GLN:HG2   | 2.41                     | 0.55              |
| 50:Ck:621:THR:HG22  | 50:Ck:623:LYS:HG3   | 1.89                     | 0.55              |
| 54:Cq:92:LEU:O      | 54:Cq:96:THR:OG1    | 2.23                     | 0.55              |
| 57:CA:197:A:O2'     | 57:CA:199:U:OP2     | 2.23                     | 0.55              |
| 64:A0:91:GLU:H      | 64:A0:137:ARG:HH22  | 1.52                     | 0.55              |
| 67:A3:61:ARG:HG2    | 67:A3:61:ARG:NH1    | 2.20                     | 0.55              |
| 87:AY:35:LYS:HD3    | 87:AY:37:GLY:H      | 1.71                     | 0.55              |
| 87:AY:279:ARG:HH12  | 128:BZ:174:SER:CB   | 2.20                     | 0.55              |
| 102:AA:43:U:H5''    | 102:AA:44:A:C8      | 2.42                     | 0.55              |
| 104:BB:87:LEU:HD13  | 104:BB:90:LYS:HZ3   | 1.72                     | 0.55              |
| 104:BB:176:LEU:HB3  | 104:BB:234:ILE:HG21 | 1.88                     | 0.55              |
| 114:BL:196:THR:HG21 | 114:BL:304:VAL:HG22 | 1.89                     | 0.55              |
| 115:BM:133:MET:HE1  | 115:BM:195:VAL:HG13 | 1.88                     | 0.55              |
| 125:BW:68:PHE:CE2   | 125:BW:75:ARG:NH1   | 2.74                     | 0.55              |
| 130:Bb:120:ARG:HG2  | 130:Bb:120:ARG:HH11 | 1.72                     | 0.55              |
| 1:DA:65:ILE:HD11    | 2:DD:164:ARG:HG3    | 1.89                     | 0.55              |
| 5:DM:266:ALA:HB2    | 29:CE:61:PHE:CE2    | 2.42                     | 0.55              |
| 13:DZ:34:LYS:HG3    | 13:DZ:35:LYS:H      | 1.72                     | 0.55              |
| 15:DB:1154:LYS:CD   | 89:Ad:150:ARG:CD    | 2.67                     | 0.55              |
| 19:DG:15:ARG:HG2    | 19:DG:15:ARG:HH11   | 1.72                     | 0.55              |
| 23:DT:65:VAL:HG13   | 23:DT:69:ASP:HB2    | 1.88                     | 0.55              |
| 25:DW:50:LYS:HD3    | 25:DW:136:THR:HG21  | 1.89                     | 0.55              |
| 29:CE:83:MET:CE     | 29:CE:83:MET:H      | 2.20                     | 0.55              |
| 31:CH:249:ARG:HD3   | 31:CH:266:ILE:HD13  | 1.88                     | 0.55              |
| 34:CK:26:ARG:HB2    | 57:CA:460:U:C5      | 2.40                     | 0.55              |
| 34:CK:284:PHE:O     | 42:CU:71:ARG:NH2    | 2.34                     | 0.55              |
| 39:CQ:103:MET:HB2   | 39:CQ:106:THR:HB    | 1.89                     | 0.55              |
| 49:Cj:94:ILE:HG23   | 49:Cj:98:LYS:HG3    | 1.89                     | 0.55              |
| 65:A1:51:ARG:HH22   | 98:Av:60:ARG:HB3    | 1.71                     | 0.55              |
| 102:AA:947:U:OP1    | 127:BY:162:ARG:NH2  | 2.35                     | 0.55              |
| 104:BB:85:TYR:O     | 104:BB:89:THR:OG1   | 2.15                     | 0.55              |
| 105:BC:98:ASN:HA    | 105:BC:101:ALA:HB3  | 1.88                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 105:BC:442:ARG:HD3 | 105:BC:512:ARG:NH1  | 2.22                     | 0.55              |
| 109:BG:103:LEU:HB2 | 109:BG:318:ALA:HB1  | 1.89                     | 0.55              |
| 124:BV:49:ARG:NH1  | 124:BV:73:LEU:HD23  | 2.22                     | 0.55              |
| 1:DA:90:MET:HE1    | 2:DD:122:GLN:NE2    | 2.17                     | 0.54              |
| 1:DA:247:ASP:OD1   | 44:Ca:553:ARG:NH1   | 2.36                     | 0.54              |
| 1:DA:584:PHE:HB3   | 1:DA:759:GLY:HA3    | 1.89                     | 0.54              |
| 2:DD:339:ARG:NH2   | 57:CA:85:U:O2       | 2.41                     | 0.54              |
| 15:DB:1042:TYR:HA  | 33:CJ:263:ASP:OD1   | 2.07                     | 0.54              |
| 15:DB:1125:HIS:CG  | 15:DB:1126:PRO:HD2  | 2.42                     | 0.54              |
| 16:DC:56:ALA:HB2   | 22:DK:267:ARG:HD3   | 1.88                     | 0.54              |
| 17:DE:618:ARG:NH1  | 17:DE:628:HIS:CE1   | 2.75                     | 0.54              |
| 19:DG:50:LEU:CD2   | 32:CI:249:GLU:OE1   | 2.54                     | 0.54              |
| 19:DG:399:ARG:HH21 | 19:DG:457:ARG:NH1   | 2.05                     | 0.54              |
| 29:CE:42:ARG:NH1   | 29:CE:105:GLN:NE2   | 2.52                     | 0.54              |
| 44:Ca:569:ARG:NH1  | 57:CA:143:U:H5''    | 2.21                     | 0.54              |
| 46:Cd:13:ARG:CZ    | 46:Cd:26:ARG:HH21   | 2.20                     | 0.54              |
| 56:Cv:738:ARG:HH21 | 56:Cv:788:ARG:HD2   | 1.72                     | 0.54              |
| 56:Cv:847:ARG:NE   | 56:Cv:938:ASP:OD2   | 2.38                     | 0.54              |
| 70:A6:43:GLU:OE2   | 98:Av:183:ARG:NE    | 2.27                     | 0.54              |
| 77:AK:62:ALA:HB2   | 77:AK:86:PHE:CD2    | 2.42                     | 0.54              |
| 81:AR:104:ALA:HA   | 81:AR:129:PHE:CE1   | 2.42                     | 0.54              |
| 88:Ab:99:ASP:OD2   | 105:BC:239:ARG:NH1  | 2.40                     | 0.54              |
| 88:Ab:123:ARG:HH11 | 88:Ab:203:THR:HG21  | 1.72                     | 0.54              |
| 102:AA:1166:A:H4'  | 102:AA:1167:A:H5'   | 1.89                     | 0.54              |
| 103:BA:585:HIS:HD2 | 103:BA:587:SER:H    | 1.54                     | 0.54              |
| 104:BB:317:SER:HB3 | 104:BB:432:HIS:HE1  | 1.72                     | 0.54              |
| 104:BB:356:ASN:HA  | 104:BB:363:ARG:HH21 | 1.71                     | 0.54              |
| 116:BN:111:PHE:HB3 | 116:BN:120:TRP:HE1  | 1.71                     | 0.54              |
| 126:BX:70:PRO:HB2  | 126:BX:72:VAL:HG13  | 1.88                     | 0.54              |
| 134:Bf:106:SER:HB3 | 134:Bf:107:PRO:HD2  | 1.89                     | 0.54              |
| 1:DA:80:PRO:HB3    | 57:CA:153:A:N1      | 2.22                     | 0.54              |
| 1:DA:1278:THR:HG21 | 54:Cq:152:GLU:HB2   | 1.89                     | 0.54              |
| 2:DD:741:ARG:CB    | 2:DD:741:ARG:HH11   | 2.20                     | 0.54              |
| 5:DM:43:GLN:NE2    | 29:CE:313:MET:H     | 2.05                     | 0.54              |
| 18:DF:222:TYR:OH   | 18:DF:256:ASP:OD1   | 2.22                     | 0.54              |
| 19:DG:186:ARG:HH12 | 19:DG:189:LYS:HD3   | 1.71                     | 0.54              |
| 19:DG:399:ARG:NH2  | 19:DG:457:ARG:HH12  | 2.03                     | 0.54              |
| 31:CH:107:ARG:HH11 | 31:CH:107:ARG:HG3   | 1.72                     | 0.54              |
| 44:Ca:570:THR:HG21 | 53:Cp:16:HIS:CD2    | 2.42                     | 0.54              |
| 45:Cb:19:PRO:HD2   | 51:Cm:156:THR:CG2   | 2.37                     | 0.54              |
| 50:Ck:132:TYR:CZ   | 50:Ck:140:ARG:HG3   | 2.43                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 51:Cm:146:TRP:CD1   | 51:Cm:150:ASN:HD22  | 2.25                     | 0.54              |
| 57:CA:217:U:H3'     | 57:CA:218:A:H8      | 1.71                     | 0.54              |
| 63:UT:30:UNK:O      | 63:UT:32:UNK:N      | 2.40                     | 0.54              |
| 66:A2:376:ARG:HH22  | 87:AY:269:GLN:HE21  | 1.53                     | 0.54              |
| 71:A8:104:LYS:O     | 71:A8:107:ARG:NH1   | 2.40                     | 0.54              |
| 75:AI:48:ARG:HH11   | 75:AI:48:ARG:HG3    | 1.72                     | 0.54              |
| 75:AI:48:ARG:CG     | 75:AI:48:ARG:NH1    | 2.69                     | 0.54              |
| 76:AJ:24:THR:HG21   | 76:AJ:33:ARG:HD2    | 1.89                     | 0.54              |
| 78:AN:31:ASP:N      | 78:AN:31:ASP:OD1    | 2.40                     | 0.54              |
| 81:AR:84:ILE:HG22   | 81:AR:160:MET:HE3   | 1.89                     | 0.54              |
| 88:Ab:456:ALA:HB3   | 88:Ab:479:THR:HG21  | 1.88                     | 0.54              |
| 89:Ad:131:PRO:HB2   | 93:Aj:134:GLU:HG2   | 1.88                     | 0.54              |
| 93:Aj:104:ARG:NH1   | 93:Aj:113:ASN:OD1   | 2.38                     | 0.54              |
| 97:At:136:ARG:HH11  | 97:At:136:ARG:CB    | 2.13                     | 0.54              |
| 105:BC:60:LEU:N     | 105:BC:292:ASN:HD21 | 2.01                     | 0.54              |
| 114:BL:222:ARG:HH21 | 114:BL:241:ASP:HB3  | 1.70                     | 0.54              |
| 116:BN:53:ARG:HB3   | 116:BN:95:HIS:ND1   | 2.21                     | 0.54              |
| 132:Bd:91:ARG:HB3   | 132:Bd:97:GLN:NE2   | 2.22                     | 0.54              |
| 20:DH:440:VAL:HG22  | 28:CC:77:THR:HG23   | 1.88                     | 0.54              |
| 21:DJ:322:SER:OG    | 23:DT:187:LYS:O     | 2.25                     | 0.54              |
| 33:CJ:54:MET:HE2    | 57:CA:463:A:N6      | 2.23                     | 0.54              |
| 33:CJ:553:ARG:O     | 33:CJ:583:LYS:HD2   | 2.08                     | 0.54              |
| 37:CO:138:LEU:HD23  | 37:CO:138:LEU:H     | 1.72                     | 0.54              |
| 41:CS:62:HIS:O      | 41:CS:65:ASN:HB2    | 2.07                     | 0.54              |
| 43:CZ:250:PRO:HB3   | 43:CZ:321:MET:HE2   | 1.90                     | 0.54              |
| 56:Cv:945:VAL:HG13  | 56:Cv:946:PRO:HD3   | 1.88                     | 0.54              |
| 57:CA:233:C:H4'     | 57:CA:234:C:H5''    | 1.88                     | 0.54              |
| 77:AK:302:THR:O     | 77:AK:305:GLU:HG2   | 2.07                     | 0.54              |
| 79:AP:196:THR:H     | 79:AP:199:HIS:CD2   | 2.25                     | 0.54              |
| 80:AQ:74:LEU:HD11   | 80:AQ:124:ILE:HD12  | 1.89                     | 0.54              |
| 92:Ag:158:GLU:HA    | 92:Ag:158:GLU:OE2   | 2.06                     | 0.54              |
| 104:BB:422:MET:HB3  | 104:BB:427:PHE:CE1  | 2.37                     | 0.54              |
| 109:BG:148:LEU:HD23 | 109:BG:174:MET:HB2  | 1.88                     | 0.54              |
| 133:Be:37:SER:HB2   | 143:UI:9:UNK:HA     | 1.89                     | 0.54              |
| 1:DA:502:LYS:HB3    | 1:DA:502:LYS:HZ2    | 1.72                     | 0.54              |
| 1:DA:1012:THR:O     | 4:DL:77:LEU:HD11    | 2.02                     | 0.54              |
| 2:DD:347:GLU:OE1    | 2:DD:347:GLU:N      | 2.39                     | 0.54              |
| 3:DI:351:LEU:O      | 3:DI:381:TYR:OH     | 2.23                     | 0.54              |
| 11:DS:238:ARG:HG3   | 11:DS:239:SER:N     | 2.21                     | 0.54              |
| 20:DH:393:GLY:HA3   | 50:Ck:691:GLN:HG2   | 1.88                     | 0.54              |
| 25:DW:140:TRP:HE3   | 25:DW:143:MET:HE3   | 1.73                     | 0.54              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:CH:150:THR:HG22  | 31:CH:151:PRO:HD2  | 1.89                     | 0.54              |
| 51:Cm:137:SER:HB3   | 57:CA:394:A:C2     | 2.41                     | 0.54              |
| 56:Cv:392:HIS:HB3   | 56:Cv:417:THR:HG21 | 1.90                     | 0.54              |
| 74:AF:38:ARG:CZ     | 92:Ag:50:ARG:HH12  | 2.20                     | 0.54              |
| 78:AN:164:HIS:HD2   | 78:AN:166:HIS:HB2  | 1.72                     | 0.54              |
| 81:AR:173:ASN:HB3   | 81:AR:202:PRO:HD2  | 1.88                     | 0.54              |
| 104:BB:111:ILE:HD11 | 112:BJ:194:SER:HB3 | 1.90                     | 0.54              |
| 104:BB:427:PHE:HA   | 104:BB:430:TYR:CE2 | 2.41                     | 0.54              |
| 112:BJ:264:LEU:HA   | 112:BJ:267:GLU:HB3 | 1.89                     | 0.54              |
| 120:BR:35:PHE:CE2   | 120:BR:38:GLU:HB3  | 2.42                     | 0.54              |
| 133:Be:62:ARG:HB3   | 133:Be:69:VAL:HG22 | 1.89                     | 0.54              |
| 137:UA:21:UNK:HB2   | 137:UA:26:UNK:HB1  | 1.88                     | 0.54              |
| 7:DO:139:GLU:HB3    | 7:DO:176:THR:HG23  | 1.90                     | 0.54              |
| 11:DS:56:LEU:HG     | 11:DS:88:TRP:HA    | 1.90                     | 0.54              |
| 15:DB:388:VAL:HB    | 20:DH:509:TYR:HA   | 1.90                     | 0.54              |
| 15:DB:867:THR:HG21  | 33:CJ:343:VAL:HG21 | 1.89                     | 0.54              |
| 19:DG:445:LEU:HD22  | 19:DG:531:ASP:HB3  | 1.89                     | 0.54              |
| 34:CK:176:TYR:CZ    | 34:CK:180:ASP:HB3  | 2.43                     | 0.54              |
| 40:CR:142:MET:HE1   | 40:CR:155:VAL:HG13 | 1.89                     | 0.54              |
| 45:Cb:168:ALA:HB2   | 55:Cr:144:ARG:HD3  | 1.89                     | 0.54              |
| 45:Cb:222:SER:OG    | 45:Cb:273:VAL:O    | 2.22                     | 0.54              |
| 51:Cm:53:THR:H      | 51:Cm:56:ASN:HB3   | 1.72                     | 0.54              |
| 53:Cp:93:ARG:HH12   | 57:CA:187:A:H2     | 1.55                     | 0.54              |
| 64:A0:165:PRO:HB2   | 89:Ad:207:THR:HG22 | 1.89                     | 0.54              |
| 69:A5:54:TRP:CH2    | 85:AW:245:ARG:HG3  | 2.43                     | 0.54              |
| 75:AI:212:ASP:OD1   | 75:AI:212:ASP:N    | 2.41                     | 0.54              |
| 79:AP:282:ARG:NH2   | 79:AP:286:GLU:OE2  | 2.40                     | 0.54              |
| 96:Ap:227:HIS:CE1   | 99:AB:18:ALA:HB1   | 2.43                     | 0.54              |
| 102:AA:404:U:OP1    | 124:BV:22:LYS:NZ   | 2.34                     | 0.54              |
| 105:BC:108:GLN:NE2  | 105:BC:242:LEU:H   | 2.05                     | 0.54              |
| 130:Bb:64:PRO:HA    | 130:Bb:67:ARG:NH1  | 2.21                     | 0.54              |
| 3:DI:88:GLN:OE1     | 3:DI:92:GLU:OE2    | 2.25                     | 0.54              |
| 4:DL:114:SER:CB     | 4:DL:254:ARG:HE    | 2.11                     | 0.54              |
| 6:DN:113:ALA:O      | 6:DN:131:PRO:HD2   | 2.08                     | 0.54              |
| 8:DP:143:ASN:ND2    | 49:Cj:142:ASN:OD1  | 2.41                     | 0.54              |
| 17:DE:299:LYS:HB2   | 17:DE:336:ILE:HD13 | 1.90                     | 0.54              |
| 32:CI:293:ARG:NH2   | 32:CI:407:ARG:NH1  | 2.47                     | 0.54              |
| 34:CK:207:VAL:HG22  | 34:CK:219:THR:HG23 | 1.88                     | 0.54              |
| 34:CK:307:PHE:HE1   | 42:CU:61:ILE:HD12  | 1.72                     | 0.54              |
| 34:CK:321:PRO:HD3   | 42:CU:16:HIS:CE1   | 2.42                     | 0.54              |
| 40:CR:75:GLN:HB3    | 40:CR:94:MET:HE3   | 1.89                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:CU:104:LEU:O     | 42:CU:107:SER:OG    | 2.24                     | 0.54              |
| 50:Ck:264:ASN:HD22  | 50:Ck:267:TYR:H     | 1.55                     | 0.54              |
| 52:Cn:179:ARG:HG3   | 52:Cn:183:ARG:HD3   | 1.89                     | 0.54              |
| 65:A1:80:GLU:HG3    | 65:A1:123:VAL:HG11  | 1.88                     | 0.54              |
| 69:A5:51:MET:HE1    | 85:AW:155:LEU:HD11  | 1.90                     | 0.54              |
| 77:AK:304:GLU:OE2   | 77:AK:307:ARG:HD2   | 2.07                     | 0.54              |
| 85:AW:109:ASN:HB2   | 114:BL:152:ASP:OD2  | 2.08                     | 0.54              |
| 89:Ad:227:ARG:NH1   | 132:Bd:40:PHE:HE1   | 2.05                     | 0.54              |
| 95:Ao:97:SER:HB2    | 95:Ao:100:ARG:H     | 1.72                     | 0.54              |
| 98:Av:207:ARG:HG2   | 98:Av:207:ARG:HH11  | 1.73                     | 0.54              |
| 102:AA:526:G:N3     | 102:AA:526:G:H2'    | 2.23                     | 0.54              |
| 104:BB:111:ILE:HG13 | 104:BB:413:LEU:HD21 | 1.90                     | 0.54              |
| 109:BG:180:LEU:H    | 109:BG:287:HIS:CE1  | 2.23                     | 0.54              |
| 116:BN:22:ARG:CA    | 116:BN:191:ARG:HH12 | 2.20                     | 0.54              |
| 120:BR:68:TRP:CZ3   | 120:BR:80:PHE:HB2   | 2.43                     | 0.54              |
| 120:BR:118:GLN:HG3  | 120:BR:119:GLY:H    | 1.71                     | 0.54              |
| 1:DA:651:ARG:HG2    | 1:DA:727:SER:HB3    | 1.90                     | 0.54              |
| 4:DL:119:MET:HE3    | 4:DL:153:ALA:HB2    | 1.90                     | 0.54              |
| 11:DS:76:GLU:OE1    | 11:DS:76:GLU:N      | 2.40                     | 0.54              |
| 11:DS:216:TRP:CZ2   | 11:DS:220:MET:HE3   | 2.43                     | 0.54              |
| 11:DS:238:ARG:HG3   | 11:DS:239:SER:H     | 1.73                     | 0.54              |
| 18:DF:55:ARG:HB2    | 18:DF:59:GLY:HA3    | 1.89                     | 0.54              |
| 25:DW:42:SER:HB2    | 57:CA:519:U:OP1     | 2.08                     | 0.54              |
| 25:DW:53:VAL:HG12   | 25:DW:54:GLU:O      | 2.08                     | 0.54              |
| 25:DW:89:ILE:HG23   | 27:DY:109:PHE:HE2   | 1.72                     | 0.54              |
| 33:CJ:585:SER:C     | 33:CJ:594:GLU:HB2   | 2.32                     | 0.54              |
| 37:CO:261:HIS:O     | 37:CO:265:ARG:HG3   | 2.08                     | 0.54              |
| 37:CO:353:GLU:HB3   | 39:CQ:104:LEU:HD21  | 1.90                     | 0.54              |
| 49:Cj:47:VAL:HG22   | 49:Cj:48:PRO:HD2    | 1.90                     | 0.54              |
| 55:Cr:168:MET:HE1   | 55:Cr:177:LEU:HD12  | 1.88                     | 0.54              |
| 56:Cv:78:ILE:HD11   | 56:Cv:80:TYR:CZ     | 2.43                     | 0.54              |
| 57:CA:461:A:C2      | 57:CA:463:A:H2'     | 2.43                     | 0.54              |
| 65:A1:97:ARG:NH1    | 98:Av:30:MET:O      | 2.41                     | 0.54              |
| 66:A2:57:GLU:HB3    | 66:A2:87:ILE:HD11   | 1.89                     | 0.54              |
| 77:AK:126:LEU:HD21  | 77:AK:187:MET:HE1   | 1.89                     | 0.54              |
| 96:Ap:253:GLN:HE21  | 111:BI:290:LEU:HD12 | 1.72                     | 0.54              |
| 103:BA:197:GLU:H    | 103:BA:197:GLU:CD   | 2.16                     | 0.54              |
| 105:BC:353:ILE:HA   | 105:BC:356:LEU:HD23 | 1.90                     | 0.54              |
| 109:BG:244:ARG:HD3  | 109:BG:257:ARG:NH1  | 2.23                     | 0.54              |
| 112:BJ:257:PRO:HB2  | 129:Ba:45:MET:HE2   | 1.88                     | 0.54              |
| 1:DA:945:ILE:HB     | 5:DM:128:ILE:HD11   | 1.89                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:DA:1003:PHE:HA    | 4:DL:78:ALA:CA      | 2.38                     | 0.54              |
| 3:DI:113:VAL:HG22   | 3:DI:114:PRO:HD2    | 1.88                     | 0.54              |
| 5:DM:289:GLU:OE1    | 5:DM:289:GLU:N      | 2.39                     | 0.54              |
| 23:DT:109:GLU:OE1   | 23:DT:109:GLU:N     | 2.39                     | 0.54              |
| 40:CR:199:TYR:CZ    | 42:CU:106:LYS:NZ    | 2.76                     | 0.54              |
| 47:Cg:325:LEU:HB3   | 47:Cg:326:PRO:HD2   | 1.90                     | 0.54              |
| 65:A1:193:ASP:OD1   | 65:A1:194:GLY:N     | 2.41                     | 0.54              |
| 65:A1:223:LYS:HB2   | 65:A1:223:LYS:NZ    | 2.23                     | 0.54              |
| 74:AF:263:VAL:HG12  | 74:AF:299:ASN:HB3   | 1.89                     | 0.54              |
| 85:AW:78:ASP:OD2    | 85:AW:81:ARG:HB2    | 2.07                     | 0.54              |
| 85:AW:193:LYS:HZ3   | 107:BE:390:SER:HG   | 1.47                     | 0.54              |
| 110:BH:130:VAL:HG22 | 110:BH:182:VAL:HG22 | 1.88                     | 0.54              |
| 2:DD:17:ALA:O       | 29:CE:223:ARG:NH1   | 2.41                     | 0.54              |
| 5:DM:130:ASP:O      | 5:DM:164:ILE:HD11   | 2.08                     | 0.54              |
| 6:DN:141:MET:HB2    | 6:DN:149:ASP:HB3    | 1.89                     | 0.54              |
| 7:DO:60:MET:HE1     | 7:DO:111:ARG:HB3    | 1.89                     | 0.54              |
| 9:DQ:135:GLN:HA     | 9:DQ:138:MET:HE2    | 1.89                     | 0.54              |
| 15:DB:1012:THR:HG22 | 15:DB:1013:ARG:H    | 1.72                     | 0.54              |
| 15:DB:1102:TYR:O    | 15:DB:1106:VAL:HG23 | 2.08                     | 0.54              |
| 16:DC:410:ARG:HE    | 16:DC:453:LEU:HD23  | 1.71                     | 0.54              |
| 23:DT:82:HIS:CD2    | 23:DT:128:PRO:HB3   | 2.43                     | 0.54              |
| 29:CE:88:ASP:OD2    | 29:CE:302:PRO:HB2   | 2.08                     | 0.54              |
| 37:CO:82:ASN:ND2    | 52:Cn:142:TRP:H     | 2.04                     | 0.54              |
| 40:CR:122:MET:HE1   | 56:Cv:192:LEU:HA    | 1.90                     | 0.54              |
| 40:CR:313:PRO:O     | 40:CR:318:LYS:HB2   | 2.07                     | 0.54              |
| 77:AK:334:TYR:CD1   | 92:Ag:218:GLU:HA    | 2.43                     | 0.54              |
| 93:Aj:124:MET:HE3   | 109:BG:345:MET:HE1  | 1.90                     | 0.54              |
| 102:AA:165:A:N7     | 118:BP:112:ARG:NH2  | 2.55                     | 0.54              |
| 102:AA:387:A:N6     | 102:AA:448:A:O4'    | 2.41                     | 0.54              |
| 107:BE:287:LEU:HD11 | 107:BE:325:ALA:HB3  | 1.90                     | 0.54              |
| 113:BK:295:ARG:HB3  | 113:BK:295:ARG:NH1  | 2.22                     | 0.54              |
| 116:BN:142:ALA:O    | 116:BN:145:SER:OG   | 2.25                     | 0.54              |
| 1:DA:131:ASP:O      | 1:DA:133:SER:N      | 2.41                     | 0.54              |
| 1:DA:216:LEU:HB3    | 1:DA:238:VAL:HG22   | 1.89                     | 0.54              |
| 1:DA:1002:PRO:O     | 4:DL:78:ALA:CA      | 2.55                     | 0.54              |
| 4:DL:96:SER:OG      | 4:DL:98:ASP:OD1     | 2.26                     | 0.54              |
| 11:DS:150:GLN:HE22  | 11:DS:176:ARG:NH2   | 2.05                     | 0.54              |
| 15:DB:641:ARG:HD2   | 50:Ck:555:PHE:CD2   | 2.43                     | 0.54              |
| 29:CE:10:LYS:N      | 57:CA:11:U:O4'      | 2.41                     | 0.54              |
| 32:CI:202:LEU:HA    | 32:CI:211:ASN:HD21  | 1.73                     | 0.54              |
| 33:CJ:572:CYS:SG    | 33:CJ:600:PRO:HA    | 2.48                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 39:CQ:140:VAL:HG21 | 39:CQ:172:ARG:HG3   | 1.88                     | 0.54              |
| 40:CR:315:LEU:HD11 | 57:CA:390:U:O2'     | 2.08                     | 0.54              |
| 47:Cg:435:SER:O    | 47:Cg:440:LYS:HE3   | 2.07                     | 0.54              |
| 52:Cn:163:ARG:NH1  | 57:CA:591:A:O2'     | 2.41                     | 0.54              |
| 56:Cv:827:ALA:HB3  | 56:Cv:830:ASN:HD22  | 1.73                     | 0.54              |
| 65:A1:142:LYS:HZ1  | 65:A1:143:ARG:NH1   | 2.06                     | 0.54              |
| 66:A2:394:LYS:NZ   | 102:AA:33:G:OP1     | 2.25                     | 0.54              |
| 67:A3:130:ILE:HG22 | 79:AP:28:ALA:N      | 2.23                     | 0.54              |
| 67:A3:154:ALA:HB2  | 102:AA:333:U:OP2    | 2.08                     | 0.54              |
| 69:A5:51:MET:HE3   | 103:BA:752:ARG:HH21 | 1.71                     | 0.54              |
| 71:A8:172:LYS:HZ2  | 79:AP:259:HIS:CD2   | 2.23                     | 0.54              |
| 77:AK:185:ARG:NH2  | 124:BV:115:GLN:HA   | 2.23                     | 0.54              |
| 81:AR:185:ARG:HH21 | 107:BE:411:LYS:NZ   | 2.06                     | 0.54              |
| 84:AV:144:LYS:HE3  | 84:AV:146:MET:HE3   | 1.90                     | 0.54              |
| 103:BA:714:ASN:HB3 | 103:BA:717:VAL:HG22 | 1.90                     | 0.54              |
| 107:BE:447:GLU:O   | 107:BE:448:ARG:HB2  | 2.06                     | 0.54              |
| 110:BH:122:HIS:HD2 | 110:BH:124:PHE:HB2  | 1.73                     | 0.54              |
| 112:BJ:221:ARG:NH1 | 137:UA:29:UNK:HG1   | 2.22                     | 0.54              |
| 116:BN:64:LEU:HD11 | 116:BN:108:PHE:CD2  | 2.42                     | 0.54              |
| 128:BZ:19:ARG:HD2  | 128:BZ:162:VAL:HG13 | 1.88                     | 0.54              |
| 1:DA:1244:LYS:NZ   | 1:DA:1296:GLU:HB3   | 2.23                     | 0.53              |
| 2:DD:535:ASP:OD2   | 2:DD:538:THR:OG1    | 2.23                     | 0.53              |
| 5:DM:52:VAL:HG22   | 5:DM:63:VAL:HG22    | 1.90                     | 0.53              |
| 8:DP:132:LEU:HD21  | 8:DP:154:PHE:CE1    | 2.43                     | 0.53              |
| 18:DF:426:LEU:CB   | 20:DH:200:THR:CG2   | 2.71                     | 0.53              |
| 19:DG:530:PHE:HZ   | 19:DG:596:VAL:HG12  | 1.73                     | 0.53              |
| 25:DW:83:THR:HG21  | 25:DW:163:GLU:HG3   | 1.90                     | 0.53              |
| 28:CC:17:GLN:O     | 28:CC:19:TYR:N      | 2.42                     | 0.53              |
| 45:Cb:52:TYR:O     | 45:Cb:56:ARG:HB2    | 2.08                     | 0.53              |
| 51:Cm:56:ASN:HD21  | 51:Cm:62:ALA:HB2    | 1.73                     | 0.53              |
| 56:Cv:27:LYS:HE3   | 56:Cv:29:LEU:HB2    | 1.89                     | 0.53              |
| 56:Cv:559:GLN:OE1  | 56:Cv:565:ILE:HG12  | 2.08                     | 0.53              |
| 65:A1:85:ARG:HH12  | 102:AA:891:G:H5'    | 1.73                     | 0.53              |
| 69:A5:71:ARG:NH1   | 81:AR:84:ILE:HD11   | 2.23                     | 0.53              |
| 85:AW:134:LEU:HD13 | 85:AW:231:VAL:HG22  | 1.89                     | 0.53              |
| 87:AY:75:THR:HG23  | 107:BE:58:PRO:O     | 2.07                     | 0.53              |
| 87:AY:227:ASP:OD2  | 87:AY:230:LYS:HB2   | 2.08                     | 0.53              |
| 105:BC:272:ASP:OD2 | 105:BC:275:PRO:HA   | 2.07                     | 0.53              |
| 105:BC:510:ASP:HB3 | 105:BC:514:GLN:HB3  | 1.90                     | 0.53              |
| 110:BH:127:SER:HB2 | 110:BH:185:HIS:HB2  | 1.89                     | 0.53              |
| 113:BK:97:ALA:O    | 113:BK:146:ARG:NH2  | 2.37                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 115:BM:245:LEU:HD12 | 120:BR:180:ASN:HB2  | 1.90                     | 0.53              |
| 121:BS:110:LEU:HD23 | 121:BS:113:ARG:HD3  | 1.90                     | 0.53              |
| 122:BT:105:VAL:O    | 122:BT:108:LEU:HG   | 2.08                     | 0.53              |
| 125:BW:27:TYR:CE2   | 125:BW:29:SER:HA    | 2.43                     | 0.53              |
| 129:Ba:49:ARG:HD2   | 129:Ba:83:PHE:CE2   | 2.43                     | 0.53              |
| 1:DA:565:ASN:HA     | 6:DN:144:ARG:NH1    | 2.23                     | 0.53              |
| 2:DD:605:ARG:HH12   | 2:DD:642:ASP:CG     | 2.14                     | 0.53              |
| 4:DL:181:ARG:HG3    | 4:DL:181:ARG:NH1    | 2.17                     | 0.53              |
| 19:DG:80:LEU:N      | 19:DG:81:PRO:HD2    | 2.23                     | 0.53              |
| 65:A1:179:MET:HE1   | 112:BJ:243:LYS:HG3  | 1.88                     | 0.53              |
| 73:AE:139:GLY:HA3   | 73:AE:339:PHE:O     | 2.09                     | 0.53              |
| 85:AW:59:ILE:HG23   | 108:BF:394:GLY:HA3  | 1.90                     | 0.53              |
| 85:AW:158:ARG:NH1   | 85:AW:242:LEU:HD13  | 2.22                     | 0.53              |
| 88:Ab:85:GLU:O      | 88:Ab:88:THR:N      | 2.36                     | 0.53              |
| 88:Ab:200:PHE:O     | 88:Ab:203:THR:HG23  | 2.08                     | 0.53              |
| 90:Ae:59:ASP:OD2    | 90:Ae:61:THR:HG22   | 2.06                     | 0.53              |
| 96:Ap:264:TRP:CD1   | 96:Ap:285:TYR:HH    | 2.25                     | 0.53              |
| 103:BA:311:PHE:CE1  | 131:Bc:22:PRO:HB3   | 2.43                     | 0.53              |
| 106:BD:346:LYS:CB   | 106:BD:364:CYS:N    | 2.71                     | 0.53              |
| 126:BX:164:HIS:ND1  | 126:BX:164:HIS:O    | 2.41                     | 0.53              |
| 140:UD:59:UNK:O     | 140:UD:63:UNK:HB1   | 2.08                     | 0.53              |
| 1:DA:834:PRO:HA     | 1:DA:837:ARG:HD2    | 1.90                     | 0.53              |
| 1:DA:1510:GLU:OE1   | 1:DA:1510:GLU:N     | 2.42                     | 0.53              |
| 4:DL:91:PHE:CE1     | 4:DL:106:PHE:HB2    | 2.43                     | 0.53              |
| 9:DQ:181:VAL:O      | 9:DQ:184:ILE:HG13   | 2.08                     | 0.53              |
| 16:DC:302:ARG:HH11  | 16:DC:356:TRP:CD1   | 2.25                     | 0.53              |
| 16:DC:381:LEU:CD1   | 16:DC:385:THR:HG21  | 2.38                     | 0.53              |
| 16:DC:899:GLN:HG3   | 16:DC:933:ARG:HH22  | 1.74                     | 0.53              |
| 18:DF:349:ASP:N     | 18:DF:349:ASP:OD1   | 2.40                     | 0.53              |
| 66:A2:176:LYS:NZ    | 66:A2:176:LYS:HB3   | 2.23                     | 0.53              |
| 67:A3:87:GLU:HG2    | 102:AA:333:U:H1'    | 1.90                     | 0.53              |
| 75:AI:31:GLU:OE2    | 75:AI:74:SER:HB2    | 2.09                     | 0.53              |
| 77:AK:301:MET:HA    | 77:AK:305:GLU:OE2   | 2.07                     | 0.53              |
| 85:AW:112:LEU:O     | 85:AW:116:ARG:HB2   | 2.08                     | 0.53              |
| 92:Ag:125:ARG:NH1   | 92:Ag:129:ALA:HA    | 2.22                     | 0.53              |
| 102:AA:485:A:O2'    | 102:AA:486:A:OP1    | 2.25                     | 0.53              |
| 104:BB:218:HIS:O    | 126:BX:118:LYS:NZ   | 2.41                     | 0.53              |
| 105:BC:319:PRO:HB3  | 105:BC:323:ILE:HD12 | 1.90                     | 0.53              |
| 114:BL:241:ASP:N    | 114:BL:241:ASP:OD1  | 2.41                     | 0.53              |
| 6:DN:23:VAL:HG12    | 6:DN:116:VAL:CG1    | 2.39                     | 0.53              |
| 12:DU:206:PRO:HB3   | 37:CO:387:VAL:HG13  | 1.91                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:DU:207:ARG:HB2   | 57:CA:160:U:C6      | 2.42                     | 0.53              |
| 44:Ca:225:PRO:HD2   | 44:Ca:228:LYS:HD2   | 1.91                     | 0.53              |
| 57:CA:153:A:C4      | 57:CA:154:G:C8      | 2.97                     | 0.53              |
| 92:Ag:14:ILE:HG12   | 92:Ag:57:ILE:HD11   | 1.90                     | 0.53              |
| 102:AA:1115:A:OP2   | 111:BI:26:ASN:ND2   | 2.42                     | 0.53              |
| 104:BB:166:LEU:HD11 | 104:BB:240:HIS:CE1  | 2.44                     | 0.53              |
| 127:BY:129:ASP:N    | 127:BY:129:ASP:OD1  | 2.41                     | 0.53              |
| 132:Bd:125:GLN:HE21 | 132:Bd:129:MET:HE3  | 1.73                     | 0.53              |
| 2:DD:421:PHE:HB3    | 2:DD:531:LYS:HG3    | 1.89                     | 0.53              |
| 3:DI:161:MET:O      | 3:DI:165:ARG:HG3    | 2.08                     | 0.53              |
| 9:DQ:146:GLN:CG     | 9:DQ:176:ARG:HH12   | 2.21                     | 0.53              |
| 32:CI:139:ASP:OD1   | 32:CI:139:ASP:N     | 2.41                     | 0.53              |
| 32:CI:303:THR:HB    | 32:CI:305:ILE:HG13  | 1.89                     | 0.53              |
| 57:CA:88:A:H3'      | 57:CA:88:A:OP2      | 2.08                     | 0.53              |
| 85:AW:240:MET:HE3   | 85:AW:242:LEU:HD21  | 1.90                     | 0.53              |
| 94:Al:146:LEU:HD12  | 94:Al:147:PRO:HD3   | 1.89                     | 0.53              |
| 96:Ap:45:LEU:HD23   | 96:Ap:48:TYR:HB3    | 1.91                     | 0.53              |
| 98:Av:47:ARG:HG2    | 98:Av:48:ALA:N      | 2.23                     | 0.53              |
| 108:BF:123:LEU:HA   | 108:BF:126:VAL:HG22 | 1.89                     | 0.53              |
| 114:BL:180:LEU:HD21 | 114:BL:256:ARG:HD3  | 1.91                     | 0.53              |
| 3:DI:25:PRO:HB3     | 3:DI:79:ILE:HD11    | 1.90                     | 0.53              |
| 4:DL:271:PRO:C      | 4:DL:274:THR:HG23   | 2.32                     | 0.53              |
| 6:DN:129:LEU:HD21   | 6:DN:156:ALA:HB2    | 1.91                     | 0.53              |
| 8:DP:48:GLN:OE1     | 8:DP:75:ARG:NH2     | 2.34                     | 0.53              |
| 9:DQ:218:ARG:HD2    | 9:DQ:223:ASP:OD1    | 2.07                     | 0.53              |
| 10:DR:60:VAL:HG22   | 10:DR:63:ILE:HG12   | 1.90                     | 0.53              |
| 11:DS:111:VAL:HG12  | 11:DS:117:ALA:HB3   | 1.90                     | 0.53              |
| 18:DF:275:MET:O     | 18:DF:279:ILE:HG12  | 2.08                     | 0.53              |
| 19:DG:204:SER:OG    | 19:DG:205:GLY:N     | 2.39                     | 0.53              |
| 19:DG:395:TRP:HA    | 19:DG:451:ARG:HH12  | 1.74                     | 0.53              |
| 25:DW:115:ASN:ND2   | 40:CR:296:PHE:CE2   | 2.76                     | 0.53              |
| 27:DY:35:PRO:HB3    | 47:Cg:464:VAL:HG11  | 1.90                     | 0.53              |
| 33:CJ:53:PRO:HG2    | 33:CJ:56:ILE:HD12   | 1.91                     | 0.53              |
| 33:CJ:555:TRP:HA    | 33:CJ:583:LYS:NZ    | 2.23                     | 0.53              |
| 38:CP:88:LEU:HD21   | 53:Cp:33:ILE:HD13   | 1.90                     | 0.53              |
| 44:Ca:507:MET:O     | 44:Ca:513:ASN:ND2   | 2.42                     | 0.53              |
| 73:AE:102:ASP:HB3   | 96:Ap:145:VAL:HG11  | 1.91                     | 0.53              |
| 75:AI:196:GLU:HG3   | 127:BY:137:ALA:HB3  | 1.91                     | 0.53              |
| 76:AJ:74:ARG:HH22   | 77:AK:239:ILE:HD13  | 1.73                     | 0.53              |
| 88:Ab:329:SER:O     | 88:Ab:372:ARG:NH2   | 2.41                     | 0.53              |
| 102:AA:830:A:H2'    | 102:AA:831:A:C8     | 2.44                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 108:BF:321:PHE:HA   | 108:BF:324:MET:HE3  | 1.90                     | 0.53              |
| 110:BH:228:VAL:HG12 | 110:BH:229:ALA:O    | 2.09                     | 0.53              |
| 116:BN:197:GLU:OE2  | 116:BN:219:ARG:HG2  | 2.08                     | 0.53              |
| 121:BS:85:ASP:HA    | 121:BS:88:LYS:HG2   | 1.90                     | 0.53              |
| 1:DA:1606:THR:HG22  | 1:DA:1607:MET:HG3   | 1.91                     | 0.53              |
| 2:DD:13:GLY:O       | 52:Cn:155:ARG:NH2   | 2.42                     | 0.53              |
| 16:DC:50:GLU:OE1    | 16:DC:405:ILE:CD1   | 2.57                     | 0.53              |
| 18:DF:425:ILE:CD1   | 20:DH:196:LEU:CD1   | 2.87                     | 0.53              |
| 26:DX:85:LYS:HA     | 26:DX:87:PHE:H      | 1.73                     | 0.53              |
| 33:CJ:37:ASN:ND2    | 51:Cm:49:GLY:O      | 2.32                     | 0.53              |
| 33:CJ:233:THR:HG22  | 33:CJ:235:GLU:H     | 1.74                     | 0.53              |
| 37:CO:259:LEU:HD22  | 37:CO:286:ILE:HD11  | 1.90                     | 0.53              |
| 41:CS:152:ASP:OD1   | 41:CS:152:ASP:N     | 2.34                     | 0.53              |
| 42:CU:52:GLU:HG3    | 46:Cd:250:LEU:HD21  | 1.91                     | 0.53              |
| 45:Cb:168:ALA:HB1   | 45:Cb:174:PHE:CD2   | 2.43                     | 0.53              |
| 56:Cv:470:PHE:HD1   | 56:Cv:556:PHE:CE2   | 2.26                     | 0.53              |
| 57:CA:394:A:H2'     | 57:CA:394:A:OP2     | 2.09                     | 0.53              |
| 71:A8:143:THR:OG1   | 71:A8:144:ASN:N     | 2.42                     | 0.53              |
| 74:AF:118:PHE:HE1   | 74:AF:124:VAL:HG22  | 1.73                     | 0.53              |
| 74:AF:192:ASN:O     | 74:AF:198:GLY:HA3   | 2.08                     | 0.53              |
| 94:Al:88:ARG:HG2    | 94:Al:88:ARG:HH11   | 1.74                     | 0.53              |
| 97:At:100:ALA:O     | 97:At:104:ARG:NH2   | 2.42                     | 0.53              |
| 102:AA:440:U:P      | 115:BM:277:LYS:HZ1  | 2.32                     | 0.53              |
| 105:BC:83:ILE:HG12  | 105:BC:338:HIS:HB2  | 1.89                     | 0.53              |
| 111:BI:265:THR:HG21 | 111:BI:305:LYS:HZ2  | 1.72                     | 0.53              |
| 119:BQ:86:VAL:HG22  | 119:BQ:92:VAL:HG13  | 1.91                     | 0.53              |
| 119:BQ:222:GLU:O    | 119:BQ:226:ILE:HG22 | 2.08                     | 0.53              |
| 2:DD:27:MET:HE1     | 31:CH:239:ARG:HD2   | 1.90                     | 0.53              |
| 2:DD:576:MET:HE3    | 10:DR:221:ARG:HB2   | 1.91                     | 0.53              |
| 4:DL:139:ARG:HH22   | 4:DL:203:ARG:NH1    | 2.06                     | 0.53              |
| 10:DR:30:TRP:CE3    | 12:DU:98:MET:HB2    | 2.44                     | 0.53              |
| 10:DR:87:LEU:HB2    | 10:DR:178:TYR:HE2   | 1.74                     | 0.53              |
| 10:DR:112:ARG:HD2   | 49:Cj:158:THR:HG23  | 1.91                     | 0.53              |
| 17:DE:174:VAL:HG11  | 17:DE:550:ALA:HB2   | 1.90                     | 0.53              |
| 19:DG:399:ARG:NH2   | 19:DG:457:ARG:NH1   | 2.57                     | 0.53              |
| 26:DX:103:MET:HG2   | 26:DX:124:ILE:HG13  | 1.91                     | 0.53              |
| 30:CF:35:LEU:HD21   | 37:CO:187:LYS:HD3   | 1.91                     | 0.53              |
| 44:Ca:191:MET:SD    | 44:Ca:195:ARG:NH2   | 2.80                     | 0.53              |
| 49:Cj:112:ARG:NH1   | 49:Cj:183:PHE:HA    | 2.23                     | 0.53              |
| 50:Ck:188:LEU:HD21  | 50:Ck:224:LYS:HD3   | 1.91                     | 0.53              |
| 64:A0:149:ARG:NH1   | 120:BR:19:TYR:O     | 2.41                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 75:AI:70:ARG:HD2    | 75:AI:75:GLU:HG3    | 1.91                     | 0.53              |
| 75:AI:205:TYR:O     | 75:AI:208:ARG:HG3   | 2.08                     | 0.53              |
| 86:AX:168:SER:HB3   | 86:AX:171:GLU:HG3   | 1.91                     | 0.53              |
| 87:AY:72:GLN:O      | 107:BE:54:LEU:HD13  | 2.07                     | 0.53              |
| 92:Ag:159:ILE:HD13  | 111:BI:276:ILE:HG23 | 1.91                     | 0.53              |
| 102:AA:10:A:N6      | 102:AA:104:A:O2'    | 2.39                     | 0.53              |
| 102:AA:572:U:H2'    | 102:AA:573:U:H5'    | 1.91                     | 0.53              |
| 106:BD:108:TYR:O    | 106:BD:109:CYS:CB   | 2.56                     | 0.53              |
| 109:BG:65:MET:HE2   | 109:BG:67:HIS:N     | 2.24                     | 0.53              |
| 110:BH:122:HIS:CD2  | 110:BH:124:PHE:H    | 2.27                     | 0.53              |
| 113:BK:373:PRO:HG2  | 113:BK:376:MET:HB2  | 1.89                     | 0.53              |
| 118:BP:177:ARG:HB2  | 118:BP:180:ASP:OD2  | 2.09                     | 0.53              |
| 129:Ba:89:PRO:HG2   | 129:Ba:92:TYR:CD2   | 2.40                     | 0.53              |
| 1:DA:410:ASP:OD1    | 1:DA:494:ARG:NH1    | 2.41                     | 0.53              |
| 1:DA:1280:GLU:OE2   | 54:Cq:151:ARG:HB3   | 2.09                     | 0.53              |
| 2:DD:283:MET:HG3    | 3:DI:65:MET:HE3     | 1.91                     | 0.53              |
| 10:DR:117:ILE:HG22  | 10:DR:118:VAL:H     | 1.74                     | 0.53              |
| 15:DB:517:GLU:HG2   | 15:DB:841:ARG:NH2   | 2.24                     | 0.53              |
| 18:DF:585:TYR:CD1   | 20:DH:195:TYR:CD1   | 2.97                     | 0.53              |
| 33:CJ:631:LEU:HD13  | 33:CJ:656:VAL:HG13  | 1.91                     | 0.53              |
| 40:CR:37:PRO:HD3    | 45:Cb:110:MET:HG3   | 1.91                     | 0.53              |
| 40:CR:319:LYS:HZ1   | 46:Cd:281:MET:C     | 2.09                     | 0.53              |
| 42:CU:62:MET:HB3    | 42:CU:171:VAL:HG11  | 1.90                     | 0.53              |
| 56:Cv:441:PRO:HD3   | 56:Cv:447:PRO:HD3   | 1.91                     | 0.53              |
| 56:Cv:690:GLU:HB2   | 56:Cv:798:TYR:CE1   | 2.44                     | 0.53              |
| 64:A0:65:ARG:HH21   | 64:A0:98:TYR:HB3    | 1.74                     | 0.53              |
| 75:AI:48:ARG:HH11   | 75:AI:48:ARG:HG2    | 1.73                     | 0.53              |
| 103:BA:585:HIS:CD2  | 103:BA:587:SER:H    | 2.27                     | 0.53              |
| 104:BB:102:ILE:HG21 | 104:BB:393:LEU:HD11 | 1.91                     | 0.53              |
| 107:BE:439:PHE:HB3  | 135:Bg:26:PHE:HB3   | 1.90                     | 0.53              |
| 109:BG:189:MET:HE1  | 109:BG:253:ARG:HH11 | 1.74                     | 0.53              |
| 116:BN:121:LEU:HD23 | 116:BN:123:PHE:CZ   | 2.44                     | 0.53              |
| 121:BS:44:ASP:O     | 121:BS:45:ILE:HG13  | 2.09                     | 0.53              |
| 1:DA:135:ASP:OD2    | 46:Cd:109:MET:HE2   | 2.09                     | 0.53              |
| 2:DD:106:ALA:HB2    | 44:Ca:457:LYS:HD3   | 1.91                     | 0.53              |
| 2:DD:527:THR:HG21   | 10:DR:224:ALA:H     | 1.73                     | 0.53              |
| 10:DR:128:PRO:HD3   | 10:DR:133:LEU:C     | 2.30                     | 0.53              |
| 13:DZ:11:LYS:O      | 44:Ca:89:ARG:NH1    | 2.42                     | 0.53              |
| 13:DZ:74:MET:HE3    | 44:Ca:194:LEU:HD13  | 1.91                     | 0.53              |
| 15:DB:917:LEU:HD13  | 15:DB:930:GLU:HB3   | 1.90                     | 0.53              |
| 16:DC:1008:GLY:O    | 22:DK:157:ALA:HB3   | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:DH:26:PRO:HB3   | 21:DJ:17:PRO:HB2   | 1.90                     | 0.53              |
| 31:CH:107:ARG:NH1  | 31:CH:133:ARG:NE   | 2.57                     | 0.53              |
| 37:CO:301:TRP:HZ2  | 39:CQ:182:VAL:HG21 | 1.73                     | 0.53              |
| 40:CR:319:LYS:NZ   | 46:Cd:281:MET:C    | 2.67                     | 0.53              |
| 42:CU:142:PRO:HD3  | 42:CU:154:LYS:HE2  | 1.91                     | 0.53              |
| 43:CZ:341:LYS:HD2  | 57:CA:578:C:P      | 2.49                     | 0.53              |
| 46:Cd:137:ARG:HG2  | 46:Cd:137:ARG:NH1  | 2.22                     | 0.53              |
| 51:Cm:211:LEU:HD23 | 51:Cm:212:PRO:HD2  | 1.90                     | 0.53              |
| 66:A2:64:MET:HE2   | 66:A2:64:MET:HA    | 1.91                     | 0.53              |
| 69:A5:28:ARG:HD2   | 102:AA:813:U:H5    | 1.74                     | 0.53              |
| 73:AE:317:ASP:OD1  | 73:AE:380:GLN:NE2  | 2.42                     | 0.53              |
| 74:AF:38:ARG:CZ    | 92:Ag:50:ARG:NH1   | 2.71                     | 0.53              |
| 79:AP:43:LYS:HG3   | 108:BF:135:TYR:CE1 | 2.44                     | 0.53              |
| 85:AW:99:VAL:HG11  | 114:BL:159:TYR:CZ  | 2.44                     | 0.53              |
| 108:BF:207:GLU:OE2 | 108:BF:281:ARG:HB3 | 2.08                     | 0.53              |
| 112:BJ:267:GLU:HA  | 112:BJ:270:ARG:HD3 | 1.90                     | 0.53              |
| 132:Bd:17:GLN:O    | 132:Bd:20:ARG:HG2  | 2.09                     | 0.53              |
| 140:UD:82:UNK:HG3  | 140:UD:136:UNK:N   | 2.24                     | 0.53              |
| 1:DA:1524:ARG:HH21 | 1:DA:1601:ARG:HH21 | 1.57                     | 0.52              |
| 2:DD:21:ARG:NH2    | 57:CA:274:A:N7     | 2.53                     | 0.52              |
| 5:DM:56:TRP:O      | 5:DM:59:ARG:HG2    | 2.08                     | 0.52              |
| 9:DQ:77:LEU:HB2    | 9:DQ:115:ILE:HB    | 1.90                     | 0.52              |
| 15:DB:123:ILE:H    | 15:DB:123:ILE:HD12 | 1.73                     | 0.52              |
| 16:DC:589:VAL:HG21 | 16:DC:604:VAL:O    | 2.10                     | 0.52              |
| 16:DC:1104:MET:HE1 | 20:DH:146:GLN:HE21 | 1.73                     | 0.52              |
| 23:DT:162:TYR:CE2  | 23:DT:165:GLY:HA2  | 2.43                     | 0.52              |
| 27:DY:20:PRO:HG2   | 27:DY:23:SER:OG    | 2.09                     | 0.52              |
| 37:CO:214:HIS:CD2  | 37:CO:216:PHE:H    | 2.28                     | 0.52              |
| 37:CO:264:ARG:NH1  | 37:CO:303:TYR:HB3  | 2.24                     | 0.52              |
| 40:CR:23:TRP:CD2   | 56:Cv:494:THR:HG21 | 2.43                     | 0.52              |
| 44:Ca:89:ARG:HD2   | 44:Ca:177:GLN:HE21 | 1.74                     | 0.52              |
| 68:A4:50:ARG:HH21  | 105:BC:215:GLN:CB  | 2.22                     | 0.52              |
| 68:A4:164:ARG:NH1  | 93:Aj:26:PRO:HB3   | 2.24                     | 0.52              |
| 74:AF:207:TRP:O    | 74:AF:327:LYS:HG3  | 2.08                     | 0.52              |
| 76:Aj:12:LEU:O     | 76:Aj:41:ARG:NH2   | 2.42                     | 0.52              |
| 79:AP:233:GLU:OE2  | 125:BW:12:SER:HB2  | 2.09                     | 0.52              |
| 81:AR:154:ARG:HD3  | 107:BE:406:ASP:CG  | 2.33                     | 0.52              |
| 85:AW:90:ARG:HH11  | 108:BF:398:ARG:NH2 | 2.07                     | 0.52              |
| 96:Ap:123:LYS:NZ   | 146:UM:6:UNK:HA    | 2.25                     | 0.52              |
| 98:Av:118:ASN:ND2  | 98:Av:121:THR:OG1  | 2.42                     | 0.52              |
| 102:AA:948:A:OP2   | 127:BY:165:ARG:NH2 | 2.42                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 105:BC:470:ARG:NH1  | 105:BC:518:HIS:HB3  | 2.24                     | 0.52              |
| 107:BE:239:ILE:HD12 | 107:BE:265:ALA:HB1  | 1.91                     | 0.52              |
| 107:BE:350:ASN:O    | 107:BE:354:GLU:N    | 2.41                     | 0.52              |
| 115:BM:82:ASN:ND2   | 119:BQ:217:THR:HA   | 2.24                     | 0.52              |
| 115:BM:216:HIS:CE1  | 115:BM:221:LEU:HA   | 2.45                     | 0.52              |
| 118:BP:91:GLU:HG2   | 118:BP:99:VAL:HB    | 1.91                     | 0.52              |
| 140:UD:34:UNK:O     | 140:UD:38:UNK:HG3   | 2.10                     | 0.52              |
| 1:DA:130:ALA:N      | 31:CH:260:ASN:HD21  | 2.07                     | 0.52              |
| 2:DD:133:GLU:OE2    | 12:DU:50:SER:OG     | 2.25                     | 0.52              |
| 2:DD:631:ALA:HB1    | 2:DD:635:LEU:HD23   | 1.90                     | 0.52              |
| 15:DB:511:ARG:CG    | 15:DB:511:ARG:NH1   | 2.66                     | 0.52              |
| 15:DB:815:ASP:OD2   | 18:DF:555:ARG:HA    | 2.09                     | 0.52              |
| 16:DC:119:THR:HG21  | 16:DC:136:TRP:CD1   | 2.44                     | 0.52              |
| 16:DC:638:ASP:HB3   | 16:DC:652:ARG:HH22  | 1.74                     | 0.52              |
| 17:DE:199:SER:H     | 17:DE:202:HIS:HD2   | 1.56                     | 0.52              |
| 18:DF:228:VAL:HG22  | 18:DF:261:LEU:HD22  | 1.91                     | 0.52              |
| 18:DF:383:ASP:O     | 18:DF:387:VAL:HG23  | 2.09                     | 0.52              |
| 30:CF:123:ARG:HG3   | 30:CF:127:GLU:CD    | 2.33                     | 0.52              |
| 31:CH:138:LYS:NZ    | 31:CH:138:LYS:HB2   | 2.23                     | 0.52              |
| 33:CJ:441:HIS:CD2   | 50:Ck:768:SER:HB2   | 2.44                     | 0.52              |
| 33:CJ:541:LEU:O     | 33:CJ:544:THR:HG22  | 2.08                     | 0.52              |
| 33:CJ:555:TRP:HA    | 33:CJ:583:LYS:HZ2   | 1.74                     | 0.52              |
| 33:CJ:800:LEU:HB2   | 33:CJ:803:ILE:HD12  | 1.89                     | 0.52              |
| 51:Cm:77:PRO:HB3    | 51:Cm:155:HIS:HE1   | 1.73                     | 0.52              |
| 54:Cq:146:PRO:HG3   | 54:Cq:167:MET:HE2   | 1.91                     | 0.52              |
| 55:Cr:103:VAL:HG23  | 55:Cr:184:VAL:HG13  | 1.91                     | 0.52              |
| 56:Cv:592:TYR:HE1   | 56:Cv:785:ILE:HD11  | 1.74                     | 0.52              |
| 56:Cv:1108:GLN:HA   | 56:Cv:1108:GLN:HE21 | 1.74                     | 0.52              |
| 71:A8:135:ARG:HG2   | 102:AA:178:A:C2     | 2.44                     | 0.52              |
| 102:AA:318:A:H61    | 102:AA:343:U:H3     | 1.58                     | 0.52              |
| 109:BG:72:GLY:HA3   | 109:BG:107:TYR:HD2  | 1.75                     | 0.52              |
| 110:BH:85:ASP:OD1   | 110:BH:85:ASP:N     | 2.41                     | 0.52              |
| 111:BI:187:LEU:HD22 | 134:Bf:99:ILE:HD11  | 1.91                     | 0.52              |
| 115:BM:217:GLU:OE1  | 115:BM:217:GLU:N    | 2.42                     | 0.52              |
| 116:BN:179:LEU:HD11 | 140:UD:212:UNK:HG1  | 1.90                     | 0.52              |
| 122:BT:72:LEU:HD12  | 122:BT:76:GLY:HA2   | 1.91                     | 0.52              |
| 2:DD:608:ASP:O      | 10:DR:227:ARG:NH1   | 2.36                     | 0.52              |
| 8:DP:171:LEU:HD11   | 8:DP:187:ARG:HA     | 1.91                     | 0.52              |
| 15:DB:452:ARG:HG3   | 15:DB:462:ASP:OD1   | 2.09                     | 0.52              |
| 20:DH:175:ALA:HB1   | 20:DH:206:ILE:HD13  | 1.91                     | 0.52              |
| 26:DX:136:ARG:HB3   | 26:DX:136:ARG:HH11  | 1.74                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 36:CN:76:TYR:HA     | 41:CS:86:GLU:OE2    | 2.10                     | 0.52              |
| 40:CR:36:THR:HG23   | 40:CR:99:ASN:HD22   | 1.75                     | 0.52              |
| 40:CR:306:LYS:HZ3   | 57:CA:390:U:P       | 2.31                     | 0.52              |
| 57:CA:43:A:H62      | 57:CA:173:A:H62     | 1.57                     | 0.52              |
| 68:A4:29:HIS:CE1    | 68:A4:31:ARG:HE     | 2.28                     | 0.52              |
| 68:A4:61:ARG:HE     | 89:Ad:49:ARG:NH1    | 2.07                     | 0.52              |
| 75:AI:99:LEU:HD12   | 75:AI:100:LEU:HB2   | 1.91                     | 0.52              |
| 78:AN:176:TRP:CZ2   | 78:AN:178:ASP:HB3   | 2.44                     | 0.52              |
| 84:AV:162:ARG:HG2   | 84:AV:164:VAL:HG23  | 1.91                     | 0.52              |
| 86:AX:87:ASP:HB2    | 87:AY:82:ARG:HG2    | 1.90                     | 0.52              |
| 91:Af:58:ARG:NH1    | 102:AA:381:U:P      | 2.83                     | 0.52              |
| 96:Ap:168:THR:HG21  | 96:Ap:285:TYR:HA    | 1.92                     | 0.52              |
| 104:BB:359:HIS:HD2  | 104:BB:363:ARG:NH1  | 2.06                     | 0.52              |
| 113:BK:227:GLN:HA   | 113:BK:230:GLU:OE2  | 2.10                     | 0.52              |
| 113:BK:360:GLU:H    | 113:BK:360:GLU:CD   | 2.18                     | 0.52              |
| 116:BN:193:PHE:CE2  | 140:UD:222:UNK:HG1  | 2.44                     | 0.52              |
| 122:BT:173:LEU:HD13 | 122:BT:176:GLY:HA3  | 1.91                     | 0.52              |
| 131:Bc:56:TRP:HD1   | 131:Bc:64:PHE:HZ    | 1.56                     | 0.52              |
| 140:UD:193:UNK:O    | 140:UD:197:UNK:HB1  | 2.10                     | 0.52              |
| 1:DA:617:PRO:HG2    | 1:DA:746:GLN:HE22   | 1.74                     | 0.52              |
| 1:DA:1038:HIS:CG    | 1:DA:1045:ILE:HD11  | 2.45                     | 0.52              |
| 2:DD:610:VAL:HG21   | 10:DR:229:ARG:O     | 2.08                     | 0.52              |
| 17:DE:229:ARG:NH1   | 17:DE:255:PHE:HE1   | 2.07                     | 0.52              |
| 20:DH:156:LEU:HD13  | 20:DH:216:THR:HG23  | 1.91                     | 0.52              |
| 33:CJ:544:THR:CG2   | 33:CJ:552:ILE:H     | 2.15                     | 0.52              |
| 34:CK:156:LYS:HB2   | 34:CK:156:LYS:HZ3   | 1.74                     | 0.52              |
| 37:CO:82:ASN:HD21   | 52:Cn:142:TRP:H     | 1.57                     | 0.52              |
| 44:Ca:272:PHE:CE1   | 44:Ca:309:ALA:HB1   | 2.45                     | 0.52              |
| 45:Cb:12:PRO:HG2    | 45:Cb:15:MET:HG2    | 1.91                     | 0.52              |
| 54:Cq:104:HIS:HB3   | 54:Cq:108:THR:OG1   | 2.09                     | 0.52              |
| 57:CA:309:A:H2'     | 57:CA:309:A:N3      | 2.24                     | 0.52              |
| 57:CA:360:C:C2'     | 57:CA:361:A:H5'     | 2.39                     | 0.52              |
| 66:A2:92:ARG:NH1    | 113:BK:365:CYS:SG   | 2.82                     | 0.52              |
| 89:Ad:173:SER:HB2   | 89:Ad:176:LEU:HB2   | 1.90                     | 0.52              |
| 89:Ad:277:TYR:CE1   | 105:BC:237:PRO:HG2  | 2.43                     | 0.52              |
| 90:Ae:100:HIS:HB2   | 90:Ae:106:LEU:HD23  | 1.92                     | 0.52              |
| 105:BC:109:THR:HB   | 105:BC:165:HIS:HE1  | 1.73                     | 0.52              |
| 105:BC:306:GLU:HA   | 105:BC:335:VAL:HG23 | 1.90                     | 0.52              |
| 107:BE:38:PRO:CB    | 107:BE:43:PRO:HB3   | 2.40                     | 0.52              |
| 108:BF:362:HIS:CD2  | 125:BW:177:VAL:H    | 2.26                     | 0.52              |
| 114:BL:162:HIS:ND1  | 114:BL:239:VAL:HG12 | 2.23                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 140:UD:164:UNK:HA  | 140:UD:167:UNK:HG3  | 1.92                     | 0.52              |
| 1:DA:1414:LEU:HD23 | 1:DA:1424:VAL:HG21  | 1.90                     | 0.52              |
| 3:DI:307:ASN:OD1   | 46:CD:107:GLN:HG2   | 2.10                     | 0.52              |
| 6:DN:74:HIS:O      | 6:DN:109:ASN:OD1    | 2.27                     | 0.52              |
| 14:Da:25:ARG:C     | 14:Da:25:ARG:HD3    | 2.34                     | 0.52              |
| 16:DC:61:ILE:HB    | 16:DC:536:SER:HB2   | 1.91                     | 0.52              |
| 17:DE:570:GLU:HG3  | 20:DH:526:ASN:CG    | 2.35                     | 0.52              |
| 30:CF:15:ARG:NH1   | 46:CD:165:ASP:OD1   | 2.39                     | 0.52              |
| 40:CR:60:PHE:CE2   | 40:CR:62:GLN:HB3    | 2.44                     | 0.52              |
| 40:CR:136:LEU:HD13 | 40:CR:140:GLY:O     | 2.10                     | 0.52              |
| 51:Cm:95:MET:N     | 51:Cm:95:MET:SD     | 2.81                     | 0.52              |
| 68:A4:28:THR:O     | 68:A4:33:ARG:NH2    | 2.42                     | 0.52              |
| 68:A4:161:LYS:HA   | 89:Ad:176:LEU:HD13  | 1.92                     | 0.52              |
| 70:A6:37:MET:HE3   | 71:A8:97:VAL:HG21   | 1.91                     | 0.52              |
| 71:A8:66:ARG:HD3   | 71:A8:71:GLN:NE2    | 2.25                     | 0.52              |
| 74:AF:118:PHE:CE1  | 74:AF:124:VAL:HG22  | 2.45                     | 0.52              |
| 78:AN:141:HIS:CE1  | 91:Af:57:PHE:HA     | 2.43                     | 0.52              |
| 81:AR:61:ARG:HH21  | 102:AA:571:U:H3'    | 1.74                     | 0.52              |
| 85:AW:90:ARG:NH1   | 108:BF:398:ARG:NH2  | 2.57                     | 0.52              |
| 103:BA:698:SER:HA  | 103:BA:703:ARG:CZ   | 2.40                     | 0.52              |
| 103:BA:791:PHE:CD2 | 103:BA:796:LEU:HA   | 2.45                     | 0.52              |
| 104:BB:219:ASN:HB2 | 126:BX:157:HIS:CD2  | 2.44                     | 0.52              |
| 115:BM:133:MET:HG2 | 115:BM:198:LEU:HD23 | 1.91                     | 0.52              |
| 119:BQ:95:GLY:HA3  | 119:BQ:143:GLN:HA   | 1.91                     | 0.52              |
| 132:Bd:25:LEU:HB3  | 132:Bd:36:MET:HE1   | 1.90                     | 0.52              |
| 1:DA:1012:THR:O    | 4:DL:77:LEU:CD2     | 2.47                     | 0.52              |
| 1:DA:1045:ILE:HD12 | 5:DM:291:ILE:HG23   | 1.92                     | 0.52              |
| 6:DN:118:LEU:HB3   | 6:DN:127:VAL:HG23   | 1.90                     | 0.52              |
| 8:DP:206:TYR:O     | 8:DP:212:ASN:HB2    | 2.09                     | 0.52              |
| 19:DG:295:VAL:HG22 | 19:DG:336:MET:CE    | 2.40                     | 0.52              |
| 23:DT:36:GLU:OE2   | 23:DT:36:GLU:HA     | 2.10                     | 0.52              |
| 29:CE:240:ASP:HA   | 29:CE:243:CYS:HB2   | 1.91                     | 0.52              |
| 31:CH:107:ARG:HH12 | 31:CH:133:ARG:NE    | 2.08                     | 0.52              |
| 31:CH:173:PRO:O    | 31:CH:178:THR:HG21  | 2.10                     | 0.52              |
| 47:Cg:233:THR:HG23 | 47:Cg:237:GLU:HB3   | 1.90                     | 0.52              |
| 48:Ci:69:THR:HG21  | 48:Ci:73:MET:HE3    | 1.91                     | 0.52              |
| 50:Ck:119:GLU:OE1  | 50:Ck:132:TYR:OH    | 2.25                     | 0.52              |
| 51:Cm:153:ASP:OD1  | 51:Cm:153:ASP:N     | 2.42                     | 0.52              |
| 56:Cv:454:LEU:HA   | 56:Cv:457:ARG:HD2   | 1.91                     | 0.52              |
| 65:A1:56:ARG:HH12  | 143:UI:14:UNK:HG3   | 1.74                     | 0.52              |
| 67:A3:109:ILE:HG22 | 97:At:44:LEU:HD21   | 1.91                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 70:A6:92:MET:HE2    | 98:Av:169:ARG:HE    | 1.74                     | 0.52              |
| 74:AF:72:ILE:HD13   | 74:AF:72:ILE:H      | 1.74                     | 0.52              |
| 78:AN:131:TRP:HD1   | 131:Bc:12:PHE:CE1   | 2.28                     | 0.52              |
| 93:Aj:192:GLU:O     | 93:Aj:205:ARG:NH2   | 2.43                     | 0.52              |
| 98:Av:45:LEU:HD11   | 102:AA:49:A:N6      | 2.24                     | 0.52              |
| 98:Av:101:PRO:HG2   | 98:Av:104:ILE:HG12  | 1.92                     | 0.52              |
| 103:BA:207:SER:HB3  | 103:BA:276:LEU:HD23 | 1.91                     | 0.52              |
| 103:BA:220:LEU:HD23 | 103:BA:232:TYR:HB3  | 1.91                     | 0.52              |
| 105:BC:405:ASP:HB3  | 105:BC:436:ARG:HH22 | 1.75                     | 0.52              |
| 107:BE:332:ASP:HA   | 107:BE:379:ARG:NH1  | 2.24                     | 0.52              |
| 109:BG:183:ARG:HH12 | 109:BG:187:ARG:HB3  | 1.74                     | 0.52              |
| 117:BO:185:LEU:HD22 | 117:BO:222:ILE:HD11 | 1.91                     | 0.52              |
| 121:BS:97:ASP:N     | 121:BS:97:ASP:OD1   | 2.43                     | 0.52              |
| 127:BY:150:GLN:OE1  | 139:UC:1:UNK:N      | 2.43                     | 0.52              |
| 1:DA:182:ARG:HH12   | 44:Ca:414:THR:CG2   | 2.23                     | 0.52              |
| 1:DA:1650:MET:HE1   | 29:CE:425:PRO:HD2   | 1.91                     | 0.52              |
| 3:DI:66:ARG:HA      | 3:DI:177:THR:HG21   | 1.91                     | 0.52              |
| 11:DS:17:SER:OG     | 11:DS:18:ARG:N      | 2.43                     | 0.52              |
| 12:DU:115:LYS:O     | 12:DU:119:ILE:HG13  | 2.09                     | 0.52              |
| 16:DC:1028:THR:HG22 | 16:DC:1032:ASP:HB2  | 1.91                     | 0.52              |
| 19:DG:447:ALA:HA    | 19:DG:450:MET:HE2   | 1.91                     | 0.52              |
| 29:CE:124:THR:O     | 29:CE:124:THR:OG1   | 2.19                     | 0.52              |
| 34:CK:73:GLN:HG3    | 45:Cb:178:ARG:NH2   | 2.24                     | 0.52              |
| 56:Cv:1003:HIS:HB3  | 56:Cv:1006:GLU:O    | 2.10                     | 0.52              |
| 65:A1:172:VAL:O     | 65:A1:176:GLN:HG2   | 2.10                     | 0.52              |
| 66:A2:167:HIS:HD2   | 66:A2:169:GLY:H     | 1.57                     | 0.52              |
| 80:AQ:74:LEU:HD23   | 80:AQ:75:PRO:HD2    | 1.92                     | 0.52              |
| 89:Ad:34:GLU:CD     | 89:Ad:34:GLU:H      | 2.18                     | 0.52              |
| 90:Ae:131:GLY:HA3   | 102:AA:540:U:H5''   | 1.92                     | 0.52              |
| 102:AA:492:U:H4'    | 102:AA:492:U:OP2    | 2.09                     | 0.52              |
| 117:BO:88:ARG:HB2   | 117:BO:93:ILE:HD11  | 1.91                     | 0.52              |
| 1:DA:1029:LYS:NZ    | 5:DM:254:HIS:ND1    | 2.46                     | 0.52              |
| 2:DD:763:TYR:CD1    | 44:Ca:387:GLN:HG2   | 2.44                     | 0.52              |
| 15:DB:731:TYR:CE1   | 15:DB:820:GLU:HB2   | 2.45                     | 0.52              |
| 16:DC:381:LEU:HD12  | 16:DC:385:THR:HG21  | 1.91                     | 0.52              |
| 18:DF:495:GLU:OE2   | 20:DH:243:SER:HB3   | 2.09                     | 0.52              |
| 36:CN:150:HIS:CD2   | 48:Ci:67:THR:HG23   | 2.45                     | 0.52              |
| 38:CP:69:PRO:HA     | 38:CP:90:MET:HE1    | 1.91                     | 0.52              |
| 56:Cv:604:LEU:HD23  | 56:Cv:766:THR:HG22  | 1.91                     | 0.52              |
| 65:A1:88:THR:HG21   | 65:A1:92:VAL:HG13   | 1.92                     | 0.52              |
| 66:A2:17:VAL:HG13   | 86:AX:148:LEU:HD11  | 1.92                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 66:A2:271:PRO:HG3  | 113:BK:324:LYS:HD3  | 1.91                     | 0.52              |
| 74:AF:211:MET:HG3  | 74:AF:212:PRO:HD2   | 1.91                     | 0.52              |
| 77:AK:42:PRO:HD2   | 77:AK:115:THR:HG22  | 1.92                     | 0.52              |
| 84:AV:189:ASP:HB2  | 84:AV:196:LEU:HD13  | 1.91                     | 0.52              |
| 98:Av:79:GLU:H     | 98:Av:79:GLU:CD     | 2.18                     | 0.52              |
| 107:BE:25:HIS:HD2  | 107:BE:27:THR:H     | 1.58                     | 0.52              |
| 107:BE:280:ALA:O   | 107:BE:283:SER:OG   | 2.24                     | 0.52              |
| 125:BW:26:PHE:HB2  | 125:BW:107:VAL:HG11 | 1.92                     | 0.52              |
| 140:UD:39:UNK:O    | 140:UD:41:UNK:HG2   | 2.10                     | 0.52              |
| 140:UD:200:UNK:HA  | 140:UD:203:UNK:HG3  | 1.92                     | 0.52              |
| 1:DA:1060:LEU:O    | 54:Cq:140:ARG:NE    | 2.36                     | 0.52              |
| 3:DI:307:ASN:HB2   | 3:DI:310:LEU:HB2    | 1.90                     | 0.52              |
| 9:DQ:63:PRO:HB3    | 12:DU:34:TYR:HD2    | 1.74                     | 0.52              |
| 10:DR:128:PRO:CG   | 10:DR:133:LEU:O     | 2.56                     | 0.52              |
| 11:DS:142:GLN:O    | 11:DS:145:PRO:HD3   | 2.09                     | 0.52              |
| 14:Da:36:SER:OG    | 14:Da:38:ASP:OD1    | 2.26                     | 0.52              |
| 16:DC:361:ASP:O    | 16:DC:365:LYS:HB2   | 2.10                     | 0.52              |
| 18:DF:589:GLN:HB3  | 20:DH:192:PHE:HE1   | 1.74                     | 0.52              |
| 27:DY:111:ARG:HH11 | 27:DY:125:THR:HG23  | 1.74                     | 0.52              |
| 30:CF:34:GLY:HA2   | 37:CO:193:MET:HE1   | 1.91                     | 0.52              |
| 37:CO:211:TYR:CD2  | 37:CO:226:VAL:HG21  | 2.45                     | 0.52              |
| 40:CR:315:LEU:CD1  | 57:CA:390:U:O2'     | 2.57                     | 0.52              |
| 55:Cr:172:ARG:HH21 | 55:Cr:176:LEU:CD2   | 2.19                     | 0.52              |
| 55:Cr:246:GLU:O    | 55:Cr:249:GLU:HG3   | 2.10                     | 0.52              |
| 57:CA:63:G:N2      | 57:CA:156:U:HO2'    | 2.08                     | 0.52              |
| 72:A9:100:TRP:CG   | 72:A9:101:LEU:N     | 2.78                     | 0.52              |
| 77:AK:205:MET:HE3  | 77:AK:209:GLN:HB3   | 1.92                     | 0.52              |
| 79:AP:315:ARG:NH1  | 105:BC:506:GLU:OE2  | 2.43                     | 0.52              |
| 88:Ab:113:SER:HB3  | 105:BC:244:TRP:CE3  | 2.44                     | 0.52              |
| 92:Ag:204:HIS:HD2  | 92:Ag:209:LEU:HD11  | 1.75                     | 0.52              |
| 107:BE:235:GLU:O   | 107:BE:239:ILE:HG22 | 2.10                     | 0.52              |
| 108:BF:153:ALA:O   | 108:BF:157:ASN:HB2  | 2.08                     | 0.52              |
| 111:BI:262:TRP:N   | 111:BI:266:GLU:OE1  | 2.28                     | 0.52              |
| 114:BL:162:HIS:HE1 | 114:BL:239:VAL:H    | 1.56                     | 0.52              |
| 117:BO:219:ARG:H   | 117:BO:219:ARG:HD2  | 1.75                     | 0.52              |
| 129:Ba:48:PRO:HG3  | 129:Ba:96:TYR:CE1   | 2.44                     | 0.52              |
| 130:Bb:45:LYS:HB3  | 130:Bb:49:LYS:NZ    | 2.25                     | 0.52              |
| 137:UA:29:UNK:O    | 137:UA:33:UNK:HB2   | 2.10                     | 0.52              |
| 2:DD:296:LEU:HD13  | 2:DD:392:SER:HB2    | 1.90                     | 0.52              |
| 2:DD:797:PHE:HB2   | 2:DD:803:GLN:HE21   | 1.75                     | 0.52              |
| 3:DI:48:LEU:HD23   | 3:DI:165:ARG:HH21   | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:DL:104:ARG:NH1   | 33:CJ:48:ILE:HD12  | 2.25                     | 0.52              |
| 14:Da:11:ALA:HB2   | 57:CA:149:U:H5''   | 1.92                     | 0.52              |
| 16:DC:330:ARG:HB2  | 16:DC:344:MET:HE1  | 1.91                     | 0.52              |
| 23:DT:60:LEU:HD13  | 23:DT:149:TRP:HB3  | 1.91                     | 0.52              |
| 25:DW:168:MET:CE   | 47:Cg:16:ARG:HH12  | 2.23                     | 0.52              |
| 26:DX:89:ARG:CG    | 26:DX:89:ARG:NH1   | 2.71                     | 0.52              |
| 37:CO:264:ARG:HH12 | 37:CO:303:TYR:HB3  | 1.75                     | 0.52              |
| 39:CQ:197:LYS:NZ   | 39:CQ:199:ASN:O    | 2.41                     | 0.52              |
| 40:CR:12:ALA:HB1   | 56:Cv:803:GLN:HB2  | 1.92                     | 0.52              |
| 47:Cg:61:PRO:HG2   | 47:Cg:79:CYS:SG    | 2.50                     | 0.52              |
| 54:Cq:78:ASP:O     | 54:Cq:82:SER:OG    | 2.27                     | 0.52              |
| 68:A4:66:GLU:O     | 89:Ad:65:ARG:HD3   | 2.09                     | 0.52              |
| 75:AI:58:SER:HB2   | 75:AI:63:ARG:HE    | 1.76                     | 0.52              |
| 77:AK:249:PRO:HG2  | 77:AK:310:PHE:CE1  | 2.45                     | 0.52              |
| 83:AU:65:ASN:HD22  | 83:AU:97:GLN:HE21  | 1.56                     | 0.52              |
| 83:AU:106:ALA:HB2  | 92:Ag:110:GLN:HE22 | 1.75                     | 0.52              |
| 94:Al:92:HIS:CE1   | 94:Al:128:ALA:HA   | 2.45                     | 0.52              |
| 105:BC:271:GLU:HG3 | 105:BC:282:HIS:CE1 | 2.45                     | 0.52              |
| 124:BV:100:PRO:HG2 | 124:BV:103:THR:OG1 | 2.09                     | 0.52              |
| 126:BX:133:SER:H   | 140:UD:48:UNK:HB2  | 1.75                     | 0.52              |
| 129:Ba:125:ARG:HD2 | 129:Ba:135:LYS:NZ  | 2.25                     | 0.52              |
| 130:Bb:46:LEU:HD13 | 130:Bb:137:ALA:HA  | 1.92                     | 0.52              |
| 1:DA:501:GLU:HG2   | 1:DA:889:VAL:HB    | 1.92                     | 0.51              |
| 2:DD:140:SER:HB2   | 57:CA:86:G:H22     | 1.74                     | 0.51              |
| 2:DD:150:GLY:HA3   | 57:CA:80:U:C4      | 2.45                     | 0.51              |
| 10:DR:113:LEU:HD21 | 10:DR:140:PHE:HE1  | 1.76                     | 0.51              |
| 16:DC:1102:GLY:HA2 | 20:DH:59:MET:CE    | 2.39                     | 0.51              |
| 18:DF:237:LEU:HB3  | 18:DF:253:ILE:HD13 | 1.91                     | 0.51              |
| 29:CE:253:ARG:NH1  | 29:CE:256:LEU:O    | 2.43                     | 0.51              |
| 33:CJ:119:ARG:HG2  | 33:CJ:119:ARG:NH1  | 2.26                     | 0.51              |
| 35:CL:128:ASP:OD2  | 57:CA:237:C:N4     | 2.43                     | 0.51              |
| 44:Ca:38:TRP:CH2   | 63:UT:25:UNK:HA    | 2.44                     | 0.51              |
| 44:Ca:233:ARG:NH1  | 44:Ca:233:ARG:HB3  | 2.24                     | 0.51              |
| 46:Cd:10:ARG:HE    | 57:CA:47:U:H4'     | 1.75                     | 0.51              |
| 56:Cv:636:ALA:HB3  | 56:Cv:650:HIS:CE1  | 2.46                     | 0.51              |
| 57:CA:261:U:OP2    | 149:CA:736:SPD:H42 | 2.10                     | 0.51              |
| 67:A3:74:PRO:HG3   | 67:A3:91:GLU:O     | 2.10                     | 0.51              |
| 73:AE:349:THR:HG22 | 73:AE:351:TRP:H    | 1.75                     | 0.51              |
| 74:AF:315:ASN:HD21 | 74:AF:323:MET:HE3  | 1.75                     | 0.51              |
| 75:AI:205:TYR:CE2  | 75:AI:208:ARG:NH1  | 2.78                     | 0.51              |
| 77:AK:244:ARG:HH12 | 77:AK:314:ARG:CZ   | 2.23                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 87:AY:255:ARG:HG2  | 87:AY:255:ARG:HH11  | 1.74                     | 0.51              |
| 88:Ab:212:LEU:HD23 | 88:Ab:415:ASP:HB3   | 1.92                     | 0.51              |
| 88:Ab:251:THR:OG1  | 88:Ab:351:GLN:NE2   | 2.35                     | 0.51              |
| 89:Ad:214:TRP:CD2  | 132:Bd:54:MET:HE2   | 2.44                     | 0.51              |
| 97:At:30:GLU:HA    | 97:At:30:GLU:OE2    | 2.09                     | 0.51              |
| 103:BA:688:PRO:O   | 114:BL:79:LYS:HD3   | 2.10                     | 0.51              |
| 113:BK:114:HIS:CE1 | 113:BK:194:ARG:HH22 | 2.28                     | 0.51              |
| 116:BN:26:MET:HE3  | 116:BN:53:ARG:NH1   | 2.25                     | 0.51              |
| 122:BT:64:GLN:NE2  | 129:Ba:144:VAL:HG13 | 2.25                     | 0.51              |
| 133:Be:14:GLY:HA3  | 133:Be:72:HIS:CD2   | 2.45                     | 0.51              |
| 1:DA:650:LEU:HB3   | 1:DA:728:VAL:HG12   | 1.91                     | 0.51              |
| 3:DI:405:LEU:HD13  | 31:CH:116:HIS:CD2   | 2.45                     | 0.51              |
| 4:DL:109:VAL:CG1   | 32:CI:234:PHE:CE2   | 2.89                     | 0.51              |
| 9:DQ:33:VAL:HA     | 9:DQ:37:GLU:HG3     | 1.92                     | 0.51              |
| 9:DQ:72:THR:O      | 9:DQ:251:MET:HG3    | 2.09                     | 0.51              |
| 12:DU:62:ARG:HG2   | 12:DU:64:TYR:CZ     | 2.45                     | 0.51              |
| 20:DH:76:LEU:HD23  | 20:DH:93:LEU:HD22   | 1.91                     | 0.51              |
| 26:DX:64:SER:HB3   | 26:DX:163:TYR:H     | 1.75                     | 0.51              |
| 32:CI:439:ARG:NH2  | 57:CA:406:U:O2'     | 2.42                     | 0.51              |
| 40:CR:295:LYS:HE2  | 40:CR:299:LEU:HA    | 1.90                     | 0.51              |
| 44:Ca:365:LEU:HD13 | 56:Cv:287:ASN:HB3   | 1.92                     | 0.51              |
| 50:Ck:414:MET:SD   | 50:Ck:541:ARG:HG2   | 2.49                     | 0.51              |
| 55:Cr:247:ILE:HG13 | 55:Cr:248:ARG:N     | 2.24                     | 0.51              |
| 68:A4:61:ARG:HH21  | 89:Ad:49:ARG:NH1    | 2.06                     | 0.51              |
| 68:A4:128:LYS:HE3  | 68:A4:130:ARG:HE    | 1.75                     | 0.51              |
| 73:AE:207:ALA:HA   | 103:BA:185:ALA:HB1  | 1.93                     | 0.51              |
| 76:AJ:43:GLU:HA    | 76:AJ:46:LYS:HD3    | 1.92                     | 0.51              |
| 78:AN:55:PRO:HG2   | 78:AN:184:TRP:CD2   | 2.45                     | 0.51              |
| 78:AN:144:ARG:NE   | 102:AA:113:A:H62    | 2.08                     | 0.51              |
| 79:AP:176:ARG:HG2  | 79:AP:221:ASN:HD22  | 1.74                     | 0.51              |
| 79:AP:328:ASP:H    | 110:BH:239:ASN:ND2  | 2.08                     | 0.51              |
| 84:AV:191:TYR:CE1  | 92:Ag:126:ARG:NH1   | 2.79                     | 0.51              |
| 88:Ab:415:ASP:CG   | 88:Ab:416:ILE:H     | 2.18                     | 0.51              |
| 91:Af:91:ALA:HB1   | 95:Ao:34:TRP:CE2    | 2.46                     | 0.51              |
| 93:Aj:290:ALA:HA   | 132:Bd:15:PHE:CZ    | 2.45                     | 0.51              |
| 103:BA:638:ARG:HD3 | 107:BE:120:GLY:O    | 2.10                     | 0.51              |
| 107:BE:69:GLU:HG3  | 113:BK:380:TYR:HE2  | 1.75                     | 0.51              |
| 112:BJ:240:VAL:HA  | 112:BJ:243:LYS:HZ1  | 1.74                     | 0.51              |
| 113:BK:135:GLU:HG3 | 113:BK:192:PHE:CG   | 2.45                     | 0.51              |
| 114:BL:222:ARG:NH2 | 114:BL:241:ASP:HB3  | 2.25                     | 0.51              |
| 114:BL:255:HIS:HA  | 114:BL:258:ARG:NH1  | 2.25                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:222:GLU:CD    | 1:DA:222:GLU:H     | 2.18                     | 0.51              |
| 1:DA:1658:GLU:HB3  | 29:CE:394:ARG:HG3  | 1.93                     | 0.51              |
| 4:DL:84:GLU:HA     | 4:DL:112:VAL:HG11  | 1.93                     | 0.51              |
| 4:DL:287:TRP:CD2   | 33:CJ:75:TYR:HA    | 2.45                     | 0.51              |
| 11:DS:215:SER:O    | 11:DS:218:PRO:HD2  | 2.10                     | 0.51              |
| 15:DB:114:ASN:HD22 | 15:DB:686:GLN:HG2  | 1.75                     | 0.51              |
| 15:DB:479:VAL:O    | 15:DB:483:VAL:HG12 | 2.10                     | 0.51              |
| 15:DB:513:TYR:CE1  | 50:Ck:31:LEU:HD23  | 2.45                     | 0.51              |
| 15:DB:522:MET:HB2  | 15:DB:526:PRO:HB3  | 1.91                     | 0.51              |
| 15:DB:580:PHE:HZ   | 15:DB:585:MET:CE   | 2.22                     | 0.51              |
| 23:DT:74:MET:HG3   | 23:DT:98:PRO:CG    | 2.40                     | 0.51              |
| 27:DY:62:GLN:OE1   | 27:DY:99:GLN:NE2   | 2.44                     | 0.51              |
| 29:CE:173:LYS:HB3  | 45:Cb:45:PHE:CE2   | 2.45                     | 0.51              |
| 51:Cm:191:LYS:NZ   | 57:CA:337:U:OP2    | 2.43                     | 0.51              |
| 56:Cv:584:SER:HB2  | 56:Cv:790:THR:CG2  | 2.40                     | 0.51              |
| 64:A0:94:ILE:HD13  | 120:BR:15:LEU:HD13 | 1.92                     | 0.51              |
| 73:AE:100:LYS:NZ   | 134:Bf:43:ALA:HA   | 2.24                     | 0.51              |
| 74:AF:27:TRP:HE1   | 114:BL:68:THR:HA   | 1.75                     | 0.51              |
| 77:AK:51:HIS:HB2   | 77:AK:106:VAL:HB   | 1.92                     | 0.51              |
| 78:AN:161:ASP:OD1  | 78:AN:161:ASP:N    | 2.43                     | 0.51              |
| 83:AU:137:TRP:HZ2  | 83:AU:163:LEU:HB3  | 1.75                     | 0.51              |
| 84:AV:213:ASP:HB2  | 84:AV:215:TYR:H    | 1.75                     | 0.51              |
| 93:Aj:18:GLY:N     | 132:Bd:78:CYS:O    | 2.43                     | 0.51              |
| 102:AA:455:U:H2'   | 102:AA:456:U:H4'   | 1.91                     | 0.51              |
| 111:BI:225:TRP:CZ2 | 134:Bf:107:PRO:HD3 | 2.46                     | 0.51              |
| 118:BP:54:GLY:H    | 132:Bd:77:HIS:CE1  | 2.28                     | 0.51              |
| 125:BW:2:SER:OG    | 125:BW:3:GLY:N     | 2.41                     | 0.51              |
| 140:UD:52:UNK:HB2  | 140:UD:152:UNK:HG1 | 1.92                     | 0.51              |
| 6:DN:214:MET:HE2   | 6:DN:217:MET:HE2   | 1.91                     | 0.51              |
| 7:DO:63:ALA:O      | 7:DO:67:ARG:HG2    | 2.11                     | 0.51              |
| 9:DQ:142:PHE:HB3   | 9:DQ:267:LEU:HD21  | 1.91                     | 0.51              |
| 10:DR:127:VAL:HG22 | 10:DR:134:LEU:HD23 | 1.92                     | 0.51              |
| 15:DB:641:ARG:HD2  | 50:Ck:555:PHE:CG   | 2.45                     | 0.51              |
| 15:DB:1055:GLN:NE2 | 20:DH:33:VAL:H     | 2.09                     | 0.51              |
| 19:DG:248:LEU:HD11 | 19:DG:313:SER:HB2  | 1.93                     | 0.51              |
| 19:DG:447:ALA:O    | 19:DG:451:ARG:HD2  | 2.10                     | 0.51              |
| 24:DV:31:HIS:HE1   | 24:DV:48:HIS:HE1   | 1.57                     | 0.51              |
| 25:DW:99:HIS:HE1   | 40:CR:270:TYR:OH   | 1.91                     | 0.51              |
| 26:DX:48:LYS:O     | 26:DX:52:GLU:HG2   | 2.11                     | 0.51              |
| 33:CJ:457:THR:HB   | 33:CJ:459:GLU:H    | 1.75                     | 0.51              |
| 33:CJ:460:HIS:CE1  | 36:CN:57:LYS:HG3   | 2.44                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 37:CO:334:ARG:HD2   | 39:CQ:164:ILE:HG12  | 1.92                     | 0.51              |
| 43:CZ:276:HIS:HB3   | 43:CZ:305:HIS:NE2   | 2.25                     | 0.51              |
| 47:Cg:195:PRO:HD3   | 50:Ck:817:LEU:HD12  | 1.92                     | 0.51              |
| 55:Cr:243:LYS:O     | 55:Cr:247:ILE:HG23  | 2.10                     | 0.51              |
| 56:Cv:977:LYS:HZ1   | 56:Cv:979:GLU:CD    | 2.19                     | 0.51              |
| 65:A1:113:VAL:HG12  | 65:A1:137:ASP:OD2   | 2.11                     | 0.51              |
| 66:A2:14:TYR:CE1    | 86:AX:224:VAL:HG13  | 2.45                     | 0.51              |
| 66:A2:24:ASN:O      | 144:UK:2:UNK:HB1    | 2.10                     | 0.51              |
| 66:A2:149:VAL:HG11  | 66:A2:345:ILE:HD12  | 1.92                     | 0.51              |
| 67:A3:163:LYS:NZ    | 102:AA:326:U:OP2    | 2.43                     | 0.51              |
| 73:AE:110:LYS:HB3   | 142:UN:13:UNK:CG    | 2.40                     | 0.51              |
| 78:AN:82:HIS:CD2    | 78:AN:157:TRP:HE1   | 2.22                     | 0.51              |
| 81:AR:222:HIS:ND1   | 81:AR:248:PRO:HB3   | 2.25                     | 0.51              |
| 83:AU:112:GLU:OE1   | 84:AV:190:LYS:NZ    | 2.43                     | 0.51              |
| 87:AY:25:ASP:OD2    | 87:AY:31:ARG:NH2    | 2.43                     | 0.51              |
| 87:AY:278:ARG:HD3   | 87:AY:279:ARG:N     | 2.25                     | 0.51              |
| 98:Av:181:THR:OG1   | 105:BC:159:ASN:OD1  | 2.28                     | 0.51              |
| 102:AA:440:U:H3'    | 115:BM:277:LYS:HZ3  | 1.75                     | 0.51              |
| 103:BA:701:THR:HG23 | 103:BA:708:PHE:CD2  | 2.45                     | 0.51              |
| 105:BC:83:ILE:HD12  | 105:BC:125:CYS:HB2  | 1.93                     | 0.51              |
| 109:BG:264:LEU:O    | 109:BG:267:VAL:HG22 | 2.10                     | 0.51              |
| 115:BM:109:VAL:HG13 | 115:BM:193:GLN:NE2  | 2.26                     | 0.51              |
| 120:BR:126:LEU:HB2  | 120:BR:159:ILE:HB   | 1.92                     | 0.51              |
| 1:DA:1003:PHE:HA    | 4:DL:78:ALA:HA      | 1.91                     | 0.51              |
| 2:DD:339:ARG:NH2    | 57:CA:85:U:C2       | 2.78                     | 0.51              |
| 5:DM:174:ASP:OD1    | 5:DM:177:ARG:NH2    | 2.43                     | 0.51              |
| 19:DG:15:ARG:NH1    | 19:DG:18:TRP:CH2    | 2.78                     | 0.51              |
| 19:DG:294:MET:SD    | 19:DG:310:LEU:HG    | 2.50                     | 0.51              |
| 33:CJ:182:VAL:HG12  | 33:CJ:184:ARG:HG3   | 1.92                     | 0.51              |
| 35:CL:122:GLU:OE2   | 35:CL:137:ARG:NE    | 2.43                     | 0.51              |
| 37:CO:127:THR:HG22  | 37:CO:131:LYS:HZ1   | 1.76                     | 0.51              |
| 37:CO:131:LYS:HA    | 37:CO:134:GLU:HG2   | 1.93                     | 0.51              |
| 38:CP:32:ARG:NH1    | 38:CP:52:LYS:HD3    | 2.25                     | 0.51              |
| 42:CU:16:HIS:CD2    | 42:CU:18:LYS:H      | 2.25                     | 0.51              |
| 44:Ca:577:PRO:HG2   | 44:Ca:579:VAL:HG12  | 1.91                     | 0.51              |
| 47:Cg:65:THR:HG22   | 47:Cg:67:THR:H      | 1.74                     | 0.51              |
| 50:Ck:132:TYR:CE2   | 50:Ck:140:ARG:HG3   | 2.45                     | 0.51              |
| 55:Cr:65:LYS:NZ     | 55:Cr:65:LYS:HB2    | 2.26                     | 0.51              |
| 76:AJ:27:ARG:NH2    | 111:BI:278:GLU:HB2  | 2.25                     | 0.51              |
| 78:AN:96:ASP:HB2    | 111:BI:314:TYR:OH   | 2.11                     | 0.51              |
| 79:AP:132:ASP:OD1   | 79:AP:135:ARG:NH2   | 2.43                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 89:Ad:39:GLN:OE1    | 98:Av:204:TRP:NE1   | 2.37                     | 0.51              |
| 89:Ad:125:ARG:H     | 93:Aj:54:GLN:HE22   | 1.59                     | 0.51              |
| 89:Ad:214:TRP:CG    | 132:Bd:54:MET:HE2   | 2.45                     | 0.51              |
| 103:BA:141:GLU:OE1  | 103:BA:141:GLU:N    | 2.42                     | 0.51              |
| 103:BA:162:ARG:HG2  | 103:BA:162:ARG:NH1  | 2.22                     | 0.51              |
| 103:BA:223:LYS:HD3  | 103:BA:232:TYR:CE1  | 2.44                     | 0.51              |
| 103:BA:304:GLY:HA2  | 103:BA:307:HIS:CE1  | 2.46                     | 0.51              |
| 103:BA:593:THR:HG21 | 103:BA:638:ARG:HG2  | 1.93                     | 0.51              |
| 103:BA:799:ASP:OD2  | 103:BA:799:ASP:C    | 2.54                     | 0.51              |
| 104:BB:184:ARG:HA   | 104:BB:187:GLU:HB2  | 1.91                     | 0.51              |
| 104:BB:355:GLU:O    | 104:BB:363:ARG:NH2  | 2.43                     | 0.51              |
| 116:BN:53:ARG:HH21  | 136:Bh:92:TRP:HZ3   | 1.58                     | 0.51              |
| 132:Bd:95:LEU:HD13  | 132:Bd:121:LEU:HD11 | 1.92                     | 0.51              |
| 132:Bd:102:LEU:HB2  | 132:Bd:112:VAL:HG21 | 1.92                     | 0.51              |
| 134:Bf:86:ILE:HG23  | 134:Bf:109:HIS:NE2  | 2.26                     | 0.51              |
| 1:DA:907:GLN:NE2    | 44:Ca:399:ASN:HD22  | 2.08                     | 0.51              |
| 1:DA:1066:LEU:HD22  | 1:DA:1143:LEU:HD21  | 1.93                     | 0.51              |
| 2:DD:347:GLU:OE2    | 10:DR:188:LYS:NZ    | 2.40                     | 0.51              |
| 7:DO:59:ALA:HA      | 7:DO:62:LEU:HD23    | 1.92                     | 0.51              |
| 8:DP:101:PHE:O      | 49:Cj:139:ARG:HD2   | 2.10                     | 0.51              |
| 8:DP:188:ARG:HH11   | 8:DP:194:GLN:NE2    | 2.09                     | 0.51              |
| 13:DZ:13:ALA:H      | 44:Ca:177:GLN:NE2   | 2.09                     | 0.51              |
| 16:DC:46:ARG:NH1    | 16:DC:475:LEU:HB3   | 2.26                     | 0.51              |
| 16:DC:295:VAL:HG21  | 16:DC:367:MET:HE3   | 1.93                     | 0.51              |
| 17:DE:572:VAL:HA    | 17:DE:575:CYS:HB3   | 1.92                     | 0.51              |
| 19:DG:334:MET:HE1   | 19:DG:384:VAL:O     | 2.10                     | 0.51              |
| 31:CH:167:LYS:HD3   | 56:Cv:102:ASP:OD1   | 2.10                     | 0.51              |
| 46:Cd:188:ASP:HB3   | 46:Cd:194:VAL:HG21  | 1.92                     | 0.51              |
| 55:Cr:10:ARG:O      | 55:Cr:10:ARG:HD3    | 2.10                     | 0.51              |
| 65:A1:142:LYS:NZ    | 65:A1:143:ARG:NH1   | 2.59                     | 0.51              |
| 74:AF:80:GLN:HE22   | 125:BW:162:LYS:HG3  | 1.76                     | 0.51              |
| 76:AJ:45:GLN:CD     | 96:Ap:231:ARG:NH1   | 2.68                     | 0.51              |
| 92:Ag:242:GLU:HA    | 92:Ag:245:ASN:ND2   | 2.25                     | 0.51              |
| 94:Al:81:GLU:HG3    | 94:Al:84:LYS:HE3    | 1.93                     | 0.51              |
| 104:BB:77:HIS:HA    | 104:BB:80:ILE:HG22  | 1.92                     | 0.51              |
| 108:BF:218:ILE:HG12 | 108:BF:292:ARG:NH1  | 2.25                     | 0.51              |
| 116:BN:54:ASP:HB2   | 116:BN:214:TRP:CE2  | 2.45                     | 0.51              |
| 116:BN:108:PHE:HE1  | 116:BN:128:ARG:HD2  | 1.75                     | 0.51              |
| 119:BQ:117:SER:HB2  | 119:BQ:119:GLU:HG2  | 1.91                     | 0.51              |
| 1:DA:1077:ARG:NH2   | 1:DA:1085:GLU:OE1   | 2.43                     | 0.51              |
| 1:DA:1278:THR:CA    | 54:Cq:152:GLU:OE1   | 2.56                     | 0.51              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:DA:1647:SER:OG   | 1:DA:1648:ALA:N     | 2.44                     | 0.51              |
| 2:DD:91:TYR:CE1    | 39:CQ:25:MET:HG3    | 2.45                     | 0.51              |
| 2:DD:465:PHE:CG    | 2:DD:479:ARG:NH1    | 2.79                     | 0.51              |
| 13:DZ:62:ASP:OD1   | 13:DZ:62:ASP:N      | 2.29                     | 0.51              |
| 16:DC:419:TYR:O    | 16:DC:422:VAL:HG12  | 2.11                     | 0.51              |
| 18:DF:119:HIS:CG   | 18:DF:120:ASP:H     | 2.29                     | 0.51              |
| 19:DG:240:HIS:CG   | 19:DG:241:PRO:HD2   | 2.46                     | 0.51              |
| 19:DG:399:ARG:HG3  | 19:DG:411:TYR:CE1   | 2.46                     | 0.51              |
| 23:DT:55:ALA:HA    | 23:DT:58:HIS:CD2    | 2.46                     | 0.51              |
| 26:DX:31:LYS:HD3   | 26:DX:32:PRO:HD2    | 1.93                     | 0.51              |
| 26:DX:57:ARG:NH2   | 41:CS:64:MET:HG3    | 2.25                     | 0.51              |
| 40:CR:190:TYR:HB3  | 40:CR:192:GLU:HG2   | 1.93                     | 0.51              |
| 44:Ca:14:ASN:HD22  | 44:Ca:14:ASN:H      | 1.59                     | 0.51              |
| 44:Ca:205:LEU:HA   | 44:Ca:208:VAL:HG22  | 1.93                     | 0.51              |
| 50:Ck:611:ASN:H    | 50:Ck:611:ASN:HD22  | 1.57                     | 0.51              |
| 56:Cv:292:LYS:HZ1  | 56:Cv:509:THR:HG22  | 1.76                     | 0.51              |
| 68:A4:161:LYS:HE3  | 89:Ad:173:SER:HB3   | 1.92                     | 0.51              |
| 74:AF:56:HIS:HB2   | 108:BF:364:VAL:HG22 | 1.92                     | 0.51              |
| 74:AF:78:SER:HB2   | 108:BF:361:ILE:HD11 | 1.93                     | 0.51              |
| 81:AR:219:GLU:OE2  | 81:AR:219:GLU:HA    | 2.10                     | 0.51              |
| 89:Ad:151:GLN:HE22 | 132:Bd:123:ASN:HB3  | 1.74                     | 0.51              |
| 95:Ao:153:VAL:HG12 | 115:BM:213:LYS:HG2  | 1.93                     | 0.51              |
| 102:AA:86:U:H5''   | 113:BK:340:ARG:HH12 | 1.76                     | 0.51              |
| 103:BA:600:VAL:HA  | 103:BA:603:LEU:HG   | 1.93                     | 0.51              |
| 104:BB:185:ARG:HE  | 104:BB:193:ASN:H    | 1.58                     | 0.51              |
| 117:BO:96:LEU:HB3  | 117:BO:220:MET:HE3  | 1.93                     | 0.51              |
| 137:UA:14:UNK:HA   | 137:UA:17:UNK:HG3   | 1.93                     | 0.51              |
| 1:DA:164:TRP:HZ3   | 2:DD:201:GLU:HG2    | 1.75                     | 0.51              |
| 2:DD:395:GLU:OE2   | 2:DD:398:ARG:NH2    | 2.29                     | 0.51              |
| 5:DM:55:GLU:HB2    | 5:DM:94:ALA:HB2     | 1.92                     | 0.51              |
| 15:DB:194:GLN:HE22 | 17:DE:470:LYS:HB2   | 1.76                     | 0.51              |
| 15:DB:308:PRO:HG3  | 17:DE:496:LEU:HD13  | 1.92                     | 0.51              |
| 15:DB:519:PHE:CD2  | 15:DB:522:MET:HE2   | 2.46                     | 0.51              |
| 15:DB:558:ASN:HB2  | 50:Ck:113:ASN:HB3   | 1.93                     | 0.51              |
| 16:DC:307:LEU:O    | 16:DC:310:ARG:HG2   | 2.10                     | 0.51              |
| 17:DE:725:PRO:HG2  | 22:DK:146:TYR:CZ    | 2.45                     | 0.51              |
| 19:DG:133:ARG:HG3  | 33:CJ:189:LEU:HD13  | 1.91                     | 0.51              |
| 19:DG:186:ARG:HD2  | 34:CK:54:LEU:HB3    | 1.93                     | 0.51              |
| 24:DV:95:LEU:HD21  | 33:CJ:771:PRO:HB3   | 1.93                     | 0.51              |
| 48:Ci:28:ALA:HB3   | 50:Ck:785:PRO:HA    | 1.92                     | 0.51              |
| 51:Cm:47:ASN:ND2   | 57:CA:387:U:H4'     | 2.25                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 51:Cm:83:LYS:HZ1    | 57:CA:393:U:H5'     | 1.75                     | 0.51              |
| 53:Cp:10:ASP:N      | 57:CA:29:A:OP2      | 2.44                     | 0.51              |
| 56:Cv:681:HIS:O     | 56:Cv:781:PRO:HA    | 2.11                     | 0.51              |
| 56:Cv:719:THR:O     | 56:Cv:723:ARG:HG3   | 2.11                     | 0.51              |
| 70:A6:44:ALA:HB2    | 98:Av:177:LEU:HD13  | 1.92                     | 0.51              |
| 73:AE:108:ARG:HA    | 73:AE:115:TYR:HD2   | 1.75                     | 0.51              |
| 78:AN:28:LEU:HG     | 131:Bc:18:ARG:NH2   | 2.22                     | 0.51              |
| 79:AP:113:ILE:HG21  | 102:AA:342:U:H1'    | 1.93                     | 0.51              |
| 79:AP:327:ARG:HH22  | 110:BH:243:LEU:HD12 | 1.76                     | 0.51              |
| 87:AY:309:ASN:OD1   | 87:AY:310:ALA:N     | 2.44                     | 0.51              |
| 88:Ab:120:GLU:O     | 88:Ab:120:GLU:HG2   | 2.11                     | 0.51              |
| 88:Ab:127:PRO:HD2   | 88:Ab:226:THR:HG22  | 1.93                     | 0.51              |
| 97:At:51:ILE:O      | 130:Bb:90:PRO:HG2   | 2.10                     | 0.51              |
| 102:AA:45:U:O2      | 129:Ba:35:ILE:HG22  | 2.10                     | 0.51              |
| 103:BA:408:ASN:HD22 | 103:BA:411:ILE:HG13 | 1.75                     | 0.51              |
| 104:BB:439:ASP:O    | 104:BB:443:ARG:HG2  | 2.11                     | 0.51              |
| 113:BK:311:GLU:H    | 113:BK:311:GLU:CD   | 2.19                     | 0.51              |
| 127:BY:117:PRO:HA   | 127:BY:127:GLU:OE2  | 2.10                     | 0.51              |
| 2:DD:26:ARG:NH1     | 57:CA:145:A:H2      | 2.08                     | 0.51              |
| 4:DL:114:SER:HB3    | 4:DL:254:ARG:CD     | 2.40                     | 0.51              |
| 8:DP:101:PHE:CD2    | 8:DP:110:PRO:HG3    | 2.45                     | 0.51              |
| 9:DQ:65:TRP:HA      | 9:DQ:68:ARG:NH1     | 2.26                     | 0.51              |
| 11:DS:89:ASN:O      | 11:DS:110:SER:HB3   | 2.11                     | 0.51              |
| 12:DU:83:ARG:HD3    | 12:DU:159:ASP:OD1   | 2.11                     | 0.51              |
| 15:DB:214:ARG:CZ    | 17:DE:539:ARG:HH12  | 2.24                     | 0.51              |
| 15:DB:962:MET:HE2   | 15:DB:962:MET:HA    | 1.93                     | 0.51              |
| 21:DJ:22:MET:HE3    | 33:CJ:74:TRP:CH2    | 2.46                     | 0.51              |
| 21:DJ:69:PHE:CZ     | 21:DJ:71:MET:HG3    | 2.46                     | 0.51              |
| 22:DK:4:ARG:NH2     | 23:DT:131:SER:O     | 2.42                     | 0.51              |
| 24:DV:127:THR:HG23  | 50:Ck:742:GLY:HA2   | 1.92                     | 0.51              |
| 27:DY:51:ASP:HB3    | 47:Cg:424:GLY:O     | 2.11                     | 0.51              |
| 31:CH:218:VAL:HG22  | 31:CH:282:HIS:CE1   | 2.46                     | 0.51              |
| 43:CZ:223:VAL:O     | 43:CZ:227:SER:OG    | 2.21                     | 0.51              |
| 43:CZ:306:ILE:HG12  | 43:CZ:308:TYR:HE1   | 1.75                     | 0.51              |
| 73:AE:171:VAL:HG22  | 73:AE:210:VAL:HG11  | 1.93                     | 0.51              |
| 74:AF:257:ARG:NE    | 108:BF:420:ARG:HH11 | 2.09                     | 0.51              |
| 88:Ab:459:ARG:HH12  | 88:Ab:472:PHE:HA    | 1.76                     | 0.51              |
| 89:Ad:220:LEU:HB3   | 132:Bd:47:ARG:HB3   | 1.92                     | 0.51              |
| 114:BL:88:ASN:H     | 114:BL:91:CYS:HB2   | 1.75                     | 0.51              |
| 124:BV:147:ARG:O    | 124:BV:150:LYS:HB3  | 2.11                     | 0.51              |
| 2:DD:275:ASP:OD1    | 2:DD:275:ASP:N      | 2.37                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:DL:74:ARG:CZ      | 29:CE:110:LEU:HD11  | 2.40                     | 0.51              |
| 5:DM:10:ARG:NH1     | 29:CE:325:LEU:HB2   | 2.26                     | 0.51              |
| 8:DP:196:TRP:CD1    | 8:DP:196:TRP:H      | 2.26                     | 0.51              |
| 10:DR:250:ARG:NH2   | 49:Cj:23:GLY:O      | 2.44                     | 0.51              |
| 11:DS:34:SER:HA     | 11:DS:39:ARG:HB3    | 1.93                     | 0.51              |
| 12:DU:107:LYS:HB3   | 12:DU:107:LYS:HZ3   | 1.75                     | 0.51              |
| 15:DB:1051:GLN:NE2  | 21:DJ:42:HIS:H      | 2.09                     | 0.51              |
| 34:CK:78:ASP:HB2    | 45:Cb:178:ARG:HH11  | 1.76                     | 0.51              |
| 64:A0:49:GLN:NE2    | 64:A0:64:TYR:O      | 2.43                     | 0.51              |
| 77:AK:206:THR:HG23  | 77:AK:209:GLN:H     | 1.76                     | 0.51              |
| 79:AP:21:ILE:HG23   | 95:Ao:110:LEU:HD13  | 1.93                     | 0.51              |
| 79:AP:79:TRP:HB2    | 79:AP:84:GLN:HE21   | 1.76                     | 0.51              |
| 86:AX:152:LEU:O     | 86:AX:154:ASN:N     | 2.44                     | 0.51              |
| 88:Ab:144:TYR:CE1   | 118:BP:74:GLU:HB3   | 2.46                     | 0.51              |
| 90:Ae:116:PRO:HA    | 90:Ae:119:HIS:CD2   | 2.46                     | 0.51              |
| 93:Aj:181:GLU:HG3   | 93:Aj:259:ILE:HG12  | 1.93                     | 0.51              |
| 94:Al:141:SER:OG    | 94:Al:142:SER:N     | 2.44                     | 0.51              |
| 95:Ao:54:GLN:HG3    | 142:UF:16:UNK:CA    | 2.41                     | 0.51              |
| 105:BC:295:PHE:HB2  | 105:BC:331:THR:HG21 | 1.93                     | 0.51              |
| 108:BF:232:ALA:O    | 108:BF:235:GLU:HG2  | 2.11                     | 0.51              |
| 111:BI:103:THR:HG22 | 111:BI:104:ARG:H    | 1.75                     | 0.51              |
| 111:BI:299:ARG:H    | 111:BI:299:ARG:HD3  | 1.76                     | 0.51              |
| 114:BL:173:GLY:C    | 114:BL:256:ARG:HH12 | 2.19                     | 0.51              |
| 114:BL:239:VAL:HG23 | 114:BL:245:ARG:NH1  | 2.26                     | 0.51              |
| 124:BV:87:ILE:HD11  | 124:BV:96:PRO:HG2   | 1.93                     | 0.51              |
| 140:UD:7:UNK:HG2    | 140:UD:8:UNK:HG3    | 1.93                     | 0.51              |
| 1:DA:907:GLN:HE22   | 44:Ca:399:ASN:HD22  | 1.59                     | 0.50              |
| 1:DA:1645:GLU:HG2   | 29:CE:425:PRO:HB2   | 1.93                     | 0.50              |
| 4:DL:271:PRO:HG3    | 57:CA:456:A:H5"     | 1.92                     | 0.50              |
| 12:DU:73:ARG:HD3    | 12:DU:73:ARG:H      | 1.76                     | 0.50              |
| 14:Da:10:ILE:N      | 57:CA:270:U:OP1     | 2.44                     | 0.50              |
| 15:DB:572:ASP:OD1   | 15:DB:647:SER:OG    | 2.26                     | 0.50              |
| 15:DB:635:MET:HE1   | 50:Ck:374:ARG:HE    | 1.76                     | 0.50              |
| 16:DC:121:LEU:H     | 16:DC:530:GLN:HE22  | 1.60                     | 0.50              |
| 16:DC:903:THR:HB    | 16:DC:906:GLN:HG3   | 1.92                     | 0.50              |
| 20:DH:518:LYS:HG3   | 20:DH:523:ARG:HH12  | 1.77                     | 0.50              |
| 29:CE:376:LEU:O     | 29:CE:380:GLN:HG2   | 2.11                     | 0.50              |
| 32:CI:194:THR:HG23  | 32:CI:218:ARG:NH1   | 2.26                     | 0.50              |
| 35:CL:78:MET:HG2    | 35:CL:129:LEU:HD11  | 1.93                     | 0.50              |
| 37:CO:73:ILE:HD13   | 52:Ch:226:LEU:HD23  | 1.93                     | 0.50              |
| 37:CO:183:ASP:OD1   | 37:CO:183:ASP:N     | 2.44                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 39:CQ:56:ARG:HH11   | 39:CQ:56:ARG:CG     | 2.12                     | 0.50              |
| 44:Ca:11:TYR:O      | 44:Ca:14:ASN:ND2    | 2.44                     | 0.50              |
| 47:Cg:286:ASP:HA    | 47:Cg:356:CYS:HB3   | 1.93                     | 0.50              |
| 53:Cp:65:ILE:O      | 53:Cp:124:LYS:HG3   | 2.11                     | 0.50              |
| 55:Cr:67:PRO:HG2    | 55:Cr:70:GLU:HB2    | 1.92                     | 0.50              |
| 57:CA:460:U:O2      | 57:CA:461:A:N6      | 2.43                     | 0.50              |
| 71:A8:92:MET:HB3    | 71:A8:107:ARG:NE    | 2.26                     | 0.50              |
| 73:AE:102:ASP:OD2   | 96:Ap:115:VAL:HG21  | 2.09                     | 0.50              |
| 80:AQ:44:ILE:O      | 80:AQ:44:ILE:HG13   | 2.09                     | 0.50              |
| 97:At:34:ARG:HD3    | 120:BR:127:ARG:NH1  | 2.26                     | 0.50              |
| 102:AA:454:U:O2'    | 102:AA:455:U:H5''   | 2.11                     | 0.50              |
| 109:BG:182:THR:HG23 | 109:BG:224:LEU:HD23 | 1.93                     | 0.50              |
| 110:BH:196:LEU:HD13 | 110:BH:197:PRO:HD2  | 1.94                     | 0.50              |
| 115:BM:55:TRP:CD1   | 115:BM:55:TRP:H     | 2.28                     | 0.50              |
| 119:BQ:96:ASP:OD2   | 119:BQ:100:LYS:HA   | 2.11                     | 0.50              |
| 123:BU:135:ARG:HH22 | 123:BU:139:ARG:NH2  | 2.05                     | 0.50              |
| 125:BW:56:ASN:N     | 125:BW:65:ASN:HD21  | 2.03                     | 0.50              |
| 6:DN:75:VAL:HG12    | 6:DN:110:ALA:HB3    | 1.89                     | 0.50              |
| 14:Da:32:SER:O      | 31:CH:144:ARG:NH1   | 2.45                     | 0.50              |
| 15:DB:141:HIS:HA    | 16:DC:903:THR:HG21  | 1.92                     | 0.50              |
| 15:DB:975:LYS:HA    | 19:DG:92:GLN:HE22   | 1.76                     | 0.50              |
| 18:DF:341:VAL:HG22  | 18:DF:346:LEU:HD11  | 1.92                     | 0.50              |
| 19:DG:99:VAL:HG22   | 19:DG:133:ARG:O     | 2.11                     | 0.50              |
| 19:DG:236:VAL:HG12  | 19:DG:237:PRO:HD2   | 1.93                     | 0.50              |
| 21:DJ:101:ILE:HG23  | 21:DJ:139:LEU:HD11  | 1.93                     | 0.50              |
| 32:CI:203:ASP:N     | 32:CI:203:ASP:OD1   | 2.44                     | 0.50              |
| 33:CJ:632:GLN:HB3   | 33:CJ:661:ARG:HD2   | 1.93                     | 0.50              |
| 34:CK:77:MET:HG2    | 45:Cb:286:LEU:HD13  | 1.92                     | 0.50              |
| 37:CO:71:PRO:HB3    | 52:Cn:192:ASN:ND2   | 2.26                     | 0.50              |
| 40:CR:237:ARG:HD2   | 40:CR:237:ARG:O     | 2.11                     | 0.50              |
| 45:Cb:298:ASP:HB3   | 55:Cr:40:HIS:ND1    | 2.27                     | 0.50              |
| 45:Cb:303:GLU:OE2   | 55:Cr:267:GLN:NE2   | 2.44                     | 0.50              |
| 47:Cg:283:ILE:HD11  | 47:Cg:342:MET:HE1   | 1.93                     | 0.50              |
| 70:A6:67:VAL:HG22   | 70:A6:84:GLU:HB2    | 1.92                     | 0.50              |
| 73:AE:117:ASP:OD1   | 73:AE:117:ASP:N     | 2.41                     | 0.50              |
| 77:AK:327:ALA:O     | 77:AK:330:SER:OG    | 2.28                     | 0.50              |
| 79:AP:300:ARG:NH2   | 138:UB:5:UNK:HB1    | 2.25                     | 0.50              |
| 81:AR:154:ARG:HD3   | 107:BE:406:ASP:OD1  | 2.12                     | 0.50              |
| 88:Ab:98:PRO:HD2    | 105:BC:238:MET:HB2  | 1.92                     | 0.50              |
| 89:Ad:95:GLU:HA     | 89:Ad:98:GLU:HG2    | 1.92                     | 0.50              |
| 98:Av:231:ILE:O     | 98:Av:233:THR:N     | 2.44                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 129:Ba:104:ARG:O    | 129:Ba:132:ALA:HB2  | 2.11                     | 0.50              |
| 1:DA:651:ARG:HG3    | 1:DA:726:GLU:HB3    | 1.94                     | 0.50              |
| 1:DA:853:LYS:HE3    | 56:Cv:1005:TRP:CE2  | 2.46                     | 0.50              |
| 6:DN:45:ARG:HB3     | 6:DN:132:TYR:CE2    | 2.46                     | 0.50              |
| 8:DP:103:SER:O      | 49:Cj:139:ARG:NH2   | 2.35                     | 0.50              |
| 12:DU:207:ARG:NH2   | 57:CA:159:G:H4'     | 2.26                     | 0.50              |
| 17:DE:195:ILE:HG21  | 17:DE:203:LEU:HD11  | 1.93                     | 0.50              |
| 17:DE:543:ARG:HG2   | 17:DE:543:ARG:NH1   | 2.26                     | 0.50              |
| 33:CJ:260:LEU:HD21  | 33:CJ:423:LEU:HD22  | 1.93                     | 0.50              |
| 34:CK:153:ASP:N     | 34:CK:153:ASP:OD1   | 2.44                     | 0.50              |
| 39:CQ:58:HIS:CD2    | 57:CA:132:G:H21     | 2.29                     | 0.50              |
| 43:CZ:360:ASP:OD1   | 43:CZ:360:ASP:N     | 2.40                     | 0.50              |
| 47:Cg:260:ASP:OD1   | 50:Ck:825:LYS:HE2   | 2.10                     | 0.50              |
| 47:Cg:294:GLU:HA    | 47:Cg:329:PRO:HA    | 1.93                     | 0.50              |
| 55:Cr:10:ARG:HH12   | 55:Cr:13:ARG:HB3    | 1.75                     | 0.50              |
| 73:AE:133:PHE:O     | 96:Ap:44:PRO:HG2    | 2.11                     | 0.50              |
| 74:AF:224:ARG:NH2   | 102:AA:156:U:O4     | 2.36                     | 0.50              |
| 75:AI:143:PHE:HE1   | 145:UL:8:UNK:HG1    | 1.76                     | 0.50              |
| 76:AJ:27:ARG:HH21   | 111:BI:278:GLU:HB2  | 1.77                     | 0.50              |
| 77:AK:103:ARG:NH2   | 102:AA:402:A:OP1    | 2.45                     | 0.50              |
| 78:AN:172:ARG:NH1   | 92:Ag:119:ASN:OD1   | 2.44                     | 0.50              |
| 93:Aj:99:ILE:O      | 132:Bd:117:THR:HA   | 2.12                     | 0.50              |
| 93:Aj:139:PRO:HA    | 93:Aj:142:LEU:HD23  | 1.94                     | 0.50              |
| 95:Ao:160:ALA:HB2   | 115:BM:234:HIS:CE1  | 2.46                     | 0.50              |
| 102:AA:161:G:O2'    | 102:AA:162:A:H5''   | 2.12                     | 0.50              |
| 107:BE:135:MET:HE2  | 107:BE:139:GLU:OE2  | 2.11                     | 0.50              |
| 111:BI:115:LEU:HD22 | 111:BI:156:PHE:HD2  | 1.76                     | 0.50              |
| 112:BJ:177:THR:HG22 | 112:BJ:181:ARG:HH11 | 1.76                     | 0.50              |
| 112:BJ:210:ILE:HD11 | 137:UA:17:UNK:HA    | 1.93                     | 0.50              |
| 119:BQ:134:HIS:HB2  | 119:BQ:139:GLN:O    | 2.11                     | 0.50              |
| 138:UB:14:UNK:HA    | 138:UB:17:UNK:HG3   | 1.93                     | 0.50              |
| 2:DD:115:GLU:O      | 31:CH:53:ARG:NH2    | 2.44                     | 0.50              |
| 2:DD:704:ASP:OD1    | 2:DD:704:ASP:N      | 2.31                     | 0.50              |
| 2:DD:774:VAL:HG23   | 29:CE:294:HIS:CE1   | 2.46                     | 0.50              |
| 3:DI:104:ILE:HG12   | 3:DI:152:LEU:HD21   | 1.93                     | 0.50              |
| 5:DM:198:THR:HG22   | 5:DM:199:LEU:H      | 1.75                     | 0.50              |
| 6:DN:144:ARG:HA     | 6:DN:144:ARG:HE     | 1.76                     | 0.50              |
| 9:DQ:31:PRO:HB3     | 57:CA:86:G:OP1      | 2.12                     | 0.50              |
| 18:DF:39:ARG:NH2    | 18:DF:163:ARG:HD3   | 2.26                     | 0.50              |
| 20:DH:193:VAL:N     | 20:DH:194:PRO:CD    | 2.74                     | 0.50              |
| 26:DX:33:LYS:NZ     | 41:CS:32:LYS:HG2    | 2.27                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:283:VAL:HG21 | 33:CJ:330:LEU:HD13 | 1.94                     | 0.50              |
| 33:CJ:372:GLU:HG2  | 33:CJ:391:HIS:CD2  | 2.47                     | 0.50              |
| 33:CJ:618:VAL:HG13 | 33:CJ:627:ILE:HD11 | 1.92                     | 0.50              |
| 41:CS:109:GLN:OE1  | 41:CS:109:GLN:N    | 2.44                     | 0.50              |
| 49:Cj:53:ASN:O     | 49:Cj:55:ARG:HG3   | 2.11                     | 0.50              |
| 50:Ck:316:ASP:OD1  | 50:Ck:316:ASP:N    | 2.30                     | 0.50              |
| 50:Ck:606:THR:HG23 | 50:Ck:613:VAL:HG21 | 1.93                     | 0.50              |
| 50:Ck:728:GLN:HG3  | 50:Ck:784:TRP:CE2  | 2.46                     | 0.50              |
| 65:A1:76:ILE:O     | 65:A1:123:VAL:HG23 | 2.11                     | 0.50              |
| 67:A3:54:ILE:HG21  | 130:Bb:76:VAL:HG21 | 1.92                     | 0.50              |
| 73:AE:122:ASP:O    | 96:Ap:109:GLN:NE2  | 2.44                     | 0.50              |
| 75:AI:83:ILE:HB    | 75:AI:89:PRO:O     | 2.11                     | 0.50              |
| 79:AP:358:TRP:O    | 79:AP:359:HIS:CG   | 2.64                     | 0.50              |
| 87:AY:279:ARG:NH1  | 128:BZ:174:SER:HA  | 2.26                     | 0.50              |
| 89:Ad:100:ILE:HG22 | 93:Aj:238:PHE:CZ   | 2.46                     | 0.50              |
| 89:Ad:255:TRP:HA   | 89:Ad:260:MET:HE3  | 1.93                     | 0.50              |
| 92:Ag:17:CYS:SG    | 92:Ag:20:ASN:HB2   | 2.51                     | 0.50              |
| 111:BI:190:ARG:NH1 | 111:BI:230:GLU:HB3 | 2.25                     | 0.50              |
| 116:BN:90:LEU:HA   | 116:BN:95:HIS:CD2  | 2.46                     | 0.50              |
| 129:Ba:55:SER:HB3  | 129:Ba:71:TRP:HZ3  | 1.76                     | 0.50              |
| 131:Bc:56:TRP:HD1  | 131:Bc:64:PHE:CZ   | 2.30                     | 0.50              |
| 134:Bf:41:SER:O    | 134:Bf:45:ARG:HB2  | 2.12                     | 0.50              |
| 140:UD:182:UNK:HA  | 140:UD:185:UNK:HG3 | 1.94                     | 0.50              |
| 1:DA:774:GLY:H     | 5:DM:206:ALA:HA    | 1.76                     | 0.50              |
| 5:DM:176:VAL:HG21  | 5:DM:226:PRO:HD3   | 1.93                     | 0.50              |
| 8:DP:143:ASN:HB2   | 49:Cj:141:GLY:HA3  | 1.93                     | 0.50              |
| 9:DQ:250:ARG:NE    | 9:DQ:252:LYS:CE    | 2.65                     | 0.50              |
| 10:DR:189:GLU:HA   | 10:DR:191:GLN:HE21 | 1.76                     | 0.50              |
| 17:DE:461:MET:N    | 17:DE:461:MET:SD   | 2.84                     | 0.50              |
| 20:DH:111:ASP:OD1  | 20:DH:170:ARG:NH2  | 2.45                     | 0.50              |
| 25:DW:109:GLU:OE1  | 27:DY:96:ARG:NH1   | 2.42                     | 0.50              |
| 33:CJ:552:ILE:HG22 | 33:CJ:557:GLU:CD   | 2.37                     | 0.50              |
| 36:CN:120:LYS:NZ   | 57:CA:474:U:O2     | 2.38                     | 0.50              |
| 39:CQ:152:LYS:HD2  | 39:CQ:154:SER:O    | 2.12                     | 0.50              |
| 40:CR:306:LYS:NZ   | 57:CA:390:U:OP2    | 2.44                     | 0.50              |
| 43:CZ:216:ASP:HB2  | 43:CZ:247:PHE:HA   | 1.93                     | 0.50              |
| 44:Ca:14:ASN:HD22  | 44:Ca:14:ASN:N     | 2.09                     | 0.50              |
| 45:Cb:294:THR:HG23 | 55:Cr:283:LYS:HB3  | 1.92                     | 0.50              |
| 47:Cg:85:LEU:HD22  | 47:Cg:107:ARG:HG2  | 1.92                     | 0.50              |
| 55:Cr:281:GLY:O    | 55:Cr:285:ARG:HG3  | 2.11                     | 0.50              |
| 66:A2:221:VAL:HG12 | 74:AF:397:LEU:HD13 | 1.92                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 68:A4:44:ARG:NH1    | 68:A4:44:ARG:HB3    | 2.26                     | 0.50              |
| 73:AE:100:LYS:HZ2   | 134:Bf:43:ALA:HA    | 1.75                     | 0.50              |
| 74:AF:418:SER:CB    | 98:Av:78:ARG:HH12   | 2.24                     | 0.50              |
| 75:AI:95:ARG:HH22   | 133:Be:53:GLY:HA3   | 1.77                     | 0.50              |
| 88:Ab:419:GLN:HE21  | 105:BC:73:ARG:NH1   | 2.04                     | 0.50              |
| 89:Ad:131:PRO:HD3   | 93:Aj:136:ARG:HB2   | 1.93                     | 0.50              |
| 92:Ag:180:ARG:HB3   | 92:Ag:221:LEU:HD11  | 1.92                     | 0.50              |
| 93:Aj:255:ARG:O     | 93:Aj:257:LYS:N     | 2.43                     | 0.50              |
| 102:AA:1:A:H5'      | 103:BA:631:LYS:HZ1  | 1.75                     | 0.50              |
| 125:BW:45:ARG:HB3   | 125:BW:45:ARG:NH1   | 2.27                     | 0.50              |
| 128:BZ:24:LYS:HD3   | 128:BZ:155:GLN:HE21 | 1.76                     | 0.50              |
| 130:Bb:120:ARG:HG2  | 130:Bb:120:ARG:NH1  | 2.26                     | 0.50              |
| 1:DA:825:GLU:OE1    | 1:DA:825:GLU:N      | 2.45                     | 0.50              |
| 2:DD:647:ARG:HH22   | 10:DR:230:ARG:NH1   | 2.03                     | 0.50              |
| 2:DD:778:PRO:HB3    | 29:CE:32:TRP:CD2    | 2.46                     | 0.50              |
| 3:DI:280:SER:OG     | 3:DI:281:GLY:N      | 2.44                     | 0.50              |
| 6:DN:293:PRO:HB3    | 29:CE:109:LYS:HZ3   | 1.76                     | 0.50              |
| 7:DO:209:ARG:O      | 7:DO:213:GLU:HG2    | 2.10                     | 0.50              |
| 8:DP:200:SER:O      | 8:DP:204:ASN:N      | 2.44                     | 0.50              |
| 15:DB:146:MET:HE1   | 15:DB:214:ARG:HB3   | 1.94                     | 0.50              |
| 19:DG:173:MET:HE1   | 19:DG:209:THR:HG22  | 1.93                     | 0.50              |
| 22:DK:273:LEU:HD11  | 23:DT:99:HIS:CE1    | 2.46                     | 0.50              |
| 29:CE:286:ALA:HB2   | 44:Ca:355:PHE:CE1   | 2.46                     | 0.50              |
| 32:CI:313:ASP:C     | 32:CI:315:GLU:H     | 2.19                     | 0.50              |
| 33:CJ:724:THR:HG21  | 47:Cg:302:PRO:HG3   | 1.94                     | 0.50              |
| 40:CR:308:MET:HE3   | 57:CA:388:U:H4'     | 0.50                     | 0.50              |
| 44:Ca:124:ILE:HD11  | 56:Cv:1033:GLU:HA   | 1.93                     | 0.50              |
| 44:Ca:228:LYS:O     | 44:Ca:232:GLN:HG2   | 2.12                     | 0.50              |
| 46:Cd:13:ARG:NH2    | 46:Cd:28:MET:O      | 2.45                     | 0.50              |
| 56:Cv:112:ILE:HD11  | 56:Cv:150:LEU:HB3   | 1.94                     | 0.50              |
| 66:A2:160:ARG:NH1   | 66:A2:330:ARG:NH1   | 2.59                     | 0.50              |
| 71:A8:66:ARG:HD3    | 71:A8:71:GLN:HE22   | 1.75                     | 0.50              |
| 71:A8:66:ARG:HH12   | 71:A8:142:ALA:HB2   | 1.77                     | 0.50              |
| 78:AN:124:ARG:O     | 96:Ap:61:ASN:ND2    | 2.39                     | 0.50              |
| 89:Ad:70:ALA:HA     | 89:Ad:73:ARG:NH1    | 2.26                     | 0.50              |
| 91:Af:83:LEU:HB2    | 92:Ag:121:GLU:OE2   | 2.12                     | 0.50              |
| 96:Ap:176:MET:HG2   | 96:Ap:177:HIS:HD1   | 1.77                     | 0.50              |
| 102:AA:117:U:OP2    | 114:BL:62:ARG:NH2   | 2.45                     | 0.50              |
| 104:BB:202:VAL:HG11 | 104:BB:378:MET:HB3  | 1.94                     | 0.50              |
| 112:BJ:192:ARG:HH22 | 137:UA:34:UNK:HB2   | 1.77                     | 0.50              |
| 119:BQ:174:VAL:O    | 119:BQ:178:SER:OG   | 2.19                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:DA:303:TYR:HB2   | 1:DA:306:GLU:HG3    | 1.93                     | 0.50              |
| 1:DA:319:ARG:HG2   | 1:DA:319:ARG:NH1    | 2.22                     | 0.50              |
| 1:DA:971:GLU:HG2   | 1:DA:972:PRO:HD3    | 1.92                     | 0.50              |
| 4:DL:278:ARG:NH1   | 4:DL:296:PRO:O      | 2.44                     | 0.50              |
| 6:DN:68:PHE:CD2    | 6:DN:69:VAL:HG23    | 2.47                     | 0.50              |
| 6:DN:212:THR:C     | 44:Ca:193:ARG:HH12  | 2.20                     | 0.50              |
| 8:DP:62:LYS:NZ     | 12:DU:206:PRO:O     | 2.45                     | 0.50              |
| 10:DR:246:GLY:HA2  | 46:Cd:32:LEU:HD12   | 1.93                     | 0.50              |
| 15:DB:72:TRP:CD1   | 15:DB:72:TRP:H      | 2.29                     | 0.50              |
| 16:DC:218:TYR:CG   | 16:DC:256:ILE:HD11  | 2.47                     | 0.50              |
| 16:DC:903:THR:HG22 | 16:DC:905:ALA:H     | 1.77                     | 0.50              |
| 18:DF:411:VAL:HG11 | 18:DF:586:TYR:CD2   | 2.47                     | 0.50              |
| 18:DF:502:ARG:HD2  | 18:DF:579:GLU:HG3   | 1.93                     | 0.50              |
| 19:DG:160:ARG:NH2  | 50:Ck:406:ARG:HE    | 2.09                     | 0.50              |
| 50:Ck:275:TRP:CG   | 50:Ck:314:LEU:HD13  | 2.47                     | 0.50              |
| 50:Ck:362:TYR:CD2  | 50:Ck:365:ILE:HB    | 2.46                     | 0.50              |
| 53:Cp:93:ARG:HG3   | 53:Cp:102:ARG:NH1   | 2.27                     | 0.50              |
| 66:A2:18:ASP:HA    | 66:A2:60:MET:HE2    | 1.94                     | 0.50              |
| 66:A2:164:PHE:HB2  | 112:BJ:310:PHE:CD2  | 2.46                     | 0.50              |
| 72:A9:104:THR:HG1  | 78:AN:117:ARG:HH12  | 1.60                     | 0.50              |
| 74:AF:262:ASP:OD2  | 74:AF:267:GLY:HA3   | 2.11                     | 0.50              |
| 75:AI:210:TYR:HB2  | 110:BH:153:ARG:HH22 | 1.77                     | 0.50              |
| 84:AV:200:THR:HG22 | 84:AV:202:GLY:H     | 1.76                     | 0.50              |
| 92:Ag:137:SER:OG   | 92:Ag:138:GLU:N     | 2.44                     | 0.50              |
| 96:Ap:141:TRP:CZ3  | 141:UE:4:UNK:HG3    | 2.47                     | 0.50              |
| 98:Av:52:GLU:HG3   | 98:Av:53:LYS:N      | 2.26                     | 0.50              |
| 113:BK:137:TYR:CZ  | 113:BK:141:ILE:HG13 | 2.47                     | 0.50              |
| 117:BO:141:ASP:CB  | 117:BO:153:ARG:H    | 2.24                     | 0.50              |
| 127:BY:85:TRP:CD2  | 139:UC:11:UNK:HB2   | 2.47                     | 0.50              |
| 135:Bg:47:ARG:NH1  | 135:Bg:47:ARG:HB3   | 2.27                     | 0.50              |
| 1:DA:1014:TYR:CE1  | 4:DL:67:ASN:O       | 2.65                     | 0.50              |
| 2:DD:21:ARG:HB2    | 2:DD:26:ARG:HH21    | 1.77                     | 0.50              |
| 15:DB:544:ARG:NH1  | 15:DB:849:ASP:OD2   | 2.42                     | 0.50              |
| 18:DF:192:LEU:HD12 | 18:DF:264:VAL:HG13  | 1.93                     | 0.50              |
| 23:DT:16:HIS:HD2   | 23:DT:28:GLU:OE1    | 1.93                     | 0.50              |
| 32:CI:203:ASP:OD1  | 32:CI:211:ASN:ND2   | 2.44                     | 0.50              |
| 32:CI:320:THR:OG1  | 32:CI:375:GLU:OE1   | 2.28                     | 0.50              |
| 34:CK:71:SER:HB3   | 45:Cb:280:ASN:HD22  | 1.76                     | 0.50              |
| 39:CQ:56:ARG:NH1   | 57:CA:97:U:H2'      | 2.27                     | 0.50              |
| 41:CS:45:ARG:HB2   | 41:CS:48:ARG:HD2    | 1.94                     | 0.50              |
| 44:Ca:444:PHE:HB2  | 44:Ca:472:VAL:HG12  | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Ck:728:GLN:HE22 | 50:Ck:731:ARG:NH1  | 2.10                     | 0.50              |
| 54:Cq:175:TRP:HZ3  | 54:Cq:235:LEU:HD23 | 1.76                     | 0.50              |
| 56:Cv:893:GLU:OE2  | 56:Cv:898:ARG:NH1  | 2.45                     | 0.50              |
| 66:A2:396:GLU:HB3  | 66:A2:400:TYR:CE2  | 2.47                     | 0.50              |
| 67:A3:64:ASN:HB2   | 67:A3:101:ASP:OD2  | 2.11                     | 0.50              |
| 69:A5:64:LYS:NZ    | 69:A5:80:PRO:C     | 2.70                     | 0.50              |
| 73:AE:384:PRO:HD3  | 131:Bc:96:PRO:HB2  | 1.93                     | 0.50              |
| 77:AK:38:ILE:HD11  | 124:BV:90:PHE:CE1  | 2.47                     | 0.50              |
| 77:AK:312:ASN:HD22 | 77:AK:315:LEU:HB2  | 1.77                     | 0.50              |
| 78:AN:80:GLY:H     | 78:AN:155:LYS:HZ3  | 1.60                     | 0.50              |
| 79:AP:106:MET:HE1  | 85:AW:25:LEU:HD22  | 1.92                     | 0.50              |
| 80:AQ:164:HIS:CD2  | 115:BM:251:GLU:HG3 | 2.46                     | 0.50              |
| 88:Ab:347:MET:HE1  | 115:BM:98:PHE:CD2  | 2.47                     | 0.50              |
| 102:AA:380:G:H1    | 147:UU:4:UNK:CB    | 2.24                     | 0.50              |
| 103:BA:138:SER:N   | 103:BA:141:GLU:OE2 | 2.37                     | 0.50              |
| 103:BA:223:LYS:HZ3 | 103:BA:232:TYR:HD1 | 1.50                     | 0.50              |
| 104:BB:87:LEU:HD13 | 104:BB:90:LYS:NZ   | 2.26                     | 0.50              |
| 109:BG:244:ARG:NH1 | 109:BG:257:ARG:NH2 | 2.60                     | 0.50              |
| 120:BR:26:ARG:HG2  | 120:BR:70:TYR:CE1  | 2.46                     | 0.50              |
| 120:BR:40:ARG:CZ   | 120:BR:95:ARG:NH1  | 2.68                     | 0.50              |
| 130:Bb:44:HIS:O    | 130:Bb:47:ARG:HD2  | 2.12                     | 0.50              |
| 133:Be:21:ARG:NH1  | 133:Be:98:TRP:CG   | 2.80                     | 0.50              |
| 136:Bh:25:LEU:HD13 | 140:UD:14:UNK:HG2  | 1.93                     | 0.50              |
| 1:DA:715:GLY:HA3   | 1:DA:721:ILE:HG12  | 1.94                     | 0.50              |
| 1:DA:751:GLU:HG3   | 5:DM:197:LEU:HD22  | 1.93                     | 0.50              |
| 8:DP:36:GLN:HG2    | 12:DU:204:LEU:HG   | 1.94                     | 0.50              |
| 15:DB:281:GLN:HB3  | 15:DB:285:MET:HE3  | 1.93                     | 0.50              |
| 16:DC:635:MET:HE3  | 16:DC:656:ILE:HG12 | 1.94                     | 0.50              |
| 16:DC:946:GLU:HG2  | 16:DC:986:LEU:HD21 | 1.92                     | 0.50              |
| 17:DE:152:ALA:N    | 17:DE:157:ARG:HH11 | 2.09                     | 0.50              |
| 17:DE:406:ASP:OD1  | 17:DE:406:ASP:N    | 2.26                     | 0.50              |
| 23:DT:87:ARG:HB2   | 23:DT:93:MET:HE2   | 1.94                     | 0.50              |
| 25:DW:99:HIS:CG    | 40:CR:274:VAL:HG11 | 2.47                     | 0.50              |
| 29:CE:42:ARG:HG3   | 29:CE:105:GLN:NE2  | 2.26                     | 0.50              |
| 29:CE:109:LYS:HB3  | 29:CE:113:GLU:HB2  | 1.94                     | 0.50              |
| 32:CI:420:ARG:O    | 34:CK:27:ARG:HB3   | 2.12                     | 0.50              |
| 43:CZ:278:THR:HG22 | 43:CZ:279:SER:OG   | 2.12                     | 0.50              |
| 43:CZ:315:THR:O    | 43:CZ:318:LEU:HB2  | 2.12                     | 0.50              |
| 46:Cd:102:ARG:HG3  | 46:Cd:103:ILE:N    | 2.26                     | 0.50              |
| 50:Ck:37:ILE:HG22  | 50:Ck:38:ILE:HD12  | 1.94                     | 0.50              |
| 54:Cq:227:ILE:HG22 | 54:Cq:228:LEU:HD12 | 1.93                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 56:Cv:902:ILE:HG22  | 56:Cv:903:ASP:OD1   | 2.12                     | 0.50              |
| 56:Cv:975:ASP:HB3   | 56:Cv:979:GLU:HG3   | 1.94                     | 0.50              |
| 57:CA:350:U:H5'     | 57:CA:351:A:H5''    | 1.92                     | 0.50              |
| 73:AE:235:VAL:HG21  | 73:AE:321:SER:HA    | 1.94                     | 0.50              |
| 85:AW:165:LYS:NZ    | 107:BE:396:GLY:HA3  | 2.27                     | 0.50              |
| 86:AX:72:HIS:HD2    | 102:AA:55:A:OP1     | 1.95                     | 0.50              |
| 88:Ab:54:LEU:HD21   | 98:Av:213:ARG:HD2   | 1.93                     | 0.50              |
| 88:Ab:175:ARG:HH11  | 105:BC:93:ALA:HB3   | 1.75                     | 0.50              |
| 94:Al:41:VAL:O      | 94:Al:45:ILE:HG23   | 2.11                     | 0.50              |
| 96:Ap:74:ARG:HD3    | 96:Ap:90:TYR:HB2    | 1.93                     | 0.50              |
| 97:At:34:ARG:NH1    | 120:BR:127:ARG:NH1  | 2.60                     | 0.50              |
| 102:AA:546:A:H62    | 135:Bg:77:GLN:NE2   | 2.10                     | 0.50              |
| 110:BH:71:LYS:HB3   | 127:BY:149:ILE:HD11 | 1.94                     | 0.50              |
| 111:BI:160:PHE:N    | 111:BI:161:PRO:HD2  | 2.27                     | 0.50              |
| 113:BK:360:GLU:OE1  | 113:BK:360:GLU:N    | 2.39                     | 0.50              |
| 114:BL:141:ASN:HD22 | 114:BL:141:ASN:H    | 1.58                     | 0.50              |
| 116:BN:37:ASN:HB3   | 121:BS:48:GLY:HA3   | 1.93                     | 0.50              |
| 120:BR:95:ARG:HA    | 120:BR:95:ARG:HE    | 1.77                     | 0.50              |
| 127:BY:163:ASP:N    | 127:BY:163:ASP:OD1  | 2.44                     | 0.50              |
| 1:DA:779:LEU:O      | 1:DA:812:PRO:HD3    | 2.12                     | 0.49              |
| 6:DN:267:GLU:CD     | 6:DN:267:GLU:H      | 2.20                     | 0.49              |
| 8:DP:27:ASP:OD1     | 8:DP:27:ASP:N       | 2.41                     | 0.49              |
| 8:DP:189:TYR:CE1    | 8:DP:208:PRO:HD3    | 2.46                     | 0.49              |
| 9:DQ:227:GLN:HG3    | 9:DQ:230:TRP:CZ2    | 2.46                     | 0.49              |
| 15:DB:861:GLU:HG2   | 15:DB:941:ARG:HA    | 1.93                     | 0.49              |
| 16:DC:282:GLY:O     | 16:DC:286:GLN:HG2   | 2.12                     | 0.49              |
| 16:DC:934:ARG:HH11  | 16:DC:934:ARG:CG    | 2.25                     | 0.49              |
| 21:DJ:31:HIS:HD2    | 21:DJ:33:ASN:N      | 2.06                     | 0.49              |
| 23:DT:158:HIS:HB3   | 23:DT:160:TYR:HE1   | 1.77                     | 0.49              |
| 24:DV:25:SER:OG     | 24:DV:29:PHE:CZ     | 2.65                     | 0.49              |
| 29:CE:257:LYS:HB3   | 29:CE:260:ASN:ND2   | 2.27                     | 0.49              |
| 29:CE:408:ARG:HH11  | 29:CE:408:ARG:HG3   | 1.77                     | 0.49              |
| 33:CJ:141:ASP:N     | 33:CJ:141:ASP:OD1   | 2.43                     | 0.49              |
| 35:CL:111:PHE:HB3   | 44:Ca:15:LYS:HA     | 1.94                     | 0.49              |
| 44:Ca:46:ARG:NH2    | 56:Cv:1113:TYR:O    | 2.44                     | 0.49              |
| 48:CI:27:CYS:SG     | 48:CI:29:GLN:NE2    | 2.85                     | 0.49              |
| 66:A2:387:TRP:CD1   | 66:A2:388:PRO:HA    | 2.47                     | 0.49              |
| 69:A5:78:ILE:O      | 69:A5:80:PRO:HD3    | 2.12                     | 0.49              |
| 73:AE:82:ARG:HB2    | 111:BI:77:ASN:ND2   | 2.27                     | 0.49              |
| 73:AE:246:ILE:HD11  | 73:AE:339:PHE:CZ    | 2.47                     | 0.49              |
| 92:Ag:125:ARG:HH11  | 92:Ag:129:ALA:HB2   | 1.77                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 103:BA:221:THR:HG23 | 103:BA:222:VAL:H    | 1.77                     | 0.49              |
| 103:BA:373:ALA:HA   | 103:BA:376:ARG:HH11 | 1.77                     | 0.49              |
| 103:BA:797:LYS:HE2  | 103:BA:823:LEU:HD23 | 1.94                     | 0.49              |
| 104:BB:83:ASN:HA    | 104:BB:87:LEU:HD23  | 1.94                     | 0.49              |
| 104:BB:347:LYS:NZ   | 104:BB:405:TRP:CD2  | 2.80                     | 0.49              |
| 105:BC:56:ASP:O     | 118:BP:200:ARG:NH1  | 2.45                     | 0.49              |
| 110:BH:194:ARG:HB3  | 110:BH:194:ARG:NH1  | 2.27                     | 0.49              |
| 140:UD:211:UNK:O    | 140:UD:215:UNK:HG3  | 2.12                     | 0.49              |
| 1:DA:349:PRO:HG2    | 1:DA:350:TYR:CD2    | 2.47                     | 0.49              |
| 2:DD:368:LEU:O      | 2:DD:589:GLN:O      | 2.31                     | 0.49              |
| 3:DI:74:ASP:OD1     | 3:DI:75:GLN:N       | 2.42                     | 0.49              |
| 15:DB:876:LEU:HD11  | 15:DB:949:THR:HG21  | 1.93                     | 0.49              |
| 15:DB:881:ARG:HG2   | 15:DB:881:ARG:NH1   | 2.24                     | 0.49              |
| 20:DH:413:ASP:OD1   | 20:DH:413:ASP:N     | 2.37                     | 0.49              |
| 24:DV:31:HIS:HE1    | 24:DV:48:HIS:CE1    | 2.29                     | 0.49              |
| 25:DW:137:PRO:HA    | 25:DW:140:TRP:CD2   | 2.47                     | 0.49              |
| 29:CE:21:MET:HG2    | 29:CE:23:GLY:H      | 1.77                     | 0.49              |
| 29:CE:340:LYS:HA    | 29:CE:343:TYR:HB2   | 1.93                     | 0.49              |
| 31:CH:105:ILE:HD12  | 56:Cv:226:PHE:CE1   | 2.48                     | 0.49              |
| 40:CR:202:LYS:NZ    | 40:CR:202:LYS:HB3   | 2.27                     | 0.49              |
| 42:CU:10:GLY:HA3    | 57:CA:344:C:OP1     | 2.11                     | 0.49              |
| 43:CZ:216:ASP:O     | 43:CZ:256:LYS:HG3   | 2.13                     | 0.49              |
| 44:Ca:568:ARG:NH2   | 57:CA:144:A:OP2     | 2.41                     | 0.49              |
| 55:Cr:9:LEU:HG      | 55:Cr:100:TYR:CG    | 2.46                     | 0.49              |
| 56:Cv:977:LYS:NZ    | 56:Cv:979:GLU:CD    | 2.71                     | 0.49              |
| 67:A3:171:ARG:HG2   | 67:A3:171:ARG:NH1   | 2.23                     | 0.49              |
| 68:A4:69:SER:O      | 118:BP:61:LEU:HD22  | 2.12                     | 0.49              |
| 68:A4:161:LYS:HD2   | 89:Ad:176:LEU:HD12  | 1.94                     | 0.49              |
| 76:AJ:51:HIS:ND1    | 96:Ap:222:PHE:HZ    | 2.10                     | 0.49              |
| 81:AR:61:ARG:H      | 81:AR:65:HIS:CD2    | 2.22                     | 0.49              |
| 88:Ab:87:ASP:HB2    | 88:Ab:144:TYR:CE1   | 2.47                     | 0.49              |
| 89:Ad:174:PHE:O     | 89:Ad:177:VAL:HG23  | 2.12                     | 0.49              |
| 95:Ao:148:LEU:HD22  | 115:BM:223:THR:HG23 | 1.94                     | 0.49              |
| 102:AA:389:A:H3'    | 102:AA:390:A:C8     | 2.46                     | 0.49              |
| 104:BB:79:ARG:HG3   | 104:BB:79:ARG:NH1   | 2.27                     | 0.49              |
| 105:BC:397:ASP:OD1  | 105:BC:398:ALA:N    | 2.45                     | 0.49              |
| 111:BI:48:PHE:O     | 111:BI:50:ARG:N     | 2.45                     | 0.49              |
| 115:BM:150:ILE:HG23 | 115:BM:191:LEU:HD21 | 1.94                     | 0.49              |
| 116:BN:64:LEU:HD11  | 116:BN:108:PHE:HD2  | 1.77                     | 0.49              |
| 117:BO:134:PRO:HA   | 121:BS:26:ARG:CZ    | 2.42                     | 0.49              |
| 128:BZ:96:GLN:HB3   | 128:BZ:132:GLY:HA3  | 1.93                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 132:Bd:57:LEU:HD11 | 132:Bd:103:GLY:HA3  | 1.94                     | 0.49              |
| 1:DA:212:ARG:HA    | 11:DS:134:GLN:NE2   | 2.22                     | 0.49              |
| 1:DA:285:TYR:OH    | 1:DA:292:PRO:O      | 2.19                     | 0.49              |
| 1:DA:1589:ALA:HB3  | 1:DA:1591:ARG:O     | 2.12                     | 0.49              |
| 4:DL:85:PHE:HB2    | 32:CI:270:PHE:CE2   | 2.46                     | 0.49              |
| 8:DP:30:LYS:HG3    | 53:Cp:144:PRO:HG2   | 1.94                     | 0.49              |
| 15:DB:1030:ARG:CG  | 15:DB:1030:ARG:NH1  | 2.72                     | 0.49              |
| 16:DC:854:LEU:HD22 | 16:DC:859:LEU:HD12  | 1.92                     | 0.49              |
| 25:DW:44:ASN:O     | 25:DW:58:ARG:NH2    | 2.45                     | 0.49              |
| 37:CO:251:VAL:HG22 | 57:CA:285:A:C5      | 2.47                     | 0.49              |
| 37:CO:327:CYS:HB3  | 37:CO:330:THR:HB    | 1.94                     | 0.49              |
| 43:CZ:305:HIS:CD2  | 43:CZ:307:LYS:HB2   | 2.39                     | 0.49              |
| 43:CZ:314:TRP:O    | 43:CZ:318:LEU:HD23  | 2.12                     | 0.49              |
| 47:Cg:205:ARG:HH21 | 47:Cg:259:ILE:HG12  | 1.77                     | 0.49              |
| 68:A4:44:ARG:HB3   | 68:A4:44:ARG:HH11   | 1.77                     | 0.49              |
| 75:AI:118:LEU:HD11 | 75:AI:155:ILE:HG12  | 1.94                     | 0.49              |
| 77:AK:134:ARG:NH1  | 102:AA:406:U:OP2    | 2.45                     | 0.49              |
| 77:AK:218:ARG:HH22 | 124:BV:112:ILE:HG13 | 1.78                     | 0.49              |
| 88:Ab:271:THR:HG22 | 88:Ab:273:ARG:H     | 1.77                     | 0.49              |
| 91:Af:58:ARG:HH11  | 102:AA:381:U:P      | 2.35                     | 0.49              |
| 91:Af:171:TRP:NE1  | 103:BA:426:ASP:OD1  | 2.45                     | 0.49              |
| 93:Aj:24:ARG:NH1   | 132:Bd:139:PRO:HG3  | 2.27                     | 0.49              |
| 97:At:57:PRO:O     | 97:At:60:VAL:HG23   | 2.13                     | 0.49              |
| 98:Av:37:MET:HE1   | 98:Av:43:ARG:HD2    | 1.95                     | 0.49              |
| 104:BB:148:LYS:HB2 | 104:BB:148:LYS:NZ   | 2.26                     | 0.49              |
| 108:BF:60:LEU:HD13 | 108:BF:63:ARG:HD2   | 1.93                     | 0.49              |
| 112:BJ:195:PRO:HG2 | 112:BJ:200:ARG:HE   | 1.76                     | 0.49              |
| 115:BM:81:TRP:O    | 115:BM:82:ASN:HB2   | 2.13                     | 0.49              |
| 122:BT:99:THR:HG22 | 122:BT:103:MET:HE2  | 1.94                     | 0.49              |
| 1:DA:364:LEU:HD23  | 1:DA:380:PHE:CE1    | 2.48                     | 0.49              |
| 1:DA:1566:ARG:O    | 1:DA:1570:ASN:ND2   | 2.44                     | 0.49              |
| 2:DD:593:ASP:OD2   | 2:DD:595:ARG:NE     | 2.35                     | 0.49              |
| 4:DL:228:MET:HG3   | 4:DL:229:THR:HG22   | 1.95                     | 0.49              |
| 4:DL:270:THR:H     | 4:DL:271:PRO:HD2    | 1.77                     | 0.49              |
| 9:DQ:29:ILE:HD13   | 9:DQ:40:VAL:HG21    | 1.93                     | 0.49              |
| 11:DS:127:PRO:O    | 11:DS:168:LYS:HE2   | 2.13                     | 0.49              |
| 18:DF:56:TYR:OH    | 57:CA:485:U:H5'     | 2.12                     | 0.49              |
| 18:DF:389:PRO:HA   | 18:DF:439:THR:HG21  | 1.94                     | 0.49              |
| 18:DF:467:LEU:HB3  | 18:DF:475:TYR:HB2   | 1.94                     | 0.49              |
| 26:DX:136:ARG:HH11 | 26:DX:136:ARG:CG    | 2.25                     | 0.49              |
| 27:DY:58:THR:HG23  | 27:DY:99:GLN:HG2    | 1.94                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:CR:18:VAL:HG21  | 56:Cv:543:ALA:HA    | 1.94                     | 0.49              |
| 44:Ca:295:PHE:CD2  | 44:Ca:299:ARG:NH1   | 2.80                     | 0.49              |
| 64:A0:166:ASN:OD1  | 64:A0:166:ASN:N     | 2.30                     | 0.49              |
| 65:A1:11:SER:OG    | 65:A1:16:ASN:ND2    | 2.45                     | 0.49              |
| 74:AF:192:ASN:ND2  | 102:AA:185:U:O3'    | 2.45                     | 0.49              |
| 77:AK:42:PRO:HB2   | 77:AK:113:LEU:HD13  | 1.94                     | 0.49              |
| 79:AP:158:SER:O    | 79:AP:160:GLY:N     | 2.46                     | 0.49              |
| 87:AY:51:ARG:NH1   | 107:BE:42:GLY:O     | 2.45                     | 0.49              |
| 93:Aj:24:ARG:NH2   | 132:Bd:136:GLU:O    | 2.45                     | 0.49              |
| 111:BI:76:TYR:CE1  | 111:BI:82:PHE:HB2   | 2.48                     | 0.49              |
| 120:BR:13:PRO:HG2  | 120:BR:14:GLU:OE2   | 2.12                     | 0.49              |
| 126:BX:91:VAL:HB   | 126:BX:93:SER:H     | 1.77                     | 0.49              |
| 133:Be:31:ASN:HD21 | 133:Be:34:LEU:HB2   | 1.75                     | 0.49              |
| 137:UA:17:UNK:O    | 137:UA:21:UNK:HB1   | 2.11                     | 0.49              |
| 2:DD:647:ARG:HH21  | 10:DR:230:ARG:NH1   | 2.10                     | 0.49              |
| 10:DR:228:THR:HG22 | 10:DR:228:THR:O     | 2.11                     | 0.49              |
| 16:DC:112:TYR:HB3  | 16:DC:960:VAL:HG12  | 1.93                     | 0.49              |
| 16:DC:475:LEU:HB2  | 16:DC:476:PHE:CD2   | 2.46                     | 0.49              |
| 18:DF:387:VAL:HG11 | 18:DF:475:TYR:HE2   | 1.77                     | 0.49              |
| 34:CK:70:ILE:HD12  | 45:Cb:189:LYS:HD3   | 1.94                     | 0.49              |
| 39:CQ:79:ASP:O     | 39:CQ:83:LEU:HB2    | 2.12                     | 0.49              |
| 42:CU:85:SER:HB3   | 57:CA:609:A:H5''    | 1.94                     | 0.49              |
| 44:Ca:399:ASN:OD1  | 44:Ca:399:ASN:N     | 2.41                     | 0.49              |
| 50:Ck:80:GLU:O     | 50:Ck:92:ARG:NH1    | 2.45                     | 0.49              |
| 68:A4:154:CYS:HB2  | 89:Ad:228:GLN:NE2   | 2.27                     | 0.49              |
| 73:AE:104:PHE:CE2  | 73:AE:108:ARG:HD2   | 2.47                     | 0.49              |
| 79:AP:251:SER:HB2  | 118:BP:189:THR:HG21 | 1.95                     | 0.49              |
| 81:AR:156:ASP:OD1  | 81:AR:156:ASP:N     | 2.46                     | 0.49              |
| 85:AW:165:LYS:HZ1  | 107:BE:396:GLY:HA3  | 1.77                     | 0.49              |
| 87:AY:120:VAL:HG21 | 87:AY:176:ARG:HG3   | 1.94                     | 0.49              |
| 87:AY:243:ASP:OD2  | 87:AY:246:ALA:HB3   | 2.11                     | 0.49              |
| 88:Ab:61:HIS:CE1   | 89:Ad:204:ALA:HB2   | 2.47                     | 0.49              |
| 88:Ab:444:TYR:O    | 88:Ab:447:ARG:HG2   | 2.12                     | 0.49              |
| 94:Al:99:PRO:HG2   | 94:Al:120:GLY:HA2   | 1.94                     | 0.49              |
| 102:AA:301:A:O2'   | 102:AA:335:G:O6     | 2.30                     | 0.49              |
| 102:AA:488:U:O2'   | 102:AA:489:G:OP1    | 2.22                     | 0.49              |
| 102:AA:561:U:O5'   | 126:BX:154:ARG:NH2  | 2.40                     | 0.49              |
| 103:BA:761:TYR:H   | 103:BA:798:HIS:HE1  | 1.59                     | 0.49              |
| 119:BQ:69:ARG:HD3  | 119:BQ:108:VAL:HB   | 1.93                     | 0.49              |
| 128:BZ:22:VAL:HB   | 128:BZ:158:ASP:HB3  | 1.93                     | 0.49              |
| 132:Bd:67:HIS:CD2  | 132:Bd:68:GLN:HG2   | 2.46                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:DA:618:TYR:CE2    | 1:DA:711:ILE:HD11  | 2.47                     | 0.49              |
| 12:DU:211:ARG:HB2   | 12:DU:211:ARG:HH11 | 1.77                     | 0.49              |
| 16:DC:635:MET:HE2   | 16:DC:659:LEU:HD12 | 1.94                     | 0.49              |
| 19:DG:68:TYR:CZ     | 40:CR:250:GLN:NE2  | 2.59                     | 0.49              |
| 19:DG:70:TYR:HB3    | 19:DG:90:MET:HE2   | 1.95                     | 0.49              |
| 20:DH:194:PRO:HG2   | 20:DH:195:TYR:CE2  | 2.48                     | 0.49              |
| 29:CE:22:ARG:NH2    | 29:CE:240:ASP:HB3  | 2.25                     | 0.49              |
| 30:CF:63:ARG:NH2    | 46:CD:187:GLU:OE2  | 2.45                     | 0.49              |
| 35:CL:71:LEU:HD23   | 35:CL:118:LEU:HB3  | 1.95                     | 0.49              |
| 37:CO:424:LYS:NZ    | 57:CA:66:U:OP1     | 2.29                     | 0.49              |
| 39:CQ:191:VAL:HG21  | 39:CQ:195:ILE:HD11 | 1.93                     | 0.49              |
| 48:CI:34:ARG:HH21   | 48:CI:45:ILE:HG12  | 1.77                     | 0.49              |
| 56:CV:813:ARG:HG2   | 56:CV:813:ARG:NH1  | 2.27                     | 0.49              |
| 66:A2:100:GLU:O     | 66:A2:103:GLU:HG3  | 2.12                     | 0.49              |
| 73:AE:364:ILE:HD12  | 131:BC:85:PRO:HG2  | 1.94                     | 0.49              |
| 74:AF:34:ASP:OD1    | 114:BL:44:ASN:ND2  | 2.45                     | 0.49              |
| 77:AK:27:PRO:HB2    | 77:AK:31:VAL:HG11  | 1.94                     | 0.49              |
| 77:AK:136:THR:O     | 102:AA:405:U:H5'   | 2.13                     | 0.49              |
| 93:AJ:229:PRO:HB3   | 93:AJ:236:TRP:CZ3  | 2.48                     | 0.49              |
| 94:AI:88:ARG:HH11   | 94:AI:88:ARG:CG    | 2.26                     | 0.49              |
| 97:AT:116:GLN:HE21  | 97:AT:119:SER:H    | 1.59                     | 0.49              |
| 102:AA:12:U:H3'     | 102:AA:13:A:H5''   | 1.94                     | 0.49              |
| 103:BA:334:ILE:HG13 | 103:BA:335:PRO:HD2 | 1.94                     | 0.49              |
| 105:BC:187:MET:SD   | 105:BC:192:MET:HE1 | 2.53                     | 0.49              |
| 108:BF:362:HIS:CD2  | 125:BW:176:ARG:HG3 | 2.48                     | 0.49              |
| 110:BH:252:TYR:HB3  | 110:BH:255:PHE:O   | 2.13                     | 0.49              |
| 1:DA:1107:ARG:O     | 1:DA:1109:ARG:HG2  | 2.13                     | 0.49              |
| 5:DM:104:LYS:HB2    | 5:DM:104:LYS:NZ    | 2.27                     | 0.49              |
| 7:DO:114:GLY:H      | 56:CV:780:PRO:HG3  | 1.77                     | 0.49              |
| 10:DR:100:ARG:HG3   | 10:DR:102:LEU:HG   | 1.94                     | 0.49              |
| 16:DC:211:LYS:NZ    | 16:DC:439:ALA:HA   | 2.28                     | 0.49              |
| 17:DE:729:ARG:HH22  | 50:CK:92:ARG:NH1   | 2.10                     | 0.49              |
| 18:DF:186:LEU:HD23  | 18:DF:193:PRO:HD3  | 1.94                     | 0.49              |
| 18:DF:426:LEU:C     | 20:DH:200:THR:CG2  | 2.85                     | 0.49              |
| 18:DF:543:HIS:HD2   | 20:DH:266:SER:OG   | 1.96                     | 0.49              |
| 24:DV:31:HIS:NE2    | 24:DV:82:VAL:HG11  | 2.27                     | 0.49              |
| 24:DV:99:TRP:CE2    | 33:CJ:771:PRO:HG2  | 2.48                     | 0.49              |
| 33:CJ:258:MET:HE2   | 33:CJ:259:LYS:HG2  | 1.95                     | 0.49              |
| 44:CA:102:TRP:CE2   | 44:CA:159:LEU:HD13 | 2.48                     | 0.49              |
| 46:CD:217:GLU:H     | 46:CD:217:GLU:CD   | 2.21                     | 0.49              |
| 47:CG:462:GLU:HA    | 47:CG:465:TRP:NE1  | 2.28                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:A0:68:ASN:N      | 64:A0:102:ASP:OD1   | 2.44                     | 0.49              |
| 66:A2:160:ARG:CZ    | 66:A2:330:ARG:HH11  | 2.25                     | 0.49              |
| 77:AK:139:VAL:O     | 77:AK:143:GLY:N     | 2.44                     | 0.49              |
| 77:AK:262:PRO:HG3   | 92:Ag:169:VAL:HG21  | 1.93                     | 0.49              |
| 79:AP:216:PHE:H     | 79:AP:235:GLN:HG3   | 1.76                     | 0.49              |
| 80:AQ:130:ARG:HD3   | 102:AA:418:G:H5'    | 1.95                     | 0.49              |
| 84:AV:213:ASP:HB2   | 84:AV:215:TYR:HB2   | 1.95                     | 0.49              |
| 87:AY:69:ASP:HB3    | 107:BE:36:ARG:HH22  | 1.78                     | 0.49              |
| 88:Ab:92:PHE:O      | 88:Ab:94:ILE:HG13   | 2.12                     | 0.49              |
| 88:Ab:352:ARG:NH2   | 88:Ab:398:GLN:O     | 2.46                     | 0.49              |
| 98:Av:45:LEU:HD11   | 102:AA:49:A:C6      | 2.48                     | 0.49              |
| 102:AA:134:U:O2'    | 102:AA:135:G:H8     | 1.95                     | 0.49              |
| 102:AA:534:U:HO2'   | 102:AA:535:U:P      | 2.34                     | 0.49              |
| 104:BB:359:HIS:CD2  | 112:BJ:200:ARG:HH12 | 2.31                     | 0.49              |
| 105:BC:300:LEU:HD11 | 105:BC:447:PRO:HD2  | 1.94                     | 0.49              |
| 107:BE:133:VAL:HB   | 107:BE:134:PRO:HD3  | 1.94                     | 0.49              |
| 108:BF:240:VAL:O    | 108:BF:244:HIS:HB3  | 2.13                     | 0.49              |
| 112:BJ:182:VAL:HG12 | 112:BJ:183:ILE:HD12 | 1.93                     | 0.49              |
| 116:BN:13:VAL:HG13  | 116:BN:14:HIS:H     | 1.78                     | 0.49              |
| 116:BN:108:PHE:CE1  | 116:BN:128:ARG:HD2  | 2.48                     | 0.49              |
| 123:BU:154:LYS:O    | 123:BU:158:VAL:HG23 | 2.13                     | 0.49              |
| 131:Bc:33:GLN:HA    | 131:Bc:36:LEU:HD12  | 1.95                     | 0.49              |
| 1:DA:591:LEU:HD13   | 1:DA:598:ALA:HA     | 1.94                     | 0.49              |
| 4:DL:95:ALA:HB3     | 32:CI:248:PHE:CD2   | 2.48                     | 0.49              |
| 5:DM:106:MET:HE3    | 29:CE:313:MET:HG2   | 1.95                     | 0.49              |
| 5:DM:169:ALA:HB2    | 29:CE:343:TYR:CE2   | 2.47                     | 0.49              |
| 6:DN:26:ARG:NH1     | 44:Ca:407:PHE:CE2   | 2.80                     | 0.49              |
| 15:DB:285:MET:HE2   | 50:Ck:36:ARG:NH2    | 2.27                     | 0.49              |
| 15:DB:684:GLN:HB2   | 15:DB:689:LEU:HD13  | 1.95                     | 0.49              |
| 17:DE:503:ASP:N     | 17:DE:503:ASP:OD1   | 2.46                     | 0.49              |
| 20:DH:495:THR:HG22  | 20:DH:498:ASN:HD22  | 1.77                     | 0.49              |
| 24:DV:95:LEU:HD22   | 48:CI:55:LEU:HD23   | 1.94                     | 0.49              |
| 35:CL:135:TYR:CG    | 44:Ca:10:ARG:NH1    | 2.81                     | 0.49              |
| 37:CO:376:GLU:OE2   | 37:CO:379:ARG:NH2   | 2.45                     | 0.49              |
| 46:Cd:58:ARG:HH11   | 46:Cd:58:ARG:HG3    | 1.76                     | 0.49              |
| 46:Cd:284:THR:HG22  | 46:Cd:285:ASP:H     | 1.77                     | 0.49              |
| 47:Cg:102:PRO:HG2   | 47:Cg:105:HIS:HB2   | 1.95                     | 0.49              |
| 57:CA:370:A:O2'     | 57:CA:371:U:H5'     | 2.12                     | 0.49              |
| 67:A3:72:ASP:HB3    | 67:A3:115:ILE:HG23  | 1.95                     | 0.49              |
| 69:A5:28:ARG:HD2    | 102:AA:813:U:C5     | 2.48                     | 0.49              |
| 75:Al:70:ARG:NH2    | 133:Be:83:ASP:OD2   | 2.45                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 84:AV:92:ALA:HB3    | 92:Ag:107:ARG:HH11  | 1.78                     | 0.49              |
| 105:BC:82:ARG:NH1   | 105:BC:308:ARG:NH2  | 2.60                     | 0.49              |
| 106:BD:428:SER:O    | 106:BD:432:THR:N    | 2.45                     | 0.49              |
| 108:BF:28:ARG:CG    | 59:UW:1:UNK:H2      | 2.21                     | 0.49              |
| 120:BR:128:LYS:HE2  | 142:UF:21:UNK:HA    | 1.94                     | 0.49              |
| 122:BT:96:LEU:HD22  | 125:BW:50:ARG:NH2   | 2.26                     | 0.49              |
| 124:BV:49:ARG:HH12  | 124:BV:73:LEU:HD23  | 1.78                     | 0.49              |
| 128:BZ:2:ARG:HD3    | 128:BZ:28:ARG:NE    | 2.28                     | 0.49              |
| 1:DA:222:GLU:O      | 1:DA:233:ARG:HD3    | 2.12                     | 0.49              |
| 1:DA:1417:PHE:C     | 1:DA:1419:GLY:H     | 2.20                     | 0.49              |
| 3:DI:190:PRO:O      | 3:DI:193:ASN:N      | 2.39                     | 0.49              |
| 6:DN:128:VAL:HB     | 44:Ca:405:ARG:HB3   | 1.94                     | 0.49              |
| 6:DN:224:ARG:HB3    | 6:DN:287:ARG:HD2    | 1.93                     | 0.49              |
| 10:DR:26:ASN:ND2    | 49:Cj:37:ARG:NH1    | 2.61                     | 0.49              |
| 15:DB:910:PHE:CD2   | 33:CJ:112:ARG:HG2   | 2.47                     | 0.49              |
| 18:DF:170:ARG:NH2   | 36:CN:33:GLU:OE1    | 2.45                     | 0.49              |
| 19:DG:46:TRP:CZ2    | 19:DG:93:ARG:HB2    | 2.48                     | 0.49              |
| 19:DG:540:VAL:HG13  | 19:DG:569:LEU:HD22  | 1.94                     | 0.49              |
| 20:DH:341:ASN:O     | 20:DH:344:VAL:HG23  | 2.12                     | 0.49              |
| 29:CE:308:ARG:C     | 29:CE:311:LYS:HZ2   | 2.21                     | 0.49              |
| 36:CN:93:ASP:OD1    | 36:CN:114:SER:N     | 2.41                     | 0.49              |
| 40:CR:168:ILE:HG23  | 40:CR:170:LEU:HG    | 1.94                     | 0.49              |
| 49:Cj:209:TYR:CE1   | 49:Cj:212:TYR:HB2   | 2.47                     | 0.49              |
| 67:A3:163:LYS:HA    | 67:A3:166:PHE:HB3   | 1.95                     | 0.49              |
| 69:A5:50:LYS:HD2    | 102:AA:1161:A:OP2   | 2.13                     | 0.49              |
| 74:AF:221:LYS:NZ    | 102:AA:155:U:O2     | 2.44                     | 0.49              |
| 74:AF:259:MET:HE2   | 74:AF:259:MET:HB3   | 1.67                     | 0.49              |
| 74:AF:394:VAL:HG22  | 74:AF:395:PRO:HD2   | 1.95                     | 0.49              |
| 78:AN:36:TRP:CZ2    | 78:AN:147:LYS:HD2   | 2.48                     | 0.49              |
| 85:AW:73:LYS:HD2    | 102:AA:17:A:N7      | 2.28                     | 0.49              |
| 89:Ad:72:ASP:OD2    | 118:BP:60:HIS:HA    | 2.12                     | 0.49              |
| 92:Ag:28:PHE:HZ     | 92:Ag:83:LEU:HD22   | 1.78                     | 0.49              |
| 93:Aj:228:VAL:HG23  | 93:Aj:237:LEU:HB3   | 1.94                     | 0.49              |
| 102:AA:43:U:H5''    | 102:AA:44:A:N7      | 2.27                     | 0.49              |
| 102:AA:392:A:H2'    | 111:BI:299:ARG:HH12 | 1.78                     | 0.49              |
| 103:BA:206:ILE:HG23 | 103:BA:241:TYR:HE1  | 1.78                     | 0.49              |
| 103:BA:618:ARG:HH11 | 103:BA:618:ARG:HG3  | 1.78                     | 0.49              |
| 106:BD:270:ALA:HB1  | 106:BD:406:ALA:CB   | 2.26                     | 0.49              |
| 107:BE:38:PRO:HB2   | 107:BE:43:PRO:HB3   | 1.94                     | 0.49              |
| 108:BF:59:ILE:HB    | 108:BF:63:ARG:NH1   | 2.28                     | 0.49              |
| 113:BK:384:ARG:HH21 | 135:Bg:69:ARG:C     | 2.21                     | 0.49              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 115:BM:87:ARG:O     | 115:BM:90:GLN:HG2  | 2.13                     | 0.49              |
| 116:BN:26:MET:HE3   | 116:BN:53:ARG:HH11 | 1.77                     | 0.49              |
| 1:DA:1003:PHE:N     | 4:DL:78:ALA:HB1    | 2.16                     | 0.49              |
| 3:DI:251:VAL:HG13   | 3:DI:258:VAL:HG13  | 1.95                     | 0.49              |
| 4:DL:85:PHE:N       | 32:CI:270:PHE:CZ   | 2.79                     | 0.49              |
| 4:DL:114:SER:CA     | 4:DL:254:ARG:HE    | 2.24                     | 0.49              |
| 7:DO:236:PRO:HG2    | 7:DO:239:LYS:HG3   | 1.94                     | 0.49              |
| 11:DS:207:TRP:CZ2   | 38:CP:134:ILE:HG23 | 2.47                     | 0.49              |
| 15:DB:1069:THR:HG21 | 50:Ck:764:THR:HG21 | 1.95                     | 0.49              |
| 16:DC:666:GLU:OE1   | 16:DC:790:ARG:HD2  | 2.12                     | 0.49              |
| 19:DG:392:ARG:HH11  | 19:DG:392:ARG:CG   | 2.26                     | 0.49              |
| 20:DH:480:ASP:OD1   | 33:CJ:16:ARG:NH1   | 2.46                     | 0.49              |
| 30:CF:16:ARG:HB2    | 30:CF:16:ARG:NH1   | 2.27                     | 0.49              |
| 33:CJ:27:PRO:HG3    | 51:Cm:28:GLN:NE2   | 2.28                     | 0.49              |
| 40:CR:319:LYS:HB3   | 46:Cd:281:MET:C    | 2.13                     | 0.49              |
| 47:Cg:60:HIS:ND1    | 47:Cg:419:SER:HB2  | 2.28                     | 0.49              |
| 47:Cg:153:CYS:HA    | 47:Cg:452:PRO:HG2  | 1.95                     | 0.49              |
| 67:A3:122:ASP:OD1   | 67:A3:122:ASP:N    | 2.41                     | 0.49              |
| 73:AE:183:ASP:HB3   | 73:AE:226:TYR:OH   | 2.13                     | 0.49              |
| 97:At:59:ALA:HB1    | 97:At:62:ARG:NH1   | 2.27                     | 0.49              |
| 97:At:128:THR:O     | 108:BF:292:ARG:NH2 | 2.46                     | 0.49              |
| 102:AA:105:G:H5"    | 102:AA:105:G:N3    | 2.28                     | 0.49              |
| 103:BA:357:MET:HE3  | 103:BA:358:PRO:HD2 | 1.95                     | 0.49              |
| 103:BA:618:ARG:HG3  | 103:BA:618:ARG:NH1 | 2.27                     | 0.49              |
| 112:BJ:192:ARG:HH22 | 137:UA:34:UNK:HB1  | 1.77                     | 0.49              |
| 130:Bb:53:ARG:HD3   | 130:Bb:53:ARG:N    | 2.28                     | 0.49              |
| 2:DD:177:TYR:CE2    | 2:DD:200:MET:HG3   | 2.49                     | 0.48              |
| 2:DD:543:LEU:O      | 2:DD:547:VAL:HG23  | 2.13                     | 0.48              |
| 9:DQ:127:ARG:HH12   | 9:DQ:262:GLU:CD    | 2.21                     | 0.48              |
| 9:DQ:154:GLY:HA2    | 9:DQ:234:GLN:O     | 2.13                     | 0.48              |
| 10:DR:128:PRO:HB2   | 10:DR:130:ASP:OD1  | 2.13                     | 0.48              |
| 10:DR:189:GLU:HA    | 10:DR:191:GLN:NE2  | 2.28                     | 0.48              |
| 15:DB:981:HIS:HD2   | 15:DB:983:LEU:HB2  | 1.77                     | 0.48              |
| 15:DB:1047:TRP:CD2  | 21:DJ:41:PRO:HD3   | 2.48                     | 0.48              |
| 15:DB:1160:LYS:O    | 26:DX:59:ARG:HD2   | 2.13                     | 0.48              |
| 18:DF:532:LEU:HB2   | 18:DF:537:GLU:OE1  | 2.13                     | 0.48              |
| 19:DG:208:PRO:HG3   | 19:DG:282:ASP:OD1  | 2.13                     | 0.48              |
| 19:DG:497:ARG:HH11  | 19:DG:497:ARG:CG   | 2.26                     | 0.48              |
| 21:DJ:71:MET:HG2    | 21:DJ:119:LEU:HD23 | 1.93                     | 0.48              |
| 29:CE:83:MET:H      | 29:CE:83:MET:HE2   | 1.77                     | 0.48              |
| 32:CI:256:LYS:H     | 32:CI:256:LYS:HD2  | 1.77                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:CO:214:HIS:HD2  | 37:CO:216:PHE:H    | 1.60                     | 0.48              |
| 38:CP:173:LYS:NZ   | 38:CP:181:GLU:CD   | 2.71                     | 0.48              |
| 43:CZ:277:PHE:CG   | 43:CZ:309:PRO:HD3  | 2.48                     | 0.48              |
| 54:Cq:76:GLN:OE1   | 54:Cq:228:LEU:HB2  | 2.13                     | 0.48              |
| 77:AK:34:LYS:HE2   | 124:BV:90:PHE:CG   | 2.48                     | 0.48              |
| 77:AK:127:ARG:HD3  | 124:BV:23:PRO:HB3  | 1.94                     | 0.48              |
| 78:AN:66:THR:HG21  | 78:AN:68:GLN:HE21  | 1.78                     | 0.48              |
| 96:Ap:55:HIS:HD2   | 96:Ap:57:LYS:H     | 1.60                     | 0.48              |
| 96:Ap:288:ASP:OD1  | 96:Ap:288:ASP:N    | 2.34                     | 0.48              |
| 97:At:86:MET:HE2   | 97:At:86:MET:HA    | 1.95                     | 0.48              |
| 102:AA:437:U:H2'   | 102:AA:438:U:H5''  | 1.94                     | 0.48              |
| 108:BF:63:ARG:HE   | 108:BF:235:GLU:HB2 | 1.76                     | 0.48              |
| 109:BG:164:GLN:O   | 109:BG:165:GLU:HG3 | 2.12                     | 0.48              |
| 128:BZ:9:MET:HG3   | 128:BZ:23:PHE:HE2  | 1.78                     | 0.48              |
| 135:Bg:47:ARG:HB3  | 135:Bg:47:ARG:HH11 | 1.78                     | 0.48              |
| 1:DA:897:SER:OG    | 1:DA:898:VAL:N     | 2.46                     | 0.48              |
| 8:DP:67:GLN:HE22   | 8:DP:75:ARG:NH1    | 2.11                     | 0.48              |
| 15:DB:1080:ARG:NH1 | 18:DF:177:ASP:OD1  | 2.46                     | 0.48              |
| 15:DB:1109:TRP:CZ3 | 36:CN:66:MET:HG3   | 2.49                     | 0.48              |
| 16:DC:200:VAL:HG11 | 16:DC:206:PHE:HB2  | 1.94                     | 0.48              |
| 16:DC:231:THR:HG21 | 16:DC:518:CYS:SG   | 2.53                     | 0.48              |
| 17:DE:539:ARG:HG2  | 17:DE:539:ARG:NH1  | 2.28                     | 0.48              |
| 21:DJ:137:MET:HE2  | 21:DJ:169:CYS:SG   | 2.53                     | 0.48              |
| 22:DK:254:GLU:HG3  | 22:DK:261:SER:CB   | 2.37                     | 0.48              |
| 23:DT:74:MET:HG3   | 23:DT:98:PRO:HG3   | 1.94                     | 0.48              |
| 29:CE:222:VAL:HG21 | 29:CE:267:HIS:HB3  | 1.94                     | 0.48              |
| 29:CE:311:LYS:HD2  | 29:CE:311:LYS:N    | 2.24                     | 0.48              |
| 32:CI:9:THR:HG22   | 32:CI:10:ALA:H     | 1.78                     | 0.48              |
| 33:CJ:463:MET:HG2  | 48:Ci:89:MET:HG3   | 1.95                     | 0.48              |
| 40:CR:317:ILE:CA   | 46:Cd:283:GLU:CD   | 2.81                     | 0.48              |
| 44:Ca:521:GLN:HG3  | 44:Ca:586:ILE:O    | 2.13                     | 0.48              |
| 49:Cj:50:VAL:O     | 49:Cj:54:ALA:HB2   | 2.14                     | 0.48              |
| 53:Cp:23:TYR:CE2   | 53:Cp:25:PRO:HD3   | 2.48                     | 0.48              |
| 66:A2:293:PHE:O    | 66:A2:294:PRO:C    | 2.55                     | 0.48              |
| 67:A3:107:LYS:HE2  | 67:A3:111:ARG:NH2  | 2.28                     | 0.48              |
| 71:A8:42:MET:N     | 71:A8:42:MET:SD    | 2.87                     | 0.48              |
| 73:AE:94:ASP:O     | 73:AE:98:GLU:HB2   | 2.14                     | 0.48              |
| 73:AE:373:LYS:C    | 117:BO:232:GLU:HG2 | 2.38                     | 0.48              |
| 76:AJ:17:ILE:HG12  | 76:AJ:38:VAL:HG12  | 1.94                     | 0.48              |
| 83:AU:27:ARG:HE    | 83:AU:31:GLU:CD    | 2.21                     | 0.48              |
| 85:AW:36:TRP:CH2   | 85:AW:46:PRO:HG3   | 2.48                     | 0.48              |

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| Atom-1                | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|---------------------|--------------------------|-------------------|
| 85:AW:102:GLU:HB3     | 114:BL:230:ARG:NH2  | 2.28                     | 0.48              |
| 88:Ab:333:PRO:HB3     | 88:Ab:344:HIS:NE2   | 2.28                     | 0.48              |
| 93:Aj:53:ARG:NH1      | 93:Aj:174:LEU:HD12  | 2.28                     | 0.48              |
| 96:Ap:39:LYS:HA       | 96:Ap:39:LYS:HD2    | 1.58                     | 0.48              |
| 96:Ap:106:LYS:HB3     | 96:Ap:106:LYS:HZ2   | 1.77                     | 0.48              |
| 103:BA:791:PHE:CE1    | 103:BA:801:ARG:HD3  | 2.48                     | 0.48              |
| 104:BB:359:HIS:HD2    | 104:BB:363:ARG:HH12 | 1.59                     | 0.48              |
| 111:BI:263:HIS:HB2    | 111:BI:302:PRO:CB   | 2.42                     | 0.48              |
| 112:BJ:259:ASP:OD1    | 112:BJ:259:ASP:N    | 2.44                     | 0.48              |
| 116:BN:16:PRO:O       | 116:BN:19:VAL:HG12  | 2.13                     | 0.48              |
| 1:DA:385:ARG:HD3      | 6:DN:195:TYR:CD1    | 2.48                     | 0.48              |
| 1:DA:557:SER:CB       | 1:DA:562:LYS:HZ2    | 2.21                     | 0.48              |
| 10:DR:60:VAL:HG23     | 10:DR:61:PRO:HD2    | 1.95                     | 0.48              |
| 11:DS:200:LEU:HD22    | 53:Cp:40:GLU:HB3    | 1.94                     | 0.48              |
| 16:DC:909:ILE:HD13    | 16:DC:941:MET:HE2   | 1.94                     | 0.48              |
| 16:DC:961:THR:HG21    | 17:DE:563:ASP:CG    | 2.39                     | 0.48              |
| 16:DC:1156:PRO:O      | 20:DH:41:LYS:NZ     | 2.46                     | 0.48              |
| 19:DG:50:LEU:HD13     | 32:CI:249:GLU:OE1   | 2.12                     | 0.48              |
| 31:CH:24:GLY:HA3      | 31:CH:29:HIS:ND1    | 2.29                     | 0.48              |
| 33:CJ:151:ASN:HD21    | 33:CJ:209:GLN:HB3   | 1.77                     | 0.48              |
| 50:Ck:414:MET:O       | 50:Ck:541:ARG:NH2   | 2.46                     | 0.48              |
| 65:A1:113:VAL:HG13    | 65:A1:114:LEU:HD23  | 1.95                     | 0.48              |
| 68:A4:74:ARG:HH12     | 132:Bd:52:ARG:HD2   | 1.78                     | 0.48              |
| 71:A8:95:ARG:HH11     | 71:A8:99:ARG:HH22   | 1.61                     | 0.48              |
| 73:AE:77:ILE:HG23     | 73:AE:90:GLN:HG2    | 1.94                     | 0.48              |
| 84:AV:143:GLN:HB2     | 92:Ag:88:SER:OG     | 2.13                     | 0.48              |
| 85:AW:204:TYR:HB2     | 85:AW:205:PRO:HD2   | 1.96                     | 0.48              |
| 86:AX:66:ARG:N        | 102:AA:284:U:OP1    | 2.39                     | 0.48              |
| 87:AY:206:MET:HE3     | 87:AY:208:LEU:HD23  | 1.96                     | 0.48              |
| 96:Ap:55:HIS:CD2      | 96:Ap:57:LYS:HB2    | 2.47                     | 0.48              |
| 102:AA:84:A:H2'       | 102:AA:84:A:N3      | 2.28                     | 0.48              |
| 102:AA:86:U:H5''      | 113:BK:340:ARG:NH1  | 2.28                     | 0.48              |
| 104:BB:194:TYR:CE2    | 104:BB:196:TRP:HB2  | 2.48                     | 0.48              |
| 127:BY:79(G):LEU:HD23 | 139:UC:10:UNK:HG1   | 1.95                     | 0.48              |
| 136:Bh:56:LYS:NZ      | 136:Bh:57:PRO:HD2   | 2.28                     | 0.48              |
| 139:UC:9:UNK:HG3      | 139:UC:10:UNK:HG3   | 1.95                     | 0.48              |
| 1:DA:155:ILE:HG21     | 46:Cd:84:LYS:HE2    | 1.93                     | 0.48              |
| 4:DL:113:LEU:HD13     | 32:CI:231:LEU:O     | 2.13                     | 0.48              |
| 6:DN:73:VAL:HG21      | 6:DN:132:TYR:CD1    | 2.47                     | 0.48              |
| 7:DO:114:GLY:HA3      | 56:Cv:780:PRO:HB3   | 1.96                     | 0.48              |
| 8:DP:130:TYR:OH       | 49:Cj:71:ILE:O      | 2.21                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:DS:131:ARG:HB2   | 11:DS:134:GLN:HB2   | 1.95                     | 0.48              |
| 15:DB:91:ALA:HB2    | 17:DE:529:ASP:O     | 2.13                     | 0.48              |
| 19:DG:71:ASN:ND2    | 19:DG:101:THR:OG1   | 2.39                     | 0.48              |
| 20:DH:78:GLY:O      | 20:DH:81:LYS:HD2    | 2.13                     | 0.48              |
| 23:DT:44:ARG:H      | 23:DT:218:MET:HE1   | 1.79                     | 0.48              |
| 23:DT:139:HIS:HB2   | 23:DT:176:ASP:OD1   | 2.13                     | 0.48              |
| 29:CE:34:ARG:HD3    | 29:CE:205:ASP:OD1   | 2.14                     | 0.48              |
| 33:CJ:790:MET:HE2   | 33:CJ:790:MET:HB3   | 1.78                     | 0.48              |
| 37:CO:429:ASN:ND2   | 57:CA:92:A:OP1      | 2.46                     | 0.48              |
| 45:Cb:291:GLU:HB3   | 45:Cb:296:PHE:O     | 2.14                     | 0.48              |
| 46:Cd:20:SER:HB3    | 46:Cd:29:THR:HG23   | 1.94                     | 0.48              |
| 47:Cg:139:THR:HG22  | 47:Cg:145:PHE:CZ    | 2.48                     | 0.48              |
| 50:Ck:392:PHE:CD1   | 50:Ck:408:VAL:HG11  | 2.48                     | 0.48              |
| 56:Cv:744:TRP:HZ2   | 56:Cv:767:ASP:HB2   | 1.78                     | 0.48              |
| 56:Cv:930:ARG:HB3   | 56:Cv:930:ARG:HH11  | 1.78                     | 0.48              |
| 64:A0:75:ASN:OD1    | 64:A0:75:ASN:N      | 2.44                     | 0.48              |
| 65:A1:71:GLN:HG2    | 129:Ba:98:TRP:CE3   | 2.48                     | 0.48              |
| 71:A8:102:ASP:OD1   | 71:A8:103:VAL:N     | 2.42                     | 0.48              |
| 78:AN:98:TRP:NE1    | 111:BI:49:PRO:O     | 2.46                     | 0.48              |
| 81:AR:79:ARG:NH1    | 107:BE:448:ARG:HH22 | 2.10                     | 0.48              |
| 83:AU:20:ILE:O      | 83:AU:22:SER:N      | 2.47                     | 0.48              |
| 86:AX:199:LYS:HE2   | 86:AX:205:ILE:HG12  | 1.94                     | 0.48              |
| 107:BE:166:ASP:OD1  | 107:BE:167:ASP:N    | 2.46                     | 0.48              |
| 111:BI:253:PRO:HG2  | 111:BI:256:MET:HE1  | 1.95                     | 0.48              |
| 113:BK:136:ALA:O    | 113:BK:140:LEU:HB2  | 2.13                     | 0.48              |
| 123:BU:146:LEU:HD12 | 136:Bh:38:LEU:HD23  | 1.95                     | 0.48              |
| 1:DA:387:SER:OG     | 1:DA:389:GLU:OE1    | 2.28                     | 0.48              |
| 1:DA:551:LYS:HA     | 1:DA:554:GLU:HG2    | 1.95                     | 0.48              |
| 1:DA:914:THR:HG21   | 1:DA:917:ARG:HH21   | 1.77                     | 0.48              |
| 2:DD:17:ALA:HB2     | 57:CA:273:A:H5''    | 1.95                     | 0.48              |
| 3:DI:27:THR:N       | 3:DI:30:GLN:HE21    | 2.07                     | 0.48              |
| 5:DM:272:GLN:HB2    | 54:Cq:9:TYR:HB3     | 1.95                     | 0.48              |
| 13:DZ:13:ALA:HB2    | 44:Ca:89:ARG:HA     | 1.95                     | 0.48              |
| 17:DE:181:LEU:HD22  | 17:DE:538:VAL:HG21  | 1.96                     | 0.48              |
| 19:DG:399:ARG:HB2   | 19:DG:409:LYS:O     | 2.13                     | 0.48              |
| 19:DG:578:ASP:HA    | 19:DG:581:VAL:HG22  | 1.94                     | 0.48              |
| 20:DH:14:TYR:OH     | 48:Ci:136:HIS:HD2   | 1.95                     | 0.48              |
| 40:CR:319:LYS:CE    | 46:Cd:283:GLU:O     | 2.61                     | 0.48              |
| 44:Ca:335:ARG:NH2   | 44:Ca:391:ASP:OD1   | 2.41                     | 0.48              |
| 49:Cj:195:THR:OG1   | 49:Cj:196:ASP:N     | 2.47                     | 0.48              |
| 51:Cm:184:HIS:HE1   | 57:CA:282:A:N3      | 2.11                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:Cq:223:GLU:HG2   | 54:Cq:227:ILE:HG13  | 1.96                     | 0.48              |
| 56:Cv:1123:GLN:CD   | 56:Cv:1124:PRO:HD2  | 2.38                     | 0.48              |
| 57:CA:617:U:H5'     | 57:CA:618:U:OP2     | 2.13                     | 0.48              |
| 64:A0:165:PRO:O     | 64:A0:168:PHE:N     | 2.47                     | 0.48              |
| 65:A1:208:LYS:HE3   | 65:A1:212:LEU:HD11  | 1.94                     | 0.48              |
| 79:AP:107:ARG:HH22  | 102:AA:150:A:H5''   | 1.78                     | 0.48              |
| 79:AP:258:THR:HG21  | 79:AP:278:GLU:OE1   | 2.13                     | 0.48              |
| 80:AQ:33:ASP:HB3    | 142:UG:17:UNK:HB2   | 1.96                     | 0.48              |
| 87:AY:87:LYS:HZ3    | 87:AY:87:LYS:HB2    | 1.78                     | 0.48              |
| 88:Ab:283:ASN:H     | 88:Ab:351:GLN:NE2   | 2.11                     | 0.48              |
| 88:Ab:421:PHE:O     | 88:Ab:425:ARG:HG3   | 2.13                     | 0.48              |
| 104:BB:351:LEU:HD12 | 104:BB:409:LEU:HD11 | 1.96                     | 0.48              |
| 110:BH:78:LEU:HD22  | 110:BH:83:GLU:HB3   | 1.95                     | 0.48              |
| 110:BH:106:GLU:HA   | 110:BH:249:ARG:HH11 | 1.78                     | 0.48              |
| 116:BN:219:ARG:HH11 | 116:BN:221:VAL:HG22 | 1.78                     | 0.48              |
| 126:BX:132:TYR:CD1  | 140:UD:48:UNK:HA    | 2.48                     | 0.48              |
| 1:DA:79:LEU:HD21    | 38:CP:53:ARG:NH1    | 2.28                     | 0.48              |
| 2:DD:323:LEU:HD22   | 2:DD:448:ARG:HH21   | 1.79                     | 0.48              |
| 3:DI:234:SER:O      | 3:DI:237:ARG:HG3    | 2.13                     | 0.48              |
| 6:DN:73:VAL:HG21    | 6:DN:132:TYR:HE1    | 1.79                     | 0.48              |
| 7:DO:74:TRP:CE2     | 7:DO:259:THR:HG23   | 2.48                     | 0.48              |
| 9:DQ:250:ARG:CZ     | 9:DQ:252:LYS:CE     | 2.92                     | 0.48              |
| 16:DC:1119:GLN:OE1  | 16:DC:1125:SER:OG   | 2.20                     | 0.48              |
| 16:DC:1119:GLN:HA   | 16:DC:1120:PRO:HD3  | 1.74                     | 0.48              |
| 18:DF:119:HIS:CG    | 18:DF:120:ASP:N     | 2.82                     | 0.48              |
| 19:DG:245:ILE:HG22  | 19:DG:248:LEU:H     | 1.77                     | 0.48              |
| 26:DX:76:ARG:NH1    | 26:DX:146:PRO:HA    | 2.28                     | 0.48              |
| 31:CH:16:VAL:CB     | 31:CH:17:PRO:HD2    | 2.38                     | 0.48              |
| 35:CL:111:PHE:CB    | 44:Ca:15:LYS:HA     | 2.43                     | 0.48              |
| 41:CS:48:ARG:HH11   | 41:CS:48:ARG:CG     | 2.23                     | 0.48              |
| 44:Ca:359:ARG:NH2   | 56:Cv:257:LYS:HD3   | 2.29                     | 0.48              |
| 45:Cb:161:ALA:HA    | 54:Cq:121:VAL:HG21  | 1.94                     | 0.48              |
| 50:Ck:201:THR:HG23  | 50:Ck:600:LEU:HD11  | 1.95                     | 0.48              |
| 50:Ck:704:ASN:HB2   | 50:Ck:751:ASP:OD1   | 2.13                     | 0.48              |
| 51:Cm:178:GLU:HG3   | 51:Cm:183:GLY:HA2   | 1.95                     | 0.48              |
| 52:Cn:169:PHE:CZ    | 56:Cv:26:LEU:HD11   | 2.48                     | 0.48              |
| 56:Cv:509:THR:HG23  | 56:Cv:520:GLN:NE2   | 2.28                     | 0.48              |
| 56:Cv:930:ARG:HB3   | 56:Cv:930:ARG:NH1   | 2.29                     | 0.48              |
| 65:A1:156:ILE:HG23  | 112:BJ:279:GLY:HA2  | 1.95                     | 0.48              |
| 73:AE:166:PRO:CG    | 73:AE:190:MET:HG2   | 2.44                     | 0.48              |
| 77:AK:25:ARG:HB3    | 77:AK:26:LEU:HD12   | 1.96                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 77:AK:48:ARG:HG2    | 96:Ap:211:ARG:HA    | 1.95                     | 0.48              |
| 79:AP:73:ARG:NH2    | 92:Ag:82:ARG:NH1    | 2.62                     | 0.48              |
| 90:Ae:71:HIS:HB2    | 90:Ae:121:TYR:CD2   | 2.48                     | 0.48              |
| 96:Ap:123:LYS:HZ1   | 146:UM:6:UNK:HA     | 1.78                     | 0.48              |
| 108:BF:392:ASP:OD1  | 108:BF:392:ASP:N    | 2.47                     | 0.48              |
| 109:BG:149:THR:HB   | 109:BG:154:ALA:HB2  | 1.95                     | 0.48              |
| 115:BM:109:VAL:HG13 | 115:BM:193:GLN:HE22 | 1.78                     | 0.48              |
| 128:BZ:89:VAL:HG23  | 128:BZ:90:THR:HG22  | 1.95                     | 0.48              |
| 1:DA:251:SER:OG     | 1:DA:253:ASP:OD1    | 2.15                     | 0.48              |
| 1:DA:751:GLU:HG2    | 5:DM:197:LEU:HB3    | 1.95                     | 0.48              |
| 1:DA:1185:ARG:O     | 1:DA:1185:ARG:HG2   | 2.14                     | 0.48              |
| 2:DD:181:MET:HE1    | 2:DD:215:TYR:HA     | 1.95                     | 0.48              |
| 2:DD:353:HIS:HE1    | 10:DR:196:TYR:OH    | 1.96                     | 0.48              |
| 8:DP:19:TRP:CZ3     | 8:DP:20:MET:HG2     | 2.49                     | 0.48              |
| 10:DR:39:GLN:O      | 10:DR:42:MET:HB3    | 2.14                     | 0.48              |
| 13:DZ:90:VAL:HG22   | 44:Ca:149:ARG:HH12  | 1.78                     | 0.48              |
| 15:DB:968:VAL:CG1   | 19:DG:42:PRO:HG2    | 2.43                     | 0.48              |
| 16:DC:910:GLU:HG3   | 16:DC:937:LEU:HD11  | 1.96                     | 0.48              |
| 31:CH:225:ASP:HB3   | 31:CH:227:ARG:H     | 1.78                     | 0.48              |
| 32:CI:400:VAL:HG23  | 32:CI:410:LEU:HD12  | 1.96                     | 0.48              |
| 33:CJ:278:GLU:O     | 33:CJ:281:VAL:HG12  | 2.13                     | 0.48              |
| 35:CL:111:PHE:HB2   | 44:Ca:15:LYS:HB2    | 1.94                     | 0.48              |
| 38:CP:102:TRP:HB3   | 38:CP:108:CYS:SG    | 2.53                     | 0.48              |
| 46:Cd:103:ILE:O     | 46:Cd:107:GLN:HG3   | 2.13                     | 0.48              |
| 46:Cd:264:ILE:HG22  | 51:Cm:104:ARG:CZ    | 2.44                     | 0.48              |
| 53:Cp:93:ARG:NH1    | 57:CA:187:A:H2      | 2.12                     | 0.48              |
| 56:Cv:458:PRO:HG3   | 56:Cv:828:ALA:HA    | 1.95                     | 0.48              |
| 56:Cv:490:ASP:HB3   | 56:Cv:491:LEU:HD12  | 1.96                     | 0.48              |
| 57:CA:469:A:OP1     | 149:CA:735:SPD:N1   | 2.46                     | 0.48              |
| 64:A0:167:LEU:HB3   | 64:A0:173:VAL:HG12  | 1.95                     | 0.48              |
| 65:A1:78:LEU:H      | 65:A1:78:LEU:CD2    | 2.27                     | 0.48              |
| 66:A2:270:ASN:ND2   | 66:A2:272:LEU:H     | 2.08                     | 0.48              |
| 66:A2:389:HIS:HD2   | 102:AA:32:U:C2      | 2.32                     | 0.48              |
| 68:A4:90:LEU:HD23   | 89:Ad:130:THR:OG1   | 2.13                     | 0.48              |
| 68:A4:116:ARG:HG3   | 68:A4:169:LEU:HD21  | 1.95                     | 0.48              |
| 73:AE:132:MET:HE3   | 73:AE:133:PHE:CE2   | 2.49                     | 0.48              |
| 74:AF:91:PRO:O      | 122:BT:131:LEU:HD12 | 2.14                     | 0.48              |
| 79:AP:13:LEU:HD22   | 102:AA:378:A:C2     | 2.48                     | 0.48              |
| 79:AP:257:MET:CE    | 125:BW:11:ARG:HH12  | 2.23                     | 0.48              |
| 81:AR:253:LYS:O     | 81:AR:256:GLU:HG3   | 2.13                     | 0.48              |
| 85:AW:109:ASN:ND2   | 85:AW:112:LEU:HG    | 2.25                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 88:Ab:56:ARG:HD3   | 98:Av:230:PRO:HB2   | 1.96                     | 0.48              |
| 102:AA:180:U:O2    | 102:AA:180:U:H2'    | 2.13                     | 0.48              |
| 110:BH:91:LYS:HB3  | 110:BH:91:LYS:NZ    | 2.29                     | 0.48              |
| 113:BK:194:ARG:NH1 | 113:BK:198:ASP:HB2  | 2.28                     | 0.48              |
| 115:BM:274:GLY:H   | 115:BM:279:ASN:ND2  | 2.12                     | 0.48              |
| 116:BN:71:GLN:OE1  | 140:UD:197:UNK:HB2  | 2.12                     | 0.48              |
| 139:UC:9:UNK:CG    | 139:UC:10:UNK:HG3   | 2.43                     | 0.48              |
| 1:DA:1131:ASN:HA   | 1:DA:1134:ILE:HD12  | 1.94                     | 0.48              |
| 6:DN:73:VAL:CG1    | 6:DN:112:ILE:HD12   | 2.43                     | 0.48              |
| 9:DQ:254:SER:H     | 9:DQ:255:PRO:CD     | 2.25                     | 0.48              |
| 10:DR:244:LEU:HD22 | 10:DR:269:TRP:CE2   | 2.48                     | 0.48              |
| 19:DG:100:ASP:OD2  | 40:CR:245:ALA:HB3   | 2.14                     | 0.48              |
| 29:CE:171:SER:C    | 29:CE:173:LYS:H     | 2.22                     | 0.48              |
| 32:CI:106:LEU:HD11 | 34:CK:107:GLN:NE2   | 2.23                     | 0.48              |
| 33:CJ:484:HIS:HB2  | 33:CJ:487:GLU:HG3   | 1.95                     | 0.48              |
| 33:CJ:616:GLU:OE1  | 33:CJ:630:ARG:NH1   | 2.43                     | 0.48              |
| 33:CJ:793:HIS:HB2  | 48:CI:90:LYS:O      | 2.14                     | 0.48              |
| 37:CO:296:ARG:NH2  | 57:CA:124:U:OP2     | 2.47                     | 0.48              |
| 40:CR:320:VAL:C    | 46:CD:281:MET:HE2   | 2.39                     | 0.48              |
| 42:CU:77:ARG:NH1   | 56:Cv:175:ARG:HH22  | 2.11                     | 0.48              |
| 44:Ca:272:PHE:O    | 44:Ca:276:SER:OG    | 2.30                     | 0.48              |
| 46:CD:10:ARG:HA    | 57:CA:177:A:OP2     | 2.14                     | 0.48              |
| 52:Cn:152:PHE:O    | 52:Cn:152:PHE:CG    | 2.66                     | 0.48              |
| 56:Cv:172:THR:HG21 | 56:Cv:178:GLU:HB3   | 1.95                     | 0.48              |
| 64:A0:145:GLU:HG2  | 64:A0:151:ARG:HH21  | 1.77                     | 0.48              |
| 66:A2:131:PRO:HG2  | 66:A2:134:ALA:HB2   | 1.96                     | 0.48              |
| 66:A2:177:LEU:HD22 | 66:A2:181:VAL:HG11  | 1.95                     | 0.48              |
| 71:A8:56:LEU:HD13  | 74:AF:207:TRP:HB2   | 1.96                     | 0.48              |
| 73:AE:351:TRP:CE3  | 73:AE:358:PRO:HD3   | 2.49                     | 0.48              |
| 74:AF:257:ARG:NE   | 108:BF:420:ARG:NH1  | 2.62                     | 0.48              |
| 86:AX:128:GLN:HB3  | 86:AX:137:ARG:HH21  | 1.79                     | 0.48              |
| 88:Ab:135:LYS:NZ   | 88:Ab:135:LYS:HB3   | 2.29                     | 0.48              |
| 95:Ao:218:PHE:CG   | 115:BM:241:MET:HE3  | 2.48                     | 0.48              |
| 102:AA:830:A:H2'   | 102:AA:831:A:H8     | 1.78                     | 0.48              |
| 104:BB:213:LEU:O   | 104:BB:215:ARG:HG2  | 2.14                     | 0.48              |
| 104:BB:443:ARG:HG2 | 104:BB:443:ARG:HH11 | 1.79                     | 0.48              |
| 105:BC:101:ALA:HB1 | 105:BC:243:VAL:O    | 2.14                     | 0.48              |
| 105:BC:510:ASP:CB  | 105:BC:514:GLN:HB3  | 2.44                     | 0.48              |
| 120:BR:29:LEU:HD21 | 120:BR:184:TYR:CE1  | 2.49                     | 0.48              |
| 122:BT:145:SER:HB3 | 122:BT:174:ILE:HG22 | 1.96                     | 0.48              |
| 132:Bd:136:GLU:H   | 132:Bd:136:GLU:CD   | 2.22                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 133:Be:19:ILE:HD13 | 133:Be:76:MET:HE1   | 1.95                     | 0.48              |
| 1:DA:48:GLN:OE1    | 39:CQ:29:ALA:HB1    | 2.14                     | 0.48              |
| 2:DD:683:ASP:O     | 46:Cd:64:GLN:NE2    | 2.47                     | 0.48              |
| 4:DL:65:PRO:HG2    | 29:CE:133:ARG:HH22  | 1.79                     | 0.48              |
| 4:DL:85:PHE:HA     | 32:CI:270:PHE:CZ    | 2.49                     | 0.48              |
| 4:DL:214:TYR:CD2   | 32:CI:219:LEU:HD11  | 2.49                     | 0.48              |
| 5:DM:254:HIS:CG    | 29:CE:47:ARG:HH11   | 2.32                     | 0.48              |
| 7:DO:85:LYS:HE3    | 7:DO:85:LYS:HB3     | 1.76                     | 0.48              |
| 13:DZ:73:HIS:HA    | 13:DZ:76:TYR:CE2    | 2.48                     | 0.48              |
| 15:DB:78:ARG:NH1   | 15:DB:78:ARG:CG     | 2.76                     | 0.48              |
| 15:DB:1127:MET:HE3 | 15:DB:1144:LEU:HB3  | 1.94                     | 0.48              |
| 16:DC:430:ILE:HG23 | 16:DC:442:LEU:HD11  | 1.94                     | 0.48              |
| 19:DG:199:LEU:HD12 | 19:DG:206:LEU:HD13  | 1.94                     | 0.48              |
| 19:DG:214:TYR:C    | 19:DG:214:TYR:HD1   | 2.22                     | 0.48              |
| 20:DH:257:ASN:ND2  | 20:DH:260:GLU:HG3   | 2.29                     | 0.48              |
| 21:DJ:71:MET:HB3   | 21:DJ:71:MET:HE2    | 1.62                     | 0.48              |
| 23:DT:144:SER:OG   | 23:DT:161:ASN:ND2   | 2.46                     | 0.48              |
| 32:CI:40:TRP:CE2   | 33:CJ:163:MET:HE2   | 2.49                     | 0.48              |
| 37:CO:151:LYS:HD2  | 37:CO:156:TRP:HZ3   | 1.78                     | 0.48              |
| 51:Cm:56:ASN:HD21  | 51:Cm:62:ALA:CB     | 2.26                     | 0.48              |
| 51:Cm:85:ILE:HG12  | 51:Cm:140:CYS:HB2   | 1.96                     | 0.48              |
| 51:Cm:181:GLN:OE1  | 51:Cm:212:PRO:HG2   | 2.14                     | 0.48              |
| 53:Cp:93:ARG:HG3   | 53:Cp:102:ARG:HH12  | 1.79                     | 0.48              |
| 56:Cv:531:MET:HG2  | 56:Cv:535:HIS:CD2   | 2.48                     | 0.48              |
| 71:A8:95:ARG:HH11  | 71:A8:99:ARG:NH2    | 2.12                     | 0.48              |
| 71:A8:107:ARG:NH2  | 71:A8:108:TYR:OH    | 2.47                     | 0.48              |
| 79:AP:38:ASN:HB3   | 97:At:105:LEU:HA    | 1.96                     | 0.48              |
| 92:Ag:16:TYR:O     | 92:Ag:49:PRO:HA     | 2.14                     | 0.48              |
| 95:Ao:131:PRO:HD2  | 97:At:48:TYR:CD2    | 2.49                     | 0.48              |
| 95:Ao:158:ARG:HB3  | 115:BM:217:GLU:HG3  | 1.94                     | 0.48              |
| 96:Ap:217:ASP:OD1  | 96:Ap:217:ASP:N     | 2.44                     | 0.48              |
| 102:AA:520:U:H3'   | 102:AA:521:G:C8     | 2.48                     | 0.48              |
| 103:BA:211:SER:HB2 | 103:BA:628:PRO:HG3  | 1.94                     | 0.48              |
| 103:BA:350:LEU:HB2 | 103:BA:370:ILE:HG21 | 1.96                     | 0.48              |
| 105:BC:364:MET:HE3 | 105:BC:364:MET:HB2  | 1.71                     | 0.48              |
| 117:BO:224:TYR:HH  | 117:BO:226:GLU:CD   | 2.21                     | 0.48              |
| 120:BR:84:ASN:ND2  | 120:BR:86:GLU:HG2   | 2.26                     | 0.48              |
| 1:DA:344:ARG:NH1   | 44:Ca:546:PHE:O     | 2.47                     | 0.48              |
| 2:DD:361:ASN:OD1   | 2:DD:366:LEU:HA     | 2.14                     | 0.48              |
| 2:DD:687:HIS:HE1   | 2:DD:691:PHE:O      | 1.95                     | 0.48              |
| 7:DO:138:LEU:HD23  | 7:DO:176:THR:HG21   | 1.94                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:DR:39:GLN:HG2    | 10:DR:42:MET:HE2    | 1.96                     | 0.48              |
| 16:DC:855:ARG:HH12  | 17:DE:202:HIS:CE1   | 2.32                     | 0.48              |
| 16:DC:866:GLU:OE2   | 17:DE:202:HIS:HE1   | 1.96                     | 0.48              |
| 29:CE:396:LEU:HD22  | 29:CE:415:ILE:HD13  | 1.96                     | 0.48              |
| 37:CO:122:VAL:O     | 37:CO:191:LYS:NZ    | 2.38                     | 0.48              |
| 40:CR:12:ALA:HA     | 56:Cv:689:CYS:SG    | 2.54                     | 0.48              |
| 44:Ca:294:ASP:OD1   | 44:Ca:297:LEU:HB2   | 2.14                     | 0.48              |
| 44:Ca:443:MET:HG2   | 44:Ca:473:ILE:HG12  | 1.95                     | 0.48              |
| 47:Cg:270:MET:HE1   | 47:Cg:335:PHE:CD1   | 2.49                     | 0.48              |
| 49:Cj:90:ARG:NE     | 49:Cj:94:ILE:HD11   | 2.29                     | 0.48              |
| 54:Cq:25:PHE:O      | 54:Cq:27:PRO:HD3    | 2.14                     | 0.48              |
| 56:Cv:233:LYS:HG3   | 56:Cv:500:TYR:CD2   | 2.49                     | 0.48              |
| 56:Cv:686:LEU:HD21  | 56:Cv:788:ARG:HE    | 1.78                     | 0.48              |
| 57:CA:293:A:H1'     | 57:CA:315:A:H5''    | 1.96                     | 0.48              |
| 66:A2:422:ARG:NH1   | 107:BE:76:GLN:HE22  | 2.12                     | 0.48              |
| 66:A2:434:CYS:SG    | 66:A2:435:PRO:HD2   | 2.54                     | 0.48              |
| 69:A5:47:LYS:HD2    | 69:A5:48:TYR:CE2    | 2.49                     | 0.48              |
| 74:AF:215:ASP:OD1   | 74:AF:215:ASP:N     | 2.43                     | 0.48              |
| 74:AF:265:HIS:NE2   | 74:AF:296:ASN:O     | 2.47                     | 0.48              |
| 75:AI:45:ARG:NH1    | 75:AI:45:ARG:HB3    | 2.28                     | 0.48              |
| 76:AJ:76:PHE:CD2    | 77:AK:240:GLU:HG2   | 2.49                     | 0.48              |
| 77:AK:148:LEU:HD21  | 124:BV:52:PHE:CD1   | 2.49                     | 0.48              |
| 77:AK:332:GLU:OE1   | 92:Ag:216:MET:HG3   | 2.14                     | 0.48              |
| 87:AY:281:ASN:HB3   | 129:Ba:58:MET:SD    | 2.54                     | 0.48              |
| 89:Ad:165:GLU:HG3   | 89:Ad:166:PHE:N     | 2.28                     | 0.48              |
| 92:Ag:14:ILE:HG12   | 92:Ag:57:ILE:CD1    | 2.44                     | 0.48              |
| 94:Al:174:PHE:CE1   | 94:Al:191:VAL:HG21  | 2.49                     | 0.48              |
| 104:BB:136:TRP:HB2  | 104:BB:141:ILE:HD12 | 1.95                     | 0.48              |
| 105:BC:111:LEU:HD23 | 105:BC:137:ILE:HD11 | 1.96                     | 0.48              |
| 105:BC:410:LYS:HB2  | 105:BC:410:LYS:NZ   | 2.29                     | 0.48              |
| 114:BL:62:ARG:HA    | 114:BL:62:ARG:HD2   | 1.54                     | 0.48              |
| 115:BM:220:ILE:HG23 | 115:BM:228:ARG:NH1  | 2.28                     | 0.48              |
| 125:BW:20:VAL:HB    | 125:BW:21:PRO:HD3   | 1.96                     | 0.48              |
| 126:BX:133:SER:O    | 140:UD:49:UNK:HB1   | 2.13                     | 0.48              |
| 126:BX:152:PRO:HG2  | 126:BX:156:TRP:CD1  | 2.49                     | 0.48              |
| 10:DR:103:ASP:OD1   | 10:DR:104:PRO:HD2   | 2.13                     | 0.47              |
| 10:DR:108:GLN:HE22  | 49:Cj:147:TYR:HB2   | 1.78                     | 0.47              |
| 19:DG:176:VAL:HG22  | 19:DG:188:LEU:HD11  | 1.96                     | 0.47              |
| 22:DK:178:LYS:HB2   | 22:DK:256:GLY:O     | 2.14                     | 0.47              |
| 24:DV:49:ASP:OD1    | 24:DV:50:ALA:N      | 2.46                     | 0.47              |
| 24:DV:120:ARG:HH22  | 24:DV:131:GLN:HG2   | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:409:ASP:HA   | 56:Cv:1051:ARG:HD2 | 1.96                     | 0.47              |
| 33:CJ:206:PHE:CG   | 33:CJ:207:PRO:HA   | 2.49                     | 0.47              |
| 37:CO:111:GLN:HE22 | 37:CO:236:ARG:NH1  | 2.12                     | 0.47              |
| 41:CS:59:LYS:HE3   | 57:CA:411:A:OP1    | 2.14                     | 0.47              |
| 41:CS:118:ARG:HG2  | 41:CS:127:GLU:HG2  | 1.95                     | 0.47              |
| 44:Ca:400:TYR:O    | 44:Ca:404:ARG:HB3  | 2.14                     | 0.47              |
| 44:Ca:515:PRO:HG2  | 44:Ca:518:GLU:OE1  | 2.14                     | 0.47              |
| 44:Ca:548:GLU:OE1  | 44:Ca:548:GLU:N    | 2.47                     | 0.47              |
| 45:Cb:22:ASP:OD1   | 45:Cb:22:ASP:N     | 2.46                     | 0.47              |
| 46:Cd:170:GLY:O    | 46:Cd:171:LYS:HG2  | 2.14                     | 0.47              |
| 50:Ck:353:ARG:HH11 | 50:Ck:353:ARG:HG2  | 1.79                     | 0.47              |
| 56:Cv:897:GLU:HB2  | 56:Cv:912:ARG:HE   | 1.79                     | 0.47              |
| 56:Cv:1136:ASN:OD1 | 56:Cv:1136:ASN:N   | 2.47                     | 0.47              |
| 73:AE:167:ASP:O    | 73:AE:189:ALA:HA   | 2.13                     | 0.47              |
| 77:AK:148:LEU:HD12 | 77:AK:190:CYS:HB3  | 1.96                     | 0.47              |
| 77:AK:179:ARG:NH1  | 102:AA:400:U:C2    | 2.82                     | 0.47              |
| 77:AK:206:THR:HG22 | 77:AK:209:GLN:HB2  | 1.96                     | 0.47              |
| 79:AP:217:VAL:HG22 | 79:AP:236:ASN:O    | 2.14                     | 0.47              |
| 83:AU:65:ASN:HD22  | 83:AU:97:GLN:NE2   | 2.12                     | 0.47              |
| 102:AA:145:U:H2'   | 102:AA:146:A:C8    | 2.48                     | 0.47              |
| 102:AA:477:A:N6    | 102:AA:493:A:N1    | 2.62                     | 0.47              |
| 107:BE:32:LEU:CD2  | 107:BE:32:LEU:H    | 2.27                     | 0.47              |
| 107:BE:185:ARG:NH2 | 107:BE:235:GLU:OE1 | 2.47                     | 0.47              |
| 115:BM:112:TRP:CD1 | 115:BM:114:TYR:H   | 2.32                     | 0.47              |
| 120:BR:26:ARG:HG2  | 120:BR:70:TYR:CD1  | 2.49                     | 0.47              |
| 132:Bd:54:MET:HB3  | 132:Bd:55:PRO:HD2  | 1.96                     | 0.47              |
| 136:Bh:29:ASN:HB3  | 136:Bh:38:LEU:HD11 | 1.96                     | 0.47              |
| 138:UB:37:UNK:HA   | 138:UB:40:UNK:HG3  | 1.94                     | 0.47              |
| 140:UD:161:UNK:HA  | 140:UD:164:UNK:HG3 | 1.96                     | 0.47              |
| 145:UL:1:UNK:O     | 145:UL:3:UNK:N     | 2.47                     | 0.47              |
| 1:DA:794:ARG:NH1   | 1:DA:794:ARG:HB2   | 2.29                     | 0.47              |
| 1:DA:1002:PRO:O    | 4:DL:78:ALA:O      | 2.32                     | 0.47              |
| 3:DI:27:THR:H      | 3:DI:30:GLN:NE2    | 2.07                     | 0.47              |
| 11:DS:110:SER:OG   | 57:CA:206:A:OP2    | 2.27                     | 0.47              |
| 12:DU:83:ARG:HG2   | 12:DU:98:MET:HE3   | 1.95                     | 0.47              |
| 13:DZ:20:ARG:HD2   | 44:Ca:172:PHE:CE2  | 2.49                     | 0.47              |
| 15:DB:78:ARG:NH1   | 17:DE:216:LEU:HD12 | 2.29                     | 0.47              |
| 15:DB:1030:ARG:NH1 | 15:DB:1030:ARG:HG2 | 2.28                     | 0.47              |
| 16:DC:263:GLN:HB3  | 16:DC:267:LYS:NZ   | 2.29                     | 0.47              |
| 17:DE:581:THR:H    | 17:DE:585:ARG:HB2  | 1.79                     | 0.47              |
| 19:DG:229:HIS:CE1  | 19:DG:250:LEU:HD22 | 2.49                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 20:DH:309:TRP:HA    | 20:DH:310:PRO:C     | 2.39                     | 0.47              |
| 26:DX:132:THR:HB    | 33:CJ:776:GLN:HB3   | 1.97                     | 0.47              |
| 28:CC:44:LEU:HD11   | 28:CC:50:ILE:HD12   | 1.96                     | 0.47              |
| 28:CC:65:ILE:HD13   | 33:CJ:75:TYR:HD2    | 1.79                     | 0.47              |
| 33:CJ:130:ARG:NH1   | 50:Ck:710:ARG:HH21  | 2.12                     | 0.47              |
| 33:CJ:555:TRP:HE1   | 33:CJ:581:GLN:HA    | 1.79                     | 0.47              |
| 40:CR:49:ARG:HB2    | 40:CR:53:GLN:HB2    | 1.95                     | 0.47              |
| 40:CR:320:VAL:CB    | 46:Cd:281:MET:HE2   | 2.38                     | 0.47              |
| 51:Cm:77:PRO:HB3    | 51:Cm:155:HIS:CE1   | 2.48                     | 0.47              |
| 57:CA:194:A:O2'     | 57:CA:195:A:H2'     | 2.13                     | 0.47              |
| 65:A1:111:SER:OG    | 65:A1:114:LEU:HG    | 2.14                     | 0.47              |
| 66:A2:130:PRO:HA    | 128:BZ:81:TYR:CE2   | 2.50                     | 0.47              |
| 67:A3:86:ARG:NH1    | 67:A3:91:GLU:HG2    | 2.29                     | 0.47              |
| 68:A4:30:PRO:HA     | 68:A4:33:ARG:NH1    | 2.29                     | 0.47              |
| 69:A5:47:LYS:HD2    | 69:A5:48:TYR:CZ     | 2.49                     | 0.47              |
| 78:AN:93:MET:HB3    | 78:AN:98:TRP:CE2    | 2.49                     | 0.47              |
| 84:AV:190:LYS:H     | 84:AV:206:ASN:HD21  | 1.61                     | 0.47              |
| 86:AX:187:ARG:NH2   | 102:AA:536:A:H5''   | 2.30                     | 0.47              |
| 87:AY:75:THR:HG21   | 107:BE:60:GLY:HA3   | 1.95                     | 0.47              |
| 96:Ap:200:VAL:O     | 96:Ap:203:PHE:HB3   | 2.14                     | 0.47              |
| 102:AA:24:U:H2'     | 102:AA:25:A:C8      | 2.50                     | 0.47              |
| 102:AA:564:A:O2'    | 140:UD:22:UNK:HA    | 2.14                     | 0.47              |
| 102:AA:1162:G:O2'   | 102:AA:1163:A:OP1   | 2.28                     | 0.47              |
| 103:BA:373:ALA:HA   | 103:BA:376:ARG:NH1  | 2.30                     | 0.47              |
| 108:BF:60:LEU:HD22  | 108:BF:63:ARG:HH11  | 1.72                     | 0.47              |
| 110:BH:122:HIS:CD2  | 110:BH:124:PHE:HB2  | 2.49                     | 0.47              |
| 111:BI:26:ASN:HD22  | 111:BI:29:TRP:HD1   | 1.62                     | 0.47              |
| 114:BL:119:ILE:HD11 | 114:BL:150:VAL:HG22 | 1.96                     | 0.47              |
| 122:BT:86:ARG:HG2   | 122:BT:86:ARG:HH11  | 1.79                     | 0.47              |
| 131:Bc:38:ASN:HA    | 131:Bc:41:LYS:HZ2   | 1.78                     | 0.47              |
| 140:UD:27:UNK:HA    | 140:UD:30:UNK:HG3   | 1.94                     | 0.47              |
| 1:DA:1042:HIS:HD2   | 1:DA:1045:ILE:H     | 1.62                     | 0.47              |
| 1:DA:1060:LEU:HD22  | 1:DA:1163:MET:HE1   | 1.95                     | 0.47              |
| 1:DA:1662:ARG:HH22  | 29:CE:402:ARG:NH1   | 2.10                     | 0.47              |
| 2:DD:26:ARG:HH11    | 57:CA:145:A:H2      | 1.61                     | 0.47              |
| 2:DD:612:MET:O      | 2:DD:616:LEU:HB2    | 2.14                     | 0.47              |
| 15:DB:867:THR:HG22  | 15:DB:868:HIS:H     | 1.79                     | 0.47              |
| 16:DC:574:GLN:NE2   | 16:DC:807:VAL:H     | 2.07                     | 0.47              |
| 18:DF:112:ARG:HH22  | 18:DF:118:THR:HG23  | 1.80                     | 0.47              |
| 20:DH:55:ARG:HG2    | 20:DH:143:CYS:HA    | 1.95                     | 0.47              |
| 20:DH:518:LYS:O     | 20:DH:523:ARG:NH1   | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:328:ASP:OD1  | 29:CE:328:ASP:N    | 2.44                     | 0.47              |
| 32:CI:409:PRO:CD   | 40:CR:253:PHE:CE2  | 2.98                     | 0.47              |
| 34:CK:14:PRO:HA    | 40:CR:300:TYR:CE2  | 2.49                     | 0.47              |
| 37:CO:208:MET:HG2  | 37:CO:223:VAL:HG13 | 1.96                     | 0.47              |
| 38:CP:113:LYS:HB2  | 38:CP:114:PRO:HD3  | 1.96                     | 0.47              |
| 44:Ca:62:TRP:HB3   | 44:Ca:79:MET:HE1   | 1.96                     | 0.47              |
| 46:Cd:177:LEU:HD11 | 56:Cv:648:VAL:HG22 | 1.95                     | 0.47              |
| 47:Cg:159:MET:CG   | 47:Cg:356:CYS:HB2  | 2.44                     | 0.47              |
| 48:CI:155:LYS:O    | 57:CA:439:U:O2'    | 2.32                     | 0.47              |
| 50:Ck:411:CYS:HA   | 50:Ck:414:MET:HE2  | 1.96                     | 0.47              |
| 51:Cm:83:LYS:NZ    | 57:CA:393:U:H5'    | 2.29                     | 0.47              |
| 56:Cv:260:MET:HB3  | 56:Cv:299:ALA:HB2  | 1.96                     | 0.47              |
| 56:Cv:292:LYS:HE2  | 56:Cv:512:MET:HE3  | 1.95                     | 0.47              |
| 56:Cv:871:ILE:HD13 | 56:Cv:890:PRO:HG2  | 1.95                     | 0.47              |
| 57:CA:106:U:H5'    | 57:CA:107:U:OP1    | 2.15                     | 0.47              |
| 57:CA:253:U:H2'    | 57:CA:254:A:C8     | 2.49                     | 0.47              |
| 63:UT:5:UNK:O      | 63:UT:7:UNK:HG3    | 2.15                     | 0.47              |
| 63:UT:24:UNK:HG2   | 63:UT:29:UNK:HG3   | 1.96                     | 0.47              |
| 66:A2:33:SER:OG    | 66:A2:89:GLU:OE2   | 2.17                     | 0.47              |
| 69:A5:45:LYS:HB3   | 87:AY:1:MET:HA     | 1.96                     | 0.47              |
| 70:A6:65:ARG:HH22  | 98:Av:190:GLU:HB3  | 1.80                     | 0.47              |
| 73:AE:70:LYS:NZ    | 73:AE:70:LYS:HB3   | 2.30                     | 0.47              |
| 75:AI:23:THR:HG22  | 75:AI:66:GLU:OE2   | 2.14                     | 0.47              |
| 80:AQ:124:ILE:HG12 | 80:AQ:141:PHE:CZ   | 2.48                     | 0.47              |
| 88:Ab:457:ARG:HA   | 88:Ab:457:ARG:HD2  | 1.43                     | 0.47              |
| 98:Av:66:LYS:HD2   | 98:Av:120:TRP:CZ3  | 2.49                     | 0.47              |
| 102:AA:80:U:C2     | 122:BT:12:THR:HG21 | 2.48                     | 0.47              |
| 102:AA:516:U:O4    | 107:BE:431:ARG:HG2 | 2.14                     | 0.47              |
| 104:BB:287:SER:HB2 | 104:BB:331:SER:HA  | 1.95                     | 0.47              |
| 105:BC:49:SER:O    | 105:BC:49:SER:OG   | 2.33                     | 0.47              |
| 106:BD:135:LYS:O   | 106:BD:139:MET:N   | 2.45                     | 0.47              |
| 125:BW:94:MET:HB2  | 138:UB:19:UNK:HB1  | 1.96                     | 0.47              |
| 125:BW:98:LYS:O    | 125:BW:102:GLU:HG3 | 2.15                     | 0.47              |
| 137:UA:21:UNK:O    | 137:UA:26:UNK:N    | 2.46                     | 0.47              |
| 2:DD:274:PHE:CE1   | 37:CO:329:GLU:HB2  | 2.49                     | 0.47              |
| 2:DD:345:PRO:HB3   | 12:DU:98:MET:HE1   | 1.96                     | 0.47              |
| 6:DN:237:ARG:H     | 6:DN:237:ARG:HG2   | 1.46                     | 0.47              |
| 9:DQ:68:ARG:NH2    | 12:DU:29:GLU:O     | 2.37                     | 0.47              |
| 12:DU:46:THR:HG23  | 37:CO:332:ARG:HA   | 1.95                     | 0.47              |
| 13:DZ:48:ARG:H     | 44:Ca:586:ILE:HD11 | 1.80                     | 0.47              |
| 15:DB:671:VAL:HG11 | 15:DB:832:TYR:HB2  | 1.96                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:DB:908:GLN:NE2  | 15:DB:908:GLN:H     | 2.12                     | 0.47              |
| 16:DC:696:VAL:HG13 | 16:DC:703:ALA:HB2   | 1.97                     | 0.47              |
| 16:DC:801:HIS:CD2  | 16:DC:802:PRO:HD2   | 2.50                     | 0.47              |
| 19:DG:46:TRP:HB3   | 19:DG:89:GLU:OE2    | 2.15                     | 0.47              |
| 29:CE:213:TYR:HB3  | 31:CH:250:LEU:HD23  | 1.96                     | 0.47              |
| 30:CF:44:ILE:HD11  | 30:CF:63:ARG:NH1    | 2.28                     | 0.47              |
| 32:CI:104:ASN:HD22 | 32:CI:105:THR:N     | 2.12                     | 0.47              |
| 33:CJ:59:PRO:HG3   | 57:CA:462:A:C8      | 2.49                     | 0.47              |
| 33:CJ:376:SER:HB3  | 33:CJ:385:LEU:HD23  | 1.97                     | 0.47              |
| 33:CJ:712:THR:OG1  | 36:CN:52:ASP:HB2    | 2.14                     | 0.47              |
| 37:CO:248:ILE:HD11 | 57:CA:287:A:N3      | 2.29                     | 0.47              |
| 44:Ca:61:LEU:HB2   | 44:Ca:76:GLN:HE22   | 1.79                     | 0.47              |
| 51:Cm:89:GLY:O     | 51:Cm:92:GLN:HB3    | 2.15                     | 0.47              |
| 52:Cn:226:LEU:O    | 52:Cn:230:VAL:HG23  | 2.14                     | 0.47              |
| 56:Cv:566:MET:SD   | 56:Cv:918:LEU:HD13  | 2.54                     | 0.47              |
| 74:AF:240:ASP:HB3  | 74:AF:241:ARG:HG3   | 1.97                     | 0.47              |
| 75:AI:207:PHE:CE1  | 110:BH:107:VAL:HG21 | 2.49                     | 0.47              |
| 87:AY:153:ILE:HD13 | 107:BE:87:LEU:HD11  | 1.96                     | 0.47              |
| 88:Ab:490:TRP:CE3  | 88:Ab:494:THR:HG21  | 2.49                     | 0.47              |
| 97:At:148:GLN:NE2  | 108:BF:279:TYR:OH   | 2.47                     | 0.47              |
| 102:AA:440:U:P     | 115:BM:277:LYS:NZ   | 2.88                     | 0.47              |
| 102:AA:477:A:H3'   | 102:AA:477:A:N3     | 2.29                     | 0.47              |
| 103:BA:267:PHE:CZ  | 103:BA:322:MET:HB2  | 2.49                     | 0.47              |
| 104:BB:431:ARG:O   | 104:BB:434:GLU:HG2  | 2.14                     | 0.47              |
| 111:BI:144:HIS:HE1 | 111:BI:176:GLU:O    | 1.96                     | 0.47              |
| 111:BI:254:ARG:H   | 111:BI:254:ARG:HD2  | 1.79                     | 0.47              |
| 116:BN:62:PHE:CZ   | 116:BN:88:ILE:HA    | 2.49                     | 0.47              |
| 119:BQ:30:VAL:HB   | 119:BQ:198:SER:HB2  | 1.97                     | 0.47              |
| 126:BX:117:PHE:CE2 | 126:BX:126:LEU:HD12 | 2.49                     | 0.47              |
| 1:DA:1134:ILE:HG22 | 1:DA:1135:PRO:O     | 2.15                     | 0.47              |
| 1:DA:1163:MET:HE3  | 54:Cq:62:TYR:HB3    | 1.96                     | 0.47              |
| 2:DD:296:LEU:HG    | 2:DD:300:GLN:HE21   | 1.80                     | 0.47              |
| 4:DL:288:ASN:OD1   | 4:DL:288:ASN:N      | 2.46                     | 0.47              |
| 6:DN:183:ARG:CD    | 6:DN:194:ARG:HH12   | 2.26                     | 0.47              |
| 9:DQ:186:ARG:HB3   | 9:DQ:186:ARG:HH11   | 1.79                     | 0.47              |
| 12:DU:27:ARG:HB3   | 12:DU:27:ARG:NH1    | 2.29                     | 0.47              |
| 14:Da:10:ILE:HG23  | 14:Da:22:ARG:NH1    | 2.29                     | 0.47              |
| 15:DB:722:ARG:NH2  | 15:DB:802:ASP:OD2   | 2.47                     | 0.47              |
| 18:DF:286:ARG:HD3  | 18:DF:286:ARG:HA    | 1.71                     | 0.47              |
| 19:DG:296:ASP:OD2  | 32:CI:14:ARG:NH1    | 2.47                     | 0.47              |
| 20:DH:145:ALA:HA   | 20:DH:151:LEU:HD23  | 1.95                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 25:DW:61:ARG:NH1    | 47:Cg:374:GLU:OE2   | 2.47                     | 0.47              |
| 28:CC:70:TYR:CE2    | 28:CC:72:ILE:HB     | 2.49                     | 0.47              |
| 32:CI:97:GLU:OE2    | 34:CK:108:ARG:NH1   | 2.47                     | 0.47              |
| 33:CJ:94:ALA:HB2    | 33:CJ:101:PHE:HB3   | 1.95                     | 0.47              |
| 36:CN:166:ILE:HD11  | 50:Ck:766:LYS:HB2   | 1.97                     | 0.47              |
| 40:CR:307:ARG:NH1   | 57:CA:389:A:N6      | 2.62                     | 0.47              |
| 44:Ca:496:GLU:OE1   | 44:Ca:496:GLU:N     | 2.48                     | 0.47              |
| 50:Ck:176:THR:HG23  | 50:Ck:178:ASP:H     | 1.79                     | 0.47              |
| 50:Ck:259:ILE:O     | 50:Ck:263:SER:HB3   | 2.15                     | 0.47              |
| 52:Cn:243:ARG:HG3   | 52:Cn:244:PRO:HD2   | 1.96                     | 0.47              |
| 56:Cv:407:MET:HE3   | 56:Cv:407:MET:HB3   | 1.74                     | 0.47              |
| 76:AJ:73:ARG:HB3    | 76:AJ:81:ASN:O      | 2.15                     | 0.47              |
| 79:AP:110:HIS:CE1   | 85:AW:19:ASN:HB3    | 2.49                     | 0.47              |
| 89:Ad:143:ASP:OD1   | 89:Ad:148:ARG:NH2   | 2.48                     | 0.47              |
| 91:Af:101:HIS:HD2   | 91:Af:102:PRO:O     | 1.98                     | 0.47              |
| 95:Ao:127:SER:HB3   | 119:BQ:188:ARG:NH2  | 2.27                     | 0.47              |
| 98:Av:54:THR:HG22   | 98:Av:57:GLU:OE2    | 2.15                     | 0.47              |
| 102:AA:476:G:H2'    | 102:AA:476:G:N3     | 2.29                     | 0.47              |
| 108:BF:164:HIS:CD2  | 108:BF:166:GLN:H    | 2.32                     | 0.47              |
| 109:BG:244:ARG:HH11 | 109:BG:257:ARG:NH2  | 2.11                     | 0.47              |
| 111:BI:163:CYS:C    | 111:BI:185:MET:HE1  | 2.40                     | 0.47              |
| 115:BM:130:LEU:HD23 | 115:BM:166:ILE:HG12 | 1.96                     | 0.47              |
| 130:Bb:62:ARG:NH1   | 130:Bb:104:LEU:HD21 | 2.28                     | 0.47              |
| 61:UX:2:UNK:HG2     | 61:UX:3:UNK:N       | 2.22                     | 0.47              |
| 1:DA:492:ASN:HB2    | 1:DA:495:GLU:HB2    | 1.95                     | 0.47              |
| 1:DA:502:LYS:HB3    | 1:DA:502:LYS:HZ3    | 1.80                     | 0.47              |
| 1:DA:1244:LYS:NZ    | 1:DA:1298:VAL:HG23  | 2.29                     | 0.47              |
| 2:DD:118:ARG:NH1    | 44:Ca:467:LYS:HE2   | 2.29                     | 0.47              |
| 5:DM:30:ARG:HD2     | 56:Cv:1011:SER:O    | 2.15                     | 0.47              |
| 6:DN:67:TYR:HB3     | 6:DN:114:GLY:O      | 2.13                     | 0.47              |
| 9:DQ:148:LEU:HD23   | 9:DQ:176:ARG:NH2    | 2.30                     | 0.47              |
| 15:DB:905:TYR:CD1   | 15:DB:918:VAL:HG22  | 2.50                     | 0.47              |
| 16:DC:203:MET:HA    | 16:DC:203:MET:HE3   | 1.97                     | 0.47              |
| 19:DG:292:GLU:HA    | 19:DG:295:VAL:HG23  | 1.96                     | 0.47              |
| 20:DH:133:CYS:HB3   | 20:DH:136:LEU:HB3   | 1.96                     | 0.47              |
| 24:DV:70:LYS:HB3    | 57:CA:513:U:OP1     | 2.15                     | 0.47              |
| 29:CE:137:LEU:HD11  | 45:Cb:47:ILE:HG13   | 1.95                     | 0.47              |
| 32:CI:89:ARG:HE     | 40:CR:193:ASN:HD21  | 1.61                     | 0.47              |
| 44:Ca:75:LEU:O      | 44:Ca:79:MET:HG3    | 2.15                     | 0.47              |
| 44:Ca:457:LYS:HD2   | 44:Ca:492:TYR:CG    | 2.49                     | 0.47              |
| 46:Cd:129:ARG:HD3   | 56:Cv:209:VAL:O     | 2.15                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 47:Cg:37:ILE:HD13   | 47:Cg:422:LEU:HG    | 1.97                     | 0.47              |
| 47:Cg:181:VAL:HG12  | 47:Cg:203:ALA:HB2   | 1.96                     | 0.47              |
| 56:Cv:939:SER:O     | 56:Cv:939:SER:OG    | 2.29                     | 0.47              |
| 64:A0:52:ARG:HG2    | 64:A0:52:ARG:HH11   | 1.80                     | 0.47              |
| 65:A1:179:MET:HB3   | 65:A1:179:MET:HE2   | 1.72                     | 0.47              |
| 66:A2:412:ASN:ND2   | 66:A2:439:ASP:H     | 2.13                     | 0.47              |
| 70:A6:48:HIS:CD2    | 70:A6:74:PRO:HD2    | 2.49                     | 0.47              |
| 71:A8:92:MET:HB3    | 71:A8:107:ARG:HE    | 1.79                     | 0.47              |
| 73:AE:314:TRP:CE2   | 73:AE:382:LYS:NZ    | 2.82                     | 0.47              |
| 78:AN:37:LEU:HD23   | 78:AN:78:ILE:HB     | 1.97                     | 0.47              |
| 85:AW:7:ARG:N       | 102:AA:153:U:O4     | 2.42                     | 0.47              |
| 91:Af:76:LEU:HD23   | 91:Af:76:LEU:H      | 1.80                     | 0.47              |
| 94:Al:200:ASN:OD1   | 102:AA:325:A:H5''   | 2.14                     | 0.47              |
| 95:Ao:127:SER:HB3   | 119:BQ:188:ARG:HH12 | 1.78                     | 0.47              |
| 96:Ap:176:MET:HA    | 96:Ap:280:LEU:HD11  | 1.96                     | 0.47              |
| 96:Ap:177:HIS:CD2   | 96:Ap:277:LEU:HD12  | 2.50                     | 0.47              |
| 96:Ap:177:HIS:O     | 96:Ap:237:LEU:HD13  | 2.15                     | 0.47              |
| 102:AA:525:A:N1     | 135:Bg:56:ARG:NH1   | 2.62                     | 0.47              |
| 103:BA:281:GLU:HG3  | 103:BA:284:LYS:HD2  | 1.96                     | 0.47              |
| 107:BE:179:GLY:H    | 107:BE:184:ARG:HH22 | 1.62                     | 0.47              |
| 107:BE:351:GLU:CD   | 107:BE:351:GLU:H    | 2.22                     | 0.47              |
| 110:BH:128:ILE:HB   | 110:BH:168:THR:HG23 | 1.96                     | 0.47              |
| 123:BU:139:ARG:HB3  | 135:Bg:35:LEU:HD11  | 1.96                     | 0.47              |
| 124:BV:155:MET:HE2  | 124:BV:155:MET:HB3  | 1.74                     | 0.47              |
| 129:Ba:100:GLU:O    | 129:Ba:104:ARG:HG3  | 2.14                     | 0.47              |
| 131:Bc:17:HIS:HD2   | 131:Bc:24:ARG:HH22  | 1.63                     | 0.47              |
| 133:Be:30:PRO:HG2   | 133:Be:40:HIS:CD2   | 2.50                     | 0.47              |
| 136:Bh:3:LEU:HD23   | 136:Bh:14:GLU:HB2   | 1.96                     | 0.47              |
| 1:DA:828:LYS:NZ     | 6:DN:200:ASP:OD2    | 2.42                     | 0.47              |
| 1:DA:1029:LYS:NZ    | 5:DM:254:HIS:CE1    | 2.82                     | 0.47              |
| 2:DD:347:GLU:OE1    | 12:DU:83:ARG:NH2    | 2.48                     | 0.47              |
| 9:DQ:35:VAL:HG12    | 9:DQ:36:GLU:HG3     | 1.97                     | 0.47              |
| 10:DR:210:SER:HA    | 10:DR:215:ARG:NH1   | 2.29                     | 0.47              |
| 13:DZ:63:LEU:HD11   | 44:Ca:540:SER:H     | 1.80                     | 0.47              |
| 15:DB:1100:LEU:HD23 | 15:DB:1100:LEU:HA   | 1.77                     | 0.47              |
| 16:DC:88:LEU:HD23   | 16:DC:88:LEU:HA     | 1.66                     | 0.47              |
| 16:DC:104:PRO:HG2   | 16:DC:112:TYR:CE1   | 2.50                     | 0.47              |
| 18:DF:15:HIS:CE1    | 21:DJ:278:GLY:HA2   | 2.50                     | 0.47              |
| 18:DF:92:MET:HE2    | 41:CS:104:GLN:NE2   | 2.29                     | 0.47              |
| 18:DF:502:ARG:HH11  | 18:DF:579:GLU:CD    | 2.23                     | 0.47              |
| 19:DG:214:TYR:C     | 19:DG:214:TYR:CD1   | 2.92                     | 0.47              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 19:DG:334:MET:HE1 | 19:DG:388:TYR:N     | 2.30                     | 0.47              |
| 22:DK:99:ASP:C    | 22:DK:101:ASP:H     | 2.22                     | 0.47              |
| 27:DY:53:LEU:HD23 | 27:DY:53:LEU:HA     | 1.67                     | 0.47              |
| 30:CF:42:GLU:OE1  | 46:Cd:179:PHE:HD1   | 1.97                     | 0.47              |
| 32:CI:89:ARG:HA   | 34:CK:111:ASN:HD21  | 1.79                     | 0.47              |
| 32:CI:265:ASP:O   | 32:CI:266:SER:OG    | 2.30                     | 0.47              |
| 38:CP:23:ALA:CB   | 38:CP:51:HIS:ND1    | 2.69                     | 0.47              |
| 40:CR:306:LYS:NZ  | 57:CA:390:U:P       | 2.88                     | 0.47              |
| 40:CR:307:ARG:NH1 | 57:CA:389:A:H62     | 2.13                     | 0.47              |
| 44:Ca:98:PRO:HB2  | 44:Ca:174:ASP:OD2   | 2.15                     | 0.47              |
| 45:Cb:91:ARG:O    | 45:Cb:95:ARG:HG2    | 2.14                     | 0.47              |
| 46:Cd:12:ILE:HG23 | 53:Cp:120:ARG:HE    | 1.80                     | 0.47              |
| 47:Cg:362:LYS:HG3 | 47:Cg:382:LEU:O     | 2.14                     | 0.47              |
| 48:Ci:30:ARG:HH11 | 48:Ci:30:ARG:HG3    | 1.80                     | 0.47              |
| 49:Cj:217:PRO:HG2 | 49:Cj:220:PHE:CD2   | 2.50                     | 0.47              |
| 51:Cm:146:TRP:NE1 | 51:Cm:150:ASN:HD22  | 2.13                     | 0.47              |
| 51:Cm:168:HIS:CD2 | 51:Cm:168:HIS:H     | 2.33                     | 0.47              |
| 56:Cv:89:GLN:OE1  | 56:Cv:91:ARG:HD3    | 2.15                     | 0.47              |
| 56:Cv:617:ASP:HB3 | 56:Cv:663:ARG:HD2   | 1.97                     | 0.47              |
| 57:CA:232:G:H22   | 57:CA:248:A:P       | 2.38                     | 0.47              |
| 57:CA:467:A:H2'   | 149:CA:735:SPD:H52  | 1.97                     | 0.47              |
| 64:A0:164:ASP:OD1 | 64:A0:164:ASP:N     | 2.47                     | 0.47              |
| 65:A1:68:LYS:H    | 65:A1:73:MET:HE1    | 1.78                     | 0.47              |
| 65:A1:122:MET:HB3 | 65:A1:126:ALA:HB3   | 1.96                     | 0.47              |
| 66:A2:389:HIS:HB3 | 102:AA:32:U:C4      | 2.50                     | 0.47              |
| 67:A3:68:VAL:HG12 | 67:A3:90:LEU:HD11   | 1.95                     | 0.47              |
| 72:A9:91:GLN:NE2  | 96:Ap:296:VAL:HG22  | 2.30                     | 0.47              |
| 72:A9:106:MET:HE3 | 78:AN:115:ARG:HH21  | 1.80                     | 0.47              |
| 73:AE:92:THR:OG1  | 134:Bf:108:THR:O    | 2.32                     | 0.47              |
| 73:AE:106:ARG:CZ  | 142:UN:7:UNK:HG1    | 2.44                     | 0.47              |
| 74:AF:106:TYR:HA  | 94:Al:139:HIS:CE1   | 2.50                     | 0.47              |
| 74:AF:432:ASP:OD1 | 74:AF:432:ASP:N     | 2.48                     | 0.47              |
| 77:AK:336:THR:OG1 | 92:Ag:188:ARG:O     | 2.27                     | 0.47              |
| 81:AR:91:PRO:HB3  | 102:AA:1167:A:C6    | 2.50                     | 0.47              |
| 81:AR:94:ARG:NH2  | 103:BA:775:PRO:HB2  | 2.25                     | 0.47              |
| 81:AR:223:HIS:CE1 | 135:Bg:83:LEU:H     | 2.32                     | 0.47              |
| 89:Ad:96:ALA:O    | 89:Ad:99:THR:HB     | 2.15                     | 0.47              |
| 89:Ad:125:ARG:N   | 93:Aj:54:GLN:HE22   | 2.12                     | 0.47              |
| 91:Af:164:HIS:CD2 | 91:Af:166:LYS:HB2   | 2.48                     | 0.47              |
| 97:At:34:ARG:CD   | 120:BR:127:ARG:HH12 | 2.27                     | 0.47              |
| 102:AA:54:A:H2'   | 129:Ba:118:TYR:CE2  | 2.49                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 102:AA:446:A:H2'    | 102:AA:447:U:H2'    | 1.97                     | 0.47              |
| 102:AA:528:A:HO2'   | 102:AA:529:U:P      | 2.38                     | 0.47              |
| 102:AA:538:U:H4'    | 102:AA:539:A:H5'    | 1.96                     | 0.47              |
| 102:AA:1172:A:H2    | 103:BA:773:ASP:H    | 1.61                     | 0.47              |
| 103:BA:693:HIS:HA   | 103:BA:743:HIS:O    | 2.15                     | 0.47              |
| 103:BA:791:PHE:CE1  | 103:BA:801:ARG:NH1  | 2.83                     | 0.47              |
| 104:BB:117:LEU:HD12 | 104:BB:117:LEU:HA   | 1.79                     | 0.47              |
| 110:BH:88:GLU:O     | 110:BH:91:LYS:HG3   | 2.14                     | 0.47              |
| 111:BI:152:GLN:NE2  | 134:Bf:99:ILE:HA    | 2.29                     | 0.47              |
| 114:BL:122:LYS:NZ   | 114:BL:126:LYS:HB2  | 2.30                     | 0.47              |
| 116:BN:111:PHE:HE1  | 116:BN:122:CYS:HG   | 1.61                     | 0.47              |
| 120:BR:174:ALA:HB1  | 120:BR:179:ILE:HG13 | 1.96                     | 0.47              |
| 125:BW:40:HIS:ND1   | 125:BW:90:ARG:NH1   | 2.63                     | 0.47              |
| 135:Bg:80:MET:HG3   | 135:Bg:81:PHE:CD2   | 2.48                     | 0.47              |
| 138:UB:11:UNK:HB2   | 138:UB:13:UNK:HG3   | 1.97                     | 0.47              |
| 140:UD:20:UNK:O     | 140:UD:25:UNK:HG1   | 2.15                     | 0.47              |
| 140:UD:82:UNK:CG    | 140:UD:87:UNK:HG1   | 2.44                     | 0.47              |
| 1:DA:717:ASP:O      | 1:DA:721:ILE:HG13   | 2.15                     | 0.47              |
| 4:DL:92:ILE:HG22    | 32:CI:248:PHE:CD1   | 2.50                     | 0.47              |
| 5:DM:104:LYS:O      | 5:DM:107:GLU:HG2    | 2.13                     | 0.47              |
| 6:DN:258:ASP:OD2    | 6:DN:277:LYS:HG3    | 2.14                     | 0.47              |
| 6:DN:291:PRO:O      | 29:CE:114:TYR:CE1   | 2.68                     | 0.47              |
| 15:DB:517:GLU:HG2   | 15:DB:841:ARG:HH22  | 1.79                     | 0.47              |
| 15:DB:958:ASN:HD22  | 15:DB:959:PRO:HD2   | 1.80                     | 0.47              |
| 18:DF:268:GLY:HA3   | 18:DF:312:TRP:CG    | 2.49                     | 0.47              |
| 19:DG:624:ARG:NH1   | 24:DV:181:LYS:O     | 2.44                     | 0.47              |
| 26:DX:102:MET:HE2   | 26:DX:102:MET:HB3   | 1.70                     | 0.47              |
| 34:CK:316:ASN:OD1   | 34:CK:317:GLY:N     | 2.48                     | 0.47              |
| 37:CO:224:LEU:HD12  | 37:CO:224:LEU:HA    | 1.77                     | 0.47              |
| 47:Cg:40:LYS:NZ     | 47:Cg:57:THR:HA     | 2.29                     | 0.47              |
| 51:Cm:125:CYS:O     | 51:Cm:129:VAL:HG23  | 2.15                     | 0.47              |
| 56:Cv:585:ASP:OD1   | 56:Cv:586:GLU:N     | 2.48                     | 0.47              |
| 62:US:15:UNK:HB2    | 62:US:18:UNK:HG2    | 1.96                     | 0.47              |
| 70:A6:56:GLU:HA     | 70:A6:59:ARG:HB2    | 1.97                     | 0.47              |
| 72:A9:76:ARG:NH1    | 72:A9:89:PRO:HG3    | 2.30                     | 0.47              |
| 74:AF:354:GLY:O     | 74:AF:358:GLN:HG3   | 2.14                     | 0.47              |
| 87:AY:96:ARG:CZ     | 107:BE:71:LEU:HD21  | 2.45                     | 0.47              |
| 87:AY:113:PRO:HA    | 87:AY:131:ILE:HG22  | 1.97                     | 0.47              |
| 88:Ab:348:LEU:O     | 88:Ab:405:SER:N     | 2.43                     | 0.47              |
| 92:Ag:33:LEU:N      | 92:Ag:34:PRO:HD2    | 2.30                     | 0.47              |
| 102:AA:567:G:C2     | 136:Bh:23:ARG:NH1   | 2.83                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 105:BC:64:VAL:HG23  | 105:BC:287:HIS:ND1  | 2.29                     | 0.47              |
| 105:BC:309:PHE:HA   | 105:BC:363:GLY:O    | 2.15                     | 0.47              |
| 114:BL:183:TRP:CD1  | 114:BL:253:THR:HG21 | 2.50                     | 0.47              |
| 116:BN:97:ARG:HE    | 116:BN:101:LYS:HE3  | 1.80                     | 0.47              |
| 116:BN:179:LEU:HD23 | 140:UD:208:UNK:HG2  | 1.97                     | 0.47              |
| 116:BN:192:ARG:HH12 | 116:BN:193:PHE:HE1  | 1.62                     | 0.47              |
| 118:BP:145:PRO:HD2  | 118:BP:178:PRO:CG   | 2.45                     | 0.47              |
| 125:BW:45:ARG:O     | 125:BW:49:VAL:HG13  | 2.15                     | 0.47              |
| 1:DA:575:PHE:CG     | 1:DA:576:PRO:HD2    | 2.49                     | 0.47              |
| 1:DA:990:VAL:CG1    | 1:DA:1185:ARG:HG3   | 2.43                     | 0.47              |
| 2:DD:656:LEU:HD12   | 38:CP:142:LYS:HE2   | 1.97                     | 0.47              |
| 4:DL:189:THR:HB     | 40:CR:73:ASP:OD2    | 2.15                     | 0.47              |
| 5:DM:21:ARG:NH2     | 5:DM:232:PRO:O      | 2.44                     | 0.47              |
| 7:DO:67:ARG:NH1     | 56:Cv:780:PRO:HG3   | 2.29                     | 0.47              |
| 15:DB:891:GLN:HG3   | 50:Ck:310:ASP:HA    | 1.96                     | 0.47              |
| 18:DF:516:ARG:HD2   | 18:DF:542:HIS:ND1   | 2.30                     | 0.47              |
| 22:DK:99:ASP:OD2    | 22:DK:102:LYS:HD2   | 2.15                     | 0.47              |
| 29:CE:40:ARG:HD2    | 29:CE:94:ARG:HD3    | 1.96                     | 0.47              |
| 32:CI:16:PHE:HA     | 32:CI:41:VAL:HG21   | 1.97                     | 0.47              |
| 33:CJ:83:HIS:CD2    | 33:CJ:86:ASP:O      | 2.67                     | 0.47              |
| 33:CJ:769:GLN:HG3   | 48:Ci:12:VAL:HG22   | 1.97                     | 0.47              |
| 34:CK:307:PHE:CE1   | 42:CU:61:ILE:HD12   | 2.50                     | 0.47              |
| 39:CQ:66:VAL:O      | 39:CQ:67:LEU:HB2    | 2.14                     | 0.47              |
| 40:CR:47:ALA:HA     | 45:Cb:67:GLN:HE22   | 1.80                     | 0.47              |
| 43:CZ:243:THR:HG21  | 43:CZ:245:LYS:HE3   | 1.97                     | 0.47              |
| 44:Ca:46:ARG:HH11   | 44:Ca:46:ARG:HG3    | 1.80                     | 0.47              |
| 49:Cj:66:LEU:HD23   | 49:Cj:66:LEU:HA     | 1.83                     | 0.47              |
| 50:Ck:115:PRO:HB2   | 50:Ck:120:CYS:SG    | 2.55                     | 0.47              |
| 50:Ck:638:ARG:HG3   | 50:Ck:638:ARG:NH1   | 2.28                     | 0.47              |
| 55:Cr:25:LEU:HD13   | 55:Cr:83:VAL:HG22   | 1.97                     | 0.47              |
| 63:UT:6:UNK:O       | 63:UT:38:UNK:HG1    | 2.14                     | 0.47              |
| 68:A4:109:ARG:HA    | 132:Bd:132:ILE:HD11 | 1.96                     | 0.47              |
| 69:A5:51:MET:CE     | 103:BA:752:ARG:HH21 | 2.27                     | 0.47              |
| 75:AI:75:GLU:OE1    | 75:AI:75:GLU:N      | 2.40                     | 0.47              |
| 75:AI:137:VAL:HG22  | 127:BY:138:VAL:HB   | 1.95                     | 0.47              |
| 78:AN:54:LEU:HD13   | 78:AN:133:PHE:CE2   | 2.49                     | 0.47              |
| 86:AX:184:ASN:HB2   | 86:AX:219:ASP:OD2   | 2.15                     | 0.47              |
| 88:Ab:327:ILE:HD13  | 88:Ab:396:ILE:HG13  | 1.96                     | 0.47              |
| 89:Ad:214:TRP:HE3   | 132:Bd:52:ARG:HB3   | 1.80                     | 0.47              |
| 94:Al:38:PRO:HA     | 94:Al:41:VAL:HG22   | 1.96                     | 0.47              |
| 102:AA:2:U:H4'      | 103:BA:755:LYS:HE2  | 1.97                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 102:AA:564:A:O2'    | 102:AA:565:U:H5''   | 2.15                     | 0.47              |
| 103:BA:130:PRO:HB3  | 117:BO:145:LEU:HD21 | 1.97                     | 0.47              |
| 104:BB:102:ILE:HD11 | 104:BB:126:ALA:HB1  | 1.97                     | 0.47              |
| 108:BF:60:LEU:CA    | 108:BF:63:ARG:HH11  | 2.27                     | 0.47              |
| 116:BN:23:GLY:H     | 116:BN:191:ARG:HH22 | 1.62                     | 0.47              |
| 120:BR:64:ARG:HA    | 120:BR:83:ARG:HH11  | 1.80                     | 0.47              |
| 122:BT:174:ILE:H    | 122:BT:174:ILE:HG13 | 1.48                     | 0.47              |
| 126:BX:155:ARG:HH11 | 126:BX:158:THR:CG2  | 2.27                     | 0.47              |
| 136:Bh:3:LEU:HG     | 136:Bh:67:THR:HG22  | 1.97                     | 0.47              |
| 1:DA:151:PRO:CG     | 2:DD:280:LEU:HD21   | 2.44                     | 0.47              |
| 1:DA:791:THR:HA     | 1:DA:794:ARG:NH2    | 2.30                     | 0.47              |
| 1:DA:1580:ASN:O     | 1:DA:1584:GLN:HG3   | 2.14                     | 0.47              |
| 2:DD:448:ARG:HH11   | 2:DD:448:ARG:HG3    | 1.81                     | 0.47              |
| 12:DU:80:LEU:HB2    | 12:DU:103:ILE:HD12  | 1.97                     | 0.47              |
| 14:Da:46:ARG:HD2    | 57:CA:362:A:C6      | 2.50                     | 0.47              |
| 15:DB:521:LEU:HD21  | 15:DB:662:ARG:NH1   | 2.30                     | 0.47              |
| 15:DB:548:ALA:HB1   | 15:DB:553:LEU:O     | 2.15                     | 0.47              |
| 18:DF:426:LEU:CA    | 20:DH:200:THR:CG2   | 2.93                     | 0.47              |
| 24:DV:25:SER:OG     | 24:DV:29:PHE:HZ     | 1.98                     | 0.47              |
| 32:CI:265:ASP:HB3   | 32:CI:267:TYR:CE1   | 2.50                     | 0.47              |
| 34:CK:304:VAL:HG12  | 42:CU:48:VAL:HG21   | 1.97                     | 0.47              |
| 37:CO:359:HIS:CE1   | 37:CO:366:ARG:HH12  | 2.32                     | 0.47              |
| 45:Cb:97:GLU:O      | 45:Cb:101:LYS:HG3   | 2.15                     | 0.47              |
| 47:Cg:427:TRP:CE2   | 47:Cg:434:SER:HB3   | 2.50                     | 0.47              |
| 49:Cj:28:LYS:HB3    | 49:Cj:28:LYS:HZ3    | 1.79                     | 0.47              |
| 56:Cv:718:THR:OG1   | 56:Cv:719:THR:N     | 2.48                     | 0.47              |
| 56:Cv:922:ASP:OD2   | 56:Cv:924:SER:OG    | 2.32                     | 0.47              |
| 64:A0:71:ARG:HH11   | 94:Al:45:ILE:HD11   | 1.80                     | 0.47              |
| 66:A2:271:PRO:HG3   | 113:BK:324:LYS:CD   | 2.44                     | 0.47              |
| 74:AF:446:LYS:HB2   | 79:AP:274:PHE:CD2   | 2.49                     | 0.47              |
| 81:AR:94:ARG:HG2    | 81:AR:144:ALA:HB3   | 1.96                     | 0.47              |
| 81:AR:247:ASP:OD1   | 81:AR:247:ASP:N     | 2.47                     | 0.47              |
| 84:AV:193:GLY:O     | 84:AV:194:GLU:HG3   | 2.15                     | 0.47              |
| 89:Ad:196:ARG:NH1   | 132:Bd:64:GLU:HA    | 2.30                     | 0.47              |
| 93:Aj:62:HIS:ND1    | 93:Aj:63:PRO:HD2    | 2.30                     | 0.47              |
| 97:At:116:GLN:NE2   | 97:At:118:THR:HB    | 2.30                     | 0.47              |
| 102:AA:419:U:C4     | 124:BV:118:TYR:HD1  | 2.33                     | 0.47              |
| 103:BA:800:TRP:CE3  | 103:BA:803:LEU:HD12 | 2.49                     | 0.47              |
| 104:BB:209:ARG:NH1  | 126:BX:122:CYS:O    | 2.47                     | 0.47              |
| 104:BB:258:PHE:CZ   | 104:BB:372:CYS:HB3  | 2.49                     | 0.47              |
| 107:BE:409:GLU:OE2  | 107:BE:412:ASN:HA   | 2.16                     | 0.47              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 109:BG:345:MET:O   | 109:BG:349:MET:HG2   | 2.15                     | 0.47              |
| 119:BQ:114:PRO:HA  | 119:BQ:138:ASN:O     | 2.15                     | 0.47              |
| 121:BS:71:TRP:N    | 121:BS:75:GLN:OE1    | 2.48                     | 0.47              |
| 1:DA:224:VAL:HG11  | 1:DA:287:HIS:HB3     | 1.97                     | 0.46              |
| 1:DA:324:GLN:HE21  | 44:Ca:68:SER:HB3     | 1.80                     | 0.46              |
| 9:DQ:16:LEU:HD21   | 37:CO:404:PRO:O      | 2.14                     | 0.46              |
| 11:DS:57:LEU:HD21  | 11:DS:83:LEU:HD21    | 1.98                     | 0.46              |
| 16:DC:1159:ASP:OD1 | 16:DC:1159:ASP:N     | 2.48                     | 0.46              |
| 17:DE:280:LEU:HD22 | 17:DE:413:GLU:OE2    | 2.15                     | 0.46              |
| 17:DE:554:LEU:HD12 | 17:DE:554:LEU:HA     | 1.71                     | 0.46              |
| 22:DK:167:THR:HG22 | 22:DK:168:PRO:HD2    | 1.97                     | 0.46              |
| 23:DT:43:ASP:H     | 23:DT:218:MET:HE1    | 1.80                     | 0.46              |
| 25:DW:103:PRO:O    | 27:DY:90:GLN:NE2     | 2.48                     | 0.46              |
| 26:DX:94:GLY:HA2   | 47:Cg:187:TRP:CE2    | 2.50                     | 0.46              |
| 33:CJ:382:PHE:CD1  | 41:CS:48:ARG:HB2     | 2.50                     | 0.46              |
| 44:Ca:229:GLU:O    | 44:Ca:232:GLN:HB2    | 2.15                     | 0.46              |
| 50:Ck:268:LEU:O    | 50:Ck:273:SER:HB2    | 2.15                     | 0.46              |
| 53:Cp:133:PHE:CE2  | 53:Cp:142:VAL:HG13   | 2.50                     | 0.46              |
| 64:A0:49:GLN:HE21  | 64:A0:64:TYR:HB2     | 1.78                     | 0.46              |
| 65:A1:201:LEU:HD11 | 65:A1:211:LEU:HD22   | 1.97                     | 0.46              |
| 75:AI:45:ARG:O     | 75:AI:49:THR:OG1     | 2.32                     | 0.46              |
| 76:AJ:55:ARG:NH1   | 76:AJ:55:ARG:HB2     | 2.30                     | 0.46              |
| 80:AQ:78:SER:HB3   | 102:AA:418:G:OP2     | 2.15                     | 0.46              |
| 81:AR:62:SER:O     | 81:AR:65:HIS:N       | 2.48                     | 0.46              |
| 85:AW:120:GLU:O    | 85:AW:124:THR:HG23   | 2.14                     | 0.46              |
| 86:AX:61:ILE:HG13  | 98:Av:33:ILE:HA      | 1.97                     | 0.46              |
| 102:AA:518:A:N6    | 140:UD:18:UNK:HG2    | 2.30                     | 0.46              |
| 103:BA:627:SER:HB2 | 103:BA:632:GLU:OE2   | 2.15                     | 0.46              |
| 104:BB:215:ARG:NH1 | 104:BB:221:TYR:HB2   | 2.30                     | 0.46              |
| 113:BK:325:ASP:OD1 | 113:BK:325:ASP:N     | 2.48                     | 0.46              |
| 115:BM:212:ARG:CZ  | 115:BM:222:ARG:HG2   | 2.43                     | 0.46              |
| 127:BY:79(A):ALA:O | 127:BY:79(H):HIS:ND1 | 2.48                     | 0.46              |
| 133:Be:21:ARG:HG2  | 133:Be:21:ARG:NH1    | 2.27                     | 0.46              |
| 133:Be:30:PRO:O    | 133:Be:40:HIS:NE2    | 2.43                     | 0.46              |
| 1:DA:1386:ASP:HB3  | 29:CE:339:LEU:HD21   | 1.97                     | 0.46              |
| 3:DI:404:TRP:HB3   | 56:Cv:212:ARG:NH1    | 2.29                     | 0.46              |
| 8:DP:206:TYR:CE1   | 8:DP:215:LEU:HD13    | 2.46                     | 0.46              |
| 12:DU:227:SER:HA   | 49:Cj:161:VAL:HG13   | 1.98                     | 0.46              |
| 15:DB:787:LEU:HB3  | 15:DB:788:PRO:HD2    | 1.98                     | 0.46              |
| 16:DC:653:LEU:HA   | 16:DC:653:LEU:HD12   | 1.75                     | 0.46              |
| 20:DH:1:MET:HB2    | 20:DH:1:MET:HE3      | 1.47                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 21:DJ:31:HIS:CD2   | 21:DJ:33:ASN:HB2    | 2.50                     | 0.46              |
| 22:DK:237:PRO:HG2  | 22:DK:240:SER:HB2   | 1.95                     | 0.46              |
| 22:DK:273:LEU:HD12 | 22:DK:273:LEU:HA    | 1.73                     | 0.46              |
| 23:DT:183:LEU:H    | 23:DT:219:GLN:NE2   | 2.13                     | 0.46              |
| 27:DY:54:PRO:HB2   | 27:DY:102:GLU:HG2   | 1.97                     | 0.46              |
| 35:CL:81:ARG:NH2   | 35:CL:130:PRO:HB3   | 2.30                     | 0.46              |
| 37:CO:122:VAL:HG22 | 37:CO:123:ASN:H     | 1.80                     | 0.46              |
| 37:CO:194:MET:HE2  | 37:CO:198:GLU:HB3   | 1.97                     | 0.46              |
| 37:CO:409:THR:HG22 | 57:CA:69:U:OP1      | 2.14                     | 0.46              |
| 42:CU:14:MET:SD    | 42:CU:20:MET:HE3    | 2.55                     | 0.46              |
| 44:Ca:367:ASN:OD1  | 56:Cv:954:ARG:NH2   | 2.47                     | 0.46              |
| 46:Cd:55:GLU:O     | 46:Cd:58:ARG:HB2    | 2.15                     | 0.46              |
| 50:Ck:167:PHE:CE2  | 50:Ck:235:GLY:HA2   | 2.46                     | 0.46              |
| 65:A1:107:GLY:O    | 65:A1:119:GLN:HA    | 2.16                     | 0.46              |
| 78:AN:185:LYS:HE3  | 78:AN:185:LYS:HB2   | 1.64                     | 0.46              |
| 79:AP:286:GLU:OE1  | 79:AP:368:LYS:HG2   | 2.15                     | 0.46              |
| 81:AR:115:LEU:HG   | 81:AR:125:VAL:HG22  | 1.98                     | 0.46              |
| 85:AW:96:TYR:CD2   | 85:AW:107:LYS:HD2   | 2.50                     | 0.46              |
| 86:AX:164:PRO:HG2  | 86:AX:167:MET:HG3   | 1.97                     | 0.46              |
| 87:AY:198:THR:HG22 | 87:AY:200:GLU:H     | 1.80                     | 0.46              |
| 92:Ag:239:ARG:O    | 92:Ag:242:GLU:HG3   | 2.15                     | 0.46              |
| 102:AA:45:U:H6     | 129:Ba:39:ASN:HD21  | 1.62                     | 0.46              |
| 104:BB:230:THR:HB  | 104:BB:232:VAL:HG22 | 1.97                     | 0.46              |
| 115:BM:62:GLU:HA   | 115:BM:65:HIS:HB2   | 1.97                     | 0.46              |
| 116:BN:72:PRO:HB3  | 116:BN:121:LEU:HD21 | 1.98                     | 0.46              |
| 119:BQ:48:GLU:HB2  | 119:BQ:165:ILE:HD11 | 1.97                     | 0.46              |
| 120:BR:22:VAL:HG13 | 120:BR:56:ALA:HB1   | 1.97                     | 0.46              |
| 121:BS:29:ASN:N    | 121:BS:29:ASN:HD22  | 2.13                     | 0.46              |
| 124:BV:60:MET:HE2  | 124:BV:60:MET:HA    | 1.96                     | 0.46              |
| 1:DA:1235:GLY:HA3  | 1:DA:1264:LYS:HD3   | 1.98                     | 0.46              |
| 2:DD:575:THR:HG23  | 10:DR:208:PHE:CZ    | 2.50                     | 0.46              |
| 2:DD:693:ASP:OD1   | 2:DD:694:ARG:N      | 2.49                     | 0.46              |
| 3:DI:52:GLU:OE2    | 3:DI:93:TRP:NE1     | 2.33                     | 0.46              |
| 4:DL:54:GLY:HA3    | 28:CC:55:ILE:HG13   | 1.97                     | 0.46              |
| 4:DL:71:GLU:OE2    | 44:Ca:243:THR:CG2   | 2.59                     | 0.46              |
| 4:DL:294:LEU:HD11  | 36:CN:133:HIS:HB2   | 1.97                     | 0.46              |
| 7:DO:69:GLU:HA     | 7:DO:72:GLU:HB3     | 1.97                     | 0.46              |
| 9:DQ:86:THR:HG22   | 9:DQ:90:LYS:HE3     | 1.97                     | 0.46              |
| 10:DR:185:ARG:NE   | 10:DR:189:GLU:OE2   | 2.46                     | 0.46              |
| 19:DG:372:LEU:O    | 19:DG:376:VAL:HG23  | 2.15                     | 0.46              |
| 31:CH:134:VAL:HG21 | 56:Cv:97:GLN:HA     | 1.97                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 33:CJ:160:GLU:HA    | 47:Cg:407:TYR:OH    | 2.15                     | 0.46              |
| 33:CJ:544:THR:CG2   | 33:CJ:551:ARG:C     | 2.76                     | 0.46              |
| 35:CL:120:ILE:HD11  | 62:US:46:UNK:HG1    | 1.98                     | 0.46              |
| 36:CN:127:LEU:HD23  | 36:CN:127:LEU:HA    | 1.74                     | 0.46              |
| 37:CO:285:ASP:OD1   | 37:CO:285:ASP:N     | 2.30                     | 0.46              |
| 39:CQ:104:LEU:HA    | 39:CQ:104:LEU:HD23  | 1.63                     | 0.46              |
| 40:CR:153:GLU:HA    | 56:Cv:183:LEU:HD23  | 1.97                     | 0.46              |
| 44:Ca:243:THR:HG22  | 44:Ca:245:GLU:H     | 1.80                     | 0.46              |
| 48:Ci:105:ARG:HD2   | 50:Ck:685:TYR:OH    | 2.16                     | 0.46              |
| 50:Ck:379:ALA:HB3   | 50:Ck:565:LEU:HD21  | 1.98                     | 0.46              |
| 64:A0:62:PRO:HG3    | 64:A0:77:TYR:CE1    | 2.51                     | 0.46              |
| 65:A1:97:ARG:NH2    | 143:U1:14:UNK:HB2   | 2.30                     | 0.46              |
| 71:A8:140:LEU:HD23  | 71:A8:140:LEU:HA    | 1.74                     | 0.46              |
| 74:AF:369:GLN:NE2   | 125:BW:35:GLN:HE22  | 2.13                     | 0.46              |
| 76:AJ:104:VAL:HG13  | 76:AJ:107:GLU:H     | 1.80                     | 0.46              |
| 78:AN:179:PRO:HB3   | 91:Af:63:PRO:HA     | 1.96                     | 0.46              |
| 92:Ag:239:ARG:NH1   | 102:AA:441:A:N6     | 2.62                     | 0.46              |
| 92:Ag:240:ARG:NH1   | 124:BV:141:ASP:OD1  | 2.49                     | 0.46              |
| 95:Ao:230:ARG:HA    | 95:Ao:231:PRO:HD3   | 1.69                     | 0.46              |
| 102:AA:89:U:H5'     | 102:AA:90:A:H5''    | 1.97                     | 0.46              |
| 103:BA:475:LEU:HD13 | 103:BA:670:CYS:HB2  | 1.97                     | 0.46              |
| 105:BC:337:VAL:CG1  | 105:BC:359:GLU:HG2  | 2.43                     | 0.46              |
| 109:BG:72:GLY:HA3   | 109:BG:107:TYR:CD2  | 2.50                     | 0.46              |
| 109:BG:172:THR:CG2  | 109:BG:324:TRP:HE1  | 2.21                     | 0.46              |
| 116:BN:14:HIS:HB3   | 136:Bh:92:TRP:CD1   | 2.50                     | 0.46              |
| 118:BP:107:VAL:HG12 | 118:BP:114:ARG:HH12 | 1.79                     | 0.46              |
| 118:BP:194:VAL:HG12 | 118:BP:196:ALA:H    | 1.79                     | 0.46              |
| 119:BQ:22:TYR:HB2   | 119:BQ:163:GLN:NE2  | 2.29                     | 0.46              |
| 130:Bb:104:LEU:HA   | 130:Bb:129:VAL:O    | 2.15                     | 0.46              |
| 1:DA:987:LEU:HD11   | 1:DA:1173:ALA:HB1   | 1.96                     | 0.46              |
| 1:DA:1187:ASP:C     | 1:DA:1188:GLU:O     | 2.58                     | 0.46              |
| 2:DD:22:ASP:OD1     | 2:DD:24:SER:OG      | 2.34                     | 0.46              |
| 7:DO:131:ASP:OD1    | 7:DO:132:ALA:N      | 2.44                     | 0.46              |
| 14:Da:16:GLY:HA3    | 14:Da:21:HIS:ND1    | 2.30                     | 0.46              |
| 14:Da:46:ARG:HD2    | 57:CA:362:A:N6      | 2.30                     | 0.46              |
| 15:DB:154:ARG:HA    | 15:DB:157:LEU:HB2   | 1.97                     | 0.46              |
| 17:DE:405:ILE:HD13  | 17:DE:405:ILE:HA    | 1.74                     | 0.46              |
| 18:DF:18:THR:HG21   | 21:DJ:274:SER:O     | 2.14                     | 0.46              |
| 25:DW:56:LEU:O      | 25:DW:58:ARG:NH1    | 2.43                     | 0.46              |
| 25:DW:162:PRO:HB2   | 47:Cg:22:TYR:CE1    | 2.50                     | 0.46              |
| 32:CI:313:ASP:O     | 32:CI:315:GLU:N     | 2.48                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 35:CL:112:ILE:HG22  | 60:UQ:19:UNK:HB2   | 1.97                     | 0.46              |
| 37:CO:182:ASN:HB2   | 46:Cd:146:ASN:OD1  | 2.15                     | 0.46              |
| 40:CR:254:TYR:CZ    | 47:Cg:473:ARG:HD2  | 2.50                     | 0.46              |
| 56:Cv:136:TRP:HB3   | 56:Cv:225:PRO:HA   | 1.98                     | 0.46              |
| 56:Cv:238:MET:HE2   | 56:Cv:238:MET:HB3  | 1.82                     | 0.46              |
| 69:A5:68:GLU:HB3    | 81:AR:150:LYS:HA   | 1.97                     | 0.46              |
| 71:A8:156:TRP:CZ3   | 71:A8:162:ARG:NH1  | 2.83                     | 0.46              |
| 74:AF:38:ARG:NH1    | 92:Ag:50:ARG:HH12  | 2.13                     | 0.46              |
| 76:AJ:58:ASN:ND2    | 76:AJ:60:GLU:HG2   | 2.30                     | 0.46              |
| 78:AN:98:TRP:CE2    | 111:BI:49:PRO:HB2  | 2.51                     | 0.46              |
| 89:Ad:165:GLU:HG3   | 89:Ad:166:PHE:H    | 1.79                     | 0.46              |
| 97:At:27:ARG:HA     | 97:At:30:GLU:HB2   | 1.98                     | 0.46              |
| 102:AA:564:A:N7     | 140:UD:21:UNK:HB2  | 2.30                     | 0.46              |
| 103:BA:471:SER:HB2  | 103:BA:657:PHE:CE1 | 2.51                     | 0.46              |
| 105:BC:339:ILE:HG22 | 105:BC:340:HIS:H   | 1.81                     | 0.46              |
| 105:BC:434:MET:HE2  | 105:BC:434:MET:HB3 | 1.88                     | 0.46              |
| 107:BE:78:HIS:ND1   | 107:BE:78:HIS:O    | 2.49                     | 0.46              |
| 128:BZ:92:ARG:HA    | 128:BZ:92:ARG:HD2  | 1.78                     | 0.46              |
| 140:UD:139:UNK:HG3  | 140:UD:144:UNK:HB2 | 1.98                     | 0.46              |
| 1:DA:1163:MET:HE2   | 5:DM:149:LEU:HD21  | 1.96                     | 0.46              |
| 2:DD:521:ASN:HD22   | 2:DD:521:ASN:HA    | 1.59                     | 0.46              |
| 5:DM:55:GLU:CD      | 5:DM:56:TRP:H      | 2.24                     | 0.46              |
| 9:DQ:255:PRO:HG3    | 9:DQ:260:HIS:HB2   | 1.97                     | 0.46              |
| 16:DC:582:ARG:O     | 16:DC:622:TYR:HA   | 2.15                     | 0.46              |
| 18:DF:502:ARG:HB2   | 18:DF:577:ALA:O    | 2.16                     | 0.46              |
| 20:DH:348:LYS:HG3   | 20:DH:348:LYS:O    | 2.15                     | 0.46              |
| 21:DJ:205:LYS:HD3   | 21:DJ:209:ARG:HH21 | 1.80                     | 0.46              |
| 22:DK:18:LEU:HD12   | 22:DK:18:LEU:HA    | 1.74                     | 0.46              |
| 22:DK:177:LYS:NZ    | 22:DK:230:ASP:OD2  | 2.30                     | 0.46              |
| 29:CE:48:ASN:N      | 29:CE:48:ASN:OD1   | 2.45                     | 0.46              |
| 33:CJ:463:MET:HE3   | 48:Ci:89:MET:HG2   | 1.98                     | 0.46              |
| 33:CJ:469:ASP:OD2   | 36:CN:56:SER:HB2   | 2.15                     | 0.46              |
| 42:CU:169:ASN:OD1   | 42:CU:169:ASN:N    | 2.46                     | 0.46              |
| 44:Ca:397:GLY:HA3   | 44:Ca:502:PHE:CZ   | 2.51                     | 0.46              |
| 44:Ca:579:VAL:HG23  | 57:CA:259:U:O2'    | 2.15                     | 0.46              |
| 48:Ci:122:MET:HE3   | 48:Ci:122:MET:HB3  | 1.58                     | 0.46              |
| 50:Ck:817:LEU:HD22  | 50:Ck:836:THR:HG22 | 1.97                     | 0.46              |
| 53:Cp:178:GLU:HA    | 53:Cp:181:ARG:HG3  | 1.97                     | 0.46              |
| 63:UT:39:UNK:HA     | 63:UT:42:UNK:HB2   | 1.97                     | 0.46              |
| 73:AE:50:ARG:HH22   | 111:BI:41:PHE:HA   | 1.80                     | 0.46              |
| 74:AF:262:ASP:OD1   | 74:AF:264:ARG:HD3  | 2.15                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 74:AF:273:MET:HE2  | 74:AF:304:PRO:HA    | 1.98                     | 0.46              |
| 79:AP:11:TYR:HD2   | 79:AP:12:ARG:NH1    | 2.13                     | 0.46              |
| 81:AR:63:PRO:HG2   | 140:UD:5:UNK:O      | 2.15                     | 0.46              |
| 84:AV:226:MET:SD   | 92:Ag:120:TYR:HD1   | 2.39                     | 0.46              |
| 88:Ab:436:GLU:H    | 88:Ab:436:GLU:CD    | 2.23                     | 0.46              |
| 97:At:44:LEU:HD12  | 97:At:44:LEU:HA     | 1.78                     | 0.46              |
| 98:Av:157:PHE:HD1  | 105:BC:457:ARG:HH21 | 1.62                     | 0.46              |
| 103:BA:328:VAL:O   | 103:BA:335:PRO:HD3  | 2.16                     | 0.46              |
| 107:BE:300:ARG:NH1 | 107:BE:323:TRP:HZ3  | 2.05                     | 0.46              |
| 107:BE:335:LYS:HG3 | 113:BK:212:GLN:HE21 | 1.79                     | 0.46              |
| 113:BK:382:TYR:CE1 | 135:Bg:70:PRO:HD2   | 2.50                     | 0.46              |
| 129:Ba:68:ASP:OD2  | 129:Ba:70:HIS:HB2   | 2.16                     | 0.46              |
| 1:DA:1249:HIS:CE1  | 1:DA:1255:VAL:HG12  | 2.50                     | 0.46              |
| 3:DI:186:ILE:HG23  | 3:DI:195:ILE:HG23   | 1.98                     | 0.46              |
| 5:DM:292:ASN:O     | 32:CI:208:HIS:NE2   | 2.46                     | 0.46              |
| 6:DN:114:GLY:CA    | 6:DN:130:ASN:OD1    | 2.63                     | 0.46              |
| 9:DQ:147:PRO:O     | 9:DQ:176:ARG:NH2    | 2.47                     | 0.46              |
| 14:Da:45:LYS:NZ    | 14:Da:46:ARG:HH22   | 2.14                     | 0.46              |
| 15:DB:131:GLU:HG3  | 15:DB:228:THR:HG23  | 1.98                     | 0.46              |
| 15:DB:209:GLN:NE2  | 17:DE:448:PRO:HG2   | 2.30                     | 0.46              |
| 15:DB:983:LEU:HD22 | 19:DG:84:LEU:HD21   | 1.98                     | 0.46              |
| 16:DC:211:LYS:HZ2  | 16:DC:439:ALA:HA    | 1.81                     | 0.46              |
| 18:DF:18:THR:CG2   | 21:DJ:274:SER:O     | 2.63                     | 0.46              |
| 19:DG:117:VAL:HG13 | 19:DG:145:VAL:CG1   | 2.45                     | 0.46              |
| 20:DH:295:ASP:OD1  | 20:DH:295:ASP:N     | 2.48                     | 0.46              |
| 20:DH:382:PHE:CD1  | 20:DH:382:PHE:N     | 2.84                     | 0.46              |
| 20:DH:558:GLU:O    | 20:DH:565:ASN:ND2   | 2.48                     | 0.46              |
| 29:CE:30:TYR:CE2   | 29:CE:206:LEU:HB2   | 2.51                     | 0.46              |
| 29:CE:373:ARG:HD3  | 29:CE:407:THR:HG22  | 1.97                     | 0.46              |
| 31:CH:201:ARG:HG2  | 31:CH:201:ARG:HH11  | 1.81                     | 0.46              |
| 32:CI:271:TYR:CE2  | 32:CI:275:LYS:HD3   | 2.50                     | 0.46              |
| 41:CS:122:PHE:CG   | 41:CS:123:PRO:HA    | 2.51                     | 0.46              |
| 50:Ck:195:GLN:HB3  | 50:Ck:217:ILE:HD13  | 1.97                     | 0.46              |
| 65:A1:114:LEU:HD23 | 65:A1:114:LEU:H     | 1.81                     | 0.46              |
| 66:A2:142:LYS:HG3  | 66:A2:325:TYR:CE1   | 2.45                     | 0.46              |
| 71:A8:59:THR:H     | 74:AF:318:ALA:HB2   | 1.79                     | 0.46              |
| 74:AF:385:LEU:HD13 | 125:BW:33:LEU:HB2   | 1.98                     | 0.46              |
| 75:AI:17:ARG:NE    | 129:Ba:104:ARG:NH1  | 2.63                     | 0.46              |
| 75:AI:17:ARG:HG2   | 129:Ba:104:ARG:HH12 | 1.80                     | 0.46              |
| 76:AJ:83:PHE:CD2   | 96:Ap:205:ARG:HD3   | 2.48                     | 0.46              |
| 79:AP:54:ARG:HB3   | 79:AP:63:LEU:HD21   | 1.98                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 89:Ad:39:GLN:NE2   | 98:Av:200:GLN:OE1   | 2.48                     | 0.46              |
| 96:Ap:71:GLY:HA2   | 96:Ap:90:TYR:HB3    | 1.97                     | 0.46              |
| 97:At:22:LEU:HD12  | 97:At:23:PRO:HD2    | 1.98                     | 0.46              |
| 102:AA:411:A:N7    | 102:AA:433:G:O2'    | 2.38                     | 0.46              |
| 102:AA:561:U:H5'   | 102:AA:562:G:OP2    | 2.16                     | 0.46              |
| 105:BC:459:THR:OG1 | 105:BC:460:ALA:N    | 2.48                     | 0.46              |
| 107:BE:88:ARG:HA   | 107:BE:91:ILE:HG13  | 1.97                     | 0.46              |
| 107:BE:335:LYS:HG3 | 113:BK:212:GLN:NE2  | 2.31                     | 0.46              |
| 115:BM:273:ASP:HA  | 115:BM:275:PHE:CE2  | 2.50                     | 0.46              |
| 120:BR:98:LEU:HD23 | 120:BR:179:ILE:HD13 | 1.98                     | 0.46              |
| 132:Bd:57:LEU:HD12 | 132:Bd:57:LEU:HA    | 1.80                     | 0.46              |
| 140:UD:52:UNK:HA   | 140:UD:55:UNK:HG3   | 1.96                     | 0.46              |
| 1:DA:1203:CYS:HB3  | 15:DB:994:THR:HG23  | 1.97                     | 0.46              |
| 1:DA:1225:HIS:CE1  | 1:DA:1310:LEU:HD11  | 2.50                     | 0.46              |
| 1:DA:1262:PHE:HE1  | 1:DA:1305:PRO:HD3   | 1.80                     | 0.46              |
| 2:DD:368:LEU:HD13  | 2:DD:591:SER:HB3    | 1.98                     | 0.46              |
| 7:DO:206:GLN:O     | 7:DO:210:ASN:HB2    | 2.16                     | 0.46              |
| 15:DB:92:HIS:CD2   | 15:DB:94:ASP:H      | 2.19                     | 0.46              |
| 15:DB:355:GLN:O    | 15:DB:359:ILE:HG13  | 2.15                     | 0.46              |
| 16:DC:888:LEU:HD23 | 16:DC:888:LEU:HA    | 1.83                     | 0.46              |
| 17:DE:312:LEU:HD23 | 17:DE:312:LEU:HA    | 1.78                     | 0.46              |
| 20:DH:460:LEU:H    | 20:DH:460:LEU:HG    | 1.21                     | 0.46              |
| 33:CJ:238:ILE:HD11 | 33:CJ:355:HIS:HA    | 1.98                     | 0.46              |
| 33:CJ:632:GLN:HB2  | 33:CJ:661:ARG:HB2   | 1.96                     | 0.46              |
| 34:CK:315:LEU:HD21 | 57:CA:316:A:C6      | 2.51                     | 0.46              |
| 44:Ca:189:GLU:OE1  | 44:Ca:189:GLU:N     | 2.31                     | 0.46              |
| 48:Ci:157:LEU:HD12 | 48:Ci:157:LEU:HA    | 1.77                     | 0.46              |
| 50:Ck:728:GLN:NE2  | 50:Ck:731:ARG:HH11  | 2.10                     | 0.46              |
| 53:Cp:11:GLN:HG2   | 57:CA:32:A:H62      | 1.80                     | 0.46              |
| 53:Cp:53:VAL:HG11  | 53:Cp:59:PHE:CD1    | 2.44                     | 0.46              |
| 63:UT:37:UNK:HA    | 63:UT:40:UNK:HB2    | 1.98                     | 0.46              |
| 66:A2:62:LYS:HE3   | 86:AX:143:GLU:OE2   | 2.16                     | 0.46              |
| 66:A2:192:TRP:CE2  | 66:A2:314:HIS:HD2   | 2.34                     | 0.46              |
| 66:A2:393:TRP:CD1  | 66:A2:455:PRO:HD3   | 2.51                     | 0.46              |
| 71:A8:66:ARG:HH21  | 71:A8:138:MET:HE3   | 1.81                     | 0.46              |
| 73:AE:171:VAL:HG13 | 73:AE:210:VAL:HG21  | 1.97                     | 0.46              |
| 74:AF:205:LYS:HD3  | 74:AF:207:TRP:CZ2   | 2.50                     | 0.46              |
| 74:AF:250:GLU:H    | 74:AF:250:GLU:CD    | 2.22                     | 0.46              |
| 75:AI:143:PHE:HE1  | 145:UL:8:UNK:CG     | 2.29                     | 0.46              |
| 80:AQ:57:MET:HG2   | 80:AQ:114:LYS:HG2   | 1.97                     | 0.46              |
| 83:AU:108:ARG:HG2  | 91:Af:87:PHE:CZ     | 2.51                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 83:AU:190:ASN:HB2  | 83:AU:193:GLU:OE2   | 2.16                     | 0.46              |
| 84:AV:202:GLY:HA2  | 84:AV:236:LEU:HD21  | 1.97                     | 0.46              |
| 85:AW:213:ASP:HB2  | 85:AW:223:LYS:HG3   | 1.96                     | 0.46              |
| 87:AY:128:ARG:NH2  | 87:AY:183:ASN:O     | 2.44                     | 0.46              |
| 93:Aj:177:ILE:HG22 | 93:Aj:186:TRP:CE3   | 2.51                     | 0.46              |
| 97:At:21:PRO:HG3   | 120:BR:118:GLN:HE21 | 1.81                     | 0.46              |
| 102:AA:1110:A:H2   | 102:AA:1111:A:C5    | 2.34                     | 0.46              |
| 105:BC:426:PRO:HB3 | 105:BC:505:ARG:HH11 | 1.81                     | 0.46              |
| 108:BF:275:SER:HA  | 108:BF:276:PRO:HD2  | 1.80                     | 0.46              |
| 110:BH:255:PHE:CD1 | 110:BH:255:PHE:N    | 2.84                     | 0.46              |
| 111:BI:46:LEU:HD11 | 111:BI:49:PRO:HD2   | 1.98                     | 0.46              |
| 111:BI:261:GLY:HA3 | 111:BI:266:GLU:HB3  | 1.98                     | 0.46              |
| 116:BN:87:GLU:O    | 116:BN:196:ARG:NH1  | 2.49                     | 0.46              |
| 118:BP:35:ASN:HA   | 118:BP:36:ARG:NH1   | 2.30                     | 0.46              |
| 124:BV:39:ALA:HA   | 124:BV:40:PRO:HD3   | 1.71                     | 0.46              |
| 2:DD:534:PHE:CE2   | 2:DD:536:PRO:HG3    | 2.51                     | 0.46              |
| 4:DL:61:VAL:HG21   | 33:CJ:29:PRO:HA     | 1.97                     | 0.46              |
| 7:DO:67:ARG:NH2    | 56:Cv:771:GLU:OE1   | 2.49                     | 0.46              |
| 7:DO:111:ARG:HD3   | 56:Cv:673:LEU:HD11  | 1.98                     | 0.46              |
| 8:DP:153:VAL:O     | 8:DP:156:GLU:HG3    | 2.16                     | 0.46              |
| 9:DQ:115:ILE:HD11  | 9:DQ:152:PHE:HZ     | 1.81                     | 0.46              |
| 14:Da:25:ARG:O     | 14:Da:28:ARG:HB3    | 2.16                     | 0.46              |
| 16:DC:632:LEU:HA   | 16:DC:632:LEU:HD23  | 1.75                     | 0.46              |
| 17:DE:282:ALA:O    | 17:DE:403:PRO:HB3   | 2.15                     | 0.46              |
| 18:DF:421:ALA:HB1  | 18:DF:422:PRO:HD2   | 1.98                     | 0.46              |
| 26:DX:85:LYS:HB3   | 27:DY:163:LYS:HD3   | 1.98                     | 0.46              |
| 32:CI:105:THR:HG22 | 34:CK:108:ARG:O     | 2.16                     | 0.46              |
| 34:CK:315:LEU:HD12 | 34:CK:315:LEU:H     | 1.81                     | 0.46              |
| 36:CN:66:MET:HE2   | 36:CN:66:MET:HB2    | 1.61                     | 0.46              |
| 40:CR:94:MET:O     | 40:CR:98:ARG:HB2    | 2.16                     | 0.46              |
| 43:CZ:315:THR:HG22 | 43:CZ:319:ARG:HE    | 1.80                     | 0.46              |
| 44:Ca:538:ILE:HG12 | 44:Ca:539:GLN:N     | 2.31                     | 0.46              |
| 56:Cv:366:ALA:O    | 56:Cv:369:ARG:HB3   | 2.16                     | 0.46              |
| 65:A1:42:TRP:N     | 65:A1:42:TRP:CD1    | 2.83                     | 0.46              |
| 68:A4:156:PRO:HG3  | 89:Ad:232:PHE:CE1   | 2.51                     | 0.46              |
| 73:AE:353:GLU:H    | 73:AE:353:GLU:CD    | 2.24                     | 0.46              |
| 74:AF:187:VAL:HG11 | 74:AF:190:ARG:HD3   | 1.97                     | 0.46              |
| 75:AI:62:LEU:HA    | 75:AI:65:MET:HE3    | 1.98                     | 0.46              |
| 75:AI:207:PHE:CE2  | 110:BH:153:ARG:HB3  | 2.51                     | 0.46              |
| 81:AR:229:HIS:CE1  | 107:BE:415:TYR:HE1  | 2.33                     | 0.46              |
| 86:AX:94:ILE:HD12  | 90:Ae:94:MET:HE2    | 1.98                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 86:AX:152:LEU:HD23  | 86:AX:152:LEU:HA    | 1.86                     | 0.46              |
| 87:AY:300:LEU:HD23  | 87:AY:300:LEU:HA    | 1.78                     | 0.46              |
| 88:Ab:113:SER:HB3   | 105:BC:244:TRP:HE3  | 1.79                     | 0.46              |
| 89:Ad:267:ARG:HD2   | 89:Ad:269:ARG:HD2   | 1.97                     | 0.46              |
| 98:Av:56:TYR:O      | 98:Av:59:SER:HB3    | 2.16                     | 0.46              |
| 108:BF:259:LEU:HD23 | 108:BF:259:LEU:HA   | 1.78                     | 0.46              |
| 111:BI:26:ASN:ND2   | 111:BI:29:TRP:HD1   | 2.13                     | 0.46              |
| 116:BN:112:GLU:HB2  | 116:BN:123:PHE:HE2  | 1.80                     | 0.46              |
| 119:BQ:122:ALA:HA   | 119:BQ:160:VAL:HB   | 1.98                     | 0.46              |
| 121:BS:84:VAL:HG13  | 121:BS:96:MET:HG3   | 1.97                     | 0.46              |
| 126:BX:160:TYR:O    | 140:UD:41:UNK:HG1   | 2.16                     | 0.46              |
| 128:BZ:113:SER:OG   | 128:BZ:147:ASN:O    | 2.33                     | 0.46              |
| 129:Ba:150:ASP:HA   | 129:Ba:152:ARG:HH11 | 1.81                     | 0.46              |
| 140:UD:51:UNK:HG3   | 140:UD:148:UNK:HG1  | 1.98                     | 0.46              |
| 1:DA:523:LEU:HD13   | 1:DA:719:ILE:HD12   | 1.97                     | 0.46              |
| 1:DA:872:LYS:HD3    | 1:DA:872:LYS:HA     | 1.62                     | 0.46              |
| 2:DD:337:LEU:HD23   | 2:DD:337:LEU:HA     | 1.79                     | 0.46              |
| 2:DD:685:VAL:HG22   | 38:CP:100:LYS:HD2   | 1.97                     | 0.46              |
| 7:DO:131:ASP:HB3    | 7:DO:133:LYS:HG2    | 1.98                     | 0.46              |
| 9:DQ:146:GLN:HG3    | 9:DQ:176:ARG:HH12   | 1.81                     | 0.46              |
| 15:DB:867:THR:HG22  | 15:DB:868:HIS:N     | 2.31                     | 0.46              |
| 19:DG:64:ARG:HH21   | 40:CR:249:GLN:HE22  | 0.55                     | 0.46              |
| 19:DG:155:GLU:HB3   | 50:Ck:414:MET:HA    | 1.98                     | 0.46              |
| 19:DG:199:LEU:HD23  | 19:DG:199:LEU:HA    | 1.73                     | 0.46              |
| 21:DJ:22:MET:SD     | 28:CC:67:ASN:HB2    | 2.56                     | 0.46              |
| 28:CC:16:LEU:HD13   | 28:CC:18:LYS:HE3    | 1.97                     | 0.46              |
| 31:CH:186:HIS:HD2   | 56:Cv:240:ARG:HH21  | 1.64                     | 0.46              |
| 40:CR:320:VAL:C     | 46:Cd:281:MET:CE    | 2.80                     | 0.46              |
| 41:CS:75:MET:HE2    | 41:CS:75:MET:HB3    | 1.72                     | 0.46              |
| 45:Cb:168:ALA:O     | 45:Cb:171:THR:HG22  | 2.15                     | 0.46              |
| 46:Cd:185:PHE:CD2   | 46:Cd:193:ILE:HD12  | 2.50                     | 0.46              |
| 56:Cv:321:HIS:CD2   | 56:Cv:888:PRO:HG3   | 2.50                     | 0.46              |
| 56:Cv:395:LEU:HD21  | 56:Cv:421:LEU:HD12  | 1.97                     | 0.46              |
| 56:Cv:573:GLU:OE2   | 56:Cv:798:TYR:HA    | 2.16                     | 0.46              |
| 56:Cv:842:PHE:HB2   | 56:Cv:943:LEU:HD22  | 1.98                     | 0.46              |
| 57:CA:128:A:OP1     | 153:CA:738:SPM:H111 | 2.16                     | 0.46              |
| 66:A2:267:PRO:HA    | 66:A2:268:PRO:HD3   | 1.86                     | 0.46              |
| 71:A8:168:LEU:HD13  | 79:AP:165:ARG:HH11  | 1.81                     | 0.46              |
| 74:AF:253:LEU:HD23  | 74:AF:253:LEU:HA    | 1.82                     | 0.46              |
| 77:AK:134:ARG:HA    | 102:AA:405:U:H5''   | 1.97                     | 0.46              |
| 77:AK:267:THR:HG22  | 77:AK:270:ARG:NH2   | 2.31                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 85:AW:71:ILE:HG23   | 85:AW:74:LEU:HB2    | 1.98                     | 0.46              |
| 86:AX:96:ASN:ND2    | 129:Ba:29:LEU:HD22  | 2.30                     | 0.46              |
| 87:AY:285:MET:HE1   | 112:BJ:248:PRO:HG2  | 1.98                     | 0.46              |
| 89:Ad:245:ASP:CG    | 132:Bd:33:LYS:NZ    | 2.74                     | 0.46              |
| 109:BG:321:LEU:O    | 109:BG:325:MET:HG2  | 2.15                     | 0.46              |
| 129:Ba:141:TYR:HD1  | 129:Ba:141:TYR:HA   | 1.64                     | 0.46              |
| 134:Bf:44:ARG:HH11  | 141:UE:6:UNK:CA     | 2.23                     | 0.46              |
| 1:DA:205:HIS:ND1    | 38:CP:82:VAL:HG21   | 2.31                     | 0.46              |
| 1:DA:236:ARG:HH12   | 44:Ca:542:PRO:C     | 2.24                     | 0.46              |
| 2:DD:297:ARG:HH11   | 2:DD:297:ARG:HG3    | 1.81                     | 0.46              |
| 4:DL:47:GLN:HG3     | 4:DL:48:LYS:H       | 1.81                     | 0.46              |
| 5:DM:274:LEU:O      | 5:DM:278:THR:HG22   | 2.16                     | 0.46              |
| 7:DO:67:ARG:HH11    | 56:Cv:780:PRO:HG3   | 1.80                     | 0.46              |
| 9:DQ:73:HIS:ND1     | 9:DQ:250:ARG:HB2    | 2.31                     | 0.46              |
| 10:DR:96:PHE:HE1    | 10:DR:128:PRO:CD    | 2.27                     | 0.46              |
| 12:DU:147:LEU:CD2   | 12:DU:152:ILE:CD1   | 2.92                     | 0.46              |
| 16:DC:614:LEU:HB2   | 16:DC:817:ASP:HA    | 1.98                     | 0.46              |
| 17:DE:181:LEU:HD23  | 17:DE:181:LEU:HA    | 1.75                     | 0.46              |
| 33:CJ:381:SER:OG    | 33:CJ:384:GLU:HB3   | 2.16                     | 0.46              |
| 35:CL:81:ARG:NH1    | 56:Cv:29:LEU:HD11   | 2.31                     | 0.46              |
| 44:Ca:427:TRP:CE3   | 46:Cd:53:GLN:HB2    | 2.51                     | 0.46              |
| 44:Ca:588:LYS:O     | 57:CA:261:U:H5      | 1.98                     | 0.46              |
| 51:Cm:61:ARG:CZ     | 51:Cm:61:ARG:HB3    | 2.45                     | 0.46              |
| 52:Cn:151:THR:O     | 52:Cn:151:THR:OG1   | 2.32                     | 0.46              |
| 56:Cv:491:LEU:HB3   | 56:Cv:529:PHE:HB3   | 1.98                     | 0.46              |
| 56:Cv:808:SER:HB3   | 56:Cv:913:TRP:CE3   | 2.50                     | 0.46              |
| 61:UR:6:UNK:CG      | 61:UR:8:UNK:HG2     | 2.46                     | 0.46              |
| 65:A1:127:MET:O     | 65:A1:130:VAL:HG12  | 2.16                     | 0.46              |
| 66:A2:192:TRP:CD2   | 66:A2:314:HIS:HD2   | 2.34                     | 0.46              |
| 71:A8:61:TYR:HE2    | 71:A8:63:ALA:HB3    | 1.81                     | 0.46              |
| 73:AE:152:ASP:OD1   | 73:AE:156:ASN:HB2   | 2.15                     | 0.46              |
| 73:AE:169:GLN:HA    | 73:AE:231:THR:O     | 2.16                     | 0.46              |
| 78:AN:29:TYR:HA     | 78:AN:32:MET:HB2    | 1.98                     | 0.46              |
| 79:AP:11:TYR:CD2    | 79:AP:12:ARG:NH1    | 2.83                     | 0.46              |
| 79:AP:190:ASN:ND2   | 125:BW:100:GLN:OE1  | 2.37                     | 0.46              |
| 79:AP:283:ARG:HH21  | 102:AA:167:U:H5'    | 1.80                     | 0.46              |
| 84:AV:106:ILE:H     | 84:AV:106:ILE:HG13  | 1.48                     | 0.46              |
| 89:Ad:145:PRO:HA    | 89:Ad:148:ARG:NH1   | 2.31                     | 0.46              |
| 94:Al:150:VAL:HG21  | 94:Al:203:LEU:HD23  | 1.97                     | 0.46              |
| 102:AA:1:A:O2'      | 102:AA:2:U:H2'      | 2.16                     | 0.46              |
| 104:BB:111:ILE:HG21 | 112:BJ:196:THR:HG22 | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 112:BJ:267:GLU:CD  | 112:BJ:270:ARG:NH1 | 2.74                     | 0.46              |
| 123:BU:131:LYS:HB2 | 123:BU:131:LYS:NZ  | 2.31                     | 0.46              |
| 136:Bh:49:MET:HB2  | 136:Bh:61:PRO:HG3  | 1.98                     | 0.46              |
| 1:DA:43:TYR:HB3    | 2:DD:95:ARG:HA     | 1.97                     | 0.45              |
| 1:DA:164:TRP:CZ3   | 2:DD:201:GLU:HG2   | 2.51                     | 0.45              |
| 2:DD:37:LEU:HD22   | 2:DD:42:MET:HG3    | 1.97                     | 0.45              |
| 2:DD:226:THR:HG23  | 38:CP:188:LEU:HD13 | 1.97                     | 0.45              |
| 2:DD:247:VAL:HG22  | 12:DU:35:PRO:HD3   | 1.98                     | 0.45              |
| 2:DD:700:ASP:HB3   | 2:DD:704:ASP:OD1   | 2.16                     | 0.45              |
| 3:DI:50:LEU:HD12   | 3:DI:50:LEU:HA     | 1.75                     | 0.45              |
| 10:DR:26:ASN:CG    | 49:Cj:37:ARG:NH1   | 2.74                     | 0.45              |
| 15:DB:285:MET:HE2  | 50:Ck:36:ARG:HH21  | 1.80                     | 0.45              |
| 15:DB:569:HIS:CE1  | 15:DB:648:ARG:NH1  | 2.84                     | 0.45              |
| 15:DB:680:VAL:HA   | 15:DB:681:PRO:HD2  | 1.78                     | 0.45              |
| 15:DB:800:GLN:HA   | 15:DB:805:GLU:O    | 2.16                     | 0.45              |
| 19:DG:70:TYR:HB3   | 19:DG:90:MET:CE    | 2.46                     | 0.45              |
| 19:DG:577:LEU:HD21 | 19:DG:605:VAL:HG23 | 1.97                     | 0.45              |
| 20:DH:452:ARG:HA   | 20:DH:453:PRO:HD3  | 1.86                     | 0.45              |
| 21:DJ:177:TRP:CZ2  | 21:DJ:178:ARG:HG2  | 2.50                     | 0.45              |
| 21:DJ:223:MET:HE2  | 21:DJ:223:MET:HB3  | 1.71                     | 0.45              |
| 29:CE:173:LYS:HD2  | 45:Cb:45:PHE:CZ    | 2.51                     | 0.45              |
| 31:CH:229:GLU:HG2  | 31:CH:276:ARG:CD   | 2.45                     | 0.45              |
| 33:CJ:27:PRO:HB2   | 51:Cm:28:GLN:HE22  | 1.81                     | 0.45              |
| 34:CK:280:ARG:HD3  | 34:CK:308:GLU:OE2  | 2.15                     | 0.45              |
| 36:CN:108:VAL:HA   | 36:CN:109:PRO:HD3  | 1.72                     | 0.45              |
| 40:CR:138:ARG:HG3  | 40:CR:179:TRP:CG   | 2.51                     | 0.45              |
| 40:CR:209:ALA:O    | 40:CR:213:VAL:HG23 | 2.16                     | 0.45              |
| 45:Cb:288:GLU:HA   | 45:Cb:291:GLU:OE1  | 2.15                     | 0.45              |
| 49:Cj:53:ASN:O     | 49:Cj:55:ARG:N     | 2.49                     | 0.45              |
| 53:Cp:61:GLU:OE2   | 53:Cp:75:LYS:NZ    | 2.48                     | 0.45              |
| 56:Cv:922:ASP:HB3  | 56:Cv:925:ASP:OD2  | 2.16                     | 0.45              |
| 65:A1:71:GLN:HG2   | 129:Ba:98:TRP:CE2  | 2.51                     | 0.45              |
| 66:A2:282:TYR:HB3  | 66:A2:466:VAL:HG13 | 1.98                     | 0.45              |
| 71:A8:61:TYR:CE2   | 71:A8:63:ALA:HB3   | 2.51                     | 0.45              |
| 73:AE:57:TYR:OH    | 96:Ap:83:HIS:HE1   | 1.99                     | 0.45              |
| 77:AK:249:PRO:HG3  | 77:AK:309:VAL:HG12 | 1.97                     | 0.45              |
| 77:AK:264:LEU:HA   | 77:AK:264:LEU:HD23 | 1.68                     | 0.45              |
| 78:AN:121:MET:HE2  | 78:AN:121:MET:HB2  | 1.74                     | 0.45              |
| 79:AP:135:ARG:O    | 79:AP:136:VAL:HG23 | 2.17                     | 0.45              |
| 88:Ab:168:PHE:CE1  | 88:Ab:219:PRO:HG3  | 2.51                     | 0.45              |
| 95:Ao:231:PRO:HA   | 95:Ao:233:TRP:CZ3  | 2.51                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 96:Ap:175:LEU:HB2   | 96:Ap:215:PRO:HD2   | 1.98                     | 0.45              |
| 98:Av:68:ARG:HG2    | 154:Av:301:NAD:N7N  | 2.31                     | 0.45              |
| 102:AA:78:U:OP2     | 122:BT:63:THR:HG21  | 2.15                     | 0.45              |
| 102:AA:558:U:O2'    | 102:AA:559:A:O4'    | 2.25                     | 0.45              |
| 103:BA:263:SER:HA   | 103:BA:264:PRO:HD2  | 1.82                     | 0.45              |
| 103:BA:339:ASP:OD1  | 103:BA:339:ASP:N    | 2.37                     | 0.45              |
| 104:BB:165:THR:HG23 | 104:BB:238:ASN:HB3  | 1.97                     | 0.45              |
| 105:BC:463:ARG:HG3  | 105:BC:463:ARG:NH1  | 2.30                     | 0.45              |
| 108:BF:415:PHE:O    | 108:BF:419:VAL:HG23 | 2.16                     | 0.45              |
| 111:BI:260:TRP:CD1  | 111:BI:266:GLU:O    | 2.70                     | 0.45              |
| 114:BL:104:TRP:HE3  | 114:BL:171:SER:HB3  | 1.80                     | 0.45              |
| 124:BV:31:GLN:NE2   | 124:BV:33:TYR:O     | 2.49                     | 0.45              |
| 1:DA:1020:MET:HE3   | 1:DA:1020:MET:HB3   | 1.73                     | 0.45              |
| 4:DL:202:ARG:NH1    | 4:DL:203:ARG:HG3    | 2.31                     | 0.45              |
| 7:DO:70:ILE:O       | 7:DO:73:LEU:HD23    | 2.17                     | 0.45              |
| 12:DU:64:TYR:CE1    | 37:CO:330:THR:HG23  | 2.51                     | 0.45              |
| 16:DC:396:ILE:HG23  | 16:DC:402:VAL:HG11  | 1.98                     | 0.45              |
| 17:DE:248:THR:O     | 17:DE:252:ASP:HB2   | 2.16                     | 0.45              |
| 17:DE:524:PHE:N     | 17:DE:524:PHE:CD1   | 2.84                     | 0.45              |
| 18:DF:476:LEU:HD12  | 18:DF:476:LEU:HA    | 1.81                     | 0.45              |
| 24:DV:114:VAL:HG11  | 24:DV:118:GLN:HB3   | 1.99                     | 0.45              |
| 25:DW:60:VAL:CG1    | 27:DY:110:THR:HG21  | 2.46                     | 0.45              |
| 25:DW:113:PRO:CG    | 40:CR:289:THR:CG2   | 2.93                     | 0.45              |
| 27:DY:37:ARG:NH2    | 27:DY:106:GLN:NE2   | 2.63                     | 0.45              |
| 30:CF:47:PRO:HD2    | 30:CF:60:THR:O      | 2.16                     | 0.45              |
| 31:CH:107:ARG:HH22  | 31:CH:132:ASP:CG    | 2.24                     | 0.45              |
| 33:CJ:287:LEU:HD12  | 33:CJ:287:LEU:HA    | 1.64                     | 0.45              |
| 34:CK:179:LEU:HD23  | 34:CK:179:LEU:HA    | 1.79                     | 0.45              |
| 37:CO:114:ARG:NH1   | 37:CO:207:TYR:OH    | 2.50                     | 0.45              |
| 47:Cg:35:GLY:HA3    | 47:Cg:431:TRP:NE1   | 2.31                     | 0.45              |
| 49:Cj:141:GLY:C     | 49:Cj:143:LYS:H     | 2.23                     | 0.45              |
| 50:Ck:153:VAL:HG21  | 50:Ck:247:LEU:HB3   | 1.97                     | 0.45              |
| 50:Ck:775:ARG:CB    | 50:Ck:775:ARG:HH11  | 2.29                     | 0.45              |
| 52:Cn:214:ARG:H     | 52:Cn:214:ARG:HD3   | 1.81                     | 0.45              |
| 53:Cp:99:ARG:NH1    | 57:CA:187:A:H4'     | 2.31                     | 0.45              |
| 55:Cr:143:ARG:HE    | 55:Cr:143:ARG:HB3   | 1.53                     | 0.45              |
| 57:CA:504:U:H4'     | 57:CA:505:U:OP1     | 2.16                     | 0.45              |
| 65:A1:158:ARG:HA    | 65:A1:158:ARG:HD3   | 1.69                     | 0.45              |
| 66:A2:469:THR:O     | 108:BF:408:LEU:N    | 2.49                     | 0.45              |
| 74:AF:102:ILE:HD12  | 74:AF:103:VAL:N     | 2.31                     | 0.45              |
| 74:AF:271:LEU:HD12  | 74:AF:300:LYS:HB3   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:AK:48:ARG:HH12  | 96:Ap:213:PRO:HA   | 1.81                     | 0.45              |
| 77:AK:269:TRP:CE3  | 92:Ag:225:PRO:HG3  | 2.51                     | 0.45              |
| 78:AN:144:ARG:HH22 | 102:AA:123:U:H5    | 1.64                     | 0.45              |
| 81:AR:113:GLN:HE21 | 116:BN:209:LYS:NZ  | 2.14                     | 0.45              |
| 84:AV:113:LYS:HD2  | 95:Ao:84:ALA:HB3   | 1.98                     | 0.45              |
| 84:AV:180:TYR:CZ   | 84:AV:182:PRO:HB3  | 2.51                     | 0.45              |
| 85:AW:165:LYS:HB3  | 85:AW:165:LYS:HE2  | 1.68                     | 0.45              |
| 89:Ad:161:THR:HB   | 89:Ad:174:PHE:HZ   | 1.82                     | 0.45              |
| 104:BB:128:HIS:CD2 | 104:BB:132:GLU:OE2 | 2.70                     | 0.45              |
| 105:BC:289:ASN:HA  | 105:BC:479:HIS:HA  | 1.98                     | 0.45              |
| 110:BH:261:GLU:OE1 | 110:BH:261:GLU:N   | 2.49                     | 0.45              |
| 1:DA:108:TYR:OH    | 1:DA:123:HIS:HD2   | 2.00                     | 0.45              |
| 1:DA:565:ASN:HA    | 6:DN:144:ARG:HH12  | 1.80                     | 0.45              |
| 4:DL:84:GLU:C      | 32:CI:270:PHE:HZ   | 2.23                     | 0.45              |
| 5:DM:75:VAL:HG13   | 5:DM:79:VAL:HB     | 1.98                     | 0.45              |
| 8:DP:87:GLU:O      | 8:DP:92:LYS:NZ     | 2.48                     | 0.45              |
| 11:DS:49:VAL:HG23  | 44:Ca:598:ALA:HB1  | 1.98                     | 0.45              |
| 16:DC:704:HIS:NE2  | 22:DK:167:THR:HG21 | 2.32                     | 0.45              |
| 16:DC:960:VAL:HG21 | 17:DE:159:ALA:HB2  | 1.98                     | 0.45              |
| 19:DG:346:ARG:NH2  | 19:DG:497:ARG:HD3  | 2.32                     | 0.45              |
| 21:DJ:213:GLU:HB3  | 21:DJ:250:VAL:HG11 | 1.98                     | 0.45              |
| 24:DV:66:VAL:HG13  | 24:DV:71:GLN:HG2   | 1.97                     | 0.45              |
| 29:CE:356:SER:HB2  | 44:Ca:134:LEU:HD13 | 1.97                     | 0.45              |
| 36:CN:165:ARG:O    | 50:Ck:740:ARG:NH1  | 2.49                     | 0.45              |
| 38:CP:184:VAL:C    | 38:CP:188:LEU:HB3  | 2.41                     | 0.45              |
| 50:Ck:621:THR:HG21 | 50:Ck:623:LYS:HE3  | 1.98                     | 0.45              |
| 50:Ck:755:ASP:OD1  | 50:Ck:755:ASP:N    | 2.49                     | 0.45              |
| 54:Cq:79:MET:O     | 54:Cq:83:LEU:HB3   | 2.15                     | 0.45              |
| 54:Cq:85:HIS:NE2   | 54:Cq:129:HIS:HD2  | 2.14                     | 0.45              |
| 55:Cr:155:ALA:HA   | 55:Cr:158:ALA:HB2  | 1.98                     | 0.45              |
| 56:Cv:320:LEU:HD23 | 56:Cv:320:LEU:HA   | 1.76                     | 0.45              |
| 65:A1:146:PRO:HD3  | 129:Ba:97:TRP:HB2  | 1.97                     | 0.45              |
| 65:A1:198:GLU:HA   | 65:A1:201:LEU:HB2  | 1.97                     | 0.45              |
| 66:A2:189:GLU:HB2  | 66:A2:315:PRO:HG3  | 1.97                     | 0.45              |
| 66:A2:389:HIS:HD2  | 102:AA:32:U:C4     | 2.33                     | 0.45              |
| 69:A5:50:LYS:HE3   | 102:AA:1161:A:H5'  | 1.98                     | 0.45              |
| 70:A6:86:LYS:HB2   | 70:A6:86:LYS:NZ    | 2.31                     | 0.45              |
| 71:A8:118:GLN:OE1  | 88:Ab:457:ARG:NH1  | 2.50                     | 0.45              |
| 84:AV:211:VAL:HG22 | 92:Ag:125:ARG:HB2  | 1.99                     | 0.45              |
| 85:AW:71:ILE:HD13  | 85:AW:74:LEU:HD22  | 1.99                     | 0.45              |
| 92:Ag:55:MET:HE3   | 92:Ag:72:LYS:HE3   | 1.97                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 96:Ap:140:MET:HG3   | 141:UE:4:UNK:HG1    | 1.98                     | 0.45              |
| 104:BB:392:TYR:O    | 104:BB:395:GLU:HG3  | 2.16                     | 0.45              |
| 105:BC:134:CYS:HB3  | 105:BC:139:ALA:O    | 2.16                     | 0.45              |
| 105:BC:408:LEU:HD22 | 105:BC:420:VAL:HG11 | 1.97                     | 0.45              |
| 110:BH:125:THR:O    | 110:BH:166:VAL:HG22 | 2.15                     | 0.45              |
| 117:BO:78:ARG:HH11  | 121:BS:104:ARG:HH22 | 1.63                     | 0.45              |
| 136:Bh:9:CYS:SG     | 136:Bh:34:ARG:HD2   | 2.56                     | 0.45              |
| 146:UM:3:UNK:HG1    | 142:UN:2:UNK:C      | 2.47                     | 0.45              |
| 1:DA:225:GLY:H      | 1:DA:233:ARG:HD2    | 1.81                     | 0.45              |
| 1:DA:237:HIS:HE1    | 1:DA:310:ASP:HB2    | 1.81                     | 0.45              |
| 1:DA:647:ARG:HG2    | 1:DA:731:ALA:HB3    | 1.97                     | 0.45              |
| 2:DD:371:PRO:O      | 2:DD:560:ALA:HB3    | 2.16                     | 0.45              |
| 2:DD:654:ARG:NH1    | 49:Cj:15:ASN:HB2    | 2.31                     | 0.45              |
| 7:DO:132:ALA:O      | 7:DO:135:THR:HG22   | 2.17                     | 0.45              |
| 10:DR:105:THR:HG23  | 49:Cj:147:TYR:HE2   | 1.82                     | 0.45              |
| 15:DB:129:TYR:CD1   | 15:DB:129:TYR:C     | 2.94                     | 0.45              |
| 15:DB:562:GLN:HE22  | 18:DF:571:LEU:HA    | 1.82                     | 0.45              |
| 17:DE:147:MET:HE1   | 17:DE:567:HIS:CE1   | 2.52                     | 0.45              |
| 18:DF:38:GLY:H      | 18:DF:41:ASN:ND2    | 2.07                     | 0.45              |
| 18:DF:589:GLN:CD    | 20:DH:192:PHE:CE1   | 2.95                     | 0.45              |
| 21:DJ:139:LEU:HD22  | 21:DJ:143:TYR:HE2   | 1.81                     | 0.45              |
| 25:DW:22:THR:HG21   | 41:CS:149:ASP:O     | 2.16                     | 0.45              |
| 25:DW:127:PHE:HB2   | 40:CR:287:MET:SD    | 2.56                     | 0.45              |
| 38:CP:86:ARG:HH22   | 53:Cp:31:ALA:HB1    | 1.81                     | 0.45              |
| 40:CR:23:TRP:CE2    | 56:Cv:494:THR:HG21  | 2.52                     | 0.45              |
| 40:CR:320:VAL:O     | 46:Cd:278:ALA:O     | 2.34                     | 0.45              |
| 44:Ca:418:VAL:HG21  | 44:Ca:484:LYS:HG2   | 1.98                     | 0.45              |
| 50:Ck:682:ASN:H     | 50:Ck:682:ASN:ND2   | 2.13                     | 0.45              |
| 54:Cq:155:GLN:HA    | 54:Cq:166:ALA:HB2   | 1.98                     | 0.45              |
| 54:Cq:189:TYR:HB3   | 54:Cq:191:VAL:HG13  | 1.97                     | 0.45              |
| 55:Cr:143:ARG:HH12  | 55:Cr:148:TRP:N     | 2.15                     | 0.45              |
| 66:A2:314:HIS:CG    | 66:A2:315:PRO:HD2   | 2.51                     | 0.45              |
| 69:A5:57:CYS:SG     | 69:A5:60:CYS:SG     | 3.14                     | 0.45              |
| 71:A8:40:PRO:HD3    | 71:A8:41:LYS:HB2    | 1.98                     | 0.45              |
| 72:A9:68:LEU:HD23   | 72:A9:77:PHE:CE1    | 2.50                     | 0.45              |
| 75:AI:109:PRO:O     | 75:AI:111:ILE:HG13  | 2.16                     | 0.45              |
| 78:AN:53:GLN:HA     | 78:AN:92:VAL:O      | 2.17                     | 0.45              |
| 79:AP:310:HIS:CD2   | 79:AP:312:ALA:H     | 2.22                     | 0.45              |
| 80:AQ:162:GLU:HG3   | 120:BR:168:TRP:HH2  | 1.82                     | 0.45              |
| 85:AW:13:MET:HE2    | 85:AW:13:MET:HB3    | 1.84                     | 0.45              |
| 90:Ae:115:ASN:ND2   | 90:Ae:117:SER:OG    | 2.49                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 96:Ap:176:MET:HG2   | 96:Ap:177:HIS:ND1   | 2.31                     | 0.45              |
| 98:Av:67:GLY:O      | 98:Av:69:ARG:N      | 2.49                     | 0.45              |
| 102:AA:94:U:H2'     | 102:AA:95:U:C6      | 2.51                     | 0.45              |
| 103:BA:308:SER:O    | 103:BA:312:TRP:NE1  | 2.48                     | 0.45              |
| 104:BB:360:ASP:O    | 104:BB:364:VAL:HG13 | 2.17                     | 0.45              |
| 109:BG:100:LEU:HD23 | 109:BG:100:LEU:HA   | 1.78                     | 0.45              |
| 109:BG:336:LYS:HG2  | 109:BG:340:GLN:NE2  | 2.25                     | 0.45              |
| 110:BH:66:GLU:HB2   | 127:BY:85:TRP:CH2   | 2.52                     | 0.45              |
| 110:BH:194:ARG:HH12 | 110:BH:196:LEU:CD2  | 2.29                     | 0.45              |
| 115:BM:146:SER:O    | 115:BM:150:ILE:HG13 | 2.16                     | 0.45              |
| 122:BT:131:LEU:HD23 | 122:BT:131:LEU:H    | 1.81                     | 0.45              |
| 124:BV:47:ARG:HA    | 124:BV:50:ARG:NH1   | 2.31                     | 0.45              |
| 126:BX:134:LYS:HA   | 126:BX:134:LYS:HD2  | 1.73                     | 0.45              |
| 139:UH:3:UNK:HA     | 139:UH:7:UNK:HG1    | 1.99                     | 0.45              |
| 1:DA:84:PRO:HG3     | 2:DD:46:VAL:HG23    | 1.99                     | 0.45              |
| 1:DA:174:HIS:NE2    | 2:DD:685:VAL:O      | 2.49                     | 0.45              |
| 4:DL:194:ILE:HD12   | 40:CR:77:ILE:HD13   | 1.99                     | 0.45              |
| 7:DO:161:PHE:O      | 7:DO:198:ARG:NH2    | 2.49                     | 0.45              |
| 8:DP:188:ARG:HD3    | 8:DP:194:GLN:HG3    | 1.98                     | 0.45              |
| 9:DQ:152:PHE:CE1    | 9:DQ:168:VAL:HG22   | 2.51                     | 0.45              |
| 9:DQ:232:ASP:OD1    | 9:DQ:232:ASP:N      | 2.48                     | 0.45              |
| 12:DU:211:ARG:HA    | 12:DU:212:PRO:HD3   | 1.76                     | 0.45              |
| 16:DC:435:LEU:HD12  | 16:DC:435:LEU:HA    | 1.71                     | 0.45              |
| 19:DG:44:ARG:HB3    | 32:CI:253:LEU:HD11  | 1.98                     | 0.45              |
| 19:DG:67:ALA:HB2    | 19:DG:96:LYS:O      | 2.17                     | 0.45              |
| 22:DK:220:PRO:HG2   | 22:DK:223:ALA:HB2   | 1.97                     | 0.45              |
| 27:DY:37:ARG:HH21   | 27:DY:106:GLN:NE2   | 2.08                     | 0.45              |
| 32:CI:435:LYS:HG2   | 32:CI:436:VAL:HG23  | 1.97                     | 0.45              |
| 33:CJ:151:ASN:ND2   | 33:CJ:209:GLN:O     | 2.50                     | 0.45              |
| 34:CK:320:MET:HE1   | 42:CU:16:HIS:HA     | 1.97                     | 0.45              |
| 45:Cb:169:LYS:HZ2   | 45:Cb:176:THR:HG1   | 1.62                     | 0.45              |
| 50:Ck:622:LEU:HD12  | 50:Ck:622:LEU:HA    | 1.74                     | 0.45              |
| 51:Cm:175:LEU:HD11  | 56:Cv:54:ASN:HB2    | 1.99                     | 0.45              |
| 52:Cn:165:LEU:HA    | 52:Cn:165:LEU:HD23  | 1.72                     | 0.45              |
| 56:Cv:1010:SER:OG   | 56:Cv:1011:SER:N    | 2.50                     | 0.45              |
| 67:A3:86:ARG:HH12   | 67:A3:91:GLU:HG2    | 1.81                     | 0.45              |
| 68:A4:36:ASP:OD1    | 68:A4:36:ASP:N      | 2.46                     | 0.45              |
| 78:AN:121:MET:SD    | 78:AN:128:MET:HE2   | 2.56                     | 0.45              |
| 78:AN:131:TRP:CH2   | 78:AN:153:LEU:HB3   | 2.51                     | 0.45              |
| 83:AU:108:ARG:HH22  | 91:Af:81:ARG:HB3    | 1.82                     | 0.45              |
| 85:AW:129:PRO:HG3   | 107:BE:124:LEU:HD13 | 1.99                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 87:AY:42:THR:HG23   | 102:AA:102:A:C8    | 2.52                     | 0.45              |
| 87:AY:153:ILE:HG23  | 107:BE:79:VAL:HG21 | 1.98                     | 0.45              |
| 87:AY:181:SER:OG    | 87:AY:182:THR:N    | 2.49                     | 0.45              |
| 92:Ag:173:SER:HB3   | 92:Ag:224:VAL:HG21 | 1.99                     | 0.45              |
| 93:Aj:199:LEU:HD13  | 93:Aj:224:PRO:HG2  | 1.98                     | 0.45              |
| 102:AA:145:U:H2'    | 102:AA:146:A:H8    | 1.79                     | 0.45              |
| 103:BA:306:ASN:O    | 103:BA:310:ALA:HB2 | 2.16                     | 0.45              |
| 104:BB:141:ILE:HG12 | 104:BB:172:MET:HE2 | 1.97                     | 0.45              |
| 107:BE:66:ARG:HD2   | 113:BK:381:SER:HA  | 1.99                     | 0.45              |
| 108:BF:216:LEU:HD11 | 108:BF:220:ARG:CZ  | 2.46                     | 0.45              |
| 133:Be:31:ASN:HA    | 133:Be:32:PRO:HD3  | 1.63                     | 0.45              |
| 136:Bh:27:LEU:HD12  | 136:Bh:40:LEU:HD21 | 1.99                     | 0.45              |
| 1:DA:1038:HIS:CD2   | 1:DA:1045:ILE:HD11 | 2.51                     | 0.45              |
| 2:DD:20:PHE:HZ      | 29:CE:256:LEU:H    | 1.64                     | 0.45              |
| 3:DI:67:ILE:CD1     | 3:DI:80:ARG:HG2    | 2.47                     | 0.45              |
| 4:DL:88:LEU:HD21    | 32:CI:274:LEU:CD1  | 2.47                     | 0.45              |
| 6:DN:127:VAL:HG11   | 6:DN:160:CYS:SG    | 2.57                     | 0.45              |
| 7:DO:136:ASP:OD1    | 7:DO:137:ASN:N     | 2.49                     | 0.45              |
| 8:DP:120:ASP:O      | 8:DP:160:ARG:NH1   | 2.40                     | 0.45              |
| 10:DR:41:HIS:HA     | 10:DR:44:VAL:HG12  | 1.96                     | 0.45              |
| 11:DS:211:CYS:HB2   | 11:DS:214:CYS:H    | 1.82                     | 0.45              |
| 15:DB:550:LEU:HD12  | 15:DB:550:LEU:HA   | 1.74                     | 0.45              |
| 15:DB:852:TRP:HD1   | 15:DB:861:GLU:OE1  | 2.00                     | 0.45              |
| 16:DC:107:SER:OG    | 16:DC:544:GLU:OE1  | 2.31                     | 0.45              |
| 17:DE:186:ARG:NH1   | 17:DE:186:ARG:HA   | 2.31                     | 0.45              |
| 17:DE:601:ILE:HD12  | 17:DE:638:LEU:HD23 | 1.98                     | 0.45              |
| 18:DF:324:LEU:HD13  | 18:DF:332:GLU:HB2  | 1.98                     | 0.45              |
| 18:DF:549:PHE:CD1   | 18:DF:577:ALA:HB2  | 2.52                     | 0.45              |
| 19:DG:115:ILE:HG21  | 19:DG:120:VAL:HG23 | 1.99                     | 0.45              |
| 20:DH:66:ARG:HE     | 20:DH:102:LEU:HD21 | 1.81                     | 0.45              |
| 20:DH:252:LEU:HD23  | 20:DH:252:LEU:HA   | 1.82                     | 0.45              |
| 27:DY:32:TRP:O      | 27:DY:37:ARG:NH1   | 2.47                     | 0.45              |
| 27:DY:33:ALA:O      | 27:DY:38:MET:HE2   | 2.17                     | 0.45              |
| 38:CP:135:MET:HE2   | 38:CP:135:MET:HB3  | 1.79                     | 0.45              |
| 51:Cm:153:ASP:HB3   | 51:Cm:157:LYS:HE3  | 1.98                     | 0.45              |
| 56:Cv:534:SER:O     | 56:Cv:534:SER:OG   | 2.27                     | 0.45              |
| 56:Cv:577:PHE:HD2   | 56:Cv:792:TYR:CE2  | 2.35                     | 0.45              |
| 57:CA:508:A:H4'     | 57:CA:509:U:OP2    | 2.17                     | 0.45              |
| 66:A2:391:PRO:HB3   | 102:AA:32:U:H5'    | 1.99                     | 0.45              |
| 74:AF:165:GLU:HG3   | 74:AF:167:ARG:H    | 1.82                     | 0.45              |
| 77:AK:185:ARG:HH22  | 124:BV:115:GLN:HA  | 1.80                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 85:AW:110:TRP:CH2   | 87:AY:33:LYS:HB2    | 2.52                     | 0.45              |
| 88:Ab:144:TYR:CD1   | 118:BP:74:GLU:HB3   | 2.52                     | 0.45              |
| 96:Ap:67:LEU:H      | 96:Ap:70:GLU:HG3    | 1.82                     | 0.45              |
| 102:AA:442:A:C8     | 115:BM:271:ARG:HD2  | 2.51                     | 0.45              |
| 105:BC:267:ILE:H    | 105:BC:267:ILE:HG13 | 1.74                     | 0.45              |
| 114:BL:75:LEU:HD23  | 114:BL:75:LEU:HA    | 1.76                     | 0.45              |
| 124:BV:95:ASP:HA    | 124:BV:96:PRO:HD3   | 1.88                     | 0.45              |
| 126:BX:69:ARG:HA    | 126:BX:70:PRO:HD2   | 1.87                     | 0.45              |
| 129:Ba:147:ASN:HD22 | 129:Ba:147:ASN:HA   | 1.58                     | 0.45              |
| 133:Be:43:SER:O     | 133:Be:47:GLU:HB2   | 2.16                     | 0.45              |
| 1:DA:150:ILE:HG23   | 1:DA:151:PRO:O      | 2.16                     | 0.45              |
| 1:DA:1651:GLU:HA    | 1:DA:1654:ARG:NH2   | 2.32                     | 0.45              |
| 4:DL:51:PHE:HB3     | 33:CJ:29:PRO:HD2    | 1.98                     | 0.45              |
| 6:DN:224:ARG:HH11   | 6:DN:224:ARG:CB     | 2.26                     | 0.45              |
| 8:DP:189:TYR:CD1    | 8:DP:196:TRP:C      | 2.95                     | 0.45              |
| 12:DU:147:LEU:HD23  | 12:DU:152:ILE:HD12  | 1.99                     | 0.45              |
| 18:DF:257:GLY:C     | 18:DF:265:SER:HB2   | 2.42                     | 0.45              |
| 19:DG:334:MET:HG3   | 19:DG:353:VAL:HG11  | 1.98                     | 0.45              |
| 29:CE:17:THR:HG21   | 44:Ca:560:PHE:CG    | 2.52                     | 0.45              |
| 30:CF:12:PRO:HG3    | 30:CF:62:ALA:HA     | 1.98                     | 0.45              |
| 30:CF:106:SER:O     | 56:Cv:187:PRO:HA    | 2.16                     | 0.45              |
| 32:CI:100:PRO:HD3   | 40:CR:96:GLN:HG3    | 1.98                     | 0.45              |
| 33:CJ:118:MET:HA    | 33:CJ:118:MET:HE2   | 1.99                     | 0.45              |
| 35:CL:98:TYR:CZ     | 62:US:40:UNK:HG2    | 2.52                     | 0.45              |
| 36:CN:166:ILE:HG23  | 50:Ck:762:PHE:HE2   | 1.82                     | 0.45              |
| 37:CO:206:MET:HE2   | 37:CO:210:ARG:HH21  | 1.82                     | 0.45              |
| 37:CO:267:ARG:HB3   | 37:CO:274:TYR:CD2   | 2.51                     | 0.45              |
| 40:CR:125:ASN:OD1   | 40:CR:125:ASN:N     | 2.49                     | 0.45              |
| 40:CR:137:THR:HG23  | 40:CR:139:THR:N     | 2.32                     | 0.45              |
| 44:Ca:38:TRP:CZ2    | 63:UT:25:UNK:HA     | 2.52                     | 0.45              |
| 44:Ca:76:GLN:HG3    | 56:Cv:1120:TRP:HZ2  | 1.80                     | 0.45              |
| 44:Ca:347:ARG:O     | 44:Ca:350:GLU:HG3   | 2.17                     | 0.45              |
| 44:Ca:538:ILE:HG12  | 44:Ca:539:GLN:H     | 1.82                     | 0.45              |
| 51:Cm:93:LEU:HD22   | 51:Cm:136:MET:HE1   | 1.99                     | 0.45              |
| 53:Cp:150:TYR:H     | 53:Cp:154:GLN:NE2   | 2.14                     | 0.45              |
| 56:Cv:227:PHE:O     | 56:Cv:302:GLY:HA2   | 2.17                     | 0.45              |
| 61:UR:1:UNK:O       | 61:UR:2:UNK:HG3     | 2.16                     | 0.45              |
| 66:A2:289:GLN:HB3   | 66:A2:295:ASN:O     | 2.17                     | 0.45              |
| 68:A4:154:CYS:HB2   | 89:Ad:228:GLN:HE22  | 1.82                     | 0.45              |
| 75:AI:70:ARG:HH11   | 75:AI:70:ARG:CB     | 2.21                     | 0.45              |
| 77:AK:38:ILE:HG13   | 77:AK:39:PHE:H      | 1.81                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 87:AY:66:ARG:HG3    | 87:AY:66:ARG:HH11   | 1.81                     | 0.45              |
| 87:AY:278:ARG:NH2   | 129:Ba:63:TRP:O     | 2.50                     | 0.45              |
| 88:Ab:263:VAL:HG12  | 88:Ab:264:PRO:HD2   | 1.97                     | 0.45              |
| 97:At:31:TRP:NE1    | 120:BR:123:ASN:O    | 2.44                     | 0.45              |
| 103:BA:806:TYR:CZ   | 103:BA:808:PRO:HG3  | 2.52                     | 0.45              |
| 104:BB:87:LEU:O     | 104:BB:91:LEU:HB2   | 2.17                     | 0.45              |
| 105:BC:305:ALA:HA   | 105:BC:333:GLY:O    | 2.17                     | 0.45              |
| 108:BF:256:LEU:HD23 | 108:BF:256:LEU:HA   | 1.67                     | 0.45              |
| 128:BZ:162:VAL:O    | 128:BZ:166:ILE:HG23 | 2.16                     | 0.45              |
| 1:DA:234:HIS:HB2    | 1:DA:237:HIS:CD2    | 2.52                     | 0.45              |
| 1:DA:653:LYS:HE3    | 1:DA:653:LYS:HB3    | 1.54                     | 0.45              |
| 1:DA:935:MET:HG3    | 5:DM:118:LEU:HD12   | 1.99                     | 0.45              |
| 1:DA:1000:ASN:N     | 1:DA:1000:ASN:OD1   | 2.50                     | 0.45              |
| 1:DA:1638:LEU:O     | 1:DA:1642:LEU:HB2   | 2.16                     | 0.45              |
| 2:DD:307:GLU:OE2    | 3:DI:195:ILE:HB     | 2.17                     | 0.45              |
| 4:DL:177:GLU:OE1    | 56:Cv:501:HIS:NE2   | 2.48                     | 0.45              |
| 6:DN:144:ARG:HA     | 6:DN:144:ARG:NE     | 2.31                     | 0.45              |
| 8:DP:12:LEU:HA      | 8:DP:12:LEU:HD23    | 1.75                     | 0.45              |
| 10:DR:55:ALA:HB1    | 10:DR:154:LEU:HG    | 1.97                     | 0.45              |
| 11:DS:107:LYS:NZ    | 57:CA:208:U:OP1     | 2.43                     | 0.45              |
| 15:DB:281:GLN:CB    | 15:DB:285:MET:HE3   | 2.46                     | 0.45              |
| 16:DC:353:LEU:O     | 16:DC:357:GLN:HB2   | 2.17                     | 0.45              |
| 17:DE:49:MET:HE1    | 17:DE:91:GLY:HA2    | 1.97                     | 0.45              |
| 18:DF:533:LEU:HD23  | 18:DF:533:LEU:HA    | 1.73                     | 0.45              |
| 20:DH:20:ASN:OD1    | 21:DJ:10:VAL:N      | 2.50                     | 0.45              |
| 27:DY:163:LYS:HE2   | 27:DY:163:LYS:HB3   | 1.71                     | 0.45              |
| 29:CE:95:ILE:HD13   | 56:Cv:289:VAL:HG11  | 1.99                     | 0.45              |
| 29:CE:328:ASP:HA    | 54:Cq:21:MET:HE2    | 1.99                     | 0.45              |
| 29:CE:358:GLU:CD    | 29:CE:358:GLU:H     | 2.25                     | 0.45              |
| 31:CH:196:ASP:HA    | 31:CH:203:PHE:HB2   | 1.98                     | 0.45              |
| 32:CI:202:LEU:HA    | 32:CI:211:ASN:ND2   | 2.32                     | 0.45              |
| 32:CI:265:ASP:HB3   | 32:CI:267:TYR:CD1   | 2.52                     | 0.45              |
| 33:CJ:75:TYR:HE1    | 36:CN:123:ARG:O     | 2.00                     | 0.45              |
| 33:CJ:406:PRO:HG2   | 33:CJ:407:PHE:CD2   | 2.52                     | 0.45              |
| 37:CO:304:ASP:OD1   | 37:CO:304:ASP:N     | 2.41                     | 0.45              |
| 38:CP:32:ARG:CZ     | 38:CP:52:LYS:HD3    | 2.46                     | 0.45              |
| 40:CR:48:TYR:CE1    | 45:Cb:68:GLU:HG3    | 2.52                     | 0.45              |
| 42:CU:80:GLN:NE2    | 42:CU:180:GLN:O     | 2.49                     | 0.45              |
| 44:Ca:10:ARG:NH1    | 44:Ca:10:ARG:HB3    | 2.32                     | 0.45              |
| 46:Cd:108:MET:HE3   | 46:Cd:108:MET:HB2   | 1.85                     | 0.45              |
| 56:Cv:162:SER:H     | 56:Cv:166:HIS:CD2   | 2.35                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 56:Cv:207:PHE:C     | 56:Cv:208:LYS:HG2   | 2.42                     | 0.45              |
| 56:Cv:1037:TYR:O    | 56:Cv:1046:ASN:HB3  | 2.17                     | 0.45              |
| 57:CA:340:U:O2'     | 57:CA:355:A:N6      | 2.49                     | 0.45              |
| 66:A2:332:ASP:OD1   | 66:A2:332:ASP:N     | 2.41                     | 0.45              |
| 67:A3:141:LEU:HD22  | 79:AP:32:PHE:CE2    | 2.51                     | 0.45              |
| 76:AJ:44:GLN:O      | 76:AJ:48:VAL:HG23   | 2.17                     | 0.45              |
| 84:AV:190:LYS:H     | 84:AV:206:ASN:ND2   | 2.15                     | 0.45              |
| 85:AW:73:LYS:HD2    | 102:AA:17:A:C8      | 2.51                     | 0.45              |
| 85:AW:95:ARG:NH1    | 85:AW:110:TRP:CE2   | 2.84                     | 0.45              |
| 92:Ag:155:GLU:O     | 92:Ag:159:ILE:HG12  | 2.17                     | 0.45              |
| 93:Aj:222:ASN:O     | 93:Aj:240:TYR:OH    | 2.22                     | 0.45              |
| 93:Aj:291:ASP:OD1   | 93:Aj:292:SER:N     | 2.50                     | 0.45              |
| 96:Ap:198:LYS:HE2   | 96:Ap:202:ASP:OD2   | 2.17                     | 0.45              |
| 102:AA:798:U:C2     | 102:AA:799:A:C8     | 3.05                     | 0.45              |
| 104:BB:425:ASP:N    | 104:BB:425:ASP:OD1  | 2.49                     | 0.45              |
| 105:BC:164:HIS:ND1  | 105:BC:165:HIS:CD2  | 2.85                     | 0.45              |
| 107:BE:426:MET:HE2  | 107:BE:426:MET:HB3  | 1.75                     | 0.45              |
| 109:BG:345:MET:HB3  | 109:BG:345:MET:HE2  | 1.82                     | 0.45              |
| 111:BI:146:ILE:HG23 | 111:BI:147:TYR:HD1  | 1.82                     | 0.45              |
| 111:BI:204:ARG:O    | 111:BI:207:ILE:HG22 | 2.16                     | 0.45              |
| 126:BX:115:GLY:O    | 126:BX:118:LYS:HE3  | 2.17                     | 0.45              |
| 4:DL:28:ASN:ND2     | 33:CJ:15:TYR:O      | 2.49                     | 0.45              |
| 9:DQ:65:TRP:HA      | 9:DQ:68:ARG:HH11    | 1.82                     | 0.45              |
| 9:DQ:142:PHE:CE1    | 9:DQ:180:ALA:HB1    | 2.48                     | 0.45              |
| 10:DR:27:LYS:O      | 12:DU:97:ARG:NH2    | 2.50                     | 0.45              |
| 13:DZ:48:ARG:H      | 44:Ca:586:ILE:CD1   | 2.30                     | 0.45              |
| 15:DB:551:HIS:CD2   | 15:DB:574:ILE:HD13  | 2.52                     | 0.45              |
| 15:DB:1032:ASP:HB3  | 15:DB:1036:MET:HE2  | 1.98                     | 0.45              |
| 16:DC:540:LEU:HD12  | 16:DC:540:LEU:HA    | 1.85                     | 0.45              |
| 16:DC:1157:ALA:HA   | 20:DH:41:LYS:NZ     | 2.32                     | 0.45              |
| 20:DH:281:PHE:CD2   | 20:DH:304:LEU:HD13  | 2.52                     | 0.45              |
| 20:DH:440:VAL:HG13  | 28:CC:62:PHE:CE2    | 2.52                     | 0.45              |
| 30:CF:149:PHE:HZ    | 46:Cd:143:GLN:HB2   | 1.82                     | 0.45              |
| 31:CH:16:VAL:O      | 31:CH:17:PRO:C      | 2.59                     | 0.45              |
| 34:CK:180:ASP:HA    | 46:Cd:182:GLN:NE2   | 2.32                     | 0.45              |
| 38:CP:184:VAL:O     | 38:CP:188:LEU:HB3   | 2.17                     | 0.45              |
| 46:Cd:13:ARG:NH2    | 46:Cd:26:ARG:HE     | 2.15                     | 0.45              |
| 50:Ck:362:TYR:HD2   | 50:Ck:365:ILE:HB    | 1.82                     | 0.45              |
| 50:Ck:799:LYS:HG2   | 50:Ck:802:TYR:CE2   | 2.51                     | 0.45              |
| 51:Cm:117:ARG:NH1   | 51:Cm:117:ARG:O     | 2.44                     | 0.45              |
| 57:CA:282:A:C6      | 57:CA:283:U:O4      | 2.69                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:A0:71:ARG:HH22   | 94:A1:49:ALA:H      | 1.64                     | 0.45              |
| 66:A2:25:LYS:HB3    | 66:A2:25:LYS:NZ     | 2.31                     | 0.45              |
| 69:A5:30:LYS:HE2    | 69:A5:34:GLN:HB3    | 1.99                     | 0.45              |
| 73:AE:140:MET:HE2   | 73:AE:140:MET:HB3   | 1.72                     | 0.45              |
| 74:AF:275:GLY:HA3   | 74:AF:355:ALA:N     | 2.31                     | 0.45              |
| 77:AK:230:GLN:HG3   | 77:AK:319:GLU:CD    | 2.42                     | 0.45              |
| 79:AP:347:LEU:H     | 79:AP:347:LEU:HG    | 1.46                     | 0.45              |
| 89:Ad:151:GLN:NE2   | 132:Bd:123:ASN:HB3  | 2.32                     | 0.45              |
| 89:Ad:277:TYR:CD1   | 105:BC:237:PRO:HG2  | 2.51                     | 0.45              |
| 96:Ap:155:ILE:H     | 96:Ap:155:ILE:HG13  | 1.47                     | 0.45              |
| 103:BA:186:ASP:O    | 103:BA:190:THR:OG1  | 2.35                     | 0.45              |
| 103:BA:279:VAL:HG23 | 103:BA:280:PHE:CD1  | 2.51                     | 0.45              |
| 104:BB:108:ASP:O    | 104:BB:111:ILE:HG22 | 2.17                     | 0.45              |
| 105:BC:250:TYR:HB3  | 118:BP:81:LEU:HD13  | 1.99                     | 0.45              |
| 105:BC:297:PHE:CZ   | 105:BC:365:LEU:HD11 | 2.52                     | 0.45              |
| 106:BD:265:ARG:O    | 106:BD:269:ALA:N    | 2.49                     | 0.45              |
| 110:BH:103:GLU:O    | 110:BH:107:VAL:HG23 | 2.17                     | 0.45              |
| 118:BP:126:TYR:CZ   | 118:BP:130:LEU:HD11 | 2.52                     | 0.45              |
| 124:BV:30:LYS:HB3   | 124:BV:84:SER:OG    | 2.17                     | 0.45              |
| 1:DA:311:THR:HA     | 1:DA:312:PRO:HD3    | 1.74                     | 0.45              |
| 1:DA:1012:THR:C     | 4:DL:77:LEU:CD2     | 2.87                     | 0.45              |
| 2:DD:442:PHE:HD2    | 2:DD:486:ARG:CZ     | 2.30                     | 0.45              |
| 4:DL:44:LYS:O       | 4:DL:47:GLN:NE2     | 2.43                     | 0.45              |
| 4:DL:266:GLY:HA2    | 34:CK:22:PRO:HB3    | 1.99                     | 0.45              |
| 6:DN:109:ASN:OD1    | 6:DN:109:ASN:N      | 2.50                     | 0.45              |
| 15:DB:388:VAL:HG21  | 20:DH:508:LEU:HB2   | 1.99                     | 0.45              |
| 16:DC:381:LEU:HD12  | 16:DC:385:THR:CG2   | 2.47                     | 0.45              |
| 16:DC:605:GLU:H     | 16:DC:605:GLU:CD    | 2.25                     | 0.45              |
| 17:DE:304:ASN:HB3   | 17:DE:306:VAL:H     | 1.81                     | 0.45              |
| 18:DF:76:GLU:HB3    | 26:DX:38:VAL:HG21   | 1.98                     | 0.45              |
| 19:DG:333:LEU:O     | 19:DG:336:MET:HB2   | 2.17                     | 0.45              |
| 20:DH:17:ILE:HG12   | 48:Ci:132:THR:CG2   | 2.46                     | 0.45              |
| 24:DV:124:GLU:O     | 24:DV:127:THR:HB    | 2.17                     | 0.45              |
| 26:DX:43:HIS:CE1    | 41:CS:123:PRO:HB2   | 2.52                     | 0.45              |
| 27:DY:35:PRO:HA     | 47:Cg:464:VAL:HG11  | 1.99                     | 0.45              |
| 29:CE:257:LYS:HB3   | 29:CE:260:ASN:HD22  | 1.82                     | 0.45              |
| 33:CJ:749:ALA:HA    | 33:CJ:750:PRO:HD2   | 1.87                     | 0.45              |
| 37:CO:106:ASP:OD1   | 37:CO:107:LEU:N     | 2.50                     | 0.45              |
| 37:CO:293:VAL:HG22  | 39:CQ:189:TYR:CE2   | 2.52                     | 0.45              |
| 45:Cb:71:LEU:H      | 45:Cb:71:LEU:HG     | 1.43                     | 0.45              |
| 48:Ci:129:LEU:HD23  | 48:Ci:129:LEU:HA    | 1.78                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 50:Ck:691:GLN:HE21  | 50:Ck:691:GLN:HB2   | 1.61                     | 0.45              |
| 56:Cv:813:ARG:HH11  | 56:Cv:813:ARG:CG    | 2.29                     | 0.45              |
| 57:CA:4:A:OP2       | 57:CA:4:A:H8        | 1.99                     | 0.45              |
| 57:CA:70:U:O2'      | 57:CA:90:A:OP2      | 2.24                     | 0.45              |
| 65:A1:123:VAL:HG12  | 65:A1:124:GLU:N     | 2.31                     | 0.45              |
| 66:A2:395:TYR:CE2   | 102:AA:84:A:H5'     | 2.52                     | 0.45              |
| 68:A4:100:PRO:HB3   | 93:Aj:111:GLN:O     | 2.16                     | 0.45              |
| 71:A8:122:MET:HE2   | 71:A8:122:MET:HB2   | 1.76                     | 0.45              |
| 71:A8:179:ARG:NH1   | 71:A8:181:VAL:HG21  | 2.32                     | 0.45              |
| 73:AE:194:VAL:HG21  | 103:BA:812:GLN:HG2  | 1.99                     | 0.45              |
| 79:AP:244:LEU:HD23  | 79:AP:244:LEU:HA    | 1.84                     | 0.45              |
| 83:AU:198:TRP:HB3   | 108:BF:150:GLY:HA3  | 1.99                     | 0.45              |
| 85:AW:35:THR:O      | 85:AW:38:LYS:HB2    | 2.17                     | 0.45              |
| 85:AW:245:ARG:NH2   | 103:BA:754:ARG:O    | 2.50                     | 0.45              |
| 87:AY:261:GLU:O     | 87:AY:264:VAL:HG12  | 2.16                     | 0.45              |
| 92:Ag:238:MET:HG2   | 115:BM:257:PHE:CD1  | 2.52                     | 0.45              |
| 93:Aj:144:ASP:HA    | 93:Aj:145:PRO:HD3   | 1.82                     | 0.45              |
| 96:Ap:177:HIS:HD2   | 96:Ap:277:LEU:HD12  | 1.81                     | 0.45              |
| 102:AA:820:A:H2'    | 102:AA:821:U:C6     | 2.52                     | 0.45              |
| 103:BA:697:HIS:ND1  | 103:BA:699:ASN:HB3  | 2.32                     | 0.45              |
| 104:BB:288:SER:O    | 104:BB:294:SER:OG   | 2.32                     | 0.45              |
| 111:BI:93:TYR:CZ    | 111:BI:132:ILE:HG12 | 2.52                     | 0.45              |
| 113:BK:111:LEU:HD23 | 113:BK:111:LEU:HA   | 1.78                     | 0.45              |
| 114:BL:264:LEU:HD12 | 114:BL:264:LEU:HA   | 1.86                     | 0.45              |
| 115:BM:267:HIS:CG   | 115:BM:268:PRO:HD2  | 2.52                     | 0.45              |
| 116:BN:72:PRO:CB    | 116:BN:121:LEU:HD21 | 2.47                     | 0.45              |
| 123:BU:120:GLU:OE2  | 126:BX:155:ARG:HA   | 2.17                     | 0.45              |
| 124:BV:74:ASN:ND2   | 124:BV:77:THR:OG1   | 2.50                     | 0.45              |
| 126:BX:155:ARG:HG3  | 126:BX:158:THR:HG22 | 1.99                     | 0.45              |
| 1:DA:47:LEU:HD11    | 2:DD:38:ARG:HB3     | 1.97                     | 0.44              |
| 1:DA:562:LYS:HA     | 1:DA:567:ALA:CB     | 2.47                     | 0.44              |
| 1:DA:639:PHE:CD2    | 1:DA:696:LEU:HB2    | 2.51                     | 0.44              |
| 1:DA:946:SER:HB3    | 5:DM:10:ARG:HD2     | 1.98                     | 0.44              |
| 2:DD:88:TYR:HD1     | 2:DD:92:MET:HE2     | 1.82                     | 0.44              |
| 2:DD:237:THR:HG23   | 3:DI:184:ASN:HB3    | 1.99                     | 0.44              |
| 3:DI:178:PHE:CD1    | 3:DI:178:PHE:N      | 2.84                     | 0.44              |
| 4:DL:190:ARG:NH1    | 40:CR:71:PHE:CD1    | 2.86                     | 0.44              |
| 6:DN:23:VAL:HG13    | 6:DN:118:LEU:HD12   | 1.99                     | 0.44              |
| 14:Da:13:TRP:CZ3    | 39:CQ:39:HIS:HA     | 2.52                     | 0.44              |
| 19:DG:75:ARG:NH2    | 40:CR:244:THR:HG21  | 2.32                     | 0.44              |
| 19:DG:243:MET:HE2   | 19:DG:243:MET:HB3   | 1.92                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 19:DG:403:ASP:HB3   | 19:DG:409:LYS:NZ    | 2.32                     | 0.44              |
| 21:DJ:35:PRO:O      | 21:DJ:37:GLY:N      | 2.50                     | 0.44              |
| 29:CE:118:ARG:HD2   | 29:CE:137:LEU:HD23  | 1.98                     | 0.44              |
| 30:CF:22:LEU:HD21   | 30:CF:65:ILE:HD13   | 1.97                     | 0.44              |
| 32:CI:99:VAL:O      | 45:Cb:103:ARG:NH1   | 2.44                     | 0.44              |
| 34:CK:104:MET:CE    | 45:Cb:100:ARG:HH11  | 2.22                     | 0.44              |
| 36:CN:10:MET:HE3    | 57:CA:415:U:C6      | 2.52                     | 0.44              |
| 37:CO:250:THR:HG21  | 51:Cm:182:ASN:ND2   | 2.32                     | 0.44              |
| 38:CP:9:ALA:HB3     | 57:CA:58:A:N7       | 2.31                     | 0.44              |
| 41:CS:104:GLN:OE1   | 41:CS:110:HIS:HE1   | 1.99                     | 0.44              |
| 51:Cm:96:CYS:HB3    | 51:Cm:125:CYS:SG    | 2.57                     | 0.44              |
| 54:Cq:253:ARG:O     | 54:Cq:257:MET:HG3   | 2.17                     | 0.44              |
| 71:A8:49:ARG:NH2    | 86:AX:80:PHE:HB2    | 2.32                     | 0.44              |
| 77:AK:56:PHE:HE1    | 77:AK:101:ILE:HG12  | 1.82                     | 0.44              |
| 78:AN:164:HIS:HA    | 78:AN:165:PRO:HD3   | 1.72                     | 0.44              |
| 83:AU:23:MET:HE1    | 114:BL:64:SER:HB3   | 1.99                     | 0.44              |
| 84:AV:208:VAL:HG21  | 91:Af:85:PRO:HD3    | 1.99                     | 0.44              |
| 88:Ab:487:LEU:HD11  | 88:Ab:505:TYR:CD2   | 2.51                     | 0.44              |
| 94:Al:98:CYS:HA     | 94:Al:99:PRO:HD3    | 1.81                     | 0.44              |
| 103:BA:318:LEU:HD23 | 103:BA:318:LEU:HA   | 1.75                     | 0.44              |
| 104:BB:107:HIS:HB2  | 104:BB:358:ARG:NH1  | 2.33                     | 0.44              |
| 104:BB:124:GLU:O    | 104:BB:127:VAL:HG12 | 2.17                     | 0.44              |
| 105:BC:112:ARG:N    | 105:BC:115:GLN:HE21 | 2.15                     | 0.44              |
| 107:BE:300:ARG:HD3  | 107:BE:323:TRP:CZ3  | 2.53                     | 0.44              |
| 109:BG:60:LEU:H     | 109:BG:60:LEU:HD23  | 1.83                     | 0.44              |
| 113:BK:295:ARG:HB3  | 113:BK:295:ARG:HH11 | 1.81                     | 0.44              |
| 125:BW:45:ARG:HB3   | 125:BW:45:ARG:HH11  | 1.81                     | 0.44              |
| 136:Bh:3:LEU:HD23   | 136:Bh:3:LEU:HA     | 1.85                     | 0.44              |
| 140:UD:26:UNK:HG2   | 140:UD:29:UNK:HB2   | 2.00                     | 0.44              |
| 1:DA:1183:SER:CB    | 1:DA:1186:CYS:HB2   | 2.45                     | 0.44              |
| 2:DD:408:HIS:CE1    | 2:DD:424:THR:HG21   | 2.51                     | 0.44              |
| 2:DD:518:PHE:CE2    | 2:DD:602:VAL:HG11   | 2.52                     | 0.44              |
| 4:DL:63:ASP:OD2     | 51:Cm:21:GLN:OE1    | 2.33                     | 0.44              |
| 6:DN:43:PHE:CZ      | 6:DN:151:ARG:HD2    | 2.52                     | 0.44              |
| 6:DN:224:ARG:HH11   | 6:DN:224:ARG:CG     | 2.30                     | 0.44              |
| 9:DQ:202:ASP:OD2    | 12:DU:39:ARG:HG2    | 2.16                     | 0.44              |
| 15:DB:382:GLY:O     | 15:DB:396:ARG:NH2   | 2.32                     | 0.44              |
| 15:DB:609:PRO:HB2   | 15:DB:614:VAL:HG23  | 1.99                     | 0.44              |
| 19:DG:155:GLU:HG2   | 50:Ck:414:MET:HG3   | 2.00                     | 0.44              |
| 19:DG:334:MET:HE3   | 19:DG:334:MET:HB3   | 1.54                     | 0.44              |
| 19:DG:490:ARG:HD3   | 19:DG:571:VAL:CG1   | 2.47                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:DG:497:ARG:CG    | 19:DG:497:ARG:NH1  | 2.80                     | 0.44              |
| 22:DK:34:ASN:HA     | 22:DK:38:VAL:O     | 2.17                     | 0.44              |
| 32:CI:218:ARG:O     | 32:CI:221:GLU:HG2  | 2.18                     | 0.44              |
| 33:CJ:797:LEU:HD12  | 33:CJ:797:LEU:HA   | 1.64                     | 0.44              |
| 40:CR:258:ASN:C     | 40:CR:259:GLN:HG2  | 2.42                     | 0.44              |
| 47:Cg:112:ARG:HH21  | 47:Cg:154:GLY:HA3  | 1.81                     | 0.44              |
| 47:Cg:183:THR:OG1   | 47:Cg:184:HIS:HD2  | 2.00                     | 0.44              |
| 68:A4:42:VAL:HG13   | 68:A4:44:ARG:HH12  | 1.79                     | 0.44              |
| 71:A8:75:LYS:NZ     | 71:A8:110:TRP:CE2  | 2.85                     | 0.44              |
| 71:A8:167:MET:HG2   | 102:AA:72:A:N6     | 2.31                     | 0.44              |
| 73:AE:107:LEU:HD23  | 134:Bf:48:TRP:HB2  | 1.99                     | 0.44              |
| 74:AF:140:GLU:H     | 74:AF:225:MET:CE   | 2.28                     | 0.44              |
| 77:AK:216:ARG:O     | 77:AK:219:ARG:HG3  | 2.17                     | 0.44              |
| 79:AP:33:PRO:HB2    | 79:AP:34:LEU:HD23  | 1.99                     | 0.44              |
| 81:AR:185:ARG:HG2   | 81:AR:185:ARG:NH1  | 2.32                     | 0.44              |
| 86:AX:83:PRO:HG2    | 129:Ba:28:ARG:NH2  | 2.32                     | 0.44              |
| 88:Ab:448:LYS:HA    | 118:BP:119:ARG:HD2 | 1.99                     | 0.44              |
| 91:Af:65:LEU:HD13   | 91:Af:65:LEU:HA    | 1.81                     | 0.44              |
| 93:Aj:30:GLN:OE1    | 93:Aj:198:THR:OG1  | 2.19                     | 0.44              |
| 93:Aj:274:GLU:HG3   | 109:BG:50:ARG:HH12 | 1.82                     | 0.44              |
| 102:AA:446:A:N7     | 102:AA:448:A:N6    | 2.65                     | 0.44              |
| 113:BK:227:GLN:HE21 | 113:BK:231:LYS:HD2 | 1.81                     | 0.44              |
| 118:BP:51:MET:HE2   | 132:Bd:46:MET:HB3  | 1.99                     | 0.44              |
| 118:BP:135:CYS:SG   | 118:BP:142:LEU:HA  | 2.57                     | 0.44              |
| 129:Ba:60:VAL:HG13  | 129:Ba:63:TRP:CE2  | 2.53                     | 0.44              |
| 130:Bb:102:PHE:CD1  | 130:Bb:127:VAL:HB  | 2.52                     | 0.44              |
| 2:DD:87:MET:HE1     | 39:CQ:26:TYR:CE1   | 2.53                     | 0.44              |
| 4:DL:117:ASP:O      | 4:DL:121:ILE:HB    | 2.16                     | 0.44              |
| 4:DL:160:ARG:HD2    | 45:Cb:28:TYR:CG    | 2.53                     | 0.44              |
| 9:DQ:146:GLN:HG2    | 9:DQ:176:ARG:HH12  | 1.82                     | 0.44              |
| 10:DR:14:ARG:NH1    | 57:CA:87:U:OP2     | 2.50                     | 0.44              |
| 12:DU:196:MET:HG2   | 12:DU:208:TYR:CZ   | 2.52                     | 0.44              |
| 17:DE:406:ASP:HA    | 17:DE:409:TRP:CD1  | 2.53                     | 0.44              |
| 17:DE:463:LEU:HD23  | 17:DE:486:ILE:HG23 | 1.99                     | 0.44              |
| 18:DF:279:ILE:HD12  | 18:DF:323:TYR:HB2  | 1.98                     | 0.44              |
| 19:DG:142:LEU:HD12  | 19:DG:142:LEU:HA   | 1.86                     | 0.44              |
| 25:DW:16:PHE:CD1    | 26:DX:52:GLU:HB2   | 2.52                     | 0.44              |
| 25:DW:98:GLN:HE22   | 25:DW:154:HIS:CD2  | 2.36                     | 0.44              |
| 35:CL:106:CYS:HB2   | 35:CL:134:TYR:O    | 2.17                     | 0.44              |
| 37:CO:164:ARG:HH22  | 37:CO:201:PHE:HD1  | 1.64                     | 0.44              |
| 37:CO:259:LEU:HD13  | 37:CO:286:ILE:HD13 | 1.99                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 40:CR:319:LYS:CD    | 46:Cd:283:GLU:O     | 2.66                     | 0.44              |
| 42:CU:115:LYS:HD3   | 42:CU:115:LYS:HA    | 1.70                     | 0.44              |
| 44:Ca:10:ARG:HB3    | 44:Ca:10:ARG:CZ     | 2.47                     | 0.44              |
| 44:Ca:506:GLN:O     | 44:Ca:556:SER:HA    | 2.17                     | 0.44              |
| 44:Ca:569:ARG:HD2   | 44:Ca:569:ARG:HA    | 1.74                     | 0.44              |
| 45:Cb:57:MET:H      | 45:Cb:57:MET:HG2    | 1.56                     | 0.44              |
| 49:Cj:143:LYS:NZ    | 49:Cj:143:LYS:HB3   | 2.31                     | 0.44              |
| 53:Cp:69:ARG:HG2    | 53:Cp:104:ALA:HB2   | 1.99                     | 0.44              |
| 54:Cq:26:MET:HG2    | 54:Cq:30:ILE:HD11   | 1.99                     | 0.44              |
| 55:Cr:265:LEU:HD23  | 55:Cr:265:LEU:HA    | 1.77                     | 0.44              |
| 56:Cv:836:GLU:OE1   | 56:Cv:836:GLU:N     | 2.51                     | 0.44              |
| 57:CA:152:U:H2'     | 57:CA:153:A:O4'     | 2.17                     | 0.44              |
| 65:A1:48:LYS:HB2    | 143:UI:15:UNK:HG1   | 1.99                     | 0.44              |
| 69:A5:35:LEU:HD11   | 102:AA:505:U:H5''   | 2.00                     | 0.44              |
| 71:A8:143:THR:HG23  | 71:A8:146:ASP:H     | 1.82                     | 0.44              |
| 73:AE:74:TYR:HD1    | 73:AE:97:ARG:NH1    | 2.13                     | 0.44              |
| 73:AE:366:PRO:HB2   | 73:AE:368:ASP:OD1   | 2.16                     | 0.44              |
| 76:AJ:95:ILE:HG21   | 92:Ag:214:VAL:HG12  | 1.99                     | 0.44              |
| 77:AK:194:VAL:C     | 77:AK:196:THR:H     | 2.26                     | 0.44              |
| 77:AK:272:SER:HB3   | 77:AK:306:MET:HE2   | 1.99                     | 0.44              |
| 79:AP:328:ASP:H     | 110:BH:239:ASN:HD22 | 1.65                     | 0.44              |
| 83:AU:84:LEU:HA     | 83:AU:84:LEU:HD23   | 1.69                     | 0.44              |
| 85:AW:133:LEU:HD23  | 87:AY:46:GLU:HB2    | 1.98                     | 0.44              |
| 89:Ad:229:GLN:HG3   | 89:Ad:258:ARG:HH21  | 1.82                     | 0.44              |
| 92:Ag:183:ARG:NH1   | 92:Ag:184:HIS:NE2   | 2.61                     | 0.44              |
| 93:Aj:203:ALA:O     | 93:Aj:207:ILE:HG13  | 2.17                     | 0.44              |
| 103:BA:450:ALA:HB1  | 103:BA:466:LEU:HD21 | 1.99                     | 0.44              |
| 104:BB:101:LEU:HD22 | 104:BB:104:ILE:HD12 | 1.99                     | 0.44              |
| 104:BB:359:HIS:CG   | 112:BJ:200:ARG:NH1  | 2.85                     | 0.44              |
| 105:BC:192:MET:HE3  | 105:BC:192:MET:HB2  | 1.71                     | 0.44              |
| 107:BE:73:THR:HG23  | 107:BE:74:TYR:N     | 2.30                     | 0.44              |
| 109:BG:77:ILE:HG13  | 109:BG:145:THR:HG21 | 1.99                     | 0.44              |
| 109:BG:86:GLU:OE1   | 109:BG:86:GLU:N     | 2.50                     | 0.44              |
| 109:BG:149:THR:HG22 | 109:BG:151:SER:H    | 1.82                     | 0.44              |
| 114:BL:108:ILE:HD13 | 114:BL:108:ILE:HA   | 1.74                     | 0.44              |
| 114:BL:197:SER:HB3  | 114:BL:247:GLU:OE2  | 2.17                     | 0.44              |
| 115:BM:45:ASN:HB3   | 115:BM:67:LEU:HD12  | 1.99                     | 0.44              |
| 117:BO:100:ILE:HG13 | 117:BO:220:MET:HE1  | 1.98                     | 0.44              |
| 117:BO:142:GLU:OE2  | 117:BO:143:ARG:N    | 2.47                     | 0.44              |
| 130:Bb:93:PRO:HG2   | 130:Bb:123:TYR:HE1  | 1.83                     | 0.44              |
| 132:Bd:108:THR:HB   | 132:Bd:111:GLN:HG3  | 1.99                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 134:Bf:87:GLU:HB3   | 134:Bf:90:ARG:HG3  | 1.99                     | 0.44              |
| 1:DA:192:ASP:OD1    | 1:DA:192:ASP:N     | 2.44                     | 0.44              |
| 1:DA:864:ASP:OD1    | 1:DA:864:ASP:N     | 2.49                     | 0.44              |
| 1:DA:1094:VAL:O     | 1:DA:1098:LEU:HB2  | 2.17                     | 0.44              |
| 2:DD:390:VAL:HG13   | 2:DD:457:LEU:HD22  | 2.00                     | 0.44              |
| 9:DQ:40:VAL:HG22    | 12:DU:100:VAL:HB   | 1.99                     | 0.44              |
| 10:DR:186:PRO:C     | 10:DR:188:LYS:H    | 2.25                     | 0.44              |
| 12:DU:225:LYS:O     | 49:Cj:159:ARG:NH2  | 2.42                     | 0.44              |
| 14:Da:33:LEU:HA     | 31:CH:144:ARG:NH1  | 2.32                     | 0.44              |
| 15:DB:716:GLU:HG3   | 17:DE:474:LEU:HD21 | 2.00                     | 0.44              |
| 15:DB:983:LEU:HD11  | 19:DG:123:LEU:HD13 | 2.00                     | 0.44              |
| 15:DB:1135:VAL:HG12 | 47:Cg:320:LEU:HD22 | 1.98                     | 0.44              |
| 16:DC:71:TRP:CE2    | 16:DC:544:GLU:HG3  | 2.52                     | 0.44              |
| 16:DC:151:SER:OG    | 16:DC:230:GLN:O    | 2.35                     | 0.44              |
| 16:DC:1030:VAL:HG22 | 22:DK:98:LEU:HD21  | 1.99                     | 0.44              |
| 17:DE:648:GLU:HG3   | 17:DE:654:VAL:HG11 | 1.99                     | 0.44              |
| 20:DH:405:ARG:HG3   | 20:DH:414:LEU:HD21 | 1.99                     | 0.44              |
| 29:CE:152:VAL:HG22  | 51:Cm:42:PRO:HG2   | 1.99                     | 0.44              |
| 29:CE:296:LEU:HA    | 29:CE:296:LEU:HD23 | 1.69                     | 0.44              |
| 31:CH:103:ASP:HA    | 31:CH:104:PRO:HD3  | 1.86                     | 0.44              |
| 33:CJ:250:GLU:HB3   | 33:CJ:398:PHE:CD1  | 2.52                     | 0.44              |
| 33:CJ:258:MET:HE2   | 33:CJ:259:LYS:CG   | 2.47                     | 0.44              |
| 34:CK:32:LEU:HD12   | 34:CK:32:LEU:HA    | 1.72                     | 0.44              |
| 42:CU:182:HIS:HE1   | 42:CU:193:ASN:HA   | 1.82                     | 0.44              |
| 45:Cb:161:ALA:HA    | 54:Cq:121:VAL:CG2  | 2.47                     | 0.44              |
| 47:Cg:462:GLU:O     | 47:Cg:462:GLU:HG2  | 2.17                     | 0.44              |
| 50:Ck:288:ASN:O     | 50:Ck:294:ALA:HB1  | 2.16                     | 0.44              |
| 50:Ck:343:GLU:HG2   | 50:Ck:589:GLN:HE22 | 1.82                     | 0.44              |
| 50:Ck:373:ARG:HH21  | 50:Ck:554:SER:HA   | 1.81                     | 0.44              |
| 53:Cp:74:PHE:HE2    | 53:Cp:101:THR:HG21 | 1.82                     | 0.44              |
| 56:Cv:166:HIS:CD2   | 56:Cv:185:VAL:HG21 | 2.52                     | 0.44              |
| 57:CA:82:U:O5'      | 57:CA:82:U:H6      | 2.00                     | 0.44              |
| 65:A1:105:LYS:HD3   | 65:A1:124:GLU:OE2  | 2.16                     | 0.44              |
| 65:A1:145:GLY:HA3   | 65:A1:146:PRO:HD2  | 1.70                     | 0.44              |
| 73:AE:248:PHE:HB3   | 73:AE:337:VAL:HG22 | 1.99                     | 0.44              |
| 74:AF:455:TRP:CZ2   | 98:Av:127:TYR:HB2  | 2.52                     | 0.44              |
| 75:AI:209:LYS:HE2   | 75:AI:209:LYS:H    | 1.82                     | 0.44              |
| 75:AI:214:PRO:HD2   | 110:BH:172:MET:HE3 | 1.99                     | 0.44              |
| 76:AJ:82:ILE:HG22   | 76:AJ:83:PHE:O     | 2.18                     | 0.44              |
| 79:AP:75:THR:O      | 92:Ag:75:SER:HB3   | 2.17                     | 0.44              |
| 79:AP:163:ARG:HH11  | 79:AP:163:ARG:CG   | 2.18                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 79:AP:211:ILE:HG21 | 79:AP:266:LEU:HD11  | 2.00                     | 0.44              |
| 81:AR:211:ARG:HD2  | 123:BU:151:TRP:CZ2  | 2.52                     | 0.44              |
| 85:AW:170:LYS:HB2  | 102:AA:804:A:H5"    | 1.98                     | 0.44              |
| 86:AX:66:ARG:NH1   | 61:UX:8:UNK:HG1     | 2.31                     | 0.44              |
| 87:AY:51:ARG:HD3   | 107:BE:44:GLY:HA2   | 2.00                     | 0.44              |
| 88:Ab:136:GLN:O    | 88:Ab:140:ARG:HG3   | 2.17                     | 0.44              |
| 88:Ab:209:TYR:CZ   | 105:BC:246:PRO:HD3  | 2.53                     | 0.44              |
| 93:Aj:138:THR:HG22 | 93:Aj:140:ARG:H     | 1.82                     | 0.44              |
| 103:BA:132:GLN:HG3 | 103:BA:133:THR:O    | 2.18                     | 0.44              |
| 103:BA:368:LYS:NZ  | 103:BA:368:LYS:HB3  | 2.33                     | 0.44              |
| 103:BA:811:PRO:HG3 | 117:BO:139:LEU:CD2  | 2.47                     | 0.44              |
| 105:BC:105:GLY:O   | 105:BC:109:THR:OG1  | 2.36                     | 0.44              |
| 107:BE:93:ASP:HA   | 107:BE:94:PRO:HD2   | 1.83                     | 0.44              |
| 113:BK:98:THR:HG22 | 113:BK:99:SER:H     | 1.82                     | 0.44              |
| 113:BK:106:TYR:CD1 | 113:BK:133:VAL:HG12 | 2.53                     | 0.44              |
| 115:BM:188:PRO:HG2 | 115:BM:191:LEU:HD12 | 1.99                     | 0.44              |
| 116:BN:49:LYS:HE3  | 123:BU:184:TRP:C    | 2.42                     | 0.44              |
| 140:UD:213:UNK:O   | 140:UD:217:UNK:HB1  | 2.18                     | 0.44              |
| 2:DD:803:GLN:OE1   | 6:DN:249:LYS:HG3    | 2.17                     | 0.44              |
| 11:DS:201:HIS:HB2  | 53:Cp:41:ILE:O      | 2.17                     | 0.44              |
| 15:DB:192:ILE:HD11 | 15:DB:301:GLN:O     | 2.18                     | 0.44              |
| 15:DB:572:ASP:OD2  | 15:DB:646:SER:HB2   | 2.16                     | 0.44              |
| 15:DB:831:ASN:ND2  | 15:DB:837:TYR:HD2   | 2.16                     | 0.44              |
| 16:DC:274:VAL:O    | 16:DC:278:GLN:HG3   | 2.18                     | 0.44              |
| 17:DE:700:ASP:C    | 17:DE:700:ASP:OD1   | 2.59                     | 0.44              |
| 23:DT:82:HIS:HD2   | 23:DT:128:PRO:HB3   | 1.81                     | 0.44              |
| 23:DT:111:ALA:HA   | 23:DT:114:LEU:HD22  | 1.98                     | 0.44              |
| 24:DV:131:GLN:HB3  | 24:DV:143:ILE:HD11  | 1.99                     | 0.44              |
| 24:DV:177:MET:HB3  | 24:DV:183:LEU:HD22  | 1.98                     | 0.44              |
| 25:DW:87:ASN:ND2   | 25:DW:158:PRO:HB3   | 2.30                     | 0.44              |
| 25:DW:101:LEU:HB2  | 40:CR:277:SER:HB3   | 1.99                     | 0.44              |
| 27:DY:133:ASP:OD1  | 27:DY:133:ASP:N     | 2.50                     | 0.44              |
| 29:CE:308:ARG:C    | 29:CE:311:LYS:HZ3   | 2.16                     | 0.44              |
| 32:CI:409:PRO:CB   | 40:CR:253:PHE:CE2   | 2.94                     | 0.44              |
| 34:CK:70:ILE:HD11  | 45:Cb:186:VAL:HA    | 1.98                     | 0.44              |
| 34:CK:311:THR:HA   | 34:CK:312:PRO:HD2   | 1.85                     | 0.44              |
| 37:CO:74:TRP:CE2   | 37:CO:86:PRO:HG3    | 2.52                     | 0.44              |
| 44:Ca:467:LYS:NZ   | 46:Cd:72:ASN:ND2    | 2.65                     | 0.44              |
| 50:Ck:633:MET:HE2  | 50:Ck:633:MET:HB2   | 1.66                     | 0.44              |
| 53:Cp:128:LEU:HD23 | 53:Cp:128:LEU:HA    | 1.70                     | 0.44              |
| 54:Cq:47:LYS:O     | 54:Cq:50:GLU:HG2    | 2.17                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 54:Cq:158:TYR:OH   | 54:Cq:198:ASP:HA    | 2.17                     | 0.44              |
| 56:Cv:247:THR:HG23 | 56:Cv:263:GLU:HG3   | 2.00                     | 0.44              |
| 56:Cv:292:LYS:NZ   | 56:Cv:509:THR:CG2   | 2.80                     | 0.44              |
| 56:Cv:295:VAL:HG22 | 56:Cv:407:MET:HE3   | 2.00                     | 0.44              |
| 56:Cv:298:ALA:H    | 56:Cv:411:ASN:HD21  | 1.64                     | 0.44              |
| 68:A4:91:ASN:CG    | 89:Ad:128:THR:HG23  | 2.43                     | 0.44              |
| 72:A9:90:ALA:HB2   | 96:Ap:293:PHE:CG    | 2.52                     | 0.44              |
| 73:AE:57:TYR:HB3   | 141:UE:1:UNK:HG1    | 1.99                     | 0.44              |
| 74:AF:114:ILE:HG22 | 74:AF:127:THR:HG22  | 1.98                     | 0.44              |
| 83:AU:108:ARG:NH2  | 92:Ag:121:GLU:OE2   | 2.51                     | 0.44              |
| 85:AW:105:MET:HE2  | 85:AW:105:MET:HB3   | 1.87                     | 0.44              |
| 85:AW:181:MET:HE3  | 87:AY:48:VAL:HG21   | 1.99                     | 0.44              |
| 88:Ab:105:ASN:HB3  | 88:Ab:107:SER:H     | 1.82                     | 0.44              |
| 88:Ab:111:ARG:HD3  | 88:Ab:111:ARG:HA    | 1.86                     | 0.44              |
| 92:Ag:50:ARG:HH11  | 92:Ag:50:ARG:CB     | 2.24                     | 0.44              |
| 93:Aj:118:GLU:O    | 93:Aj:121:GLN:HB2   | 2.18                     | 0.44              |
| 93:Aj:181:GLU:N    | 93:Aj:257:LYS:O     | 2.50                     | 0.44              |
| 95:Ao:54:GLN:HG3   | 142:UF:16:UNK:N     | 2.32                     | 0.44              |
| 102:AA:440:U:O2'   | 115:BM:276:PHE:HB2  | 2.18                     | 0.44              |
| 102:AA:485:A:HO2'  | 102:AA:486:A:P      | 2.38                     | 0.44              |
| 103:BA:791:PHE:HD2 | 103:BA:796:LEU:HA   | 1.81                     | 0.44              |
| 107:BE:290:ALA:HB3 | 107:BE:391:ARG:HH22 | 1.83                     | 0.44              |
| 115:BM:233:PRO:HA  | 120:BR:96:GLN:HE21  | 1.83                     | 0.44              |
| 126:BX:66:ASP:HB3  | 126:BX:69:ARG:O     | 2.18                     | 0.44              |
| 127:BY:85:TRP:HE3  | 139:UC:8:UNK:CG     | 2.30                     | 0.44              |
| 140:UD:196:UNK:HA  | 140:UD:199:UNK:HG3  | 1.99                     | 0.44              |
| 1:DA:414:HIS:CD2   | 1:DA:416:HIS:H      | 2.36                     | 0.44              |
| 1:DA:1517:ARG:NH1  | 5:DM:179:ARG:HH11   | 2.16                     | 0.44              |
| 2:DD:689:LEU:HA    | 2:DD:690:PRO:HD3    | 1.82                     | 0.44              |
| 3:DI:290:PHE:HB2   | 3:DI:301:ILE:HB     | 1.99                     | 0.44              |
| 3:DI:328:VAL:HG22  | 7:DO:226:ILE:HD13   | 1.98                     | 0.44              |
| 4:DL:82:ASP:HA     | 4:DL:208:ARG:NE     | 2.33                     | 0.44              |
| 5:DM:7:ILE:O       | 5:DM:10:ARG:HB3     | 2.18                     | 0.44              |
| 9:DQ:39:ASP:HB2    | 10:DR:27:LYS:HE3    | 1.99                     | 0.44              |
| 15:DB:213:ASP:OD1  | 15:DB:213:ASP:N     | 2.40                     | 0.44              |
| 15:DB:495:LEU:HD23 | 15:DB:589:ASP:OD1   | 2.18                     | 0.44              |
| 15:DB:599:LEU:HD23 | 15:DB:599:LEU:HA    | 1.86                     | 0.44              |
| 16:DC:92:PHE:C     | 16:DC:94:ASN:H      | 2.24                     | 0.44              |
| 16:DC:118:GLY:HA3  | 17:DE:150:ARG:HG2   | 2.00                     | 0.44              |
| 16:DC:405:ILE:HG21 | 16:DC:460:SER:OG    | 2.18                     | 0.44              |
| 17:DE:51:ARG:HA    | 17:DE:51:ARG:HD3    | 1.89                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:DT:40:TRP:CH2    | 23:DT:214:ARG:HB3   | 2.53                     | 0.44              |
| 25:DW:85:GLU:H      | 25:DW:85:GLU:CD     | 2.26                     | 0.44              |
| 29:CE:60:TYR:HB3    | 29:CE:85:ASN:ND2    | 2.28                     | 0.44              |
| 29:CE:144:ILE:HD11  | 29:CE:190:LYS:HD2   | 1.99                     | 0.44              |
| 31:CH:263:ILE:HG22  | 31:CH:264:ASP:O     | 2.18                     | 0.44              |
| 33:CJ:83:HIS:NE2    | 33:CJ:86:ASP:O      | 2.51                     | 0.44              |
| 34:CK:198:VAL:HB    | 34:CK:205:TYR:CE1   | 2.52                     | 0.44              |
| 34:CK:232:ARG:HD2   | 34:CK:232:ARG:N     | 2.32                     | 0.44              |
| 35:CL:59:MET:HA     | 35:CL:59:MET:HE3    | 1.99                     | 0.44              |
| 42:CU:69:ARG:HA     | 42:CU:72:HIS:HD2    | 1.83                     | 0.44              |
| 45:Cb:78:GLU:HG3    | 45:Cb:79:PRO:HD2    | 1.99                     | 0.44              |
| 51:Cm:196:GLY:O     | 51:Cm:200:VAL:CG2   | 2.56                     | 0.44              |
| 53:Cp:54:PRO:HD2    | 53:Cp:58:THR:HG21   | 2.00                     | 0.44              |
| 56:Cv:413:LYS:HA    | 56:Cv:435:GLU:HB3   | 2.00                     | 0.44              |
| 57:CA:30:U:H2'      | 57:CA:31:U:C6       | 2.53                     | 0.44              |
| 64:A0:181:ARG:NH1   | 64:A0:182:TYR:OH    | 2.50                     | 0.44              |
| 81:AR:152:ARG:HD3   | 81:AR:157:ALA:O     | 2.18                     | 0.44              |
| 81:AR:222:HIS:HD1   | 81:AR:248:PRO:HB3   | 1.83                     | 0.44              |
| 83:AU:99:LEU:HD23   | 83:AU:99:LEU:HA     | 1.83                     | 0.44              |
| 94:Al:159:MET:HG3   | 102:AA:339:A:H1'    | 2.00                     | 0.44              |
| 103:BA:423:ARG:HA   | 103:BA:423:ARG:HD3  | 1.76                     | 0.44              |
| 103:BA:614:MET:HG3  | 103:BA:656:PRO:HA   | 1.99                     | 0.44              |
| 105:BC:100:GLU:HB3  | 105:BC:136:LYS:HE2  | 1.98                     | 0.44              |
| 106:BD:204:ALA:N    | 106:BD:451:ALA:HB2  | 2.29                     | 0.44              |
| 107:BE:69:GLU:H     | 107:BE:69:GLU:HG2   | 1.68                     | 0.44              |
| 108:BF:60:LEU:N     | 108:BF:63:ARG:NH1   | 2.65                     | 0.44              |
| 108:BF:148:HIS:O    | 108:BF:152:VAL:HG23 | 2.18                     | 0.44              |
| 108:BF:168:ILE:HG22 | 108:BF:197:MET:SD   | 2.58                     | 0.44              |
| 108:BF:316:MET:HE3  | 108:BF:316:MET:HB2  | 1.72                     | 0.44              |
| 1:DA:172:GLY:C      | 1:DA:174:HIS:N      | 2.75                     | 0.44              |
| 1:DA:324:GLN:HG2    | 1:DA:330:TRP:HE1    | 1.83                     | 0.44              |
| 1:DA:619:ASP:OD1    | 1:DA:626:GLN:NE2    | 2.50                     | 0.44              |
| 2:DD:393:VAL:HG21   | 2:DD:441:LEU:HD13   | 2.00                     | 0.44              |
| 12:DU:95:GLU:OE2    | 12:DU:211:ARG:NE    | 2.42                     | 0.44              |
| 15:DB:339:ARG:HH21  | 20:DH:549:SER:HB3   | 1.82                     | 0.44              |
| 15:DB:453:GLU:HB3   | 17:DE:712:MET:HE1   | 1.99                     | 0.44              |
| 15:DB:969:THR:HB    | 15:DB:1001:THR:HG21 | 1.98                     | 0.44              |
| 17:DE:647:LEU:HD23  | 17:DE:647:LEU:HA    | 1.86                     | 0.44              |
| 18:DF:189:ASP:OD1   | 18:DF:189:ASP:N     | 2.48                     | 0.44              |
| 18:DF:450:VAL:HG11  | 18:DF:486:LEU:HB3   | 1.99                     | 0.44              |
| 20:DH:136:LEU:HD21  | 20:DH:159:GLU:HG2   | 2.00                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:DT:137:LEU:HD12  | 23:DT:137:LEU:HA    | 1.68                     | 0.44              |
| 25:DW:141:LEU:HD23  | 25:DW:141:LEU:HA    | 1.75                     | 0.44              |
| 26:DX:59:ARG:HG3    | 26:DX:60:ALA:N      | 2.32                     | 0.44              |
| 26:DX:131:ILE:HB    | 33:CJ:776:GLN:OE1   | 2.17                     | 0.44              |
| 29:CE:62:ARG:HA     | 29:CE:62:ARG:HD2    | 1.80                     | 0.44              |
| 29:CE:174:GLY:HA2   | 29:CE:245:PHE:O     | 2.18                     | 0.44              |
| 33:CJ:704:GLU:H     | 33:CJ:704:GLU:HG3   | 1.50                     | 0.44              |
| 44:Ca:66:PRO:HG3    | 44:Ca:529:ASP:HB3   | 2.00                     | 0.44              |
| 53:Cp:52:TYR:CD1    | 53:Cp:62:ARG:NH1    | 2.85                     | 0.44              |
| 54:Cq:169:GLU:CD    | 54:Cq:172:ARG:HH21  | 2.25                     | 0.44              |
| 57:CA:588:U:H5''    | 57:CA:588:U:O2      | 2.17                     | 0.44              |
| 67:A3:153:LYS:HG2   | 67:A3:154:ALA:H     | 1.82                     | 0.44              |
| 74:AF:73:SER:HB2    | 74:AF:84:PRO:O      | 2.17                     | 0.44              |
| 87:AY:92:GLN:HG2    | 102:AA:18:G:OP2     | 2.18                     | 0.44              |
| 87:AY:289:GLN:HG2   | 112:BJ:241:MET:HE1  | 1.98                     | 0.44              |
| 92:Ag:12:VAL:HG11   | 92:Ag:83:LEU:HD11   | 1.98                     | 0.44              |
| 99:AB:13:ALA:HB3    | 99:AB:16:ALA:HB3    | 2.00                     | 0.44              |
| 102:AA:134:U:OP1    | 102:AA:825:A:N6     | 2.51                     | 0.44              |
| 102:AA:178:A:O2'    | 102:AA:179:A:O5'    | 2.28                     | 0.44              |
| 102:AA:1112:U:O2    | 102:AA:1112:U:H2'   | 2.18                     | 0.44              |
| 103:BA:801:ARG:HD2  | 103:BA:813:VAL:HG23 | 2.00                     | 0.44              |
| 105:BC:221:LYS:HD3  | 105:BC:221:LYS:HA   | 1.73                     | 0.44              |
| 110:BH:147:ILE:HD11 | 110:BH:206:ALA:HA   | 2.00                     | 0.44              |
| 110:BH:194:ARG:HH12 | 110:BH:196:LEU:HD21 | 1.83                     | 0.44              |
| 112:BJ:221:ARG:HH12 | 137:UA:29:UNK:CG    | 2.31                     | 0.44              |
| 115:BM:212:ARG:NH1  | 115:BM:222:ARG:HG2  | 2.33                     | 0.44              |
| 118:BP:143:GLN:HG3  | 118:BP:147:PRO:HD3  | 1.99                     | 0.44              |
| 121:BS:73:ILE:HA    | 121:BS:76:VAL:HG22  | 2.00                     | 0.44              |
| 132:Bd:9:LEU:HD23   | 132:Bd:82:GLU:OE2   | 2.18                     | 0.44              |
| 133:Be:49:ARG:HG2   | 133:Be:49:ARG:HH11  | 1.82                     | 0.44              |
| 136:Bh:56:LYS:HZ3   | 136:Bh:57:PRO:HD2   | 1.82                     | 0.44              |
| 142:UG:8:UNK:HA     | 142:UG:11:UNK:HG3   | 1.99                     | 0.44              |
| 1:DA:95:THR:OG1     | 1:DA:96:ASP:N       | 2.51                     | 0.44              |
| 1:DA:162:PRO:HA     | 1:DA:165:ARG:HE     | 1.83                     | 0.44              |
| 1:DA:695:MET:HG3    | 1:DA:713:PHE:HD2    | 1.83                     | 0.44              |
| 8:DP:84:ASP:C       | 8:DP:86:PRO:HD3     | 2.43                     | 0.44              |
| 15:DB:513:TYR:H     | 15:DB:954:SER:HG    | 1.64                     | 0.44              |
| 15:DB:562:GLN:NE2   | 18:DF:571:LEU:HA    | 2.33                     | 0.44              |
| 16:DC:29:TYR:OH     | 23:DT:45:HIS:HD2    | 2.00                     | 0.44              |
| 16:DC:934:ARG:HH11  | 16:DC:934:ARG:HG2   | 1.82                     | 0.44              |
| 19:DG:143:HIS:CE1   | 19:DG:202:LEU:HD13  | 2.53                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 21:DJ:22:MET:CG    | 28:CC:67:ASN:HB2    | 2.47                     | 0.44              |
| 27:DY:52:GLN:H     | 27:DY:52:GLN:CD     | 2.25                     | 0.44              |
| 30:CF:67:LEU:HD23  | 30:CF:67:LEU:HA     | 1.86                     | 0.44              |
| 32:CI:409:PRO:HA   | 40:CR:253:PHE:CE2   | 2.52                     | 0.44              |
| 34:CK:31:LEU:HA    | 34:CK:31:LEU:HD23   | 1.74                     | 0.44              |
| 37:CO:216:PHE:CZ   | 46:CD:124:ARG:HA    | 2.53                     | 0.44              |
| 43:CZ:240:VAL:HG23 | 43:CZ:291:PHE:O     | 2.17                     | 0.44              |
| 45:Cb:276:LYS:HE2  | 45:Cb:276:LYS:HB3   | 1.82                     | 0.44              |
| 47:Cg:155:LYS:HB2  | 152:Cg:501:GTP:O1B  | 2.17                     | 0.44              |
| 50:Ck:184:LYS:HD3  | 50:Ck:228:LEU:HD21  | 1.99                     | 0.44              |
| 51:Cm:23:ASP:OD1   | 51:Cm:24:SER:N      | 2.50                     | 0.44              |
| 52:Cn:206:GLU:OE1  | 52:Cn:206:GLU:N     | 2.50                     | 0.44              |
| 56:Cv:948:HIS:O    | 56:Cv:952:ALA:HB2   | 2.18                     | 0.44              |
| 57:CA:580:U:H5'    | 57:CA:581:G:OP2     | 2.18                     | 0.44              |
| 64:A0:61:LEU:HA    | 64:A0:62:PRO:HD3    | 1.77                     | 0.44              |
| 73:AE:94:ASP:HB3   | 73:AE:97:ARG:HG2    | 1.99                     | 0.44              |
| 74:AF:211:MET:HE3  | 74:AF:211:MET:HB2   | 1.87                     | 0.44              |
| 75:AI:61:LYS:HE2   | 75:AI:61:LYS:HB2    | 1.67                     | 0.44              |
| 78:AN:117:ARG:NH1  | 111:BI:42:VAL:HG21  | 2.33                     | 0.44              |
| 79:AP:188:ARG:NH2  | 102:AA:158:A:OP2    | 2.50                     | 0.44              |
| 79:AP:282:ARG:NH1  | 98:Av:153:PHE:CE1   | 2.86                     | 0.44              |
| 79:AP:357:PRO:O    | 98:Av:161:LYS:HD2   | 2.18                     | 0.44              |
| 81:AR:55:LEU:HD23  | 81:AR:55:LEU:H      | 1.83                     | 0.44              |
| 86:AX:167:MET:HE2  | 86:AX:167:MET:HB3   | 1.92                     | 0.44              |
| 91:Af:65:LEU:HG    | 91:Af:69:SER:HB3    | 1.99                     | 0.44              |
| 96:Ap:179:GLU:HB3  | 96:Ap:237:LEU:HD12  | 1.98                     | 0.44              |
| 102:AA:40:U:O2'    | 102:AA:41:U:OP1     | 2.34                     | 0.44              |
| 102:AA:560:G:H2'   | 102:AA:561:U:O4'    | 2.18                     | 0.44              |
| 102:AA:945:U:H3    | 102:AA:955:G:N2     | 2.15                     | 0.44              |
| 103:BA:640:LEU:HA  | 103:BA:640:LEU:HD23 | 1.84                     | 0.44              |
| 109:BG:102:GLN:O   | 109:BG:102:GLN:NE2  | 2.50                     | 0.44              |
| 109:BG:275:VAL:HB  | 109:BG:298:VAL:HG22 | 2.00                     | 0.44              |
| 112:BJ:204:ARG:H   | 112:BJ:204:ARG:HG2  | 1.66                     | 0.44              |
| 117:BO:78:ARG:HH11 | 121:BS:104:ARG:NH2  | 2.15                     | 0.44              |
| 119:BQ:80:GLY:O    | 119:BQ:230:ARG:HB3  | 2.18                     | 0.44              |
| 120:BR:146:ARG:HG3 | 142:UF:23:UNK:HB2   | 1.99                     | 0.44              |
| 122:BT:94:TYR:CD2  | 125:BW:80:MET:HE1   | 2.51                     | 0.44              |
| 124:BV:49:ARG:O    | 124:BV:53:LYS:HG3   | 2.18                     | 0.44              |
| 1:DA:74:LYS:NZ     | 57:CA:71:U:P        | 2.90                     | 0.44              |
| 5:DM:1:MET:HE1     | 29:CE:317:HIS:HA    | 1.99                     | 0.44              |
| 6:DN:183:ARG:NE    | 6:DN:194:ARG:NH1    | 2.66                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:DP:212:ASN:OD1   | 8:DP:215:LEU:HB3   | 2.18                     | 0.44              |
| 12:DU:103:ILE:H    | 12:DU:103:ILE:HG13 | 1.43                     | 0.44              |
| 15:DB:958:ASN:HA   | 15:DB:959:PRO:HD3  | 1.92                     | 0.44              |
| 16:DC:71:TRP:NE1   | 16:DC:544:GLU:HG3  | 2.33                     | 0.44              |
| 17:DE:344:ARG:O    | 17:DE:348:ILE:HG13 | 2.18                     | 0.44              |
| 21:DJ:192:THR:N    | 21:DJ:193:PRO:HD2  | 2.33                     | 0.44              |
| 23:DT:140:ASN:HB2  | 23:DT:142:ILE:HD12 | 2.00                     | 0.44              |
| 24:DV:101:GLN:HG3  | 47:Cg:385:TYR:O    | 2.18                     | 0.44              |
| 26:DX:138:LYS:HE2  | 27:DY:138:TYR:OH   | 2.17                     | 0.44              |
| 27:DY:43:LEU:HD12  | 27:DY:43:LEU:HA    | 1.83                     | 0.44              |
| 29:CE:362:GLU:OE2  | 29:CE:364:ARG:HG3  | 2.18                     | 0.44              |
| 32:CI:16:PHE:CE1   | 32:CI:38:LEU:HD13  | 2.53                     | 0.44              |
| 32:CI:82:HIS:O     | 51:Cm:128:ARG:NH2  | 2.51                     | 0.44              |
| 34:CK:14:PRO:CG    | 40:CR:300:TYR:CG   | 2.93                     | 0.44              |
| 35:CL:63:TYR:O     | 62:US:41:UNK:HB1   | 2.17                     | 0.44              |
| 36:CN:106:GLU:OE2  | 41:CS:48:ARG:NH2   | 2.50                     | 0.44              |
| 39:CQ:48:ARG:HG2   | 57:CA:565:A:C6     | 2.53                     | 0.44              |
| 40:CR:53:GLN:HB3   | 40:CR:56:GLU:OE1   | 2.18                     | 0.44              |
| 43:CZ:247:PHE:CE2  | 43:CZ:332:GLY:HA2  | 2.53                     | 0.44              |
| 44:Ca:570:THR:HG21 | 53:Cp:16:HIS:CE1   | 2.53                     | 0.44              |
| 45:Cb:56:ARG:NH1   | 45:Cb:57:MET:HE1   | 2.31                     | 0.44              |
| 46:Cd:195:GLU:HG2  | 46:Cd:214:LYS:HB2  | 2.00                     | 0.44              |
| 56:Cv:739:ASN:HB3  | 56:Cv:789:CYS:HB2  | 2.00                     | 0.44              |
| 66:A2:255:ARG:HH11 | 66:A2:255:ARG:CG   | 2.31                     | 0.44              |
| 73:AE:140:MET:HB2  | 73:AE:168:ASN:ND2  | 2.33                     | 0.44              |
| 75:AI:67:ASN:HB3   | 98:Av:112:VAL:HB   | 2.00                     | 0.44              |
| 76:AJ:55:ARG:HG3   | 96:Ap:225:ILE:HD12 | 1.99                     | 0.44              |
| 77:AK:265:LEU:HD23 | 92:Ag:230:LEU:HB3  | 1.99                     | 0.44              |
| 79:AP:134:ARG:HG3  | 102:AA:150:A:C2    | 2.53                     | 0.44              |
| 89:Ad:37:TRP:HA    | 93:Aj:97:GLN:HG2   | 2.00                     | 0.44              |
| 93:Aj:255:ARG:C    | 93:Aj:257:LYS:H    | 2.26                     | 0.44              |
| 96:Ap:52:ARG:H     | 96:Ap:52:ARG:HG3   | 1.60                     | 0.44              |
| 102:AA:516:U:O2    | 102:AA:516:U:H2'   | 2.18                     | 0.44              |
| 107:BE:66:ARG:NH1  | 107:BE:69:GLU:OE2  | 2.51                     | 0.44              |
| 111:BI:86:PRO:O    | 111:BI:87:GLN:HB3  | 2.18                     | 0.44              |
| 115:BM:175:GLU:HA  | 115:BM:178:GLU:HG2 | 2.00                     | 0.44              |
| 135:Bg:41:TYR:HA   | 135:Bg:90:LEU:HD21 | 2.00                     | 0.44              |
| 136:Bh:19:ASN:HD21 | 140:UD:8:UNK:HA    | 1.83                     | 0.44              |
| 1:DA:48:GLN:O      | 2:DD:63:GLN:NE2    | 2.37                     | 0.43              |
| 1:DA:776:GLY:O     | 1:DA:777:SER:HB2   | 2.18                     | 0.43              |
| 1:DA:1203:CYS:CB   | 15:DB:994:THR:HG23 | 2.49                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:1494:LEU:HD22 | 1:DA:1605:ARG:HB3  | 1.99                     | 0.43              |
| 2:DD:248:ASP:O     | 2:DD:249:PRO:C     | 2.59                     | 0.43              |
| 3:DI:144:LEU:HD12  | 3:DI:144:LEU:HA    | 1.85                     | 0.43              |
| 3:DI:276:GLU:HG2   | 3:DI:277:SER:N     | 2.33                     | 0.43              |
| 7:DO:162:ALA:HA    | 7:DO:198:ARG:HH21  | 1.83                     | 0.43              |
| 8:DP:17:PRO:HG2    | 8:DP:20:MET:HG3    | 2.00                     | 0.43              |
| 8:DP:64:MET:SD     | 12:DU:179:THR:HA   | 2.58                     | 0.43              |
| 14:Da:53:ARG:HB2   | 14:Da:54:TRP:CE3   | 2.53                     | 0.43              |
| 15:DB:99:VAL:HG13  | 15:DB:103:TYR:CZ   | 2.52                     | 0.43              |
| 15:DB:572:ASP:OD2  | 15:DB:648:ARG:HG2  | 2.18                     | 0.43              |
| 16:DC:435:LEU:HD13 | 16:DC:442:LEU:HD23 | 1.99                     | 0.43              |
| 17:DE:206:LEU:HA   | 17:DE:206:LEU:HD23 | 1.83                     | 0.43              |
| 18:DF:387:VAL:HG11 | 18:DF:475:TYR:CE2  | 2.53                     | 0.43              |
| 19:DG:74:LEU:HD12  | 19:DG:74:LEU:HA    | 1.82                     | 0.43              |
| 24:DV:56:ARG:C     | 24:DV:58:ALA:N     | 2.74                     | 0.43              |
| 25:DW:70:LEU:HD23  | 25:DW:70:LEU:HA    | 1.87                     | 0.43              |
| 32:CI:110:ARG:HD2  | 42:CU:143:TRP:HA   | 2.00                     | 0.43              |
| 33:CJ:54:MET:HE2   | 57:CA:463:A:C6     | 2.52                     | 0.43              |
| 36:CN:38:ASP:OD1   | 36:CN:81:LEU:HD12  | 2.18                     | 0.43              |
| 37:CO:82:ASN:HD22  | 37:CO:82:ASN:HA    | 1.58                     | 0.43              |
| 37:CO:245:ASN:ND2  | 37:CO:248:ILE:HD12 | 2.32                     | 0.43              |
| 38:CP:53:ARG:HD2   | 38:CP:58:ILE:HG21  | 1.98                     | 0.43              |
| 38:CP:177:GLU:OE1  | 38:CP:177:GLU:N    | 2.46                     | 0.43              |
| 40:CR:65:GLN:HE21  | 40:CR:70:ARG:HH22  | 1.65                     | 0.43              |
| 44:Ca:509:TRP:HA   | 44:Ca:514:THR:OG1  | 2.18                     | 0.43              |
| 46:Cd:198:GLU:OE1  | 46:Cd:198:GLU:N    | 2.50                     | 0.43              |
| 47:Cg:342:MET:CE   | 47:Cg:351:LYS:HG2  | 2.48                     | 0.43              |
| 48:CI:124:VAL:HG12 | 48:CI:125:HIS:CD2  | 2.53                     | 0.43              |
| 50:Ck:184:LYS:HD3  | 50:Ck:228:LEU:HD11 | 1.99                     | 0.43              |
| 55:Cr:192:LEU:O    | 55:Cr:196:VAL:HG23 | 2.18                     | 0.43              |
| 64:A0:181:ARG:NH1  | 64:A0:182:TYR:CZ   | 2.85                     | 0.43              |
| 65:A1:130:VAL:CG2  | 65:A1:136:PHE:HA   | 2.48                     | 0.43              |
| 68:A4:60:ASN:OD1   | 89:Ad:49:ARG:NH2   | 2.51                     | 0.43              |
| 68:A4:100:PRO:HG3  | 93:Aj:114:PHE:HB2  | 1.99                     | 0.43              |
| 72:A9:105:TRP:H    | 78:AN:100:ARG:HH12 | 1.65                     | 0.43              |
| 73:AE:78:PRO:HG2   | 73:AE:84:TRP:HD1   | 1.80                     | 0.43              |
| 76:AJ:91:ALA:HA    | 76:AJ:94:LEU:HD23  | 2.00                     | 0.43              |
| 76:AJ:92:GLN:O     | 76:AJ:96:LEU:HG    | 2.18                     | 0.43              |
| 79:AP:55:LYS:HE3   | 79:AP:55:LYS:HB2   | 1.81                     | 0.43              |
| 80:AQ:138:GLU:O    | 80:AQ:142:LEU:HB2  | 2.17                     | 0.43              |
| 81:AR:185:ARG:HG2  | 81:AR:185:ARG:HH11 | 1.83                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 89:Ad:244:TYR:HA    | 89:Ad:250:PHE:HD2   | 1.83                     | 0.43              |
| 91:Af:120:LYS:HG3   | 91:Af:121:ALA:N     | 2.33                     | 0.43              |
| 94:Al:173:MET:O     | 94:Al:176:PHE:HB3   | 2.18                     | 0.43              |
| 96:Ap:76:MET:HE2    | 111:Bl:50:ARG:HD2   | 1.99                     | 0.43              |
| 96:Ap:150:HIS:HA    | 111:Bl:216:MET:HG2  | 2.00                     | 0.43              |
| 102:AA:296:A:OP1    | 102:AA:494:U:O2'    | 2.23                     | 0.43              |
| 102:AA:478:A:C5     | 102:AA:493:A:N6     | 2.86                     | 0.43              |
| 103:BA:215:ARG:HH22 | 103:BA:289:SER:HA   | 1.83                     | 0.43              |
| 103:BA:710:LYS:HG2  | 103:BA:711:GLY:H    | 1.83                     | 0.43              |
| 105:BC:276:ALA:CB   | 105:BC:505:ARG:HE   | 2.24                     | 0.43              |
| 105:BC:426:PRO:O    | 105:BC:429:SER:OG   | 2.28                     | 0.43              |
| 107:BE:293:LYS:HD3  | 107:BE:293:LYS:HA   | 1.85                     | 0.43              |
| 117:BO:97:LYS:HG2   | 117:BO:161:MET:HE1  | 1.99                     | 0.43              |
| 120:BR:29:LEU:HD21  | 120:BR:184:TYR:HE1  | 1.82                     | 0.43              |
| 128:BZ:166:ILE:O    | 128:BZ:169:VAL:HG12 | 2.17                     | 0.43              |
| 1:DA:237:HIS:CE1    | 1:DA:310:ASP:HB2    | 2.52                     | 0.43              |
| 1:DA:587:ASP:OD1    | 1:DA:588:GLU:N      | 2.51                     | 0.43              |
| 1:DA:650:LEU:HD13   | 1:DA:725:TRP:CZ3    | 2.53                     | 0.43              |
| 1:DA:1179:GLN:HG3   | 1:DA:1181:THR:HG23  | 2.00                     | 0.43              |
| 2:DD:84:LYS:O       | 2:DD:87:MET:HB3     | 2.18                     | 0.43              |
| 2:DD:344:ALA:HB2    | 9:DQ:30:ALA:HB3     | 2.00                     | 0.43              |
| 2:DD:527:THR:CB     | 10:DR:223:GLN:HG3   | 2.46                     | 0.43              |
| 2:DD:702:TYR:HB3    | 31:CH:233:SER:HB2   | 2.00                     | 0.43              |
| 7:DO:70:ILE:HD13    | 7:DO:120:LEU:HB2    | 2.01                     | 0.43              |
| 8:DP:120:ASP:C      | 8:DP:160:ARG:HH12   | 2.25                     | 0.43              |
| 14:Da:61:ARG:HB3    | 14:Da:61:ARG:NH1    | 2.33                     | 0.43              |
| 15:DB:881:ARG:NH1   | 50:Ck:110:HIS:HE1   | 2.15                     | 0.43              |
| 16:DC:396:ILE:HD13  | 16:DC:457:LYS:HA    | 2.00                     | 0.43              |
| 17:DE:570:GLU:OE1   | 20:DH:527:VAL:N     | 2.51                     | 0.43              |
| 18:DF:118:THR:O     | 18:DF:118:THR:HG22  | 2.18                     | 0.43              |
| 19:DG:186:ARG:NH1   | 19:DG:189:LYS:HD3   | 2.33                     | 0.43              |
| 24:DV:56:ARG:O      | 24:DV:58:ALA:N      | 2.51                     | 0.43              |
| 29:CE:308:ARG:HD3   | 44:Ca:368:ARG:NH1   | 2.33                     | 0.43              |
| 33:CJ:551:ARG:HB3   | 33:CJ:553:ARG:HH21  | 1.83                     | 0.43              |
| 34:CK:195:LEU:HD12  | 34:CK:207:VAL:O     | 2.18                     | 0.43              |
| 34:CK:269:MET:HG3   | 34:CK:273:GLU:OE1   | 2.18                     | 0.43              |
| 38:CP:173:LYS:HZ1   | 38:CP:181:GLU:CD    | 2.26                     | 0.43              |
| 39:CQ:72:ARG:O      | 39:CQ:118:PRO:HD2   | 2.17                     | 0.43              |
| 50:Ck:325:LEU:HD13  | 50:Ck:632:MET:HE2   | 1.99                     | 0.43              |
| 56:Cv:60:GLN:H      | 56:Cv:60:GLN:HG3    | 1.58                     | 0.43              |
| 56:Cv:262:ASN:OD1   | 56:Cv:264:PRO:HD3   | 2.18                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 64:A0:152:VAL:O     | 120:BR:11:MET:HG2   | 2.17                     | 0.43              |
| 68:A4:59:GLU:HG3    | 68:A4:61:ARG:HD2    | 2.00                     | 0.43              |
| 68:A4:75:PHE:HB3    | 68:A4:78:PHE:CE2    | 2.53                     | 0.43              |
| 68:A4:102:ILE:HD11  | 109:BG:341:ALA:HB3  | 2.00                     | 0.43              |
| 73:AE:170:VAL:HG13  | 73:AE:185:VAL:HG13  | 1.99                     | 0.43              |
| 73:AE:314:TRP:NE1   | 73:AE:382:LYS:NZ    | 2.66                     | 0.43              |
| 74:AF:257:ARG:CZ    | 108:BF:420:ARG:HH11 | 2.31                     | 0.43              |
| 75:AI:18:HIS:HB3    | 75:AI:27:PRO:HD2    | 2.00                     | 0.43              |
| 81:AR:71:ARG:HH12   | 136:Bh:19:ASN:HB2   | 1.82                     | 0.43              |
| 83:AU:98:LEU:HD23   | 83:AU:98:LEU:HA     | 1.89                     | 0.43              |
| 84:AV:214:GLY:O     | 111:BI:251:PRO:HG3  | 2.18                     | 0.43              |
| 85:AW:271:PRO:HB3   | 107:BE:352:HIS:CE1  | 2.53                     | 0.43              |
| 86:AX:91:ARG:HD2    | 102:AA:530:U:OP1    | 2.18                     | 0.43              |
| 87:AY:55:ARG:HA     | 87:AY:55:ARG:HD2    | 1.75                     | 0.43              |
| 87:AY:87:LYS:HB2    | 87:AY:87:LYS:NZ     | 2.33                     | 0.43              |
| 88:Ab:84:ASN:OD1    | 88:Ab:84:ASN:N      | 2.48                     | 0.43              |
| 89:Ad:252:GLN:O     | 89:Ad:256:GLU:HG3   | 2.18                     | 0.43              |
| 91:Af:74:THR:HA     | 91:Af:75:PRO:HD2    | 1.87                     | 0.43              |
| 93:Aj:49:TYR:CD2    | 93:Aj:207:ILE:HG12  | 2.53                     | 0.43              |
| 102:AA:578:A:C6     | 102:AA:579:U:C4     | 3.07                     | 0.43              |
| 102:AA:948:A:N6     | 118:BP:220:ARG:H    | 2.14                     | 0.43              |
| 103:BA:401:THR:HG22 | 103:BA:406:ALA:O    | 2.18                     | 0.43              |
| 104:BB:407:LYS:HE2  | 104:BB:407:LYS:HB2  | 1.86                     | 0.43              |
| 104:BB:443:ARG:HG2  | 104:BB:443:ARG:NH1  | 2.33                     | 0.43              |
| 109:BG:284:ALA:CB   | 109:BG:296:PRO:HG3  | 2.48                     | 0.43              |
| 114:BL:80:LEU:HD23  | 114:BL:80:LEU:HA    | 1.83                     | 0.43              |
| 117:BO:220:MET:HE2  | 117:BO:220:MET:HB3  | 1.76                     | 0.43              |
| 121:BS:108:THR:HB   | 121:BS:109:PRO:HD3  | 2.00                     | 0.43              |
| 129:Ba:26:LEU:HD12  | 129:Ba:26:LEU:HA    | 1.70                     | 0.43              |
| 1:DA:287:HIS:HD2    | 1:DA:290:TYR:CD1    | 2.35                     | 0.43              |
| 4:DL:114:SER:HA     | 4:DL:254:ARG:HE     | 1.76                     | 0.43              |
| 4:DL:147:ILE:HG23   | 45:Cb:50:GLU:OE1    | 2.18                     | 0.43              |
| 5:DM:74:ARG:HB3     | 56:Cv:971:LEU:HD11  | 2.00                     | 0.43              |
| 6:DN:173:TYR:CZ     | 6:DN:182:VAL:HG13   | 2.54                     | 0.43              |
| 21:DJ:123:LYS:HD2   | 21:DJ:123:LYS:HA    | 1.61                     | 0.43              |
| 21:DJ:300:TRP:CE2   | 23:DT:224:PRO:HB3   | 2.53                     | 0.43              |
| 24:DV:129:ILE:HD13  | 33:CJ:138:PRO:HD3   | 2.00                     | 0.43              |
| 32:CI:58:GLU:OE1    | 47:Cg:436:ASP:HB2   | 2.18                     | 0.43              |
| 33:CJ:226:ARG:HD2   | 33:CJ:815:ASN:HD21  | 1.83                     | 0.43              |
| 33:CJ:713:PRO:HB3   | 57:CA:507:A:N1      | 2.33                     | 0.43              |
| 37:CO:140:ALA:O     | 37:CO:144:ARG:HB2   | 2.18                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 40:CR:101:GLN:HB3   | 40:CR:102:PRO:HD2   | 2.01                     | 0.43              |
| 44:Ca:367:ASN:HA    | 56:Cv:954:ARG:NH2   | 2.25                     | 0.43              |
| 47:Cg:193:ILE:HD11  | 47:Cg:267:LYS:HD2   | 1.99                     | 0.43              |
| 50:Ck:598:LEU:HD23  | 50:Ck:598:LEU:HA    | 1.67                     | 0.43              |
| 56:Cv:834:LEU:HD12  | 56:Cv:834:LEU:HA    | 1.81                     | 0.43              |
| 56:Cv:1005:TRP:CD1  | 56:Cv:1006:GLU:H    | 2.37                     | 0.43              |
| 64:A0:92:SER:OG     | 64:A0:95:ASN:O      | 2.36                     | 0.43              |
| 71:A8:89:GLY:N      | 71:A8:111:ARG:HH12  | 2.16                     | 0.43              |
| 73:AE:89:LEU:HB2    | 134:Bf:84:GLU:OE2   | 2.19                     | 0.43              |
| 76:AJ:89:ARG:HD3    | 76:AJ:89:ARG:HA     | 1.67                     | 0.43              |
| 89:Ad:107:HIS:CD2   | 89:Ad:111:GLU:OE2   | 2.71                     | 0.43              |
| 95:Ao:57:MET:HE2    | 95:Ao:57:MET:HB2    | 1.83                     | 0.43              |
| 95:Ao:161:PRO:HG3   | 115:BM:236:ARG:NE   | 2.33                     | 0.43              |
| 96:Ap:55:HIS:CE1    | 111:BI:28:ALA:HA    | 2.53                     | 0.43              |
| 96:Ap:66:CYS:CB     | 96:Ap:70:GLU:HB2    | 2.48                     | 0.43              |
| 98:Av:153:PHE:O     | 105:BC:463:ARG:NH2  | 2.51                     | 0.43              |
| 154:Av:301:NAD:H71N | 154:Av:301:NAD:H4N  | 1.60                     | 0.43              |
| 103:BA:317:GLU:CD   | 103:BA:317:GLU:H    | 2.27                     | 0.43              |
| 105:BC:145:PRO:HA   | 105:BC:317:VAL:HG11 | 2.00                     | 0.43              |
| 105:BC:308:ARG:O    | 105:BC:362:VAL:N    | 2.49                     | 0.43              |
| 108:BF:268:GLU:OE1  | 108:BF:268:GLU:N    | 2.41                     | 0.43              |
| 118:BP:121:ARG:HH11 | 118:BP:121:ARG:CG   | 2.26                     | 0.43              |
| 1:DA:93:TRP:O       | 1:DA:97:THR:OG1     | 2.30                     | 0.43              |
| 1:DA:733:SER:O      | 1:DA:736:VAL:HG22   | 2.18                     | 0.43              |
| 2:DD:624:THR:HG23   | 2:DD:629:ALA:O      | 2.18                     | 0.43              |
| 4:DL:106:PHE:HZ     | 32:CI:237:ARG:HG2   | 1.80                     | 0.43              |
| 4:DL:282:TRP:HZ3    | 33:CJ:33:PRO:HD3    | 1.82                     | 0.43              |
| 5:DM:62:VAL:HG13    | 5:DM:70:LEU:HD13    | 1.99                     | 0.43              |
| 6:DN:227:LYS:HE2    | 6:DN:287:ARG:NH2    | 2.32                     | 0.43              |
| 6:DN:229:THR:HB     | 29:CE:29:TYR:CE1    | 2.53                     | 0.43              |
| 7:DO:197:GLN:NE2    | 7:DO:233:ALA:HB1    | 2.33                     | 0.43              |
| 8:DP:115:LEU:HD21   | 8:DP:135:LEU:HD13   | 2.00                     | 0.43              |
| 10:DR:126:LEU:HD11  | 10:DR:137:CYS:SG    | 2.59                     | 0.43              |
| 11:DS:36:SER:O      | 11:DS:40:LYS:HG3    | 2.18                     | 0.43              |
| 12:DU:207:ARG:HD2   | 12:DU:207:ARG:N     | 2.31                     | 0.43              |
| 15:DB:944:HIS:O     | 33:CJ:342:ASN:HB3   | 2.17                     | 0.43              |
| 15:DB:1039:ILE:HD11 | 28:CC:36:LEU:HD11   | 2.01                     | 0.43              |
| 16:DC:219:LEU:HD23  | 16:DC:219:LEU:HA    | 1.86                     | 0.43              |
| 19:DG:99:VAL:HG23   | 33:CJ:187:GLY:HA2   | 2.01                     | 0.43              |
| 20:DH:99:GLN:HG2    | 20:DH:134:PRO:HD2   | 1.99                     | 0.43              |
| 20:DH:214:LEU:HD23  | 20:DH:214:LEU:HA    | 1.79                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 21:DJ:243:ASN:ND2   | 21:DJ:288:LEU:HD22  | 2.34                     | 0.43              |
| 35:CL:76:TYR:HE2    | 35:CL:78:MET:HE2    | 1.83                     | 0.43              |
| 37:CO:317:ASP:OD1   | 37:CO:318:VAL:N     | 2.52                     | 0.43              |
| 41:CS:70:TYR:CE1    | 57:CA:505:U:H2'     | 2.54                     | 0.43              |
| 42:CU:27:LYS:HG2    | 57:CA:297:G:H1      | 1.83                     | 0.43              |
| 42:CU:59:ARG:HH21   | 42:CU:170:VAL:HA    | 1.83                     | 0.43              |
| 48:CI:61:MET:HE3    | 48:CI:61:MET:HB3    | 1.92                     | 0.43              |
| 50:CK:683:LEU:HD23  | 50:CK:683:LEU:HA    | 1.81                     | 0.43              |
| 51:CM:47:ASN:HD21   | 57:CA:387:U:H4'     | 1.82                     | 0.43              |
| 53:CP:66:HIS:HB3    | 53:CP:69:ARG:HB2    | 2.01                     | 0.43              |
| 55:CR:10:ARG:HH22   | 55:CR:13:ARG:HB2    | 1.84                     | 0.43              |
| 57:CA:263:A:O2'     | 57:CA:264:A:H8      | 2.02                     | 0.43              |
| 64:A0:114:ARG:O     | 64:A0:118:ARG:HG3   | 2.18                     | 0.43              |
| 65:A1:184:MET:HE2   | 65:A1:204:TYR:CD2   | 2.53                     | 0.43              |
| 65:A1:222:LYS:HD2   | 65:A1:222:LYS:HA    | 1.83                     | 0.43              |
| 71:A8:115:PRO:CD    | 88:Ab:466:VAL:HG13  | 2.48                     | 0.43              |
| 73:AE:198:LYS:HG2   | 103:BA:761:TYR:CZ   | 2.53                     | 0.43              |
| 73:AE:314:TRP:NE1   | 73:AE:382:LYS:HZ1   | 2.15                     | 0.43              |
| 74:AF:205:LYS:HB3   | 74:AF:205:LYS:HE2   | 1.50                     | 0.43              |
| 74:AF:365:GLU:HG3   | 125:BW:38:LYS:HB3   | 2.00                     | 0.43              |
| 80:AQ:159:ARG:HH11  | 80:AQ:159:ARG:HG3   | 1.83                     | 0.43              |
| 85:AW:274:THR:H     | 107:BE:318:ARG:HH12 | 1.67                     | 0.43              |
| 88:Ab:428:LEU:HD12  | 88:Ab:428:LEU:HA    | 1.81                     | 0.43              |
| 88:Ab:437:GLU:HB2   | 118:BP:85:ARG:NH1   | 2.32                     | 0.43              |
| 92:Ag:170:GLN:NE2   | 92:Ag:227:PRO:HG2   | 2.28                     | 0.43              |
| 92:Ag:198:SER:HB3   | 92:Ag:202:ARG:HH21  | 1.84                     | 0.43              |
| 102:AA:422:A:OP1    | 124:BV:139:ILE:HD13 | 2.19                     | 0.43              |
| 102:AA:565:U:C6     | 123:BU:138:ARG:NH1  | 2.86                     | 0.43              |
| 102:AA:834:U:H2'    | 102:AA:835:A:O4'    | 2.19                     | 0.43              |
| 102:AA:1160:A:H1'   | 103:BA:763:PRO:HG2  | 1.99                     | 0.43              |
| 103:BA:374:PHE:CE2  | 103:BA:397:MET:HG2  | 2.53                     | 0.43              |
| 105:BC:248:SER:HB2  | 118:BP:84:GLU:OE1   | 2.17                     | 0.43              |
| 107:BE:81:VAL:HG13  | 107:BE:82:GLU:OE2   | 2.18                     | 0.43              |
| 109:BG:80:ASP:CG    | 109:BG:81:HIS:H     | 2.27                     | 0.43              |
| 119:BQ:31:VAL:HG11  | 119:BQ:65:CYS:SG    | 2.58                     | 0.43              |
| 119:BQ:226:ILE:HG23 | 119:BQ:227:LEU:N    | 2.33                     | 0.43              |
| 136:Bh:46:VAL:HG21  | 140:UD:12:UNK:HB2   | 2.00                     | 0.43              |
| 140:UD:60:UNK:O     | 140:UD:63:UNK:HG3   | 2.18                     | 0.43              |
| 1:DA:41:PHE:HD1     | 1:DA:42:LYS:H       | 1.67                     | 0.43              |
| 1:DA:125:LEU:HD13   | 31:CH:150:THR:HG23  | 2.01                     | 0.43              |
| 1:DA:1656:ASN:HD21  | 1:DA:1659:ARG:HD2   | 1.82                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:119:TYR:CD1   | 46:Cd:76:TYR:HD1   | 2.37                     | 0.43              |
| 4:DL:27:PRO:HB3    | 33:CJ:16:ARG:HG2   | 1.99                     | 0.43              |
| 4:DL:85:PHE:CE1    | 32:CI:269:HIS:HD2  | 2.37                     | 0.43              |
| 5:DM:83:THR:HG22   | 5:DM:85:TYR:H      | 1.83                     | 0.43              |
| 8:DP:139:ARG:HA    | 8:DP:139:ARG:HD2   | 1.84                     | 0.43              |
| 12:DU:106:PRO:HG2  | 12:DU:109:SER:HB3  | 1.99                     | 0.43              |
| 15:DB:456:LEU:HD23 | 15:DB:456:LEU:HA   | 1.76                     | 0.43              |
| 16:DC:770:LEU:HD12 | 16:DC:771:PRO:HD2  | 2.00                     | 0.43              |
| 17:DE:601:ILE:HD13 | 17:DE:601:ILE:HG21 | 1.77                     | 0.43              |
| 22:DK:263:GLU:H    | 22:DK:263:GLU:HG3  | 1.52                     | 0.43              |
| 29:CE:288:SER:OG   | 31:CH:215:THR:HG23 | 2.19                     | 0.43              |
| 32:CI:195:ILE:HG12 | 54:Cq:254:TYR:CE1  | 2.53                     | 0.43              |
| 33:CJ:100:ARG:O    | 33:CJ:101:PHE:C    | 2.61                     | 0.43              |
| 33:CJ:714:THR:OG1  | 36:CN:52:ASP:HB3   | 2.19                     | 0.43              |
| 37:CO:287:LEU:HD23 | 37:CO:287:LEU:HA   | 1.84                     | 0.43              |
| 41:CS:87:GLU:O     | 41:CS:104:GLN:HG3  | 2.17                     | 0.43              |
| 44:Ca:359:ARG:HH21 | 56:Cv:257:LYS:HD3  | 1.83                     | 0.43              |
| 45:Cb:101:LYS:HB3  | 45:Cb:101:LYS:HZ3  | 1.82                     | 0.43              |
| 47:Cg:243:LEU:HA   | 47:Cg:243:LEU:HD12 | 1.70                     | 0.43              |
| 53:Cp:20:LYS:NZ    | 57:CA:201:A:OP2    | 2.40                     | 0.43              |
| 55:Cr:177:LEU:HD23 | 55:Cr:177:LEU:HA   | 1.85                     | 0.43              |
| 64:A0:91:GLU:H     | 64:A0:137:ARG:NH2  | 2.16                     | 0.43              |
| 66:A2:127:GLY:HA2  | 128:BZ:124:ALA:HB1 | 2.01                     | 0.43              |
| 68:A4:2:VAL:O      | 71:A8:109:TYR:OH   | 2.36                     | 0.43              |
| 68:A4:29:HIS:CD2   | 68:A4:32:LEU:HD23  | 2.46                     | 0.43              |
| 69:A5:51:MET:HE1   | 85:AW:155:LEU:HD21 | 2.00                     | 0.43              |
| 71:A8:51:ALA:HB2   | 74:AF:170:TRP:HB2  | 1.99                     | 0.43              |
| 77:AK:55:PHE:HE2   | 77:AK:104:ILE:HD12 | 1.83                     | 0.43              |
| 77:AK:197:PRO:HG2  | 77:AK:198:TYR:HD2  | 1.83                     | 0.43              |
| 77:AK:250:LEU:O    | 92:Ag:241:ARG:NH1  | 2.49                     | 0.43              |
| 80:AQ:47:GLN:N     | 80:AQ:124:ILE:O    | 2.52                     | 0.43              |
| 81:AR:201:ARG:HG2  | 81:AR:201:ARG:NH1  | 2.29                     | 0.43              |
| 82:AT:37:ALA:O     | 82:AT:42:ARG:HG2   | 2.18                     | 0.43              |
| 85:AW:96:TYR:CG    | 85:AW:107:LYS:HD2  | 2.53                     | 0.43              |
| 89:Ad:118:GLU:HB3  | 93:Aj:27:VAL:HG21  | 2.01                     | 0.43              |
| 89:Ad:227:ARG:HH12 | 132:Bd:40:PHE:HE1  | 1.66                     | 0.43              |
| 93:Aj:18:GLY:HA2   | 132:Bd:129:MET:O   | 2.18                     | 0.43              |
| 94:Al:212:TRP:O    | 94:Al:216:LEU:HB2  | 2.19                     | 0.43              |
| 95:Ao:158:ARG:CB   | 115:BM:217:GLU:HG3 | 2.49                     | 0.43              |
| 97:At:152:GLU:OE2  | 97:At:153:LEU:HD22 | 2.19                     | 0.43              |
| 102:AA:389:A:C6    | 102:AA:446:A:N6    | 2.86                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 103:BA:397:MET:O   | 103:BA:401:THR:OG1 | 2.35                     | 0.43              |
| 105:BC:49:SER:HB2  | 105:BC:509:MET:HB3 | 1.99                     | 0.43              |
| 105:BC:124:ASN:HB3 | 105:BC:126:GLU:OE2 | 2.19                     | 0.43              |
| 106:BD:273:ALA:HA  | 106:BD:274:ALA:HA  | 1.72                     | 0.43              |
| 116:BN:58:ILE:HB   | 116:BN:59:PRO:HD3  | 2.00                     | 0.43              |
| 127:BY:141:GLU:OE2 | 127:BY:146:TYR:HA  | 2.18                     | 0.43              |
| 131:Bc:13:LYS:HB2  | 131:Bc:13:LYS:NZ   | 2.34                     | 0.43              |
| 136:Bh:76:GLY:H    | 136:Bh:79:ALA:HB3  | 1.83                     | 0.43              |
| 1:DA:1466:TYR:O    | 1:DA:1492:LEU:HD12 | 2.19                     | 0.43              |
| 1:DA:1557:THR:HG22 | 1:DA:1558:ASN:H    | 1.83                     | 0.43              |
| 1:DA:1591:ARG:C    | 1:DA:1593:ALA:H    | 2.27                     | 0.43              |
| 2:DD:656:LEU:HD23  | 2:DD:656:LEU:HA    | 1.90                     | 0.43              |
| 3:DI:18:HIS:CD2    | 3:DI:65:MET:HB2    | 2.54                     | 0.43              |
| 3:DI:306:ASP:OD1   | 3:DI:306:ASP:N     | 2.45                     | 0.43              |
| 5:DM:213:ARG:NH1   | 5:DM:219:GLY:HA3   | 2.34                     | 0.43              |
| 5:DM:284:ARG:NH1   | 54:Cq:46:ASP:OD2   | 2.51                     | 0.43              |
| 6:DN:74:HIS:CE1    | 6:DN:76:SER:HB2    | 2.54                     | 0.43              |
| 15:DB:494:PRO:HB3  | 15:DB:955:ARG:HD2  | 2.00                     | 0.43              |
| 15:DB:1056:PRO:HD3 | 20:DH:35:TYR:CE1   | 2.54                     | 0.43              |
| 16:DC:638:ASP:HB3  | 16:DC:652:ARG:NH2  | 2.32                     | 0.43              |
| 16:DC:649:THR:HG22 | 16:DC:651:LYS:H    | 1.84                     | 0.43              |
| 17:DE:433:ASN:HB3  | 17:DE:436:VAL:HG23 | 2.01                     | 0.43              |
| 18:DF:502:ARG:HH11 | 18:DF:579:GLU:CG   | 2.32                     | 0.43              |
| 19:DG:175:GLU:OE2  | 19:DG:191:GLN:HG3  | 2.19                     | 0.43              |
| 20:DH:46:LEU:HA    | 20:DH:46:LEU:HD12  | 1.59                     | 0.43              |
| 20:DH:148:ASP:HA   | 20:DH:149:PRO:HD2  | 1.79                     | 0.43              |
| 21:DJ:300:TRP:CZ2  | 23:DT:224:PRO:HB3  | 2.53                     | 0.43              |
| 22:DK:16:ARG:HD3   | 22:DK:16:ARG:HA    | 1.67                     | 0.43              |
| 23:DT:92:LYS:HD2   | 23:DT:174:TYR:CD1  | 2.53                     | 0.43              |
| 25:DW:153:LEU:HD23 | 25:DW:153:LEU:HA   | 1.77                     | 0.43              |
| 32:CI:241:ARG:CB   | 33:CJ:56:ILE:O     | 2.65                     | 0.43              |
| 32:CI:324:ARG:HG2  | 32:CI:325:GLU:N    | 2.32                     | 0.43              |
| 32:CI:412:LYS:HD2  | 40:CR:253:PHE:HB2  | 2.01                     | 0.43              |
| 33:CJ:36:MET:CE    | 51:Cm:52:THR:HG21  | 2.25                     | 0.43              |
| 33:CJ:130:ARG:HH12 | 50:Ck:710:ARG:HH21 | 1.65                     | 0.43              |
| 33:CJ:232:ASN:HB3  | 33:CJ:241:SER:O    | 2.19                     | 0.43              |
| 33:CJ:315:ASP:OD1  | 33:CJ:315:ASP:N    | 2.51                     | 0.43              |
| 33:CJ:575:HIS:O    | 33:CJ:579:THR:HG23 | 2.18                     | 0.43              |
| 37:CO:76:TRP:HZ2   | 52:Cn:143:ALA:HB2  | 1.83                     | 0.43              |
| 37:CO:311:ILE:O    | 37:CO:311:ILE:HG22 | 2.18                     | 0.43              |
| 44:Ca:130:TYR:HB3  | 44:Ca:131:MET:HE2  | 2.00                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 44:Ca:507:MET:HE2   | 44:Ca:507:MET:HB3   | 1.77                     | 0.43              |
| 45:Cb:298:ASP:OD1   | 45:Cb:298:ASP:N     | 2.40                     | 0.43              |
| 47:Cg:436:ASP:OD1   | 47:Cg:436:ASP:C     | 2.61                     | 0.43              |
| 50:Ck:674:LEU:HD21  | 50:Ck:707:LEU:HG    | 2.00                     | 0.43              |
| 50:Ck:775:ARG:HH11  | 50:Ck:775:ARG:HB3   | 1.83                     | 0.43              |
| 57:CA:95:U:H6       | 57:CA:95:U:H2'      | 1.66                     | 0.43              |
| 57:CA:153:A:H2'     | 57:CA:154:G:H8      | 1.83                     | 0.43              |
| 65:A1:192:GLU:HB3   | 65:A1:193:ASP:H     | 1.46                     | 0.43              |
| 66:A2:410:GLN:NE2   | 86:AX:204:GLU:OE1   | 2.51                     | 0.43              |
| 67:A3:73:HIS:HB3    | 67:A3:75:PHE:CE2    | 2.53                     | 0.43              |
| 67:A3:111:ARG:HD3   | 139:UH:11:UNK:HG1   | 2.01                     | 0.43              |
| 67:A3:114:HIS:HA    | 97:At:37:VAL:HG22   | 2.01                     | 0.43              |
| 70:A6:54:LYS:HB3    | 70:A6:58:GLU:HB2    | 2.00                     | 0.43              |
| 76:AJ:54:ALA:C      | 76:AJ:56:VAL:H      | 2.26                     | 0.43              |
| 79:AP:111:ASN:HB2   | 79:AP:117:TRP:CH2   | 2.54                     | 0.43              |
| 79:AP:282:ARG:NH2   | 105:BC:461:ASP:OD2  | 2.51                     | 0.43              |
| 85:AW:40:HIS:H      | 85:AW:43:SER:HB2    | 1.84                     | 0.43              |
| 89:Ad:164:MET:HB3   | 89:Ad:174:PHE:HE1   | 1.82                     | 0.43              |
| 93:Aj:210:ASP:HB3   | 93:Aj:254:PHE:CE1   | 2.54                     | 0.43              |
| 95:Ao:249:SER:HA    | 95:Ao:250:PRO:HD3   | 1.90                     | 0.43              |
| 98:Av:213:ARG:O     | 98:Av:213:ARG:HD3   | 2.19                     | 0.43              |
| 102:AA:483:A:OP2    | 122:BT:34:ARG:NH2   | 2.51                     | 0.43              |
| 107:BE:236:ARG:HB3  | 107:BE:236:ARG:HH11 | 1.84                     | 0.43              |
| 125:BW:46:HIS:HD2   | 125:BW:78:TYR:OH    | 2.02                     | 0.43              |
| 126:BX:125:ARG:HH12 | 126:BX:154:ARG:HB3  | 1.84                     | 0.43              |
| 132:Bd:8:ARG:HD3    | 132:Bd:8:ARG:HA     | 1.84                     | 0.43              |
| 1:DA:623:HIS:HB3    | 1:DA:625:LYS:HE3    | 2.00                     | 0.43              |
| 1:DA:955:LYS:HA     | 1:DA:956:PRO:HD3    | 1.94                     | 0.43              |
| 2:DD:323:LEU:HD11   | 2:DD:444:SER:OG     | 2.19                     | 0.43              |
| 2:DD:621:LEU:O      | 49:Cj:210:PRO:HG2   | 2.19                     | 0.43              |
| 3:DI:60:LEU:HD23    | 3:DI:60:LEU:HA      | 1.88                     | 0.43              |
| 4:DL:106:PHE:CD1    | 32:CI:239:PHE:HZ    | 2.37                     | 0.43              |
| 9:DQ:52:PHE:CE1     | 9:DQ:235:HIS:HE1    | 2.36                     | 0.43              |
| 12:DU:94:TRP:HH2    | 12:DU:196:MET:HE1   | 1.82                     | 0.43              |
| 12:DU:111:ILE:HD12  | 12:DU:142:ASP:O     | 2.19                     | 0.43              |
| 15:DB:589:ASP:OD1   | 15:DB:590:ASP:N     | 2.52                     | 0.43              |
| 15:DB:908:GLN:H     | 15:DB:908:GLN:HE21  | 1.66                     | 0.43              |
| 15:DB:908:GLN:HA    | 15:DB:909:PRO:HD3   | 1.83                     | 0.43              |
| 15:DB:1132:ARG:HD3  | 33:CJ:709:GLU:OE2   | 2.19                     | 0.43              |
| 16:DC:164:SER:HA    | 16:DC:165:PRO:HD3   | 1.71                     | 0.43              |
| 18:DF:486:LEU:HD23  | 18:DF:486:LEU:HA    | 1.73                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:DG:236:VAL:HG11 | 19:DG:240:HIS:CG   | 2.54                     | 0.43              |
| 27:DY:69:HIS:HA    | 40:CR:265:ARG:NH1  | 2.34                     | 0.43              |
| 29:CE:16:TYR:HB2   | 44:Ca:341:LEU:O    | 2.18                     | 0.43              |
| 32:CI:126:TRP:NE1  | 32:CI:133:VAL:O    | 2.39                     | 0.43              |
| 32:CI:240:ASN:N    | 32:CI:240:ASN:OD1  | 2.50                     | 0.43              |
| 33:CJ:27:PRO:CB    | 51:Cm:28:GLN:NE2   | 2.81                     | 0.43              |
| 33:CJ:668:GLU:HB3  | 33:CJ:671:LEU:HD22 | 1.99                     | 0.43              |
| 35:CL:81:ARG:NH2   | 57:CA:379:A:OP1    | 2.51                     | 0.43              |
| 35:CL:123:GLY:O    | 57:CA:266:A:O3'    | 2.37                     | 0.43              |
| 44:Ca:267:LEU:HD23 | 44:Ca:267:LEU:HA   | 1.68                     | 0.43              |
| 45:Cb:125:MET:HE3  | 45:Cb:146:VAL:HG12 | 2.00                     | 0.43              |
| 47:Cg:112:ARG:HD2  | 47:Cg:408:GLU:OE2  | 2.18                     | 0.43              |
| 47:Cg:237:GLU:HG2  | 47:Cg:238:ARG:H    | 1.83                     | 0.43              |
| 50:Ck:42:HIS:O     | 50:Ck:93:THR:HB    | 2.18                     | 0.43              |
| 50:Ck:129:THR:HG22 | 50:Ck:131:ASN:N    | 2.22                     | 0.43              |
| 50:Ck:222:LEU:HD23 | 50:Ck:239:LEU:HD12 | 2.01                     | 0.43              |
| 50:Ck:349:GLU:HG2  | 50:Ck:349:GLU:O    | 2.19                     | 0.43              |
| 51:Cm:185:ALA:HB1  | 51:Cm:188:ARG:HB2  | 2.00                     | 0.43              |
| 55:Cr:176:LEU:HA   | 55:Cr:176:LEU:HD12 | 1.72                     | 0.43              |
| 56:Cv:833:PRO:HG2  | 56:Cv:836:GLU:OE1  | 2.18                     | 0.43              |
| 57:CA:394:A:OP2    | 57:CA:394:A:C8     | 2.72                     | 0.43              |
| 62:US:25:UNK:O     | 62:US:29:UNK:HB1   | 2.19                     | 0.43              |
| 66:A2:212:ALA:HB1  | 66:A2:213:PRO:HD2  | 2.01                     | 0.43              |
| 73:AE:73:LEU:H     | 73:AE:73:LEU:CD2   | 2.31                     | 0.43              |
| 73:AE:160:CYS:HA   | 73:AE:325:LEU:O    | 2.18                     | 0.43              |
| 73:AE:377:ASP:OD1  | 73:AE:377:ASP:N    | 2.40                     | 0.43              |
| 75:AI:191:ARG:HD3  | 133:Be:58:LEU:HD23 | 2.01                     | 0.43              |
| 78:AN:54:LEU:HD13  | 78:AN:133:PHE:CD2  | 2.53                     | 0.43              |
| 79:AP:33:PRO:HD2   | 79:AP:41:LEU:O     | 2.18                     | 0.43              |
| 79:AP:87:ASN:O     | 79:AP:90:ILE:HG13  | 2.18                     | 0.43              |
| 79:AP:256:TYR:CE2  | 79:AP:284:GLY:HA3  | 2.54                     | 0.43              |
| 87:AY:35:LYS:HD3   | 87:AY:37:GLY:N     | 2.34                     | 0.43              |
| 88:Ab:447:ARG:HB2  | 88:Ab:451:GLU:HG3  | 2.01                     | 0.43              |
| 89:Ad:84:GLU:O     | 89:Ad:88:ARG:HG2   | 2.19                     | 0.43              |
| 91:Af:103:SER:OG   | 91:Af:106:GLN:HG3  | 2.19                     | 0.43              |
| 93:Aj:142:LEU:HD13 | 93:Aj:142:LEU:HA   | 1.91                     | 0.43              |
| 94:Al:74:LEU:HD22  | 94:Al:211:HIS:CD2  | 2.54                     | 0.43              |
| 95:Ao:137:ALA:HA   | 95:Ao:140:ARG:NH1  | 2.33                     | 0.43              |
| 96:Ap:117:TYR:CE2  | 111:BI:224:MET:HG2 | 2.53                     | 0.43              |
| 102:AA:1172:A:OP1  | 117:BO:130:ARG:NH2 | 2.52                     | 0.43              |
| 107:BE:13:ARG:HA   | 107:BE:13:ARG:HD3  | 1.84                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 108:BF:60:LEU:N    | 108:BF:63:ARG:HH11  | 2.17                     | 0.43              |
| 108:BF:141:MET:HE2 | 108:BF:141:MET:HB3  | 1.93                     | 0.43              |
| 109:BG:192:ARG:NH1 | 109:BG:253:ARG:HB2  | 2.33                     | 0.43              |
| 110:BH:126:LYS:HB3 | 110:BH:187:LEU:HD22 | 2.00                     | 0.43              |
| 112:BJ:195:PRO:HG2 | 112:BJ:200:ARG:HH21 | 1.84                     | 0.43              |
| 115:BM:62:GLU:O    | 115:BM:66:ARG:HG2   | 2.18                     | 0.43              |
| 120:BR:11:MET:HE2  | 120:BR:11:MET:HA    | 2.00                     | 0.43              |
| 120:BR:97:TRP:CE3  | 120:BR:179:ILE:HD12 | 2.54                     | 0.43              |
| 126:BX:131:PHE:CZ  | 140:UD:46:UNK:HB1   | 2.54                     | 0.43              |
| 128:BZ:17:ALA:HA   | 128:BZ:18:PRO:HD3   | 1.91                     | 0.43              |
| 61:UX:1:UNK:O      | 61:UX:4:UNK:HG2     | 2.19                     | 0.43              |
| 1:DA:744:GLU:O     | 1:DA:747:ARG:HG2    | 2.18                     | 0.43              |
| 1:DA:990:VAL:HG11  | 1:DA:1185:ARG:CG    | 2.46                     | 0.43              |
| 1:DA:1216:LEU:HD23 | 1:DA:1216:LEU:HA    | 1.76                     | 0.43              |
| 1:DA:1260:VAL:HA   | 1:DA:1261:PRO:HD3   | 1.66                     | 0.43              |
| 2:DD:124:TYR:CD1   | 46:Cd:84:LYS:HB2    | 2.54                     | 0.43              |
| 9:DQ:120:MET:HE3   | 9:DQ:120:MET:HB3    | 1.60                     | 0.43              |
| 15:DB:427:TRP:CH2  | 16:DC:1156:PRO:HB3  | 2.53                     | 0.43              |
| 16:DC:114:GLU:OE1  | 16:DC:118:GLY:HA2   | 2.19                     | 0.43              |
| 17:DE:162:LEU:HD12 | 17:DE:165:ARG:NH1   | 2.34                     | 0.43              |
| 19:DG:102:MET:HG3  | 19:DG:127:LEU:HD23  | 2.00                     | 0.43              |
| 19:DG:456:ARG:NH2  | 19:DG:546:ASP:OD2   | 2.52                     | 0.43              |
| 22:DK:172:LEU:HD12 | 22:DK:177:LYS:HD2   | 2.00                     | 0.43              |
| 33:CJ:293:ASP:OD1  | 33:CJ:293:ASP:N     | 2.52                     | 0.43              |
| 36:CN:115:TYR:CG   | 36:CN:116:TRP:N     | 2.87                     | 0.43              |
| 38:CP:30:ARG:HD2   | 38:CP:48:GLU:OE2    | 2.19                     | 0.43              |
| 44:Ca:32:PRO:O     | 63:UT:18:UNK:HG1    | 2.19                     | 0.43              |
| 52:Cn:204:LEU:HD12 | 52:Cn:204:LEU:HA    | 1.88                     | 0.43              |
| 55:Cr:86:LEU:HG    | 55:Cr:90:ILE:HD12   | 2.01                     | 0.43              |
| 55:Cr:164:LEU:HD13 | 55:Cr:166:VAL:HG23  | 2.01                     | 0.43              |
| 56:Cv:33:GLU:CD    | 56:Cv:33:GLU:H      | 2.25                     | 0.43              |
| 61:UR:6:UNK:HG2    | 61:UR:8:UNK:HG2     | 2.00                     | 0.43              |
| 65:A1:26:PRO:HA    | 65:A1:27:PRO:HD3    | 1.91                     | 0.43              |
| 65:A1:184:MET:HB3  | 65:A1:204:TYR:CE2   | 2.54                     | 0.43              |
| 68:A4:15:PRO:HA    | 68:A4:16:PRO:HD3    | 1.90                     | 0.43              |
| 72:A9:76:ARG:NH2   | 102:AA:392:A:H62    | 2.16                     | 0.43              |
| 74:AF:172:LYS:HA   | 86:AX:78:ARG:HD2    | 2.00                     | 0.43              |
| 74:AF:409:GLU:HB2  | 125:BW:47:PHE:CE2   | 2.52                     | 0.43              |
| 74:AF:441:ASP:OD1  | 74:AF:441:ASP:N     | 2.50                     | 0.43              |
| 79:AP:111:ASN:C    | 79:AP:111:ASN:HD22  | 2.25                     | 0.43              |
| 81:AR:194:GLU:O    | 81:AR:197:LYS:HG2   | 2.18                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 84:AV:215:TYR:CE1   | 92:Ag:132:TRP:HD1   | 2.37                     | 0.43              |
| 89:Ad:74:TYR:HE1    | 109:BG:168:HIS:HA   | 1.84                     | 0.43              |
| 93:Aj:284:VAL:O     | 93:Aj:288:ILE:HG12  | 2.18                     | 0.43              |
| 97:At:25:ARG:HG3    | 97:At:26:ALA:N      | 2.30                     | 0.43              |
| 97:At:37:VAL:O      | 97:At:40:ASN:HB2    | 2.19                     | 0.43              |
| 102:AA:1096:U:H2'   | 102:AA:1097:A:C8    | 2.51                     | 0.43              |
| 104:BB:176:LEU:HD23 | 104:BB:176:LEU:HA   | 1.81                     | 0.43              |
| 104:BB:347:LYS:HZ2  | 104:BB:405:TRP:CD1  | 2.36                     | 0.43              |
| 108:BF:310:LEU:HD23 | 108:BF:310:LEU:HA   | 1.75                     | 0.43              |
| 110:BH:95:LYS:HB2   | 110:BH:95:LYS:HE3   | 1.83                     | 0.43              |
| 111:BI:119:GLU:OE2  | 111:BI:235:PHE:HD2  | 2.02                     | 0.43              |
| 111:BI:227:ASN:HB3  | 111:BI:231:ARG:HH12 | 1.83                     | 0.43              |
| 117:BO:129:TYR:CZ   | 117:BO:139:LEU:HD21 | 2.54                     | 0.43              |
| 122:BT:57:LEU:HD23  | 122:BT:57:LEU:HA    | 1.72                     | 0.43              |
| 123:BU:147:GLU:HG3  | 123:BU:148:PHE:N    | 2.34                     | 0.43              |
| 124:BV:59:ARG:HD3   | 124:BV:116:HIS:O    | 2.18                     | 0.43              |
| 128:BZ:2:ARG:HA     | 128:BZ:2:ARG:HD2    | 1.85                     | 0.43              |
| 129:Ba:105:ARG:NH1  | 129:Ba:108:CYS:O    | 2.50                     | 0.43              |
| 1:DA:557:SER:OG     | 1:DA:562:LYS:NZ     | 2.22                     | 0.43              |
| 1:DA:1089:ASP:HB3   | 1:DA:1632:LYS:HG2   | 2.00                     | 0.43              |
| 2:DD:189:GLU:CD     | 2:DD:192:MET:HE3    | 2.44                     | 0.43              |
| 2:DD:298:MET:HG2    | 2:DD:314:PHE:CZ     | 2.54                     | 0.43              |
| 3:DI:320:GLN:NE2    | 7:DO:238:ASN:HA     | 2.33                     | 0.43              |
| 4:DL:156:GLU:OE2    | 29:CE:135:ARG:NH2   | 2.51                     | 0.43              |
| 5:DM:164:ILE:HG23   | 29:CE:343:TYR:OH    | 2.18                     | 0.43              |
| 8:DP:48:GLN:NE2     | 8:DP:67:GLN:OE1     | 2.50                     | 0.43              |
| 8:DP:78:LEU:HD23    | 8:DP:78:LEU:HA      | 1.79                     | 0.43              |
| 9:DQ:106:MET:HE2    | 9:DQ:221:LEU:HD22   | 2.00                     | 0.43              |
| 10:DR:250:ARG:HB3   | 10:DR:250:ARG:NH1   | 2.33                     | 0.43              |
| 12:DU:115:LYS:HG2   | 12:DU:132:PHE:CE2   | 2.54                     | 0.43              |
| 16:DC:87:MET:HE2    | 16:DC:957:LYS:HA    | 2.01                     | 0.43              |
| 16:DC:242:HIS:CD2   | 16:DC:242:HIS:N     | 2.87                     | 0.43              |
| 17:DE:729:ARG:HH22  | 50:Ck:92:ARG:HH12   | 1.66                     | 0.43              |
| 18:DF:43:THR:HG22   | 18:DF:44:ALA:H      | 1.84                     | 0.43              |
| 20:DH:195:TYR:CD2   | 20:DH:195:TYR:N     | 2.86                     | 0.43              |
| 24:DV:103:ASP:OD1   | 24:DV:103:ASP:N     | 2.52                     | 0.43              |
| 25:DW:61:ARG:HG2    | 47:Cg:374:GLU:OE2   | 2.19                     | 0.43              |
| 31:CH:17:PRO:HA     | 31:CH:18:PRO:HD3    | 1.76                     | 0.43              |
| 31:CH:211:GLN:HG2   | 45:Cb:31:TRP:CZ3    | 2.54                     | 0.43              |
| 33:CJ:257:VAL:HG13  | 33:CJ:399:ARG:HB2   | 2.01                     | 0.43              |
| 33:CJ:388:SER:O     | 33:CJ:388:SER:OG    | 2.30                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 33:CJ:758:TRP:CG    | 33:CJ:759:PRO:HA    | 2.53                     | 0.43              |
| 37:CO:320:ASP:OD2   | 37:CO:322:ARG:NH1   | 2.52                     | 0.43              |
| 38:CP:23:ALA:HB2    | 38:CP:51:HIS:NE2    | 2.29                     | 0.43              |
| 44:Ca:524:VAL:HA    | 44:Ca:525:PRO:HD2   | 1.77                     | 0.43              |
| 47:Cg:114:GLU:CD    | 47:Cg:401:ILE:HG12  | 2.44                     | 0.43              |
| 47:Cg:226:CYS:O     | 47:Cg:226:CYS:SG    | 2.77                     | 0.43              |
| 55:Cr:12:ALA:O      | 55:Cr:16:HIS:HB2    | 2.19                     | 0.43              |
| 56:Cv:740:ILE:HG23  | 56:Cv:786:VAL:HG13  | 2.01                     | 0.43              |
| 56:Cv:797:ALA:HA    | 56:Cv:800:VAL:HG12  | 2.01                     | 0.43              |
| 57:CA:565:A:H4'     | 57:CA:566:U:OP1     | 2.19                     | 0.43              |
| 71:A8:51:ALA:O      | 86:AX:75:PRO:HB3    | 2.18                     | 0.43              |
| 74:AF:186:ARG:NH1   | 102:AA:290:A:N6     | 2.66                     | 0.43              |
| 78:AN:116:ILE:HG23  | 78:AN:120:ASP:HB2   | 2.01                     | 0.43              |
| 85:AW:10:MET:HE2    | 85:AW:12:HIS:HD2    | 1.83                     | 0.43              |
| 85:AW:128:LEU:HD11  | 114:BL:99:HIS:HA    | 2.01                     | 0.43              |
| 85:AW:239:GLU:OE2   | 103:BA:601:ARG:NH2  | 2.52                     | 0.43              |
| 89:Ad:263:LEU:HD13  | 118:BP:38:LEU:HD21  | 2.01                     | 0.43              |
| 95:Ao:130:LEU:HA    | 95:Ao:131:PRO:HD3   | 1.79                     | 0.43              |
| 98:Av:50:TYR:CZ     | 98:Av:52:GLU:HA     | 2.53                     | 0.43              |
| 103:BA:301:HIS:CD2  | 103:BA:303:ILE:HG23 | 2.54                     | 0.43              |
| 103:BA:647:LEU:HD23 | 103:BA:647:LEU:HA   | 1.85                     | 0.43              |
| 105:BC:267:ILE:O    | 105:BC:268:LEU:HB2  | 2.19                     | 0.43              |
| 109:BG:133:ILE:HD12 | 109:BG:160:MET:HE3  | 2.00                     | 0.43              |
| 109:BG:150:TYR:HB2  | 109:BG:176:LEU:HD12 | 2.00                     | 0.43              |
| 120:BR:44:LEU:HD23  | 120:BR:44:LEU:HA    | 1.74                     | 0.43              |
| 134:Bf:76:PHE:CG    | 134:Bf:77:ALA:N     | 2.84                     | 0.43              |
| 1:DA:905:GLU:O      | 1:DA:908:ARG:HG2    | 2.18                     | 0.43              |
| 1:DA:924:TRP:CD1    | 56:Cv:1000:MET:HE2  | 2.53                     | 0.43              |
| 2:DD:679:ASN:C      | 2:DD:679:ASN:HD22   | 2.27                     | 0.43              |
| 3:DI:133:LEU:HD23   | 3:DI:133:LEU:HA     | 1.84                     | 0.43              |
| 6:DN:77:LEU:N       | 6:DN:78:PRO:CD      | 2.82                     | 0.43              |
| 13:DZ:20:ARG:HD2    | 44:Ca:172:PHE:CD2   | 2.54                     | 0.43              |
| 15:DB:720:LYS:HB2   | 15:DB:720:LYS:HE3   | 1.77                     | 0.43              |
| 16:DC:91:LYS:HG3    | 17:DE:166:ARG:HD2   | 2.01                     | 0.43              |
| 16:DC:389:GLU:HG3   | 16:DC:496:LYS:HZ1   | 1.83                     | 0.43              |
| 18:DF:192:LEU:C     | 18:DF:194:THR:H     | 2.27                     | 0.43              |
| 19:DG:143:HIS:HA    | 19:DG:164:LEU:HD21  | 2.00                     | 0.43              |
| 19:DG:293:ARG:HA    | 19:DG:293:ARG:HD2   | 1.91                     | 0.43              |
| 20:DH:14:TYR:OH     | 48:Ci:136:HIS:CD2   | 2.72                     | 0.43              |
| 24:DV:48:HIS:O      | 24:DV:61:ARG:NH1    | 2.51                     | 0.43              |
| 29:CE:417:ASN:HA    | 29:CE:418:PRO:HD3   | 1.88                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 31:CH:91:LEU:HD23   | 31:CH:91:LEU:HA    | 1.82                     | 0.43              |
| 32:CI:15:LEU:HA     | 32:CI:15:LEU:HD23  | 1.83                     | 0.43              |
| 32:CI:325:GLU:OE2   | 33:CJ:178:SER:HB2  | 2.19                     | 0.43              |
| 36:CN:51:LEU:HD12   | 36:CN:51:LEU:HA    | 1.79                     | 0.43              |
| 37:CO:88:PRO:O      | 37:CO:89:HIS:HB2   | 2.18                     | 0.43              |
| 37:CO:414:LEU:HD23  | 37:CO:414:LEU:HA   | 1.82                     | 0.43              |
| 40:CR:116:PRO:HB3   | 40:CR:135:PHE:HZ   | 1.84                     | 0.43              |
| 44:Ca:138:LYS:HZ1   | 44:Ca:141:THR:HA   | 1.84                     | 0.43              |
| 47:Cg:155:LYS:HE2   | 152:Cg:501:GTP:O1B | 2.19                     | 0.43              |
| 50:Ck:221:ALA:O     | 50:Ck:225:MET:HB2  | 2.19                     | 0.43              |
| 50:Ck:373:ARG:O     | 50:Ck:377:VAL:HG23 | 2.19                     | 0.43              |
| 50:Ck:674:LEU:CD2   | 50:Ck:707:LEU:HG   | 2.48                     | 0.43              |
| 55:Cr:102:PHE:HD2   | 55:Cr:184:VAL:HG12 | 1.83                     | 0.43              |
| 56:Cv:740:ILE:HD13  | 56:Cv:740:ILE:HA   | 1.86                     | 0.43              |
| 57:CA:309:A:O2'     | 57:CA:351:A:OP2    | 2.37                     | 0.43              |
| 64:A0:143:LEU:HD21  | 115:BM:208:LYS:HG2 | 1.99                     | 0.43              |
| 66:A2:12:ALA:O      | 66:A2:15:GLU:HG2   | 2.19                     | 0.43              |
| 66:A2:17:VAL:HG21   | 86:AX:224:VAL:HG11 | 2.00                     | 0.43              |
| 66:A2:389:HIS:HD2   | 102:AA:32:U:N3     | 2.17                     | 0.43              |
| 71:A8:168:LEU:HD23  | 71:A8:168:LEU:H    | 1.83                     | 0.43              |
| 73:AE:121:TRP:HA    | 131:Bc:56:TRP:CH2  | 2.54                     | 0.43              |
| 73:AE:169:GLN:NE2   | 73:AE:213:LYS:NZ   | 2.66                     | 0.43              |
| 75:AI:205:TYR:CZ    | 75:AI:208:ARG:NH1  | 2.87                     | 0.43              |
| 76:AJ:91:ALA:HB1    | 92:Ag:222:PHE:CD2  | 2.53                     | 0.43              |
| 78:AN:135:LYS:NZ    | 102:AA:835:A:OP1   | 2.44                     | 0.43              |
| 79:AP:45:ARG:HD2    | 79:AP:45:ARG:N     | 2.29                     | 0.43              |
| 82:AT:25:PRO:O      | 82:AT:29:VAL:HG13  | 2.19                     | 0.43              |
| 85:AW:54:GLY:O      | 102:AA:93:A:H5''   | 2.19                     | 0.43              |
| 86:AX:96:ASN:HA     | 86:AX:97:PRO:HD3   | 1.91                     | 0.43              |
| 86:AX:147:LEU:HD11  | 102:AA:532:U:H5'   | 2.01                     | 0.43              |
| 88:Ab:174:THR:HA    | 88:Ab:211:GLU:OE2  | 2.18                     | 0.43              |
| 88:Ab:348:LEU:HD12  | 88:Ab:348:LEU:HA   | 1.84                     | 0.43              |
| 91:Af:164:HIS:HD2   | 91:Af:166:LYS:HB2  | 1.84                     | 0.43              |
| 93:Aj:31:VAL:HA     | 93:Aj:32:PRO:HD3   | 1.88                     | 0.43              |
| 95:Ao:124:TYR:HE2   | 102:AA:331:C:H5'   | 1.83                     | 0.43              |
| 102:AA:135:G:O2'    | 102:AA:826:A:H2'   | 2.19                     | 0.43              |
| 102:AA:302:G:H22    | 102:AA:335:G:H2'   | 1.84                     | 0.43              |
| 102:AA:1156:A:H1'   | 102:AA:1157:A:C8   | 2.54                     | 0.43              |
| 103:BA:617:LEU:HD23 | 103:BA:617:LEU:HA  | 1.84                     | 0.43              |
| 108:BF:207:GLU:OE2  | 108:BF:281:ARG:HD3 | 2.19                     | 0.43              |
| 110:BH:102:ASN:HD21 | 110:BH:169:GLU:HG3 | 1.82                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 115:BM:86:VAL:HG12 | 115:BM:87:ARG:HD3   | 2.00                     | 0.43              |
| 133:Be:2:SER:HA    | 133:Be:3:SER:HA     | 1.60                     | 0.43              |
| 136:Bh:56:LYS:HG3  | 136:Bh:57:PRO:HD2   | 2.01                     | 0.43              |
| 4:DL:117:ASP:CA    | 4:DL:121:ILE:HG13   | 2.49                     | 0.42              |
| 4:DL:120:PHE:HE1   | 4:DL:213:SER:HA     | 1.84                     | 0.42              |
| 6:DN:27:ASP:CG     | 6:DN:29:ARG:HG2     | 2.44                     | 0.42              |
| 15:DB:528:PHE:CE2  | 15:DB:529:LEU:HG    | 2.54                     | 0.42              |
| 15:DB:891:GLN:HA   | 33:CJ:128:LYS:HE2   | 2.01                     | 0.42              |
| 17:DE:333:ASP:HA   | 17:DE:336:ILE:HD12  | 2.01                     | 0.42              |
| 18:DF:88:LEU:HD21  | 41:CS:97:LYS:HB2    | 2.01                     | 0.42              |
| 18:DF:125:TYR:N    | 18:DF:175:GLN:HE22  | 2.16                     | 0.42              |
| 19:DG:141:THR:O    | 19:DG:145:VAL:HG23  | 2.19                     | 0.42              |
| 19:DG:318:ILE:HD12 | 19:DG:329:LEU:HD21  | 2.01                     | 0.42              |
| 20:DH:354:LEU:HD12 | 20:DH:354:LEU:HA    | 1.86                     | 0.42              |
| 25:DW:102:MET:HE2  | 25:DW:102:MET:HB2   | 1.65                     | 0.42              |
| 25:DW:112:PHE:CD1  | 25:DW:113:PRO:HD2   | 2.54                     | 0.42              |
| 31:CH:67:MET:N     | 57:CA:6:U:OP2       | 2.44                     | 0.42              |
| 33:CJ:731:MET:HE2  | 33:CJ:731:MET:HB3   | 1.77                     | 0.42              |
| 34:CK:20:MET:HE2   | 34:CK:20:MET:HA     | 2.01                     | 0.42              |
| 34:CK:73:GLN:HB3   | 45:Cb:179:GLU:HG3   | 2.01                     | 0.42              |
| 35:CL:72:PHE:HB2   | 35:CL:119:PHE:CE1   | 2.49                     | 0.42              |
| 35:CL:78:MET:HE3   | 35:CL:105:ARG:NH2   | 2.28                     | 0.42              |
| 37:CO:416:THR:OG1  | 37:CO:417:LYS:N     | 2.51                     | 0.42              |
| 39:CQ:108:VAL:HG11 | 39:CQ:129:ARG:NH2   | 2.34                     | 0.42              |
| 43:CZ:277:PHE:CE1  | 43:CZ:280:ILE:HG13  | 2.53                     | 0.42              |
| 44:Ca:154:GLU:HA   | 44:Ca:157:LYS:HB2   | 2.00                     | 0.42              |
| 48:Ci:33:LEU:HD13  | 50:Ck:735:ILE:HG21  | 2.00                     | 0.42              |
| 55:Cr:14:GLU:OE1   | 55:Cr:14:GLU:N      | 2.49                     | 0.42              |
| 56:Cv:234:MET:HE2  | 56:Cv:234:MET:HB3   | 1.96                     | 0.42              |
| 57:CA:44:U:H2'     | 57:CA:45:G:H3'      | 2.01                     | 0.42              |
| 57:CA:233:C:H4'    | 57:CA:234:C:C5'     | 2.48                     | 0.42              |
| 66:A2:86:MET:O     | 66:A2:89:GLU:HG3    | 2.18                     | 0.42              |
| 66:A2:177:LEU:HD23 | 66:A2:177:LEU:HA    | 1.72                     | 0.42              |
| 76:AJ:74:ARG:HH21  | 76:AJ:85:PRO:HD3    | 1.84                     | 0.42              |
| 76:AJ:80:ARG:HG3   | 76:AJ:80:ARG:NH1    | 2.32                     | 0.42              |
| 77:AK:230:GLN:HE22 | 77:AK:318:GLY:H     | 1.68                     | 0.42              |
| 79:AP:200:LEU:HD22 | 79:AP:205:VAL:HG21  | 2.00                     | 0.42              |
| 81:AR:153:ARG:NH1  | 81:AR:158:VAL:HG11  | 2.34                     | 0.42              |
| 88:Ab:283:ASN:HD21 | 88:Ab:355:VAL:HG23  | 1.85                     | 0.42              |
| 89:Ad:266:GLU:OE2  | 118:BP:44:ARG:HA    | 2.19                     | 0.42              |
| 95:Ao:239:ALA:HB3  | 124:BV:158:VAL:HG13 | 2.01                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 96:Ap:94:GLY:O      | 96:Ap:96:GLU:N     | 2.52                     | 0.42              |
| 154:Av:301:NAD:H51A | 154:Av:301:NAD:H2B | 1.74                     | 0.42              |
| 102:AA:531:U:C5     | 135:Bg:76:SER:HB3  | 2.54                     | 0.42              |
| 102:AA:1172:A:C8    | 117:BO:125:GLU:HB2 | 2.54                     | 0.42              |
| 103:BA:477:LEU:HD23 | 103:BA:477:LEU:HA  | 1.90                     | 0.42              |
| 103:BA:532:MET:HE2  | 103:BA:532:MET:HB3 | 1.84                     | 0.42              |
| 108:BF:213:LEU:CD1  | 108:BF:236:ALA:HB2 | 2.46                     | 0.42              |
| 109:BG:39:PHE:HE1   | 109:BG:67:HIS:HD1  | 1.66                     | 0.42              |
| 111:BI:167:LEU:HG   | 111:BI:171:ARG:NH1 | 2.34                     | 0.42              |
| 114:BL:79:LYS:HG3   | 114:BL:83:HIS:CD2  | 2.53                     | 0.42              |
| 119:BQ:86:VAL:HG12  | 119:BQ:179:GLY:HA3 | 2.01                     | 0.42              |
| 133:Be:98:TRP:NE1   | 133:Be:101:ALA:HB2 | 2.34                     | 0.42              |
| 143:UI:5:UNK:HA     | 143:UI:8:UNK:HG3   | 1.99                     | 0.42              |
| 1:DA:421:GLY:HA2    | 1:DA:489:ARG:HD2   | 2.01                     | 0.42              |
| 1:DA:529:ILE:O      | 1:DA:532:ARG:N     | 2.51                     | 0.42              |
| 1:DA:1029:LYS:HE3   | 5:DM:257:GLU:OE1   | 2.19                     | 0.42              |
| 2:DD:745:ASN:OD1    | 2:DD:746:PRO:HD2   | 2.19                     | 0.42              |
| 5:DM:36:TYR:CZ      | 29:CE:314:MET:HE2  | 2.54                     | 0.42              |
| 5:DM:45:ARG:O       | 5:DM:49:MET:HE3    | 2.19                     | 0.42              |
| 6:DN:73:VAL:HG23    | 6:DN:75:VAL:HB     | 2.01                     | 0.42              |
| 6:DN:142:ARG:HG2    | 6:DN:142:ARG:HH11  | 1.83                     | 0.42              |
| 10:DR:245:MET:H     | 10:DR:245:MET:HG3  | 1.63                     | 0.42              |
| 15:DB:975:LYS:CA    | 19:DG:92:GLN:HE22  | 2.31                     | 0.42              |
| 16:DC:46:ARG:HH21   | 16:DC:401:ARG:HD2  | 1.84                     | 0.42              |
| 16:DC:317:GLU:HG2   | 16:DC:320:ARG:HH12 | 1.84                     | 0.42              |
| 16:DC:517:LEU:HD23  | 16:DC:517:LEU:HA   | 1.79                     | 0.42              |
| 16:DC:1102:GLY:HA2  | 20:DH:59:MET:HE3   | 2.01                     | 0.42              |
| 18:DF:125:TYR:H     | 18:DF:175:GLN:NE2  | 2.15                     | 0.42              |
| 21:DJ:38:MET:HE2    | 21:DJ:38:MET:HB3   | 1.76                     | 0.42              |
| 21:DJ:304:ILE:HD12  | 23:DT:42:PHE:HD2   | 1.84                     | 0.42              |
| 30:CF:81:LYS:HB2    | 30:CF:81:LYS:HE3   | 1.82                     | 0.42              |
| 32:CI:161:PHE:HA    | 32:CI:162:PRO:HD3  | 1.80                     | 0.42              |
| 32:CI:431:LEU:HA    | 32:CI:431:LEU:HD23 | 1.82                     | 0.42              |
| 33:CJ:485:GLU:HA    | 33:CJ:515:ALA:HB2  | 2.01                     | 0.42              |
| 35:CL:66:CYS:C      | 35:CL:67:LEU:HD12  | 2.44                     | 0.42              |
| 37:CO:78:PRO:HG2    | 52:Cn:185:TYR:HB3  | 2.01                     | 0.42              |
| 40:CR:9:TYR:N       | 40:CR:9:TYR:CD1    | 2.87                     | 0.42              |
| 49:Cj:99:ASN:OD1    | 49:Cj:100:ILE:N    | 2.52                     | 0.42              |
| 51:Cm:215:LYS:HE3   | 57:CA:336:U:OP2    | 2.19                     | 0.42              |
| 52:Cn:213:LYS:HE2   | 52:Cn:213:LYS:HB2  | 1.90                     | 0.42              |
| 53:Cp:151:ARG:H     | 53:Cp:154:GLN:HE21 | 1.67                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:Cq:254:TYR:HD1   | 54:Cq:254:TYR:HA    | 1.76                     | 0.42              |
| 56:Cv:169:LYS:HB3   | 56:Cv:174:ARG:HG2   | 2.00                     | 0.42              |
| 56:Cv:1106:ALA:HB3  | 56:Cv:1111:LYS:HE3  | 2.01                     | 0.42              |
| 57:CA:299:U:O2'     | 57:CA:300:G:O5'     | 2.32                     | 0.42              |
| 67:A3:164:MET:HE2   | 67:A3:164:MET:HB3   | 1.95                     | 0.42              |
| 68:A4:88:GLY:HA3    | 89:Ad:133:VAL:HG22  | 2.02                     | 0.42              |
| 72:A9:71:ARG:HB2    | 72:A9:94:HIS:ND1    | 2.33                     | 0.42              |
| 81:AR:243:PRO:O     | 81:AR:246:VAL:HG22  | 2.19                     | 0.42              |
| 87:AY:255:ARG:HG2   | 87:AY:255:ARG:NH1   | 2.34                     | 0.42              |
| 89:Ad:86:LEU:HD22   | 132:Bd:18:LEU:HD22  | 2.01                     | 0.42              |
| 95:Ao:100:ARG:HD3   | 97:At:141:TRP:CZ2   | 2.54                     | 0.42              |
| 98:Av:182:LYS:HB3   | 98:Av:182:LYS:HZ3   | 1.83                     | 0.42              |
| 102:AA:1:A:H5'      | 103:BA:631:LYS:NZ   | 2.35                     | 0.42              |
| 102:AA:15:G:H3'     | 102:AA:15:G:N3      | 2.35                     | 0.42              |
| 102:AA:538:U:O3'    | 102:AA:539:A:H8     | 2.01                     | 0.42              |
| 103:BA:365:ASP:N    | 103:BA:365:ASP:OD1  | 2.49                     | 0.42              |
| 103:BA:569:LEU:HD12 | 103:BA:569:LEU:HA   | 1.83                     | 0.42              |
| 103:BA:627:SER:OG   | 103:BA:629:SER:O    | 2.38                     | 0.42              |
| 104:BB:196:TRP:CZ2  | 104:BB:213:LEU:HD23 | 2.47                     | 0.42              |
| 108:BF:143:GLN:O    | 108:BF:146:LEU:HB3  | 2.19                     | 0.42              |
| 115:BM:136:PHE:O    | 115:BM:139:GLN:HG2  | 2.19                     | 0.42              |
| 2:DD:136:LYS:NZ     | 57:CA:87:U:O2       | 2.43                     | 0.42              |
| 2:DD:239:LEU:HD23   | 2:DD:239:LEU:HA     | 1.85                     | 0.42              |
| 2:DD:471:GLU:HB3    | 2:DD:475:ALA:HB3    | 2.01                     | 0.42              |
| 2:DD:504:ASN:N      | 2:DD:504:ASN:OD1    | 2.51                     | 0.42              |
| 2:DD:742:ASP:N      | 2:DD:742:ASP:OD1    | 2.53                     | 0.42              |
| 3:DI:47:LEU:HD23    | 3:DI:47:LEU:HA      | 1.80                     | 0.42              |
| 3:DI:286:GLY:O      | 3:DI:288:ILE:HG23   | 2.19                     | 0.42              |
| 3:DI:351:LEU:HD12   | 3:DI:351:LEU:HA     | 1.79                     | 0.42              |
| 6:DN:154:MET:HE2    | 6:DN:154:MET:HB3    | 1.78                     | 0.42              |
| 10:DR:83:MET:HE2    | 10:DR:83:MET:HB3    | 1.96                     | 0.42              |
| 11:DS:43:MET:HE1    | 57:CA:204:U:H5'     | 2.00                     | 0.42              |
| 12:DU:97:ARG:NH2    | 12:DU:211:ARG:HH21  | 2.17                     | 0.42              |
| 13:DZ:57:GLY:O      | 13:DZ:58:ASP:HB3    | 2.18                     | 0.42              |
| 15:DB:98:ASP:O      | 15:DB:103:TYR:N     | 2.51                     | 0.42              |
| 16:DC:218:TYR:CD2   | 16:DC:256:ILE:HD11  | 2.53                     | 0.42              |
| 16:DC:844:ALA:CB    | 17:DE:68:PRO:HB3    | 2.43                     | 0.42              |
| 17:DE:232:LEU:HD12  | 17:DE:420:VAL:HG13  | 2.01                     | 0.42              |
| 17:DE:725:PRO:HG2   | 22:DK:146:TYR:CE2   | 2.53                     | 0.42              |
| 18:DF:314:TYR:CZ    | 18:DF:318:MET:HG3   | 2.54                     | 0.42              |
| 19:DG:490:ARG:NH1   | 32:CI:4:LEU:HD11    | 2.34                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:DT:105:ARG:NH1   | 23:DT:146:GLN:HB3   | 2.34                     | 0.42              |
| 24:DV:93:GLN:OE1    | 24:DV:96:ARG:NH1    | 2.52                     | 0.42              |
| 26:DX:95:VAL:HG22   | 26:DX:127:MET:SD    | 2.59                     | 0.42              |
| 28:CC:74:LEU:HB3    | 28:CC:77:THR:HB     | 2.01                     | 0.42              |
| 34:CK:310:ILE:HD12  | 42:CU:38:PHE:CE1    | 2.54                     | 0.42              |
| 37:CO:90:MET:HB3    | 37:CO:91:PRO:CD     | 2.47                     | 0.42              |
| 37:CO:107:LEU:HB2   | 37:CO:112:LYS:NZ    | 2.34                     | 0.42              |
| 37:CO:266:LEU:HD13  | 37:CO:274:TYR:HA    | 2.02                     | 0.42              |
| 39:CQ:133:HIS:ND1   | 39:CQ:157:LYS:NZ    | 2.59                     | 0.42              |
| 40:CR:144:PRO:HG2   | 40:CR:147:ILE:HG12  | 2.01                     | 0.42              |
| 43:CZ:249:SER:HB3   | 43:CZ:252:CYS:SG    | 2.58                     | 0.42              |
| 44:Ca:544:LYS:HA    | 44:Ca:544:LYS:HD2   | 1.92                     | 0.42              |
| 45:Cb:10:LYS:HB2    | 57:CA:542:G:H5'     | 2.01                     | 0.42              |
| 45:Cb:14:ASN:ND2    | 51:Cm:154:ASN:O     | 2.47                     | 0.42              |
| 45:Cb:90:GLU:OE1    | 45:Cb:90:GLU:N      | 2.47                     | 0.42              |
| 45:Cb:132:LEU:HD11  | 45:Cb:145:LYS:HD3   | 2.01                     | 0.42              |
| 48:Ci:116:GLY:HA3   | 57:CA:419:U:H5'     | 2.00                     | 0.42              |
| 50:Ck:691:GLN:HG3   | 50:Ck:692:GLY:N     | 2.33                     | 0.42              |
| 56:Cv:682:VAL:O     | 56:Cv:695:SER:HA    | 2.19                     | 0.42              |
| 56:Cv:943:LEU:O     | 56:Cv:944:HIS:C     | 2.62                     | 0.42              |
| 65:A1:75:VAL:HG12   | 65:A1:121:PRO:O     | 2.19                     | 0.42              |
| 68:A4:68:LEU:HD13   | 118:BP:61:LEU:HD13  | 2.01                     | 0.42              |
| 73:AE:127:PHE:CE1   | 131:Bc:72:GLU:HA    | 2.54                     | 0.42              |
| 74:AF:165:GLU:N     | 74:AF:168:GLU:OE1   | 2.52                     | 0.42              |
| 78:AN:107:THR:HG21  | 102:AA:1115:A:O3'   | 2.20                     | 0.42              |
| 79:AP:257:MET:HG2   | 125:BW:11:ARG:HH12  | 1.84                     | 0.42              |
| 80:AQ:73:ARG:HD2    | 80:AQ:143:ALA:HB2   | 2.02                     | 0.42              |
| 88:Ab:195:MET:HG2   | 88:Ab:222:PHE:CE2   | 2.55                     | 0.42              |
| 90:Ae:83:SER:HB3    | 90:Ae:86:HIS:HD2    | 1.84                     | 0.42              |
| 91:Af:72:ASP:OD1    | 91:Af:72:ASP:N      | 2.53                     | 0.42              |
| 91:Af:162:ARG:HG3   | 103:BA:272:GLN:HE22 | 1.84                     | 0.42              |
| 96:Ap:127:LEU:HD23  | 96:Ap:127:LEU:HA    | 1.73                     | 0.42              |
| 103:BA:223:LYS:HD3  | 103:BA:232:TYR:HE1  | 1.84                     | 0.42              |
| 103:BA:466:LEU:HD12 | 103:BA:466:LEU:HA   | 1.76                     | 0.42              |
| 104:BB:252:ASP:O    | 104:BB:383:LYS:HE3  | 2.19                     | 0.42              |
| 105:BC:108:GLN:HE22 | 105:BC:242:LEU:H    | 1.67                     | 0.42              |
| 105:BC:130:LEU:HA   | 105:BC:130:LEU:HD23 | 1.82                     | 0.42              |
| 105:BC:301:MET:HE3  | 105:BC:301:MET:HB3  | 1.85                     | 0.42              |
| 105:BC:346:ASP:HB3  | 105:BC:377:HIS:CE1  | 2.54                     | 0.42              |
| 105:BC:475:LEU:HD23 | 105:BC:503:THR:HG21 | 2.01                     | 0.42              |
| 109:BG:65:MET:HG2   | 109:BG:66:TYR:N     | 2.34                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 110:BH:156:LEU:HD12 | 110:BH:156:LEU:HA  | 1.83                     | 0.42              |
| 117:BO:141:ASP:HB2  | 117:BO:153:ARG:HG3 | 2.02                     | 0.42              |
| 122:BT:86:ARG:HG2   | 122:BT:86:ARG:NH1  | 2.34                     | 0.42              |
| 123:BU:165:GLU:H    | 123:BU:165:GLU:CD  | 2.27                     | 0.42              |
| 126:BX:74:PRO:HA    | 126:BX:75:PRO:HD3  | 1.91                     | 0.42              |
| 128:BZ:117:LYS:HA   | 128:BZ:118:PRO:HD3 | 1.90                     | 0.42              |
| 129:Ba:59:ASP:HB2   | 129:Ba:66:VAL:HG22 | 2.01                     | 0.42              |
| 130:Bb:67:ARG:O     | 130:Bb:71:PRO:HB3  | 2.19                     | 0.42              |
| 132:Bd:76:GLU:HG2   | 132:Bd:77:HIS:O    | 2.19                     | 0.42              |
| 135:Bg:87:ASN:ND2   | 135:Bg:90:LEU:HD13 | 2.33                     | 0.42              |
| 136:Bh:8:ARG:HH11   | 136:Bh:37:GLN:HE21 | 1.66                     | 0.42              |
| 1:DA:702:ASP:OD2    | 1:DA:705:LYS:HG3   | 2.20                     | 0.42              |
| 2:DD:42:MET:HE3     | 2:DD:42:MET:HB3    | 1.83                     | 0.42              |
| 2:DD:150:GLY:HA3    | 57:CA:80:U:O4      | 2.19                     | 0.42              |
| 2:DD:668:ARG:HG3    | 2:DD:668:ARG:HH11  | 1.83                     | 0.42              |
| 6:DN:212:THR:OG1    | 44:Ca:193:ARG:NH1  | 2.50                     | 0.42              |
| 6:DN:235:ASN:OD1    | 6:DN:238:ASN:ND2   | 2.52                     | 0.42              |
| 8:DP:148:LYS:HB2    | 8:DP:148:LYS:HE2   | 1.84                     | 0.42              |
| 8:DP:200:SER:HB2    | 8:DP:207:TYR:HE2   | 1.84                     | 0.42              |
| 15:DB:120:TYR:O     | 15:DB:122:HIS:HD2  | 2.02                     | 0.42              |
| 16:DC:147:ARG:HH11  | 16:DC:232:GLN:HB2  | 1.84                     | 0.42              |
| 16:DC:1082:ARG:NH2  | 23:DT:75:ARG:HD3   | 2.33                     | 0.42              |
| 16:DC:1164:TRP:CG   | 16:DC:1165:SER:H   | 2.37                     | 0.42              |
| 19:DG:102:MET:HE1   | 19:DG:134:PRO:HA   | 2.01                     | 0.42              |
| 21:DJ:180:LEU:HA    | 21:DJ:180:LEU:HD23 | 1.80                     | 0.42              |
| 27:DY:35:PRO:CB     | 47:Cg:464:VAL:HG11 | 2.49                     | 0.42              |
| 33:CJ:433:THR:O     | 50:Ck:675:GLY:HA2  | 2.20                     | 0.42              |
| 35:CL:129:LEU:HA    | 35:CL:130:PRO:HD2  | 1.95                     | 0.42              |
| 36:CN:16:ASP:O      | 48:Ci:133:TYR:HB3  | 2.19                     | 0.42              |
| 37:CO:124:ILE:HA    | 37:CO:125:PRO:HD3  | 1.91                     | 0.42              |
| 37:CO:253:ALA:O     | 37:CO:257:ARG:HG3  | 2.20                     | 0.42              |
| 40:CR:184:LYS:NZ    | 40:CR:185:PHE:CE2  | 2.85                     | 0.42              |
| 40:CR:320:VAL:O     | 46:Cd:278:ALA:CA   | 2.64                     | 0.42              |
| 41:CS:106:TYR:HD2   | 41:CS:140:MET:CE   | 2.30                     | 0.42              |
| 44:Ca:293:LEU:HD13  | 44:Ca:297:LEU:HD13 | 2.01                     | 0.42              |
| 53:Cp:67:ARG:NH2    | 57:CA:45:G:N7      | 2.66                     | 0.42              |
| 53:Cp:151:ARG:O     | 53:Cp:154:GLN:HG2  | 2.19                     | 0.42              |
| 56:Cv:95:ARG:HG3    | 56:Cv:95:ARG:NH1   | 2.33                     | 0.42              |
| 56:Cv:559:GLN:HE21  | 61:UR:3:UNK:HG1    | 1.83                     | 0.42              |
| 71:A8:83:ARG:HE     | 71:A8:83:ARG:HB3   | 1.63                     | 0.42              |
| 73:AE:113:GLU:CD    | 73:AE:113:GLU:H    | 2.26                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 74:AF:72:ILE:HG12   | 74:AF:72:ILE:O      | 2.19                     | 0.42              |
| 74:AF:385:LEU:HD23  | 74:AF:385:LEU:HA    | 1.74                     | 0.42              |
| 77:AK:277:PRO:HG2   | 77:AK:332:GLU:O     | 2.19                     | 0.42              |
| 81:AR:185:ARG:HD3   | 81:AR:185:ARG:HA    | 1.85                     | 0.42              |
| 85:AW:46:PRO:HA     | 87:AY:26:PRO:HA     | 2.01                     | 0.42              |
| 85:AW:161:MET:HE1   | 107:BE:394:LEU:HG   | 2.01                     | 0.42              |
| 89:Ad:166:PHE:HE2   | 93:Aj:24:ARG:HD3    | 1.84                     | 0.42              |
| 95:Ao:111:LEU:HD23  | 95:Ao:111:LEU:HA    | 1.93                     | 0.42              |
| 97:At:34:ARG:NH1    | 120:BR:127:ARG:HH11 | 2.17                     | 0.42              |
| 102:AA:574:A:H61    | 102:AA:1167:A:H62   | 1.66                     | 0.42              |
| 103:BA:231:TYR:HE1  | 103:BA:296:ARG:NH1  | 2.17                     | 0.42              |
| 103:BA:299:TYR:CD1  | 131:Bc:18:ARG:HD3   | 2.54                     | 0.42              |
| 103:BA:528:VAL:O    | 103:BA:532:MET:HG2  | 2.20                     | 0.42              |
| 104:BB:261:VAL:HG11 | 104:BB:371:LYS:O    | 2.20                     | 0.42              |
| 105:BC:187:MET:HE3  | 105:BC:187:MET:HB2  | 1.92                     | 0.42              |
| 109:BG:169:ARG:HD3  | 109:BG:169:ARG:HA   | 1.51                     | 0.42              |
| 110:BH:99:GLN:HB3   | 110:BH:102:ASN:HB2  | 2.01                     | 0.42              |
| 112:BJ:193:LEU:HD23 | 112:BJ:193:LEU:HA   | 1.91                     | 0.42              |
| 115:BM:170:CYS:SG   | 115:BM:200:GLU:HA   | 2.60                     | 0.42              |
| 118:BP:104:LEU:HD23 | 118:BP:104:LEU:HA   | 1.84                     | 0.42              |
| 119:BQ:78:TYR:OH    | 119:BQ:142:SER:O    | 2.37                     | 0.42              |
| 120:BR:119:GLY:O    | 120:BR:121:LEU:HD13 | 2.20                     | 0.42              |
| 122:BT:66:HIS:CE1   | 122:BT:70:ARG:HE    | 2.37                     | 0.42              |
| 123:BU:162:TRP:CE2  | 123:BU:166:GLN:HG3  | 2.55                     | 0.42              |
| 127:BY:84:ARG:O     | 127:BY:88:THR:OG1   | 2.35                     | 0.42              |
| 136:Bh:5:SER:HA     | 136:Bh:11:TYR:O     | 2.19                     | 0.42              |
| 1:DA:324:GLN:HG2    | 1:DA:330:TRP:NE1    | 2.34                     | 0.42              |
| 1:DA:904:TRP:CD1    | 44:Ca:399:ASN:HB3   | 2.54                     | 0.42              |
| 2:DD:368:LEU:HD23   | 2:DD:368:LEU:HA     | 1.87                     | 0.42              |
| 3:DI:90:LEU:HD12    | 3:DI:90:LEU:HA      | 1.78                     | 0.42              |
| 4:DL:273:THR:CG2    | 4:DL:276:HIS:HB2    | 2.50                     | 0.42              |
| 6:DN:44:LYS:HD3     | 6:DN:44:LYS:HA      | 1.62                     | 0.42              |
| 15:DB:123:ILE:HG23  | 15:DB:128:GLU:HB3   | 2.00                     | 0.42              |
| 15:DB:532:GLU:H     | 15:DB:532:GLU:HG2   | 1.55                     | 0.42              |
| 16:DC:1115:ARG:NH2  | 21:DJ:193:PRO:HD3   | 2.35                     | 0.42              |
| 17:DE:77:PRO:HG3    | 20:DH:567:GLY:HA3   | 2.00                     | 0.42              |
| 17:DE:210:MET:HG3   | 17:DE:426:PHE:CZ    | 2.49                     | 0.42              |
| 20:DH:500:VAL:HG13  | 20:DH:501:PRO:HD2   | 1.99                     | 0.42              |
| 21:DJ:46:ARG:HD3    | 21:DJ:46:ARG:HA     | 1.71                     | 0.42              |
| 21:DJ:87:PRO:O      | 21:DJ:123:LYS:HE3   | 2.19                     | 0.42              |
| 30:CF:67:LEU:HD22   | 30:CF:69:LEU:HD21   | 2.01                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 32:CI:100:PRO:O     | 45:Cb:103:ARG:NH1   | 2.53                     | 0.42              |
| 33:CJ:36:MET:SD     | 51:Cm:52:THR:HG22   | 2.57                     | 0.42              |
| 33:CJ:84:MET:H      | 33:CJ:84:MET:HG2    | 1.60                     | 0.42              |
| 34:CK:318:PRO:HB2   | 57:CA:344:C:H1'     | 2.02                     | 0.42              |
| 35:CL:127:VAL:HG13  | 35:CL:129:LEU:H     | 1.83                     | 0.42              |
| 37:CO:77:TYR:HA     | 37:CO:78:PRO:HD3    | 1.82                     | 0.42              |
| 37:CO:111:GLN:HE22  | 37:CO:236:ARG:HH11  | 1.67                     | 0.42              |
| 38:CP:55:ASN:OD1    | 38:CP:58:ILE:HG13   | 2.19                     | 0.42              |
| 38:CP:87:HIS:HE1    | 53:Cp:36:THR:OG1    | 2.03                     | 0.42              |
| 38:CP:92:THR:HB     | 44:Ca:444:PHE:CE1   | 2.55                     | 0.42              |
| 39:CQ:109:VAL:HG21  | 39:CQ:147:ILE:HD11  | 2.02                     | 0.42              |
| 42:CU:86:THR:O      | 42:CU:90:LEU:HG     | 2.20                     | 0.42              |
| 49:Cj:227:ASP:OD1   | 53:Cp:117:PRO:HD3   | 2.19                     | 0.42              |
| 50:Ck:96:ASN:OD1    | 50:Ck:97:GLN:NE2    | 2.52                     | 0.42              |
| 51:Cm:177:ARG:HD2   | 51:Cm:177:ARG:HA    | 1.64                     | 0.42              |
| 52:Cn:243:ARG:HH12  | 57:CA:336:U:H6      | 1.66                     | 0.42              |
| 56:Cv:738:ARG:HH21  | 56:Cv:788:ARG:CD    | 2.31                     | 0.42              |
| 57:CA:536:U:O2'     | 57:CA:537:A:O5'     | 2.34                     | 0.42              |
| 72:A9:65:ARG:O      | 72:A9:68:LEU:HB2    | 2.19                     | 0.42              |
| 77:AK:28:GLU:HG3    | 77:AK:31:VAL:HG12   | 2.01                     | 0.42              |
| 77:AK:158:ALA:HB2   | 77:AK:180:VAL:HG21  | 2.01                     | 0.42              |
| 84:AV:225:ALA:HB3   | 91:Af:118:GLU:HB2   | 2.01                     | 0.42              |
| 87:AY:149:GLN:HB2   | 87:AY:168:HIS:CD2   | 2.53                     | 0.42              |
| 88:Ab:259:TYR:O     | 88:Ab:273:ARG:NH1   | 2.52                     | 0.42              |
| 88:Ab:393:LEU:HD23  | 88:Ab:393:LEU:HA    | 1.84                     | 0.42              |
| 91:Af:141:GLU:OE1   | 91:Af:141:GLU:N     | 2.53                     | 0.42              |
| 92:Ag:144:TYR:CE2   | 111:BI:70:PRO:HG3   | 2.54                     | 0.42              |
| 94:Al:152:SER:O     | 94:Al:155:PRO:HD3   | 2.19                     | 0.42              |
| 96:Ap:286:LYS:H     | 96:Ap:286:LYS:HG2   | 1.68                     | 0.42              |
| 103:BA:338:LEU:HD23 | 103:BA:338:LEU:HA   | 1.81                     | 0.42              |
| 103:BA:585:HIS:HE1  | 103:BA:673:ASP:OD1  | 2.02                     | 0.42              |
| 104:BB:254:ASP:O    | 104:BB:387:ALA:HB1  | 2.20                     | 0.42              |
| 109:BG:103:LEU:HD21 | 109:BG:105:TRP:HB2  | 2.00                     | 0.42              |
| 111:BI:58:GLU:O     | 111:BI:61:PHE:HB3   | 2.20                     | 0.42              |
| 111:BI:245:ASN:O    | 111:BI:245:ASN:ND2  | 2.52                     | 0.42              |
| 114:BL:239:VAL:HG23 | 114:BL:245:ARG:HH11 | 1.85                     | 0.42              |
| 115:BM:223:THR:HG22 | 115:BM:224:THR:N    | 2.32                     | 0.42              |
| 116:BN:70:HIS:HB2   | 116:BN:73:CYS:SG    | 2.58                     | 0.42              |
| 120:BR:20:MET:HG2   | 120:BR:44:LEU:HD23  | 2.02                     | 0.42              |
| 1:DA:959:LYS:HD2    | 1:DA:959:LYS:N      | 2.35                     | 0.42              |
| 1:DA:1273:GLU:HG3   | 1:DA:1282:ILE:HD13  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:208:CYS:O     | 2:DD:212:ILE:HG13  | 2.19                     | 0.42              |
| 3:DI:302:ILE:O     | 3:DI:345:LEU:HA    | 2.20                     | 0.42              |
| 4:DL:246:GLU:CD    | 51:Cm:61:ARG:NH1   | 2.77                     | 0.42              |
| 11:DS:36:SER:OG    | 57:CA:199:U:OP1    | 2.37                     | 0.42              |
| 15:DB:400:LYS:O    | 15:DB:402:THR:HG23 | 2.20                     | 0.42              |
| 15:DB:942:ARG:HE   | 15:DB:942:ARG:HB3  | 1.76                     | 0.42              |
| 15:DB:983:LEU:HD23 | 15:DB:983:LEU:HA   | 1.80                     | 0.42              |
| 18:DF:216:LYS:HB2  | 33:CJ:476:ASN:HB2  | 2.00                     | 0.42              |
| 21:DJ:213:GLU:CD   | 21:DJ:213:GLU:H    | 2.28                     | 0.42              |
| 22:DK:222:LEU:HD22 | 22:DK:226:LEU:HD22 | 2.01                     | 0.42              |
| 24:DV:133:THR:HB   | 24:DV:139:ASP:OD2  | 2.19                     | 0.42              |
| 26:DX:127:MET:HE3  | 26:DX:127:MET:HB3  | 1.82                     | 0.42              |
| 28:CC:64:LEU:HD23  | 28:CC:64:LEU:HA    | 1.82                     | 0.42              |
| 29:CE:116:GLN:HA   | 29:CE:122:TRP:CG   | 2.55                     | 0.42              |
| 29:CE:336:PRO:HD2  | 29:CE:339:LEU:HD12 | 2.02                     | 0.42              |
| 32:CI:270:PHE:O    | 32:CI:274:LEU:HB2  | 2.19                     | 0.42              |
| 33:CJ:154:THR:HG21 | 33:CJ:201:ALA:O    | 2.19                     | 0.42              |
| 33:CJ:485:GLU:HA   | 33:CJ:515:ALA:CB   | 2.49                     | 0.42              |
| 33:CJ:642:ASN:CG   | 33:CJ:654:VAL:HG12 | 2.44                     | 0.42              |
| 35:CL:114:LEU:O    | 35:CL:116:MET:HE2  | 2.20                     | 0.42              |
| 38:CP:96:ILE:HD11  | 44:Ca:470:ARG:NH2  | 2.34                     | 0.42              |
| 44:Ca:46:ARG:HG3   | 44:Ca:46:ARG:NH1   | 2.34                     | 0.42              |
| 44:Ca:359:ARG:HD2  | 57:CA:3:A:N6       | 2.33                     | 0.42              |
| 46:Cd:195:GLU:HB3  | 46:Cd:216:HIS:HB2  | 2.02                     | 0.42              |
| 47:Cg:148:ASP:OD1  | 47:Cg:357:THR:HG21 | 2.20                     | 0.42              |
| 47:Cg:443:LYS:HD3  | 47:Cg:465:TRP:CZ3  | 2.54                     | 0.42              |
| 50:Ck:716:ARG:HD3  | 50:Ck:716:ARG:HA   | 1.80                     | 0.42              |
| 53:Cp:88:ASP:O     | 53:Cp:92:LEU:HB2   | 2.19                     | 0.42              |
| 64:A0:164:ASP:HA   | 64:A0:165:PRO:HD3  | 1.79                     | 0.42              |
| 65:A1:156:ILE:H    | 65:A1:156:ILE:HG13 | 1.64                     | 0.42              |
| 66:A2:279:ARG:HD3  | 87:AY:189:GLU:OE2  | 2.20                     | 0.42              |
| 67:A3:155:VAL:HB   | 67:A3:156:PRO:HD2  | 2.01                     | 0.42              |
| 71:A8:167:MET:HB3  | 102:AA:61:A:C2     | 2.55                     | 0.42              |
| 73:AE:191:ASN:HD22 | 73:AE:191:ASN:HA   | 1.66                     | 0.42              |
| 74:AF:193:HIS:HE1  | 102:AA:184:U:O2'   | 2.03                     | 0.42              |
| 75:AI:20:ILE:H     | 75:AI:20:ILE:HG13  | 1.56                     | 0.42              |
| 75:AI:48:ARG:NH1   | 75:AI:48:ARG:HG2   | 2.32                     | 0.42              |
| 75:AI:210:TYR:HB2  | 110:BH:153:ARG:NH2 | 2.34                     | 0.42              |
| 77:AK:208:GLN:CD   | 77:AK:208:GLN:H    | 2.28                     | 0.42              |
| 77:AK:247:MET:HG2  | 92:Ag:234:ALA:HA   | 2.01                     | 0.42              |
| 87:AY:251:LEU:HD23 | 87:AY:254:LYS:HE3  | 2.01                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 88:Ab:412:THR:HG22  | 88:Ab:413:LYS:H     | 1.83                     | 0.42              |
| 88:Ab:427:MET:HE2   | 88:Ab:427:MET:HB3   | 1.74                     | 0.42              |
| 89:Ad:56:LYS:HE3    | 93:Aj:78:ARG:CZ     | 2.48                     | 0.42              |
| 91:Af:117:GLU:HG2   | 91:Af:120:LYS:HE3   | 2.02                     | 0.42              |
| 93:Aj:24:ARG:HH12   | 132:Bd:139:PRO:CG   | 2.32                     | 0.42              |
| 95:Ao:149:PHE:CE1   | 130:Bb:84:LEU:HD23  | 2.55                     | 0.42              |
| 98:Av:210:LEU:HD21  | 98:Av:231:ILE:HG13  | 2.01                     | 0.42              |
| 102:AA:422:A:O2'    | 102:AA:423:A:OP1    | 2.32                     | 0.42              |
| 102:AA:578:A:H8     | 102:AA:578:A:O5'    | 2.03                     | 0.42              |
| 102:AA:1172:A:H5''  | 117:BO:125:GLU:O    | 2.19                     | 0.42              |
| 103:BA:791:PHE:HE1  | 103:BA:801:ARG:NH1  | 2.17                     | 0.42              |
| 103:BA:811:PRO:HA   | 117:BO:152:ARG:O    | 2.20                     | 0.42              |
| 104:BB:92:ILE:HD11  | 104:BB:129:TRP:NE1  | 2.34                     | 0.42              |
| 109:BG:134:CYS:SG   | 109:BG:169:ARG:HG3  | 2.60                     | 0.42              |
| 109:BG:185:PHE:CD1  | 109:BG:253:ARG:NH1  | 2.88                     | 0.42              |
| 109:BG:191:GLN:O    | 109:BG:195:ILE:HB   | 2.20                     | 0.42              |
| 109:BG:304:ARG:HG3  | 109:BG:305:HIS:O    | 2.19                     | 0.42              |
| 111:BI:167:LEU:HG   | 111:BI:171:ARG:HH12 | 1.83                     | 0.42              |
| 114:BL:173:GLY:C    | 114:BL:256:ARG:NH1  | 2.77                     | 0.42              |
| 118:BP:144:PHE:O    | 118:BP:144:PHE:CG   | 2.71                     | 0.42              |
| 118:BP:219:VAL:HB   | 118:BP:222:SER:HB2  | 2.01                     | 0.42              |
| 133:Be:24:LYS:HB3   | 133:Be:24:LYS:HE3   | 1.82                     | 0.42              |
| 1:DA:225:GLY:O      | 1:DA:232:SER:HB2    | 2.19                     | 0.42              |
| 1:DA:418:LEU:HD23   | 1:DA:418:LEU:HA     | 1.94                     | 0.42              |
| 1:DA:683:MET:HG2    | 1:DA:698:ALA:HA     | 2.01                     | 0.42              |
| 2:DD:244:PRO:HD3    | 2:DD:326:PRO:HD3    | 2.02                     | 0.42              |
| 3:DI:71:LEU:HA      | 3:DI:71:LEU:HD23    | 1.82                     | 0.42              |
| 3:DI:284:CYS:SG     | 7:DO:238:ASN:ND2    | 2.93                     | 0.42              |
| 4:DL:164:ARG:HG2    | 4:DL:164:ARG:HH11   | 1.85                     | 0.42              |
| 8:DP:139:ARG:HH12   | 8:DP:176:PRO:C      | 2.28                     | 0.42              |
| 8:DP:148:LYS:HG3    | 8:DP:181:PHE:CD2    | 2.55                     | 0.42              |
| 9:DQ:16:LEU:HA      | 9:DQ:16:LEU:HD23    | 1.76                     | 0.42              |
| 9:DQ:23:ARG:CD      | 37:CO:397:MET:HE1   | 2.43                     | 0.42              |
| 9:DQ:129:GLU:O      | 9:DQ:133:ASN:HB2    | 2.18                     | 0.42              |
| 15:DB:1003:LYS:HG2  | 32:CI:255:SER:HB3   | 2.02                     | 0.42              |
| 15:DB:1030:ARG:HH11 | 15:DB:1030:ARG:HG2  | 1.81                     | 0.42              |
| 16:DC:148:LEU:HD12  | 16:DC:148:LEU:HA    | 1.76                     | 0.42              |
| 16:DC:977:ARG:HD3   | 16:DC:977:ARG:HA    | 1.79                     | 0.42              |
| 16:DC:1123:SER:HA   | 16:DC:1124:PRO:HD3  | 1.86                     | 0.42              |
| 20:DH:76:LEU:HG     | 20:DH:85:LEU:CD2    | 2.50                     | 0.42              |
| 25:DW:116:LEU:HD23  | 25:DW:116:LEU:HA    | 1.88                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 30:CF:71:MET:HB3    | 30:CF:71:MET:HE3   | 1.74                     | 0.42              |
| 33:CJ:105:ASN:OD1   | 33:CJ:105:ASN:N    | 2.52                     | 0.42              |
| 34:CK:53:ARG:HH22   | 40:CR:234:ALA:HB1  | 1.85                     | 0.42              |
| 34:CK:325:PHE:HE1   | 57:CA:590:A:H5'    | 1.84                     | 0.42              |
| 37:CO:222:ALA:O     | 37:CO:226:VAL:HG23 | 2.20                     | 0.42              |
| 37:CO:424:LYS:H     | 37:CO:424:LYS:HG2  | 1.68                     | 0.42              |
| 38:CP:90:MET:HE2    | 38:CP:90:MET:HB3   | 1.67                     | 0.42              |
| 39:CQ:79:ASP:OD1    | 39:CQ:81:THR:N     | 2.48                     | 0.42              |
| 43:CZ:359:MET:HA    | 43:CZ:359:MET:HE2  | 2.02                     | 0.42              |
| 44:Ca:475:GLN:HE21  | 44:Ca:481:ARG:HE   | 1.67                     | 0.42              |
| 45:Cb:122:LEU:HD12  | 45:Cb:122:LEU:HA   | 1.83                     | 0.42              |
| 45:Cb:300:TYR:CZ    | 45:Cb:302:GLY:HA3  | 2.54                     | 0.42              |
| 50:Ck:35:ASP:O      | 50:Ck:40:GLY:N     | 2.50                     | 0.42              |
| 53:Cp:135:THR:HG22  | 53:Cp:138:TYR:H    | 1.83                     | 0.42              |
| 56:Cv:544:ILE:O     | 56:Cv:544:ILE:HG22 | 2.19                     | 0.42              |
| 56:Cv:678:HIS:CD2   | 56:Cv:680:ARG:HD2  | 2.51                     | 0.42              |
| 56:Cv:959:LEU:HD13  | 56:Cv:959:LEU:HA   | 1.83                     | 0.42              |
| 65:A1:117:TRP:H     | 65:A1:117:TRP:CD1  | 2.37                     | 0.42              |
| 66:A2:273:GLU:HA    | 66:A2:276:LYS:HB2  | 2.02                     | 0.42              |
| 74:AF:274:ASP:HA    | 74:AF:352:THR:OG1  | 2.19                     | 0.42              |
| 75:AI:183:ARG:O     | 75:AI:186:GLU:HG2  | 2.20                     | 0.42              |
| 79:AP:264:GLN:HG2   | 79:AP:271:TYR:CE2  | 2.55                     | 0.42              |
| 81:AR:67:GLN:O      | 81:AR:71:ARG:HG3   | 2.20                     | 0.42              |
| 83:AU:77:TRP:CZ2    | 83:AU:81:ARG:HD3   | 2.54                     | 0.42              |
| 84:AV:101:ARG:NH1   | 102:AA:468:A:O5'   | 2.53                     | 0.42              |
| 86:AX:68:TRP:CD1    | 86:AX:69:GLU:HG3   | 2.54                     | 0.42              |
| 87:AY:166:ARG:HG3   | 87:AY:167:GLU:N    | 2.34                     | 0.42              |
| 88:Ab:139:LYS:HE2   | 88:Ab:139:LYS:HB2  | 1.84                     | 0.42              |
| 88:Ab:490:TRP:HE3   | 88:Ab:494:THR:HG21 | 1.84                     | 0.42              |
| 90:Ae:148:ILE:HG23  | 90:Ae:148:ILE:O    | 2.19                     | 0.42              |
| 95:Ao:155:GLU:OE2   | 120:BR:142:ARG:HD3 | 2.20                     | 0.42              |
| 96:Ap:52:ARG:NH1    | 96:Ap:96:GLU:OE2   | 2.53                     | 0.42              |
| 97:At:132:ARG:HA    | 97:At:132:ARG:HD2  | 1.80                     | 0.42              |
| 102:AA:420:A:H2'    | 102:AA:421:C:O4'   | 2.19                     | 0.42              |
| 103:BA:578:ILE:HD13 | 103:BA:578:ILE:HA  | 1.89                     | 0.42              |
| 104:BB:148:LYS:HB2  | 104:BB:148:LYS:HZ2 | 1.84                     | 0.42              |
| 104:BB:211:ASP:OD1  | 104:BB:212:HIS:N   | 2.53                     | 0.42              |
| 107:BE:414:LEU:HD23 | 107:BE:414:LEU:HA  | 1.91                     | 0.42              |
| 111:BI:290:LEU:HD13 | 111:BI:297:LYS:HG3 | 2.01                     | 0.42              |
| 112:BJ:320:ARG:HH11 | 112:BJ:324:MET:HE3 | 1.81                     | 0.42              |
| 121:BS:97:ASP:O     | 121:BS:101:GLU:HB2 | 2.19                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 123:BU:130:ALA:O    | 123:BU:134:ARG:HG3 | 2.20                     | 0.42              |
| 125:BW:133:ALA:HB2  | 125:BW:140:TYR:CD2 | 2.55                     | 0.42              |
| 131:Bc:34:GLN:OE1   | 131:Bc:37:ARG:NH2  | 2.52                     | 0.42              |
| 134:Bf:104:ASN:HD21 | 134:Bf:113:ARG:HB3 | 1.85                     | 0.42              |
| 1:DA:126:GLU:OE2    | 31:CH:150:THR:HG22 | 2.19                     | 0.42              |
| 1:DA:147:TYR:HB3    | 3:DI:80:ARG:HD3    | 2.02                     | 0.42              |
| 1:DA:1043:ASP:OD1   | 4:DL:140:LEU:HB2   | 2.20                     | 0.42              |
| 1:DA:1535:PHE:O     | 1:DA:1553:VAL:HA   | 2.20                     | 0.42              |
| 2:DD:10:HIS:N       | 52:Cn:154:PRO:HA   | 2.35                     | 0.42              |
| 2:DD:765:ARG:HH21   | 56:Cv:960:GLN:HE21 | 1.67                     | 0.42              |
| 3:DI:404:TRP:CE3    | 56:Cv:212:ARG:NH1  | 2.87                     | 0.42              |
| 5:DM:228:ASP:CG     | 5:DM:230:PRO:HD3   | 2.45                     | 0.42              |
| 5:DM:282:TRP:CH2    | 54:Cq:39:GLU:HG3   | 2.55                     | 0.42              |
| 6:DN:58:SER:HA      | 6:DN:59:PRO:HD2    | 1.85                     | 0.42              |
| 7:DO:74:TRP:CZ2     | 7:DO:259:THR:HG23  | 2.55                     | 0.42              |
| 10:DR:86:LEU:HD11   | 10:DR:177:LEU:HD12 | 2.01                     | 0.42              |
| 11:DS:232:GLN:CD    | 11:DS:234:LEU:HD11 | 2.44                     | 0.42              |
| 15:DB:413:PHE:HB2   | 23:DT:155:PHE:HB3  | 2.00                     | 0.42              |
| 15:DB:903:ILE:HD11  | 15:DB:921:ALA:HB2  | 2.01                     | 0.42              |
| 15:DB:1101:GLN:HB2  | 33:CJ:680:LEU:HD22 | 2.02                     | 0.42              |
| 18:DF:460:ARG:HD3   | 18:DF:461:PHE:CE2  | 2.55                     | 0.42              |
| 18:DF:502:ARG:HD3   | 18:DF:577:ALA:C    | 2.44                     | 0.42              |
| 19:DG:381:ASP:O     | 19:DG:384:VAL:HG13 | 2.19                     | 0.42              |
| 19:DG:577:LEU:O     | 19:DG:581:VAL:HG13 | 2.20                     | 0.42              |
| 23:DT:169:LEU:HD23  | 23:DT:169:LEU:HA   | 1.89                     | 0.42              |
| 26:DX:35:ARG:HG2    | 26:DX:36:PRO:HD2   | 2.01                     | 0.42              |
| 28:CC:36:LEU:HA     | 28:CC:36:LEU:HD23  | 1.87                     | 0.42              |
| 29:CE:89:LEU:HD23   | 29:CE:89:LEU:HA    | 1.94                     | 0.42              |
| 31:CH:142:ARG:HH22  | 56:Cv:74:ASN:ND2   | 2.17                     | 0.42              |
| 33:CJ:613:SER:HA    | 33:CJ:666:LEU:HD13 | 2.02                     | 0.42              |
| 33:CJ:618:VAL:HG23  | 33:CJ:652:ASP:O    | 2.19                     | 0.42              |
| 33:CJ:770:THR:HB    | 48:Ci:11:GLY:N     | 2.35                     | 0.42              |
| 37:CO:270:ASP:OD2   | 37:CO:273:LYS:HG3  | 2.20                     | 0.42              |
| 38:CP:92:THR:HB     | 44:Ca:444:PHE:CD1  | 2.54                     | 0.42              |
| 47:Cg:405:ASP:OD1   | 47:Cg:405:ASP:C    | 2.63                     | 0.42              |
| 50:Ck:214:LEU:HD23  | 50:Ck:214:LEU:HA   | 1.83                     | 0.42              |
| 55:Cr:261:TRP:CE3   | 55:Cr:264:ILE:HD12 | 2.55                     | 0.42              |
| 68:A4:130:ARG:HD2   | 68:A4:132:TRP:CH2  | 2.54                     | 0.42              |
| 68:A4:139:GLU:HG2   | 68:A4:160:LEU:HD11 | 2.00                     | 0.42              |
| 75:AI:51:TYR:CE1    | 75:AI:55:MET:HE3   | 2.55                     | 0.42              |
| 76:AJ:67:GLN:OE1    | 76:AJ:67:GLN:N     | 2.49                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 77:AK:95:LYS:HB2    | 77:AK:95:LYS:HE3    | 1.68                     | 0.42              |
| 77:AK:186:ARG:NH1   | 102:AA:403:A:C6     | 2.87                     | 0.42              |
| 79:AP:70:LEU:HA     | 79:AP:70:LEU:HD23   | 1.74                     | 0.42              |
| 79:AP:182:TRP:CE3   | 94:AI:119:VAL:HG11  | 2.46                     | 0.42              |
| 81:AR:121:ASP:HA    | 81:AR:122:PRO:HD2   | 1.85                     | 0.42              |
| 81:AR:185:ARG:O     | 81:AR:186:PHE:CD1   | 2.73                     | 0.42              |
| 81:AR:197:LYS:HB2   | 113:BK:194:ARG:HB2  | 2.02                     | 0.42              |
| 85:AW:169:ARG:HG2   | 85:AW:169:ARG:NH1   | 2.34                     | 0.42              |
| 85:AW:242:LEU:HA    | 85:AW:242:LEU:HD23  | 1.80                     | 0.42              |
| 88:Ab:76:MET:HB3    | 94:AI:29:THR:HG23   | 2.02                     | 0.42              |
| 89:Ad:40:ALA:O      | 89:Ad:43:GLU:HB2    | 2.19                     | 0.42              |
| 89:Ad:92:ARG:CZ     | 93:Aj:284:VAL:HG22  | 2.50                     | 0.42              |
| 90:Ae:71:HIS:ND1    | 90:Ae:72:PRO:HD2    | 2.34                     | 0.42              |
| 93:Aj:24:ARG:HH12   | 132:Bd:139:PRO:HG3  | 1.83                     | 0.42              |
| 102:AA:582:A:H61    | 102:AA:794:A:N6     | 2.18                     | 0.42              |
| 105:BC:115:GLN:H    | 105:BC:115:GLN:HG2  | 1.60                     | 0.42              |
| 105:BC:296:LEU:HD13 | 105:BC:296:LEU:HA   | 1.79                     | 0.42              |
| 108:BF:40:PRO:HB2   | 108:BF:256:LEU:HD11 | 2.01                     | 0.42              |
| 109:BG:336:LYS:HB2  | 109:BG:336:LYS:HE3  | 1.86                     | 0.42              |
| 118:BP:39:LEU:H     | 118:BP:39:LEU:HD12  | 1.85                     | 0.42              |
| 118:BP:94:ASP:OD1   | 118:BP:96:THR:HG23  | 2.20                     | 0.42              |
| 119:BQ:18:TYR:OH    | 119:BQ:164:VAL:O    | 2.36                     | 0.42              |
| 127:BY:79(G):LEU:O  | 127:BY:82:ARG:HG2   | 2.20                     | 0.42              |
| 132:Bd:55:PRO:C     | 132:Bd:57:LEU:H     | 2.28                     | 0.42              |
| 134:Bf:43:ALA:O     | 134:Bf:44:ARG:HB2   | 2.20                     | 0.42              |
| 135:Bg:53:PHE:HE1   | 135:Bg:90:LEU:HB3   | 1.85                     | 0.42              |
| 1:DA:493:TRP:NE1    | 1:DA:494:ARG:HG3    | 2.34                     | 0.42              |
| 1:DA:1081:GLN:HA    | 1:DA:1642:LEU:HD21  | 2.02                     | 0.42              |
| 1:DA:1530:ALA:HA    | 1:DA:1531:PRO:HD3   | 1.90                     | 0.42              |
| 2:DD:171:ASN:HA     | 2:DD:172:PRO:HD3    | 1.72                     | 0.42              |
| 4:DL:71:GLU:OE2     | 44:Ca:243:THR:CA    | 2.57                     | 0.42              |
| 4:DL:174:ALA:HB2    | 56:Cv:501:HIS:CG    | 2.55                     | 0.42              |
| 6:DN:123:GLN:N      | 6:DN:123:GLN:OE1    | 2.53                     | 0.42              |
| 8:DP:207:TYR:HA     | 8:DP:208:PRO:C      | 2.41                     | 0.42              |
| 9:DQ:31:PRO:O       | 10:DR:12:ARG:NH1    | 2.52                     | 0.42              |
| 15:DB:92:HIS:HE1    | 17:DE:447:ARG:O     | 2.02                     | 0.42              |
| 15:DB:326:THR:HA    | 15:DB:327:PRO:HD3   | 1.91                     | 0.42              |
| 15:DB:562:GLN:HE21  | 18:DF:572:HIS:H     | 1.68                     | 0.42              |
| 17:DE:659:ARG:HD2   | 17:DE:659:ARG:HA    | 1.55                     | 0.42              |
| 19:DG:64:ARG:HA     | 19:DG:64:ARG:HD2    | 1.91                     | 0.42              |
| 19:DG:117:VAL:HG21  | 19:DG:149:SER:HB2   | 2.01                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:DG:496:ARG:NH2   | 32:CI:1:MET:HG2    | 2.35                     | 0.42              |
| 21:DJ:51:PRO:HG2    | 21:DJ:53:GLN:NE2   | 2.34                     | 0.42              |
| 21:DJ:206:SER:OG    | 21:DJ:207:ILE:N    | 2.52                     | 0.42              |
| 22:DK:32:ILE:HG13   | 22:DK:41:VAL:HG22  | 2.01                     | 0.42              |
| 30:CF:11:LYS:HA     | 30:CF:12:PRO:HD3   | 1.75                     | 0.42              |
| 31:CH:195:ARG:HD3   | 57:CA:1:U:O4       | 2.19                     | 0.42              |
| 37:CO:206:MET:CE    | 37:CO:210:ARG:HH21 | 2.33                     | 0.42              |
| 47:Cg:120:LEU:HA    | 47:Cg:120:LEU:HD12 | 1.78                     | 0.42              |
| 47:Cg:205:ARG:HD3   | 47:Cg:258:SER:HB3  | 2.01                     | 0.42              |
| 56:Cv:211:ASN:HD22  | 56:Cv:211:ASN:HA   | 1.62                     | 0.42              |
| 56:Cv:278:LEU:HD22  | 56:Cv:282:ILE:HG13 | 2.02                     | 0.42              |
| 56:Cv:292:LYS:HZ1   | 56:Cv:509:THR:CG2  | 2.32                     | 0.42              |
| 56:Cv:559:GLN:NE2   | 56:Cv:568:THR:OG1  | 2.53                     | 0.42              |
| 56:Cv:975:ASP:OD1   | 56:Cv:976:ASP:N    | 2.34                     | 0.42              |
| 57:CA:88:A:C4       | 57:CA:89:U:C5      | 3.07                     | 0.42              |
| 65:A1:83:ARG:NH2    | 75:AI:100:LEU:O    | 2.53                     | 0.42              |
| 66:A2:314:HIS:HB3   | 66:A2:317:GLU:HG3  | 2.02                     | 0.42              |
| 68:A4:132:TRP:HA    | 93:Aj:201:MET:HE3  | 2.02                     | 0.42              |
| 73:AE:148:CYS:SG    | 73:AE:149:LYS:N    | 2.93                     | 0.42              |
| 74:AF:211:MET:SD    | 74:AF:332:PRO:HB3  | 2.60                     | 0.42              |
| 76:AJ:66:GLU:O      | 76:AJ:69:PHE:N     | 2.52                     | 0.42              |
| 78:AN:77:MET:HE1    | 103:BA:710:LYS:NZ  | 2.35                     | 0.42              |
| 78:AN:108:ALA:O     | 78:AN:109:TYR:CG   | 2.73                     | 0.42              |
| 85:AW:17:ARG:HD3    | 85:AW:17:ARG:HA    | 1.73                     | 0.42              |
| 96:Ap:149:GLU:O     | 111:BI:217:ARG:HG2 | 2.19                     | 0.42              |
| 102:AA:302:G:N2     | 102:AA:335:G:H2'   | 2.35                     | 0.42              |
| 102:AA:477:A:C5     | 102:AA:493:A:N6    | 2.87                     | 0.42              |
| 102:AA:889:A:H2'    | 102:AA:890:U:C6    | 2.54                     | 0.42              |
| 105:BC:61:ASP:HB2   | 105:BC:288:ARG:NH1 | 2.35                     | 0.42              |
| 105:BC:521:GLN:OE1  | 110:BH:240:GLU:HG2 | 2.19                     | 0.42              |
| 107:BE:88:ARG:HG3   | 113:BK:285:GLN:NE2 | 2.35                     | 0.42              |
| 109:BG:159:ARG:NH1  | 109:BG:258:TYR:O   | 2.52                     | 0.42              |
| 109:BG:185:PHE:O    | 109:BG:189:MET:HB2 | 2.19                     | 0.42              |
| 110:BH:271:PHE:CE1  | 133:Be:8:LYS:NZ    | 2.86                     | 0.42              |
| 112:BJ:267:GLU:OE1  | 112:BJ:270:ARG:NH1 | 2.53                     | 0.42              |
| 114:BL:158:ARG:NH2  | 114:BL:221:CYS:O   | 2.51                     | 0.42              |
| 119:BQ:224:LEU:HD23 | 119:BQ:224:LEU:HA  | 1.87                     | 0.42              |
| 120:BR:111:PHE:HE2  | 120:BR:113:ARG:NH2 | 2.18                     | 0.42              |
| 129:Ba:127:ASP:O    | 129:Ba:132:ALA:O   | 2.38                     | 0.42              |
| 1:DA:1457:HIS:HA    | 1:DA:1458:PRO:HD3  | 1.75                     | 0.42              |
| 1:DA:1556:VAL:HG21  | 1:DA:1599:PHE:CE2  | 2.55                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:15:ALA:HB2    | 57:CA:277:A:N1     | 2.35                     | 0.42              |
| 4:DL:123:LEU:HD23  | 4:DL:123:LEU:HA    | 1.77                     | 0.42              |
| 10:DR:51:LEU:HD11  | 10:DR:63:ILE:HD11  | 2.02                     | 0.42              |
| 15:DB:634:GLU:OE1  | 50:Ck:370:THR:OG1  | 2.29                     | 0.42              |
| 15:DB:898:GLN:HE21 | 50:Ck:270:TYR:HB2  | 1.85                     | 0.42              |
| 16:DC:1112:ASP:O   | 20:DH:49:LEU:HD13  | 2.20                     | 0.42              |
| 17:DE:72:ARG:HB3   | 17:DE:194:HIS:HB2  | 2.02                     | 0.42              |
| 17:DE:163:LYS:HG2  | 17:DE:556:LEU:HD11 | 2.01                     | 0.42              |
| 18:DF:13:ILE:H     | 18:DF:13:ILE:HG13  | 1.53                     | 0.42              |
| 19:DG:80:LEU:CD2   | 19:DG:115:ILE:HD11 | 2.50                     | 0.42              |
| 19:DG:293:ARG:HE   | 19:DG:299:PHE:HE1  | 1.67                     | 0.42              |
| 19:DG:569:LEU:HD23 | 19:DG:569:LEU:HA   | 1.87                     | 0.42              |
| 20:DH:269:ARG:HD2  | 33:CJ:288:GLN:OE1  | 2.20                     | 0.42              |
| 27:DY:162:ARG:HE   | 27:DY:162:ARG:HB2  | 1.56                     | 0.42              |
| 29:CE:308:ARG:HA   | 29:CE:311:LYS:HZ1  | 1.79                     | 0.42              |
| 29:CE:326:MET:HE3  | 29:CE:326:MET:HB2  | 1.88                     | 0.42              |
| 32:CI:9:THR:HG22   | 32:CI:10:ALA:N     | 2.35                     | 0.42              |
| 32:CI:142:TYR:HA   | 32:CI:145:VAL:HG22 | 2.01                     | 0.42              |
| 33:CJ:688:GLU:OE1  | 36:CN:63:HIS:NE2   | 2.52                     | 0.42              |
| 35:CL:69:PHE:HZ    | 62:US:46:UNK:CG    | 2.33                     | 0.42              |
| 37:CO:230:LEU:HD23 | 37:CO:233:ARG:HH12 | 1.85                     | 0.42              |
| 40:CR:320:VAL:HB   | 46:Cd:281:MET:CE   | 2.42                     | 0.42              |
| 44:Ca:403:TYR:OH   | 44:Ca:410:MET:HG2  | 2.20                     | 0.42              |
| 49:Cj:73:ARG:HB2   | 53:Cp:169:ASN:HA   | 2.01                     | 0.42              |
| 50:Ck:717:LEU:HD23 | 50:Ck:717:LEU:HA   | 1.74                     | 0.42              |
| 55:Cr:37:CYS:HG    | 55:Cr:40:HIS:CE1   | 2.33                     | 0.42              |
| 55:Cr:143:ARG:HH12 | 55:Cr:147:GLY:C    | 2.28                     | 0.42              |
| 56:Cv:444:GLY:HA2  | 56:Cv:808:SER:OG   | 2.19                     | 0.42              |
| 56:Cv:462:LEU:HD23 | 56:Cv:462:LEU:HA   | 1.88                     | 0.42              |
| 56:Cv:696:PHE:HB2  | 56:Cv:727:ARG:HH12 | 1.84                     | 0.42              |
| 57:CA:69:U:H4'     | 57:CA:70:U:O5'     | 2.20                     | 0.42              |
| 67:A3:68:VAL:HG13  | 67:A3:116:VAL:HG13 | 2.02                     | 0.42              |
| 67:A3:102:ILE:HD12 | 67:A3:104:GLN:NE2  | 2.35                     | 0.42              |
| 68:A4:46:PHE:HB2   | 98:Av:196:PHE:CE2  | 2.55                     | 0.42              |
| 71:A8:158:ARG:HD3  | 71:A8:158:ARG:HA   | 1.84                     | 0.42              |
| 73:AE:384:PRO:HD3  | 131:Bc:96:PRO:CB   | 2.50                     | 0.42              |
| 74:AF:33:HIS:HD2   | 92:Ag:58:THR:OG1   | 2.02                     | 0.42              |
| 77:AK:320:LYS:HE3  | 77:AK:320:LYS:HB2  | 1.73                     | 0.42              |
| 80:AQ:53:ALA:HB2   | 80:AQ:153:VAL:HG23 | 2.00                     | 0.42              |
| 83:AU:23:MET:HE3   | 102:AA:115:A:C2    | 2.55                     | 0.42              |
| 87:AY:208:LEU:HD23 | 87:AY:208:LEU:HA   | 1.92                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 91:Af:155:ARG:HD3   | 91:Af:155:ARG:HA    | 1.83                     | 0.42              |
| 93:Aj:57:VAL:HG21   | 93:Aj:136:ARG:HD2   | 2.02                     | 0.42              |
| 102:AA:572:U:C2'    | 102:AA:573:U:H5'    | 2.49                     | 0.42              |
| 103:BA:155:ILE:HD11 | 131:Bc:84:LEU:HG    | 2.02                     | 0.42              |
| 104:BB:354:MET:HE1  | 104:BB:410:ALA:HA   | 2.00                     | 0.42              |
| 105:BC:60:LEU:HB3   | 105:BC:67:TYR:CZ    | 2.55                     | 0.42              |
| 107:BE:88:ARG:HG3   | 113:BK:285:GLN:HE21 | 1.85                     | 0.42              |
| 109:BG:65:MET:SD    | 109:BG:111:TYR:N    | 2.92                     | 0.42              |
| 109:BG:347:GLN:HA   | 109:BG:350:LEU:HD23 | 2.01                     | 0.42              |
| 113:BK:278:SER:CB   | 113:BK:282:ARG:HH12 | 2.33                     | 0.42              |
| 113:BK:297:PHE:HD2  | 113:BK:300:TRP:NE1  | 2.18                     | 0.42              |
| 122:BT:33:ASN:HD22  | 122:BT:34:ARG:H     | 1.68                     | 0.42              |
| 124:BV:49:ARG:HH12  | 124:BV:73:LEU:CD2   | 2.32                     | 0.42              |
| 125:BW:114:LYS:HE3  | 125:BW:115:TYR:CZ   | 2.55                     | 0.42              |
| 132:Bd:15:PHE:O     | 132:Bd:19:MET:HG3   | 2.20                     | 0.42              |
| 136:Bh:62:GLY:HA2   | 136:Bh:63:PRO:HD2   | 1.80                     | 0.42              |
| 1:DA:148:LYS:HB2    | 1:DA:148:LYS:NZ     | 2.35                     | 0.41              |
| 1:DA:961:LYS:NZ     | 1:DA:983:GLU:OE1    | 2.49                     | 0.41              |
| 1:DA:1280:GLU:O     | 1:DA:1284:VAL:HG23  | 2.20                     | 0.41              |
| 1:DA:1312:TRP:CE2   | 1:DA:1314:GLY:HA2   | 2.54                     | 0.41              |
| 2:DD:343:TRP:CZ3    | 2:DD:345:PRO:HD3    | 2.55                     | 0.41              |
| 2:DD:620:ALA:O      | 2:DD:623:TRP:HB2    | 2.19                     | 0.41              |
| 2:DD:651:ARG:HD3    | 2:DD:651:ARG:HA     | 1.67                     | 0.41              |
| 6:DN:45:ARG:HA      | 6:DN:155:ASP:HB2    | 2.01                     | 0.41              |
| 9:DQ:27:HIS:HB2     | 12:DU:57:LEU:HD23   | 2.02                     | 0.41              |
| 12:DU:207:ARG:HG2   | 12:DU:207:ARG:O     | 2.20                     | 0.41              |
| 13:DZ:10:MET:N      | 44:Ca:181:GLU:OE1   | 2.53                     | 0.41              |
| 14:Da:33:LEU:O      | 14:Da:42:ARG:NH2    | 2.53                     | 0.41              |
| 15:DB:507:LEU:HD12  | 15:DB:507:LEU:HA    | 1.66                     | 0.41              |
| 15:DB:816:ARG:NH1   | 18:DF:571:LEU:HD11  | 2.34                     | 0.41              |
| 15:DB:923:GLN:HE21  | 15:DB:923:GLN:HB3   | 1.59                     | 0.41              |
| 16:DC:317:GLU:HG2   | 16:DC:320:ARG:NH1   | 2.35                     | 0.41              |
| 16:DC:753:LEU:HA    | 16:DC:753:LEU:HD22  | 1.83                     | 0.41              |
| 22:DK:286:LEU:HA    | 22:DK:286:LEU:HD23  | 1.72                     | 0.41              |
| 24:DV:165:LEU:HD13  | 33:CJ:748:PRO:HB3   | 2.01                     | 0.41              |
| 29:CE:136:PHE:HZ    | 29:CE:201:ILE:HD12  | 1.85                     | 0.41              |
| 32:CI:198:GLU:O     | 54:Cq:137:LYS:HE3   | 2.20                     | 0.41              |
| 33:CJ:130:ARG:O     | 33:CJ:130:ARG:HG3   | 2.20                     | 0.41              |
| 35:CL:80:PRO:HG2    | 35:CL:84:SER:O      | 2.20                     | 0.41              |
| 37:CO:82:ASN:HD21   | 52:Cn:141:ARG:HA    | 1.85                     | 0.41              |
| 37:CO:85:PRO:HA     | 37:CO:86:PRO:HD3    | 1.86                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 38:CP:163:LYS:HG2   | 38:CP:167:TYR:CE2   | 2.54                     | 0.41              |
| 44:Ca:14:ASN:O      | 44:Ca:15:LYS:HG2    | 2.20                     | 0.41              |
| 44:Ca:89:ARG:HD2    | 44:Ca:177:GLN:NE2   | 2.34                     | 0.41              |
| 44:Ca:406:MET:C     | 44:Ca:408:PRO:HD3   | 2.45                     | 0.41              |
| 47:Cg:190:PRO:O     | 50:Ck:833:PRO:HG3   | 2.20                     | 0.41              |
| 47:Cg:224:LEU:HD11  | 47:Cg:241:GLN:C     | 2.44                     | 0.41              |
| 48:Ci:88:ILE:HG22   | 48:Ci:89:MET:HE2    | 2.02                     | 0.41              |
| 48:Ci:96:ASN:HD21   | 50:Ck:697:MET:HA    | 1.84                     | 0.41              |
| 52:Cn:190:VAL:HB    | 52:Cn:193:LEU:HD12  | 2.02                     | 0.41              |
| 55:Cr:125:GLN:NE2   | 55:Cr:161:ARG:HA    | 2.35                     | 0.41              |
| 56:Cv:312:ASN:HD22  | 56:Cv:314:GLU:H     | 1.67                     | 0.41              |
| 56:Cv:914:ASN:CG    | 56:Cv:915:PRO:HD3   | 2.45                     | 0.41              |
| 66:A2:123:ARG:NH1   | 128:BZ:76:ARG:NH2   | 2.68                     | 0.41              |
| 66:A2:251:ILE:HD11  | 122:BT:119:ARG:NH2  | 2.35                     | 0.41              |
| 68:A4:3:LEU:HD21    | 71:A8:105:ASP:HB2   | 2.02                     | 0.41              |
| 68:A4:107:HIS:O     | 68:A4:107:HIS:ND1   | 2.51                     | 0.41              |
| 74:AF:193:HIS:HD2   | 102:AA:147:G:O3'    | 2.03                     | 0.41              |
| 77:AK:227:THR:HA    | 77:AK:230:GLN:HB2   | 2.01                     | 0.41              |
| 84:AV:65:LEU:HD23   | 84:AV:68:ARG:HH22   | 1.85                     | 0.41              |
| 85:AW:17:ARG:NH1    | 102:AA:149:U:OP2    | 2.52                     | 0.41              |
| 85:AW:166:LEU:HD23  | 85:AW:166:LEU:HA    | 1.86                     | 0.41              |
| 85:AW:242:LEU:HA    | 85:AW:243:PRO:HD3   | 1.94                     | 0.41              |
| 87:AY:179:ASP:HA    | 87:AY:180:PRO:HD2   | 1.90                     | 0.41              |
| 92:Ag:40:TYR:CE2    | 92:Ag:87:VAL:HG11   | 2.55                     | 0.41              |
| 93:Aj:206:ALA:O     | 93:Aj:210:ASP:HB2   | 2.20                     | 0.41              |
| 94:Al:97:LEU:HD21   | 94:Al:215:GLY:HA2   | 2.02                     | 0.41              |
| 102:AA:335:G:O2'    | 102:AA:336:U:P      | 2.77                     | 0.41              |
| 102:AA:384:U:HO2'   | 102:AA:385:A:C5'    | 2.31                     | 0.41              |
| 102:AA:539:A:OP2    | 135:Bg:100:ARG:HB3  | 2.20                     | 0.41              |
| 102:AA:1163:A:C2    | 102:AA:1166:A:C8    | 3.07                     | 0.41              |
| 103:BA:135:SER:OG   | 117:BO:140:GLY:HA3  | 2.20                     | 0.41              |
| 103:BA:177:ILE:O    | 103:BA:181:VAL:HG23 | 2.20                     | 0.41              |
| 104:BB:348:VAL:HG12 | 104:BB:426:ALA:HB1  | 2.01                     | 0.41              |
| 104:BB:352:ARG:O    | 104:BB:356:ASN:HB2  | 2.20                     | 0.41              |
| 104:BB:365:ARG:HG2  | 104:BB:377:PHE:CD2  | 2.55                     | 0.41              |
| 104:BB:417:GLU:HA   | 104:BB:420:ASN:ND2  | 2.35                     | 0.41              |
| 109:BG:39:PHE:CD2   | 109:BG:93:ALA:HB1   | 2.55                     | 0.41              |
| 112:BJ:318:GLU:HB3  | 112:BJ:322:LYS:HE3  | 2.02                     | 0.41              |
| 115:BM:280:MET:HE2  | 115:BM:280:MET:HB3  | 1.91                     | 0.41              |
| 116:BN:9:TRP:N      | 123:BU:180:ALA:O    | 2.53                     | 0.41              |
| 120:BR:13:PRO:HA    | 120:BR:16:GLN:HE21  | 1.85                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 121:BS:20:GLY:N     | 121:BS:31:ASP:OD1  | 2.52                     | 0.41              |
| 137:UA:21:UNK:CB    | 137:UA:26:UNK:HB1  | 2.49                     | 0.41              |
| 1:DA:414:HIS:HD2    | 1:DA:416:HIS:H     | 1.68                     | 0.41              |
| 2:DD:448:ARG:HG3    | 2:DD:448:ARG:NH1   | 2.35                     | 0.41              |
| 2:DD:610:VAL:O      | 2:DD:613:TRP:HB3   | 2.20                     | 0.41              |
| 2:DD:694:ARG:NH1    | 44:Ca:459:LEU:HD13 | 2.35                     | 0.41              |
| 2:DD:748:ARG:HH12   | 3:DI:147:ASP:CG    | 2.28                     | 0.41              |
| 3:DI:51:VAL:HG13    | 3:DI:182:PHE:CE2   | 2.55                     | 0.41              |
| 3:DI:227:ASN:HB3    | 3:DI:231:GLY:HA2   | 2.01                     | 0.41              |
| 5:DM:76:ASN:HD21    | 56:Cv:970:GLY:N    | 2.18                     | 0.41              |
| 7:DO:116:ALA:HA     | 7:DO:119:ARG:HG2   | 2.01                     | 0.41              |
| 8:DP:35:ILE:HD13    | 8:DP:44:GLU:OE1    | 2.19                     | 0.41              |
| 11:DS:150:GLN:HE22  | 11:DS:176:ARG:HE   | 1.68                     | 0.41              |
| 15:DB:226:LEU:HD23  | 15:DB:226:LEU:HA   | 1.87                     | 0.41              |
| 15:DB:255:LEU:HD13  | 15:DB:403:ASN:OD1  | 2.20                     | 0.41              |
| 15:DB:333:ALA:HB1   | 17:DE:33:ILE:HD13  | 2.01                     | 0.41              |
| 15:DB:1030:ARG:HH11 | 15:DB:1030:ARG:HG3 | 1.83                     | 0.41              |
| 16:DC:302:ARG:HD3   | 16:DC:359:GLU:OE1  | 2.19                     | 0.41              |
| 16:DC:327:GLU:CD    | 16:DC:410:ARG:HD2  | 2.44                     | 0.41              |
| 16:DC:775:ALA:HA    | 16:DC:777:GLY:H    | 1.84                     | 0.41              |
| 16:DC:868:GLU:OE2   | 16:DC:893:PHE:CZ   | 2.73                     | 0.41              |
| 17:DE:80:LEU:HD12   | 17:DE:80:LEU:HA    | 1.64                     | 0.41              |
| 17:DE:193:ILE:HB    | 17:DE:426:PHE:HB3  | 2.02                     | 0.41              |
| 17:DE:292:TYR:O     | 17:DE:295:TYR:HB3  | 2.20                     | 0.41              |
| 20:DH:15:TYR:OH     | 28:CC:69:GLU:OE1   | 2.28                     | 0.41              |
| 21:DJ:22:MET:HE3    | 33:CJ:74:TRP:HH2   | 1.84                     | 0.41              |
| 21:DJ:173:ASP:OD1   | 21:DJ:206:SER:HB2  | 2.20                     | 0.41              |
| 23:DT:183:LEU:H     | 23:DT:219:GLN:HE22 | 1.66                     | 0.41              |
| 25:DW:143:MET:HA    | 25:DW:144:PRO:HD3  | 1.76                     | 0.41              |
| 26:DX:78:GLU:HA     | 26:DX:79:PRO:HD3   | 1.66                     | 0.41              |
| 28:CC:69:GLU:H      | 28:CC:69:GLU:HG2   | 1.58                     | 0.41              |
| 29:CE:66:ASP:OD2    | 29:CE:69:GLU:HB2   | 2.20                     | 0.41              |
| 32:CI:104:ASN:HD22  | 32:CI:104:ASN:C    | 2.28                     | 0.41              |
| 32:CI:219:LEU:HD12  | 32:CI:219:LEU:O    | 2.20                     | 0.41              |
| 36:CN:37:ARG:NH1    | 36:CN:38:ASP:OD2   | 2.51                     | 0.41              |
| 36:CN:55:LEU:HD23   | 36:CN:55:LEU:HA    | 1.88                     | 0.41              |
| 37:CO:93:ARG:NH2    | 57:CA:358:U:H3     | 2.14                     | 0.41              |
| 40:CR:25:GLU:CB     | 56:Cv:143:THR:HG21 | 2.48                     | 0.41              |
| 40:CR:37:PRO:HG2    | 40:CR:99:ASN:HD21  | 1.85                     | 0.41              |
| 46:Cd:177:LEU:HD11  | 56:Cv:648:VAL:CG2  | 2.49                     | 0.41              |
| 47:Cg:284:VAL:HA    | 47:Cg:354:ILE:O    | 2.19                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 54:Cq:131:ASN:HB3   | 54:Cq:187:TRP:CE2   | 2.55                     | 0.41              |
| 55:Cr:27:ASP:HA     | 55:Cr:30:VAL:O      | 2.20                     | 0.41              |
| 57:CA:441:G:O2'     | 57:CA:442:A:H5'     | 2.19                     | 0.41              |
| 65:A1:97:ARG:HH21   | 143:U1:14:UNK:HB2   | 1.83                     | 0.41              |
| 66:A2:47:LEU:HA     | 66:A2:47:LEU:HD23   | 1.78                     | 0.41              |
| 66:A2:112:ILE:O     | 66:A2:115:GLU:HG3   | 2.20                     | 0.41              |
| 68:A4:71:GLU:OE1    | 132:Bd:52:ARG:NH1   | 2.53                     | 0.41              |
| 71:A8:66:ARG:NH2    | 71:A8:138:MET:HE3   | 2.33                     | 0.41              |
| 73:AE:51:GLU:HB3    | 96:Ap:70:GLU:OE1    | 2.19                     | 0.41              |
| 73:AE:82:ARG:NE     | 111:BI:247:GLU:HG2  | 2.35                     | 0.41              |
| 73:AE:114:LEU:HD11  | 142:UN:15:UNK:HG1   | 2.02                     | 0.41              |
| 75:AI:13:VAL:HA     | 75:AI:14:PRO:HD3    | 1.88                     | 0.41              |
| 77:AK:145:TYR:CG    | 77:AK:190:CYS:HB2   | 2.56                     | 0.41              |
| 77:AK:266:ASP:OD1   | 77:AK:267:THR:N     | 2.53                     | 0.41              |
| 78:AN:178:ASP:HA    | 78:AN:179:PRO:HD3   | 1.72                     | 0.41              |
| 89:Ad:245:ASP:CG    | 132:Bd:33:LYS:HZ2   | 2.28                     | 0.41              |
| 90:Ae:87:VAL:HG12   | 90:Ae:88:PRO:HD3    | 2.02                     | 0.41              |
| 90:Ae:145:MET:HA    | 90:Ae:146:PRO:HD3   | 1.79                     | 0.41              |
| 93:Aj:57:VAL:HG11   | 93:Aj:136:ARG:HD2   | 2.02                     | 0.41              |
| 93:Aj:112:SER:HA    | 109:BG:348:LEU:HD13 | 2.02                     | 0.41              |
| 96:Ap:55:HIS:CD2    | 96:Ap:57:LYS:H      | 2.37                     | 0.41              |
| 97:At:57:PRO:HA     | 97:At:58:PRO:HD3    | 1.98                     | 0.41              |
| 98:Av:180:MET:SD    | 98:Av:184:MET:HE3   | 2.60                     | 0.41              |
| 102:AA:387:A:O2'    | 102:AA:388:U:P      | 2.78                     | 0.41              |
| 102:AA:1171:A:H2'   | 102:AA:1171:A:N3    | 2.35                     | 0.41              |
| 104:BB:106:LEU:O    | 104:BB:110:THR:OG1  | 2.30                     | 0.41              |
| 107:BE:165:LEU:HD23 | 107:BE:165:LEU:HA   | 1.85                     | 0.41              |
| 108:BF:40:PRO:O     | 108:BF:43:LEU:HD12  | 2.19                     | 0.41              |
| 110:BH:116:GLU:HG2  | 133:Be:68:ARG:HA    | 2.01                     | 0.41              |
| 111:BI:122:PRO:O    | 111:BI:126:MET:HB2  | 2.21                     | 0.41              |
| 115:BM:112:TRP:HD1  | 115:BM:114:TYR:H    | 1.67                     | 0.41              |
| 122:BT:30:TYR:CE2   | 122:BT:31:LYS:HD2   | 2.55                     | 0.41              |
| 130:Bb:78:LEU:HD13  | 130:Bb:78:LEU:HA    | 1.86                     | 0.41              |
| 134:Bf:79:GLU:HA    | 134:Bf:80:PRO:HD2   | 1.94                     | 0.41              |
| 1:DA:112:GLN:CD     | 1:DA:131:ASP:OD2    | 2.62                     | 0.41              |
| 1:DA:209:TRP:HA     | 38:CP:81:PRO:HG3    | 2.01                     | 0.41              |
| 1:DA:1278:THR:CG2   | 54:Cq:152:GLU:HB2   | 2.50                     | 0.41              |
| 3:DI:304:ALA:HB2    | 3:DI:345:LEU:CD1    | 2.50                     | 0.41              |
| 8:DP:132:LEU:HD23   | 8:DP:132:LEU:HA     | 1.85                     | 0.41              |
| 8:DP:189:TYR:HD1    | 8:DP:196:TRP:C      | 2.28                     | 0.41              |
| 9:DQ:58:ARG:HH12    | 12:DU:42:THR:HB     | 1.85                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:DS:213:SER:HA   | 53:Cp:46:ILE:HB     | 2.02                     | 0.41              |
| 13:DZ:14:ASP:CG    | 44:Ca:164:ARG:HH22  | 2.28                     | 0.41              |
| 15:DB:585:MET:HE2  | 15:DB:585:MET:HB2   | 1.76                     | 0.41              |
| 15:DB:768:ALA:HB1  | 15:DB:774:ASN:HD21  | 1.86                     | 0.41              |
| 15:DB:1084:SER:HA  | 15:DB:1085:PRO:HD3  | 1.80                     | 0.41              |
| 16:DC:475:LEU:H    | 16:DC:475:LEU:HG    | 1.71                     | 0.41              |
| 18:DF:196:PHE:HD2  | 18:DF:198:HIS:CE1   | 2.38                     | 0.41              |
| 19:DG:577:LEU:HD23 | 19:DG:577:LEU:HA    | 1.77                     | 0.41              |
| 20:DH:119:LEU:HD22 | 20:DH:123:HIS:HB3   | 2.02                     | 0.41              |
| 21:DJ:230:LEU:HD23 | 21:DJ:230:LEU:HA    | 1.47                     | 0.41              |
| 22:DK:25:GLU:OE2   | 22:DK:231:SER:HB2   | 2.20                     | 0.41              |
| 33:CJ:718:PRO:HA   | 33:CJ:719:PRO:HD3   | 1.92                     | 0.41              |
| 33:CJ:798:GLN:H    | 33:CJ:798:GLN:HG3   | 1.60                     | 0.41              |
| 34:CK:102:ASP:OD2  | 45:Cb:104:LEU:HB2   | 2.19                     | 0.41              |
| 37:CO:107:LEU:HB2  | 37:CO:112:LYS:HZ2   | 1.85                     | 0.41              |
| 40:CR:306:LYS:HZ3  | 57:CA:389:A:C3'     | 2.31                     | 0.41              |
| 41:CS:140:MET:H    | 41:CS:140:MET:HG2   | 1.62                     | 0.41              |
| 45:Cb:128:GLU:HG3  | 45:Cb:146:VAL:HG22  | 2.02                     | 0.41              |
| 46:Cd:210:ASP:OD1  | 46:Cd:210:ASP:N     | 2.53                     | 0.41              |
| 49:Cj:168:VAL:HA   | 49:Cj:169:PRO:HD3   | 1.80                     | 0.41              |
| 53:Cp:90:ARG:NH1   | 57:CA:185:A:OP2     | 2.52                     | 0.41              |
| 56:Cv:39:MET:HB3   | 56:Cv:44:ARG:HD2    | 2.01                     | 0.41              |
| 56:Cv:155:ASP:HB3  | 56:Cv:158:TYR:HB2   | 2.01                     | 0.41              |
| 56:Cv:911:PRO:HG2  | 56:Cv:913:TRP:CZ2   | 2.56                     | 0.41              |
| 64:A0:36:PRO:HA    | 64:A0:87:MET:HE2    | 2.01                     | 0.41              |
| 66:A2:44:LEU:HD22  | 66:A2:44:LEU:HA     | 1.84                     | 0.41              |
| 71:A8:91:LYS:HD3   | 71:A8:91:LYS:HA     | 1.72                     | 0.41              |
| 71:A8:99:ARG:O     | 71:A8:100:GLN:HB2   | 2.20                     | 0.41              |
| 78:AN:149:ARG:NH1  | 102:AA:836:A:N6     | 2.63                     | 0.41              |
| 79:AP:234:LEU:HD23 | 79:AP:234:LEU:HA    | 1.77                     | 0.41              |
| 81:AR:212:TRP:HE1  | 107:BE:448:ARG:HH11 | 1.68                     | 0.41              |
| 84:AV:190:LYS:N    | 84:AV:206:ASN:HD21  | 2.18                     | 0.41              |
| 87:AY:35:LYS:NZ    | 102:AA:15:G:OP1     | 2.53                     | 0.41              |
| 87:AY:141:ILE:HD12 | 87:AY:172:VAL:HG13  | 2.02                     | 0.41              |
| 87:AY:243:ASP:O    | 87:AY:245:GLU:N     | 2.54                     | 0.41              |
| 89:Ad:186:THR:HG21 | 89:Ad:229:GLN:HB3   | 2.02                     | 0.41              |
| 90:Ae:72:PRO:HB3   | 102:AA:40:U:H1'     | 2.00                     | 0.41              |
| 91:Af:103:SER:OG   | 91:Af:105:GLU:OE2   | 2.21                     | 0.41              |
| 93:Aj:50:LEU:HD11  | 93:Aj:175:HIS:HB3   | 2.02                     | 0.41              |
| 97:At:129:TYR:HB3  | 97:At:133:LEU:HD23  | 2.02                     | 0.41              |
| 98:Av:84:ALA:HA    | 98:Av:87:MET:HE3    | 2.03                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 98:Av:165:ASP:HB2   | 127:BY:167:PRO:CG   | 2.49                     | 0.41              |
| 102:AA:564:A:H62    | 140:UD:39:UNK:HG3   | 1.86                     | 0.41              |
| 105:BC:375:LEU:HD23 | 105:BC:375:LEU:HA   | 1.86                     | 0.41              |
| 106:BD:304:ALA:HA   | 106:BD:350:LEU:HA   | 2.02                     | 0.41              |
| 107:BE:88:ARG:H     | 107:BE:88:ARG:HD3   | 1.84                     | 0.41              |
| 109:BG:269:HIS:O    | 109:BG:271:VAL:HG23 | 2.21                     | 0.41              |
| 112:BJ:203:LEU:HD12 | 112:BJ:203:LEU:HA   | 1.81                     | 0.41              |
| 130:Bb:83:LEU:HD12  | 130:Bb:83:LEU:HA    | 1.91                     | 0.41              |
| 134:Bf:44:ARG:CZ    | 141:UE:1:UNK:HG2    | 2.50                     | 0.41              |
| 136:Bh:48:GLY:O     | 140:UD:11:UNK:HG3   | 2.19                     | 0.41              |
| 137:UA:5:UNK:HA     | 137:UA:8:UNK:HG3    | 2.01                     | 0.41              |
| 140:UD:219:UNK:O    | 140:UD:222:UNK:HG3  | 2.20                     | 0.41              |
| 142:UG:3:UNK:HA     | 142:UG:6:UNK:HG3    | 2.01                     | 0.41              |
| 1:DA:1278:THR:CG2   | 54:Cq:152:GLU:CB    | 2.99                     | 0.41              |
| 1:DA:1656:ASN:HB2   | 1:DA:1658:GLU:OE2   | 2.20                     | 0.41              |
| 2:DD:782:ILE:HG21   | 44:Ca:303:VAL:HG11  | 2.00                     | 0.41              |
| 4:DL:269:MET:HE2    | 4:DL:272:HIS:HD2    | 1.85                     | 0.41              |
| 6:DN:226:PRO:HD2    | 6:DN:289:LEU:HB2    | 2.03                     | 0.41              |
| 6:DN:246:GLN:HE21   | 6:DN:246:GLN:HB2    | 1.59                     | 0.41              |
| 7:DO:141:LEU:HD23   | 7:DO:141:LEU:HA     | 1.89                     | 0.41              |
| 14:Da:51:THR:HG23   | 39:CQ:193:ARG:O     | 2.21                     | 0.41              |
| 15:DB:1032:ASP:OD1  | 15:DB:1032:ASP:N    | 2.31                     | 0.41              |
| 17:DE:203:LEU:HD12  | 17:DE:422:LEU:HD12  | 2.03                     | 0.41              |
| 18:DF:313:ARG:HD2   | 18:DF:339:TYR:OH    | 2.20                     | 0.41              |
| 20:DH:131:LEU:HD23  | 20:DH:131:LEU:HA    | 1.75                     | 0.41              |
| 21:DJ:31:HIS:HD2    | 21:DJ:33:ASN:HB2    | 1.84                     | 0.41              |
| 26:DX:109:LEU:HD23  | 26:DX:109:LEU:HA    | 1.70                     | 0.41              |
| 27:DY:148:ARG:NH1   | 57:CA:517:U:P       | 2.91                     | 0.41              |
| 29:CE:32:TRP:O      | 44:Ca:348:PHE:HB2   | 2.21                     | 0.41              |
| 32:CI:122:LEU:HD23  | 32:CI:122:LEU:HA    | 1.85                     | 0.41              |
| 32:CI:353:MET:O     | 32:CI:392:ARG:HG3   | 2.20                     | 0.41              |
| 33:CJ:297:LEU:HD12  | 33:CJ:319:VAL:HG21  | 2.01                     | 0.41              |
| 33:CJ:755:ASN:ND2   | 33:CJ:757:LEU:O     | 2.53                     | 0.41              |
| 34:CK:18:ALA:HB2    | 57:CA:527:A:N6      | 2.34                     | 0.41              |
| 39:CQ:173:GLU:O     | 39:CQ:177:LEU:HD13  | 2.20                     | 0.41              |
| 48:CI:83:ASN:HD22   | 57:CA:507:A:H1'     | 1.84                     | 0.41              |
| 49:Cj:46:TYR:HA     | 49:Cj:165:PHE:CE2   | 2.52                     | 0.41              |
| 56:Cv:899:ASP:OD1   | 56:Cv:906:ARG:NH1   | 2.54                     | 0.41              |
| 56:Cv:917:THR:HG22  | 56:Cv:919:GLN:H     | 1.84                     | 0.41              |
| 57:CA:414:A:O2'     | 57:CA:484:A:OP1     | 2.23                     | 0.41              |
| 67:A3:62:VAL:HG23   | 67:A3:123:LEU:HB2   | 2.02                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 69:A5:60:CYS:SG     | 69:A5:70:CYS:SG     | 3.12                     | 0.41              |
| 75:AI:151:GLN:NE2   | 145:UL:5:UNK:HB1    | 2.36                     | 0.41              |
| 77:AK:230:GLN:NE2   | 77:AK:318:GLY:H     | 2.18                     | 0.41              |
| 77:AK:275:LEU:HD22  | 77:AK:280:ARG:HG3   | 2.01                     | 0.41              |
| 85:AW:102:GLU:HB3   | 114:BL:230:ARG:HH21 | 1.86                     | 0.41              |
| 89:Ad:121:PRO:HB2   | 89:Ad:123:ASN:OD1   | 2.20                     | 0.41              |
| 92:Ag:259:PRO:HA    | 92:Ag:260:PRO:HD3   | 1.93                     | 0.41              |
| 94:AI:60:LEU:HA     | 94:AI:61:PRO:HD3    | 1.86                     | 0.41              |
| 94:AI:191:VAL:HG12  | 94:AI:196:ILE:HG12  | 2.02                     | 0.41              |
| 95:Ao:90:ASP:OD2    | 108:BF:118:ARG:NH2  | 2.54                     | 0.41              |
| 98:Av:138:LEU:HD22  | 98:Av:138:LEU:H     | 1.85                     | 0.41              |
| 98:Av:236:ILE:HD12  | 98:Av:236:ILE:H     | 1.85                     | 0.41              |
| 103:BA:166:GLU:HA   | 103:BA:169:ALA:HB3  | 2.02                     | 0.41              |
| 103:BA:174:ARG:HG2  | 103:BA:176:GLN:HE22 | 1.85                     | 0.41              |
| 104:BB:151:LEU:HB2  | 104:BB:154:GLN:OE1  | 2.19                     | 0.41              |
| 105:BC:46:LYS:HA    | 105:BC:511:GLU:O    | 2.20                     | 0.41              |
| 108:BF:171:ARG:HG3  | 108:BF:194:VAL:HG22 | 2.00                     | 0.41              |
| 112:BJ:222:PRO:HG2  | 112:BJ:227:ARG:CZ   | 2.50                     | 0.41              |
| 116:BN:62:PHE:HA    | 116:BN:139:LYS:NZ   | 2.36                     | 0.41              |
| 116:BN:207:ASN:HB3  | 136:Bh:28:ARG:NH1   | 2.32                     | 0.41              |
| 117:BO:83:VAL:HG23  | 117:BO:228:PRO:HG3  | 2.01                     | 0.41              |
| 117:BO:117:LEU:HD13 | 117:BO:162:ASP:O    | 2.19                     | 0.41              |
| 121:BS:35:TRP:CZ3   | 121:BS:102:HIS:HA   | 2.54                     | 0.41              |
| 126:BX:152:PRO:HG2  | 126:BX:156:TRP:HD1  | 1.85                     | 0.41              |
| 133:Be:63:CYS:O     | 133:Be:67:ALA:HA    | 2.19                     | 0.41              |
| 134:Bf:99:ILE:HG23  | 134:Bf:101:TYR:N    | 2.35                     | 0.41              |
| 1:DA:833:ALA:N      | 1:DA:834:PRO:HD2    | 2.36                     | 0.41              |
| 1:DA:1191:ILE:HD12  | 1:DA:1309:ILE:HG23  | 2.02                     | 0.41              |
| 3:DI:111:THR:HG21   | 3:DI:125:TRP:HZ2    | 1.86                     | 0.41              |
| 3:DI:147:ASP:O      | 3:DI:151:ARG:HG2    | 2.21                     | 0.41              |
| 8:DP:20:MET:HE2     | 8:DP:20:MET:HB3     | 1.95                     | 0.41              |
| 9:DQ:26:ASP:OD1     | 9:DQ:28:ARG:HG2     | 2.20                     | 0.41              |
| 10:DR:197:ILE:H     | 10:DR:197:ILE:HG13  | 1.64                     | 0.41              |
| 11:DS:79:LEU:HB3    | 11:DS:81:VAL:HG23   | 2.03                     | 0.41              |
| 12:DU:184:THR:OG1   | 12:DU:186:GLU:HB3   | 2.20                     | 0.41              |
| 14:Da:36:SER:O      | 14:Da:40:ARG:HG2    | 2.20                     | 0.41              |
| 15:DB:118:VAL:HG21  | 15:DB:318:LEU:HD22  | 2.02                     | 0.41              |
| 16:DC:78:PRO:HG2    | 16:DC:708:TYR:CE2   | 2.55                     | 0.41              |
| 17:DE:203:LEU:HD12  | 17:DE:203:LEU:HA    | 1.79                     | 0.41              |
| 18:DF:208:ARG:HD2   | 33:CJ:563:ASP:O     | 2.21                     | 0.41              |
| 18:DF:310:LEU:HD23  | 21:DJ:73:PRO:HB3    | 2.03                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 21:DJ:136:ALA:HB3   | 21:DJ:168:TYR:CZ    | 2.55                     | 0.41              |
| 25:DW:12:THR:HA     | 25:DW:13:PRO:HD3    | 1.77                     | 0.41              |
| 25:DW:23:HIS:HA     | 25:DW:24:PRO:HD3    | 1.86                     | 0.41              |
| 33:CJ:484:HIS:CD2   | 33:CJ:495:ARG:HH11  | 1.94                     | 0.41              |
| 33:CJ:642:ASN:ND2   | 33:CJ:654:VAL:HG12  | 2.36                     | 0.41              |
| 34:CK:14:PRO:HG3    | 40:CR:300:TYR:CD1   | 2.55                     | 0.41              |
| 35:CL:69:PHE:HZ     | 62:US:46:UNK:HG2    | 1.86                     | 0.41              |
| 36:CN:143:LEU:HD12  | 36:CN:143:LEU:HA    | 1.76                     | 0.41              |
| 46:Cd:58:ARG:HG3    | 46:Cd:58:ARG:NH1    | 2.35                     | 0.41              |
| 46:Cd:88:LEU:HD23   | 46:Cd:88:LEU:HA     | 1.89                     | 0.41              |
| 46:Cd:169:ALA:HA    | 46:Cd:186:LEU:HB3   | 2.03                     | 0.41              |
| 50:Ck:170:VAL:HG13  | 50:Ck:174:LYS:HD2   | 2.02                     | 0.41              |
| 56:Cv:493:THR:HB    | 56:Cv:529:PHE:HD1   | 1.85                     | 0.41              |
| 56:Cv:813:ARG:NH1   | 56:Cv:813:ARG:CG    | 2.83                     | 0.41              |
| 57:CA:409:A:O2'     | 57:CA:410:U:H5'     | 2.19                     | 0.41              |
| 64:A0:71:ARG:HD2    | 94:Al:45:ILE:HD11   | 2.02                     | 0.41              |
| 64:A0:151:ARG:HB3   | 64:A0:151:ARG:HH11  | 1.84                     | 0.41              |
| 64:A0:167:LEU:HD23  | 64:A0:167:LEU:HA    | 1.93                     | 0.41              |
| 66:A2:389:HIS:CD2   | 102:AA:32:U:C4      | 3.08                     | 0.41              |
| 68:A4:76:PRO:O      | 93:Aj:80:SER:HB3    | 2.20                     | 0.41              |
| 71:A8:41:LYS:O      | 71:A8:44:CYS:HB2    | 2.21                     | 0.41              |
| 73:AE:71:MET:HG3    | 96:Ap:110:LYS:HB2   | 2.03                     | 0.41              |
| 74:AF:18:SER:OG     | 74:AF:19:SER:N      | 2.51                     | 0.41              |
| 74:AF:342:ASP:O     | 74:AF:346:HIS:HD2   | 2.04                     | 0.41              |
| 75:AI:86:LEU:HD23   | 75:AI:86:LEU:HA     | 1.85                     | 0.41              |
| 75:AI:179:PRO:HG3   | 75:AI:185:TYR:HD1   | 1.86                     | 0.41              |
| 83:AU:58:GLU:O      | 83:AU:62:VAL:HG23   | 2.20                     | 0.41              |
| 86:AX:192:ASN:HD22  | 102:AA:544:G:P      | 2.44                     | 0.41              |
| 87:AY:194:ARG:HB2   | 113:BK:325:ASP:OD2  | 2.20                     | 0.41              |
| 88:Ab:114:TYR:HA    | 88:Ab:115:PRO:HD3   | 1.88                     | 0.41              |
| 89:Ad:81:ILE:HD13   | 89:Ad:81:ILE:HA     | 1.97                     | 0.41              |
| 89:Ad:89:LEU:HD22   | 132:Bd:15:PHE:HD2   | 1.86                     | 0.41              |
| 90:Ae:75:ARG:HG2    | 90:Ae:76:LEU:N      | 2.34                     | 0.41              |
| 94:Al:19:THR:HG23   | 105:BC:112:ARG:HH22 | 1.85                     | 0.41              |
| 96:Ap:238:ASP:HB2   | 96:Ap:270:MET:SD    | 2.60                     | 0.41              |
| 97:At:116:GLN:HE21  | 97:At:118:THR:HB    | 1.86                     | 0.41              |
| 98:Av:136:TRP:HA    | 98:Av:137:PRO:HD3   | 1.74                     | 0.41              |
| 103:BA:342:THR:O    | 103:BA:345:GLN:HB2  | 2.20                     | 0.41              |
| 104:BB:170:GLN:HE21 | 135:Bg:101:GLY:HA2  | 1.86                     | 0.41              |
| 104:BB:416:LEU:O    | 104:BB:419:VAL:HB   | 2.21                     | 0.41              |
| 104:BB:424:LYS:HA   | 104:BB:427:PHE:CE2  | 2.55                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 105:BC:112:ARG:H    | 105:BC:115:GLN:HE21 | 1.67                     | 0.41              |
| 105:BC:254:LEU:HD23 | 105:BC:254:LEU:HA   | 1.82                     | 0.41              |
| 105:BC:262:HIS:ND1  | 105:BC:263:PRO:HD2  | 2.35                     | 0.41              |
| 116:BN:209:LYS:HD2  | 136:Bh:15:PHE:HB2   | 2.01                     | 0.41              |
| 117:BO:89:THR:HG23  | 117:BO:91:LYS:H     | 1.85                     | 0.41              |
| 120:BR:118:GLN:HG3  | 120:BR:119:GLY:N    | 2.35                     | 0.41              |
| 122:BT:142:TYR:HE1  | 122:BT:165:ILE:HG23 | 1.85                     | 0.41              |
| 126:BX:174:PHE:H    | 140:UD:88:UNK:HB1   | 1.85                     | 0.41              |
| 127:BY:124:GLY:O    | 127:BY:125:LEU:HD13 | 2.21                     | 0.41              |
| 132:Bd:9:LEU:HD12   | 132:Bd:9:LEU:HA     | 1.81                     | 0.41              |
| 136:Bh:53:MET:HE2   | 136:Bh:56:LYS:HG2   | 2.02                     | 0.41              |
| 1:DA:115:LEU:HD13   | 39:CQ:80:LEU:CD1    | 2.50                     | 0.41              |
| 1:DA:216:LEU:HD23   | 1:DA:216:LEU:HA     | 1.92                     | 0.41              |
| 2:DD:194:ARG:HD2    | 2:DD:227:TRP:CD2    | 2.56                     | 0.41              |
| 2:DD:626:ARG:HD2    | 49:Cj:155:GLU:OE1   | 2.20                     | 0.41              |
| 2:DD:668:ARG:HG3    | 2:DD:668:ARG:NH1    | 2.36                     | 0.41              |
| 2:DD:785:MET:HE2    | 2:DD:785:MET:HB2    | 1.97                     | 0.41              |
| 3:DI:404:TRP:CZ2    | 46:Cd:122:LEU:HB3   | 2.56                     | 0.41              |
| 6:DN:75:VAL:HG12    | 6:DN:110:ALA:CB     | 2.45                     | 0.41              |
| 8:DP:199:LEU:HD23   | 8:DP:200:SER:C      | 2.45                     | 0.41              |
| 9:DQ:141:THR:HG21   | 9:DQ:184:ILE:HG23   | 2.03                     | 0.41              |
| 9:DQ:185:ARG:HH21   | 9:DQ:204:TYR:HB2    | 1.86                     | 0.41              |
| 10:DR:232:THR:O     | 49:Cj:205:ARG:NH2   | 2.47                     | 0.41              |
| 10:DR:261:ARG:NH2   | 57:CA:80:U:O3'      | 2.53                     | 0.41              |
| 11:DS:129:GLU:OE1   | 11:DS:129:GLU:N     | 2.42                     | 0.41              |
| 11:DS:196:GLY:O     | 38:CP:84:GLN:HG3    | 2.21                     | 0.41              |
| 12:DU:211:ARG:HB2   | 12:DU:211:ARG:NH1   | 2.35                     | 0.41              |
| 13:DZ:82:LYS:HA     | 44:Ca:175:TYR:OH    | 2.21                     | 0.41              |
| 15:DB:246:LEU:HD23  | 15:DB:246:LEU:HA    | 1.85                     | 0.41              |
| 15:DB:254:ASN:HB3   | 15:DB:411:MET:SD    | 2.61                     | 0.41              |
| 15:DB:623:SER:HA    | 15:DB:656:LEU:HD22  | 2.03                     | 0.41              |
| 16:DC:669:LEU:HD12  | 16:DC:669:LEU:HA    | 1.88                     | 0.41              |
| 16:DC:881:MET:HB3   | 16:DC:881:MET:HE3   | 1.72                     | 0.41              |
| 17:DE:259:ILE:H     | 17:DE:259:ILE:HG13  | 1.68                     | 0.41              |
| 19:DG:547:MET:HE3   | 19:DG:547:MET:HB3   | 1.64                     | 0.41              |
| 20:DH:69:VAL:HG22   | 20:DH:96:ARG:HH11   | 1.85                     | 0.41              |
| 22:DK:136:MET:HE2   | 22:DK:136:MET:HB3   | 1.91                     | 0.41              |
| 25:DW:119:GLN:NE2   | 57:CA:400:U:O2      | 2.48                     | 0.41              |
| 31:CH:176:ILE:HD13  | 31:CH:179:ARG:NH1   | 2.35                     | 0.41              |
| 32:CI:110:ARG:HG2   | 32:CI:110:ARG:HH11  | 1.84                     | 0.41              |
| 32:CI:335:VAL:HG13  | 32:CI:372:ILE:HB    | 2.03                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 32:CI:409:PRO:CD   | 40:CR:253:PHE:HE2   | 2.29                     | 0.41              |
| 33:CJ:23:LYS:H     | 33:CJ:23:LYS:HG2    | 1.56                     | 0.41              |
| 33:CJ:762:GLN:HB3  | 48:CI:15:VAL:HG21   | 2.03                     | 0.41              |
| 38:CP:139:LEU:HD23 | 38:CP:139:LEU:HA    | 1.88                     | 0.41              |
| 40:CR:134:ARG:NH2  | 40:CR:185:PHE:HB3   | 2.29                     | 0.41              |
| 40:CR:308:MET:HE3  | 57:CA:388:U:O3'     | 2.21                     | 0.41              |
| 44:Ca:121:ALA:HB2  | 56:Cv:1054:VAL:HG13 | 2.02                     | 0.41              |
| 44:Ca:549:SER:O    | 44:Ca:552:THR:HB    | 2.20                     | 0.41              |
| 47:Cg:153:CYS:HA   | 47:Cg:452:PRO:HD2   | 2.02                     | 0.41              |
| 48:CI:82:GLN:HA    | 48:CI:87:TYR:CD1    | 2.56                     | 0.41              |
| 49:Cj:22:LEU:HD23  | 49:Cj:22:LEU:HA     | 1.81                     | 0.41              |
| 50:Ck:552:LEU:HB3  | 50:Ck:561:SER:OG    | 2.20                     | 0.41              |
| 52:Cn:178:LYS:HE3  | 52:Cn:182:PHE:CE2   | 2.50                     | 0.41              |
| 53:Cp:10:ASP:HB2   | 57:CA:28:U:OP1      | 2.21                     | 0.41              |
| 53:Cp:66:HIS:HD2   | 53:Cp:68:LEU:H      | 1.68                     | 0.41              |
| 55:Cr:19:LEU:N     | 55:Cr:20:PRO:HD2    | 2.35                     | 0.41              |
| 56:Cv:35:ARG:HA    | 56:Cv:36:PRO:HD2    | 1.96                     | 0.41              |
| 56:Cv:613:LEU:HD12 | 56:Cv:613:LEU:HA    | 1.87                     | 0.41              |
| 65:A1:185:GLU:O    | 65:A1:189:LEU:HB2   | 2.21                     | 0.41              |
| 66:A2:222:GLU:HG3  | 66:A2:228:PHE:HE1   | 1.84                     | 0.41              |
| 66:A2:389:HIS:HB3  | 102:AA:32:U:C5      | 2.56                     | 0.41              |
| 68:A4:128:LYS:HG3  | 68:A4:130:ARG:HD3   | 2.02                     | 0.41              |
| 74:AF:120:LEU:HD23 | 74:AF:120:LEU:HA    | 1.78                     | 0.41              |
| 74:AF:397:LEU:HD12 | 122:BT:113:ARG:HH12 | 1.85                     | 0.41              |
| 75:AI:178:ILE:HA   | 75:AI:179:PRO:HD2   | 1.91                     | 0.41              |
| 75:AI:211:GLU:H    | 75:AI:211:GLU:HG2   | 1.65                     | 0.41              |
| 76:AJ:73:ARG:CZ    | 76:AJ:83:PHE:HE1    | 2.34                     | 0.41              |
| 76:AJ:73:ARG:HG2   | 76:AJ:83:PHE:CD1    | 2.56                     | 0.41              |
| 77:AK:219:ARG:NH1  | 77:AK:220:ILE:HG13  | 2.35                     | 0.41              |
| 79:AP:201:ARG:HE   | 79:AP:208:GLU:HG3   | 1.86                     | 0.41              |
| 83:AU:186:GLY:HA3  | 108:BF:158:TYR:CZ   | 2.56                     | 0.41              |
| 84:AV:66:ILE:HG13  | 84:AV:199:PHE:CD2   | 2.55                     | 0.41              |
| 86:AX:96:ASN:HB2   | 129:Ba:29:LEU:HD22  | 2.02                     | 0.41              |
| 88:Ab:211:GLU:OE2  | 105:BC:244:TRP:NE1  | 2.47                     | 0.41              |
| 88:Ab:441:ILE:HD13 | 118:BP:92:VAL:HG23  | 2.02                     | 0.41              |
| 92:Ag:202:ARG:HB3  | 92:Ag:202:ARG:CZ    | 2.51                     | 0.41              |
| 94:Al:134:ILE:HA   | 94:Al:135:PRO:HD3   | 1.78                     | 0.41              |
| 96:Ap:45:LEU:HA    | 96:Ap:46:PRO:HD3    | 1.96                     | 0.41              |
| 96:Ap:47:TYR:HB3   | 96:Ap:50:MET:HB2    | 2.03                     | 0.41              |
| 102:AA:391:U:H2'   | 102:AA:392:A:H4'    | 2.03                     | 0.41              |
| 102:AA:1106:U:OP1  | 102:AA:1160:A:N6    | 2.51                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 103:BA:231:TYR:HE1 | 103:BA:296:ARG:CZ   | 2.34                     | 0.41              |
| 103:BA:728:PRO:HG2 | 103:BA:731:SER:OG   | 2.21                     | 0.41              |
| 104:BB:90:LYS:O    | 104:BB:94:THR:OG1   | 2.34                     | 0.41              |
| 104:BB:151:LEU:H   | 104:BB:154:GLN:NE2  | 2.17                     | 0.41              |
| 107:BE:81:VAL:O    | 107:BE:85:GLU:HB2   | 2.21                     | 0.41              |
| 109:BG:74:ARG:HG2  | 109:BG:74:ARG:NH1   | 2.29                     | 0.41              |
| 109:BG:275:VAL:HA  | 109:BG:276:PRO:HD2  | 1.92                     | 0.41              |
| 114:BL:172:ILE:H   | 114:BL:172:ILE:HG13 | 1.55                     | 0.41              |
| 115:BM:256:LYS:HG3 | 115:BM:257:PHE:HD1  | 1.86                     | 0.41              |
| 130:Bb:50:LEU:C    | 130:Bb:52:SER:H     | 2.29                     | 0.41              |
| 130:Bb:93:PRO:O    | 130:Bb:123:TYR:OH   | 2.30                     | 0.41              |
| 145:UL:4:UNK:O     | 145:UL:6:UNK:HG3    | 2.20                     | 0.41              |
| 2:DD:280:LEU:HD23  | 2:DD:280:LEU:HA     | 1.71                     | 0.41              |
| 3:DI:24:VAL:HG12   | 3:DI:25:PRO:O       | 2.20                     | 0.41              |
| 4:DL:46:LYS:HB3    | 57:CA:469:A:C2      | 2.56                     | 0.41              |
| 4:DL:85:PHE:CD1    | 32:CI:269:HIS:CD2   | 3.09                     | 0.41              |
| 4:DL:282:TRP:HB3   | 4:DL:283:ILE:H      | 1.74                     | 0.41              |
| 5:DM:56:TRP:CD1    | 5:DM:56:TRP:C       | 2.98                     | 0.41              |
| 8:DP:175:GLU:CD    | 8:DP:176:PRO:HD3    | 2.45                     | 0.41              |
| 15:DB:414:GLN:HA   | 16:DC:1141:GLN:HE22 | 1.86                     | 0.41              |
| 15:DB:765:GLU:O    | 15:DB:769:VAL:HG23  | 2.20                     | 0.41              |
| 16:DC:56:ALA:HB2   | 22:DK:267:ARG:CD    | 2.49                     | 0.41              |
| 16:DC:242:HIS:CE1  | 16:DC:464:THR:HB    | 2.56                     | 0.41              |
| 16:DC:553:ALA:HA   | 16:DC:556:GLN:NE2   | 2.36                     | 0.41              |
| 18:DF:54:GLY:CA    | 18:DF:156:ALA:HB3   | 2.51                     | 0.41              |
| 18:DF:332:GLU:CD   | 18:DF:332:GLU:H     | 2.27                     | 0.41              |
| 23:DT:15:ARG:NH2   | 48:CI:174:ASP:OD2   | 2.54                     | 0.41              |
| 29:CE:306:GLU:O    | 29:CE:310:ARG:HB2   | 2.20                     | 0.41              |
| 29:CE:310:ARG:O    | 29:CE:315:ALA:HB2   | 2.21                     | 0.41              |
| 30:CF:51:PHE:HB2   | 30:CF:90:LEU:HD13   | 2.03                     | 0.41              |
| 32:CI:196:THR:HG21 | 54:Cq:106:LEU:HB3   | 2.02                     | 0.41              |
| 33:CJ:154:THR:HA   | 33:CJ:155:PRO:HD3   | 1.96                     | 0.41              |
| 34:CK:319:LYS:HB3  | 42:CU:81:GLU:HG3    | 2.03                     | 0.41              |
| 37:CO:160:TYR:CD2  | 37:CO:166:ALA:HB2   | 2.56                     | 0.41              |
| 38:CP:80:THR:HG22  | 38:CP:82:VAL:H      | 1.85                     | 0.41              |
| 39:CQ:144:LEU:HB3  | 39:CQ:166:GLU:HB3   | 2.02                     | 0.41              |
| 42:CU:43:PRO:C     | 42:CU:44:MET:HG2    | 2.45                     | 0.41              |
| 44:Ca:81:MET:HE1   | 44:Ca:89:ARG:HD3    | 2.03                     | 0.41              |
| 47:Cg:195:PRO:HA   | 50:Ck:837:TRP:CE2   | 2.56                     | 0.41              |
| 47:Cg:483:MET:HE2  | 47:Cg:483:MET:HB3   | 1.89                     | 0.41              |
| 152:Cg:501:GTP:H8  | 152:Cg:501:GTP:H5'  | 1.84                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:Ci:37:ARG:HG3   | 50:Ck:736:LEU:O    | 2.21                     | 0.41              |
| 48:Ci:69:THR:HG21  | 48:Ci:73:MET:SD    | 2.61                     | 0.41              |
| 50:Ck:60:MET:HG3   | 50:Ck:61:LEU:HG    | 2.03                     | 0.41              |
| 51:Cm:33:PRO:HB3   | 51:Cm:45:LEU:HD11  | 2.03                     | 0.41              |
| 52:Cn:144:ALA:HA   | 57:CA:280:A:N6     | 2.36                     | 0.41              |
| 56:Cv:296:LEU:HD21 | 56:Cv:421:LEU:HD21 | 2.02                     | 0.41              |
| 57:CA:293:A:H2'    | 57:CA:294:A:H8     | 1.86                     | 0.41              |
| 65:A1:56:ARG:NH1   | 143:UI:14:UNK:HG3  | 2.35                     | 0.41              |
| 69:A5:46:GLU:O     | 69:A5:50:LYS:NZ    | 2.52                     | 0.41              |
| 71:A8:69:VAL:O     | 71:A8:73:ARG:HD3   | 2.21                     | 0.41              |
| 71:A8:115:PRO:HD3  | 88:Ab:466:VAL:HG13 | 2.02                     | 0.41              |
| 73:AE:196:PHE:HE2  | 73:AE:214:HIS:CE1  | 2.38                     | 0.41              |
| 74:AF:320:LYS:HA   | 102:AA:57:A:OP2    | 2.19                     | 0.41              |
| 74:AF:388:GLU:HB2  | 74:AF:395:PRO:HA   | 2.03                     | 0.41              |
| 74:AF:423:PRO:O    | 74:AF:426:PRO:HD3  | 2.20                     | 0.41              |
| 76:AJ:14:ARG:O     | 76:AJ:41:ARG:HG3   | 2.21                     | 0.41              |
| 77:AK:31:VAL:HG23  | 124:BV:90:PHE:HE2  | 1.86                     | 0.41              |
| 77:AK:142:ARG:HB3  | 77:AK:144:HIS:CE1  | 2.56                     | 0.41              |
| 77:AK:228:LEU:HD23 | 77:AK:228:LEU:HA   | 1.94                     | 0.41              |
| 77:AK:291:TYR:O    | 77:AK:295:ARG:NH2  | 2.53                     | 0.41              |
| 79:AP:300:ARG:HH11 | 125:BW:16:GLY:HA3  | 1.86                     | 0.41              |
| 80:AQ:42:ALA:O     | 80:AQ:160:VAL:HG23 | 2.21                     | 0.41              |
| 81:AR:48:TYR:HB3   | 81:AR:57:LYS:HB3   | 2.02                     | 0.41              |
| 85:AW:258:ARG:HG2  | 103:BA:780:TYR:O   | 2.21                     | 0.41              |
| 86:AX:76:ASP:HA    | 86:AX:77:PRO:HD3   | 1.85                     | 0.41              |
| 86:AX:101:LYS:NZ   | 102:AA:33:G:OP2    | 2.54                     | 0.41              |
| 87:AY:194:ARG:HA   | 87:AY:201:MET:HA   | 2.02                     | 0.41              |
| 88:Ab:175:ARG:HH21 | 88:Ab:177:ARG:HD3  | 1.85                     | 0.41              |
| 89:Ad:260:MET:HE3  | 89:Ad:260:MET:HB2  | 1.95                     | 0.41              |
| 93:Aj:207:ILE:HG21 | 93:Aj:217:CYS:SG   | 2.60                     | 0.41              |
| 94:Al:85:LEU:HD23  | 94:Al:183:ILE:HD13 | 2.02                     | 0.41              |
| 95:Ao:51:ARG:HD3   | 95:Ao:51:ARG:HA    | 1.91                     | 0.41              |
| 102:AA:533:A:H4'   | 135:Bg:85:GLN:HE22 | 1.86                     | 0.41              |
| 103:BA:799:ASP:OD2 | 103:BA:799:ASP:O   | 2.38                     | 0.41              |
| 104:BB:154:GLN:O   | 104:BB:156:TRP:CD1 | 2.74                     | 0.41              |
| 104:BB:235:ALA:N   | 104:BB:236:PRO:HD2 | 2.35                     | 0.41              |
| 105:BC:80:PHE:CE2  | 105:BC:81:LEU:HD23 | 2.56                     | 0.41              |
| 107:BE:125:GLN:H   | 107:BE:125:GLN:HG3 | 1.68                     | 0.41              |
| 111:BI:252:MET:HE2 | 111:BI:252:MET:HB3 | 1.98                     | 0.41              |
| 112:BJ:269:GLU:HB2 | 112:BJ:274:LEU:HB3 | 2.02                     | 0.41              |
| 114:BL:242:THR:N   | 114:BL:243:PRO:HD2 | 2.36                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 116:BN:198:ILE:HG12 | 116:BN:216:TYR:CD1 | 2.56                     | 0.41              |
| 119:BQ:28:ASN:HA    | 119:BQ:29:PRO:HD3  | 1.85                     | 0.41              |
| 121:BS:28:THR:O     | 121:BS:31:ASP:HB3  | 2.20                     | 0.41              |
| 127:BY:82:ARG:O     | 127:BY:86:VAL:HG23 | 2.21                     | 0.41              |
| 129:Ba:47:ASP:O     | 129:Ba:50:LYS:HG2  | 2.20                     | 0.41              |
| 134:Bf:105:VAL:HG23 | 134:Bf:110:PHE:HE1 | 1.85                     | 0.41              |
| 135:Bg:59:LEU:HD12  | 135:Bg:59:LEU:HA   | 1.82                     | 0.41              |
| 1:DA:201:LYS:HD3    | 44:Ca:481:ARG:HD3  | 2.03                     | 0.41              |
| 1:DA:1003:PHE:CD1   | 4:DL:78:ALA:CB     | 3.04                     | 0.41              |
| 1:DA:1036:HIS:HB3   | 5:DM:294:TRP:CD1   | 2.56                     | 0.41              |
| 2:DD:741:ARG:HH11   | 2:DD:741:ARG:HB3   | 1.85                     | 0.41              |
| 5:DM:145:ILE:HG13   | 5:DM:146:GLY:N     | 2.36                     | 0.41              |
| 6:DN:12:MET:HE1     | 6:DN:17:MET:HG2    | 2.02                     | 0.41              |
| 6:DN:148:LEU:HD12   | 6:DN:148:LEU:HA    | 1.90                     | 0.41              |
| 9:DQ:151:ARG:HG2    | 9:DQ:240:ASP:OD1   | 2.20                     | 0.41              |
| 11:DS:79:LEU:HD21   | 11:DS:93:ARG:O     | 2.20                     | 0.41              |
| 15:DB:826:LEU:HA    | 15:DB:826:LEU:HD23 | 1.79                     | 0.41              |
| 16:DC:934:ARG:CG    | 16:DC:934:ARG:NH1  | 2.83                     | 0.41              |
| 17:DE:67:ASN:HA     | 17:DE:68:PRO:HD2   | 1.94                     | 0.41              |
| 17:DE:708:LEU:HD23  | 17:DE:708:LEU:HA   | 1.81                     | 0.41              |
| 18:DF:40:GLU:H      | 18:DF:40:GLU:HG2   | 1.63                     | 0.41              |
| 18:DF:88:LEU:HA     | 18:DF:88:LEU:HD12  | 1.73                     | 0.41              |
| 18:DF:94:ASP:OD1    | 18:DF:94:ASP:C     | 2.64                     | 0.41              |
| 18:DF:426:LEU:CA    | 20:DH:200:THR:HG23 | 2.50                     | 0.41              |
| 19:DG:256:ALA:HB1   | 19:DG:261:ARG:NH2  | 2.36                     | 0.41              |
| 19:DG:324:LEU:HD13  | 19:DG:373:TRP:CG   | 2.55                     | 0.41              |
| 21:DJ:147:ARG:O     | 21:DJ:155:ALA:HB3  | 2.21                     | 0.41              |
| 29:CE:69:GLU:O      | 29:CE:72:ALA:N     | 2.52                     | 0.41              |
| 29:CE:102:GLU:HG3   | 45:Cb:56:ARG:CZ    | 2.49                     | 0.41              |
| 31:CH:107:ARG:HH12  | 31:CH:133:ARG:CD   | 2.34                     | 0.41              |
| 32:CI:90:GLU:HG3    | 34:CK:107:GLN:O    | 2.20                     | 0.41              |
| 34:CK:221:THR:H     | 34:CK:224:ASN:HB3  | 1.86                     | 0.41              |
| 35:CL:112:ILE:CG2   | 60:UQ:19:UNK:HB2   | 2.49                     | 0.41              |
| 38:CP:171:MET:HE3   | 46:Cd:67:GLU:HB3   | 2.03                     | 0.41              |
| 44:Ca:299:ARG:NH1   | 44:Ca:299:ARG:CG   | 2.80                     | 0.41              |
| 46:Cd:41:LYS:HA     | 46:Cd:41:LYS:HD2   | 1.88                     | 0.41              |
| 49:Cj:147:TYR:CD1   | 49:Cj:162:GLN:HG2  | 2.56                     | 0.41              |
| 51:Cm:68:ASP:N      | 57:CA:540:A:OP1    | 2.49                     | 0.41              |
| 53:Cp:99:ARG:O      | 53:Cp:102:ARG:HG2  | 2.21                     | 0.41              |
| 57:CA:293:A:H2'     | 57:CA:294:A:C8     | 2.56                     | 0.41              |
| 64:A0:179:LEU:HD23  | 64:A0:179:LEU:HA   | 1.83                     | 0.41              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 66:A2:43:SER:H      | 87:AY:241:THR:HB     | 1.86                     | 0.41              |
| 66:A2:191:LEU:HD23  | 66:A2:191:LEU:HA     | 1.71                     | 0.41              |
| 67:A3:187:LEU:HD21  | 108:BF:311:GLN:HG3   | 2.03                     | 0.41              |
| 74:AF:458:LEU:HB2   | 98:Av:66:LYS:HE3     | 2.03                     | 0.41              |
| 79:AP:17:ARG:HD3    | 79:AP:17:ARG:HA      | 1.87                     | 0.41              |
| 79:AP:99:PRO:HD3    | 85:AW:7:ARG:NE       | 2.35                     | 0.41              |
| 79:AP:368:LYS:HD3   | 98:Av:159:GLU:HG3    | 2.03                     | 0.41              |
| 81:AR:229:HIS:HE1   | 107:BE:415:TYR:CE1   | 2.38                     | 0.41              |
| 81:AR:253:LYS:HG3   | 81:AR:254:GLU:N      | 2.35                     | 0.41              |
| 84:AV:144:LYS:HZ3   | 92:Ag:93:TYR:HE1     | 1.64                     | 0.41              |
| 85:AW:13:MET:HG2    | 85:AW:15:PRO:HD3     | 2.02                     | 0.41              |
| 87:AY:284:ASP:HA    | 87:AY:287:GLN:NE2    | 2.36                     | 0.41              |
| 89:Ad:69:PHE:HD1    | 89:Ad:69:PHE:HA      | 1.78                     | 0.41              |
| 93:Aj:59:PRO:HA     | 93:Aj:171:ASP:OD1    | 2.20                     | 0.41              |
| 96:Ap:45:LEU:HD12   | 96:Ap:46:PRO:HD2     | 2.02                     | 0.41              |
| 103:BA:183:ALA:O    | 103:BA:187:MET:HG2   | 2.20                     | 0.41              |
| 103:BA:223:LYS:NZ   | 103:BA:232:TYR:HD1   | 2.13                     | 0.41              |
| 103:BA:344:GLU:HB3  | 103:BA:393:ILE:HG12  | 2.02                     | 0.41              |
| 103:BA:603:LEU:N    | 103:BA:604:PRO:HD2   | 2.36                     | 0.41              |
| 104:BB:240:HIS:O    | 104:BB:243:ILE:HG12  | 2.21                     | 0.41              |
| 105:BC:393:VAL:HG22 | 105:BC:421:PHE:HB2   | 2.02                     | 0.41              |
| 116:BN:60:ARG:HE    | 116:BN:108:PHE:HE2   | 1.69                     | 0.41              |
| 116:BN:112:GLU:HB2  | 116:BN:123:PHE:CE2   | 2.55                     | 0.41              |
| 127:BY:79(A):ALA:HA | 127:BY:79(C):LYS:HZ3 | 1.85                     | 0.41              |
| 128:BZ:120:LEU:HD12 | 128:BZ:120:LEU:HA    | 1.83                     | 0.41              |
| 140:UD:196:UNK:O    | 140:UD:200:UNK:HB1   | 2.20                     | 0.41              |
| 1:DA:182:ARG:HH12   | 44:Ca:414:THR:HG22   | 1.86                     | 0.41              |
| 1:DA:409:LEU:HD23   | 1:DA:409:LEU:HA      | 1.88                     | 0.41              |
| 1:DA:551:LYS:HB3    | 1:DA:551:LYS:HE3     | 1.91                     | 0.41              |
| 1:DA:1526:GLY:HA3   | 1:DA:1527:PRO:HD2    | 1.97                     | 0.41              |
| 2:DD:162:LEU:HD12   | 2:DD:165:MET:HE3     | 2.02                     | 0.41              |
| 2:DD:242:LEU:HD11   | 2:DD:248:ASP:HA      | 2.03                     | 0.41              |
| 2:DD:621:LEU:C      | 49:Cj:210:PRO:HG2    | 2.46                     | 0.41              |
| 2:DD:744:ARG:NH2    | 3:DI:144:LEU:HD13    | 2.36                     | 0.41              |
| 3:DI:243:LEU:HD12   | 3:DI:243:LEU:HA      | 1.79                     | 0.41              |
| 5:DM:61:GLU:HB2     | 5:DM:74:ARG:HB2      | 2.03                     | 0.41              |
| 5:DM:186:TRP:O      | 5:DM:192:GLY:HA3     | 2.21                     | 0.41              |
| 7:DO:125:LEU:HD22   | 7:DO:125:LEU:HA      | 1.73                     | 0.41              |
| 7:DO:249:ASP:OD1    | 7:DO:249:ASP:N       | 2.53                     | 0.41              |
| 9:DQ:182:CYS:SG     | 9:DQ:203:SER:HB3     | 2.60                     | 0.41              |
| 12:DU:207:ARG:HG2   | 57:CA:161:G:N1       | 2.35                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:DZ:16:GLU:H     | 13:DZ:16:GLU:HG3    | 1.78                     | 0.41              |
| 13:DZ:90:VAL:HG22  | 44:Ca:149:ARG:NH1   | 2.36                     | 0.41              |
| 15:DB:462:ASP:HB3  | 15:DB:465:GLU:HG3   | 2.02                     | 0.41              |
| 15:DB:557:ALA:O    | 18:DF:512:ASN:ND2   | 2.54                     | 0.41              |
| 15:DB:586:ARG:HA   | 15:DB:586:ARG:HD3   | 1.85                     | 0.41              |
| 15:DB:969:THR:CB   | 15:DB:1001:THR:HG21 | 2.51                     | 0.41              |
| 16:DC:968:THR:HG22 | 16:DC:970:GLN:H     | 1.86                     | 0.41              |
| 16:DC:1090:LYS:HD3 | 16:DC:1090:LYS:HA   | 1.79                     | 0.41              |
| 17:DE:240:PRO:HD3  | 20:DH:563:HIS:NE2   | 2.36                     | 0.41              |
| 17:DE:601:ILE:HD11 | 17:DE:669:LEU:HD22  | 2.03                     | 0.41              |
| 17:DE:698:GLN:NE2  | 17:DE:699:ASN:HB2   | 2.36                     | 0.41              |
| 18:DF:23:ARG:HA    | 57:CA:435:G:N2      | 2.36                     | 0.41              |
| 18:DF:324:LEU:HA   | 18:DF:324:LEU:HD23  | 1.89                     | 0.41              |
| 18:DF:353:ARG:HH12 | 18:DF:380:LEU:HD21  | 1.85                     | 0.41              |
| 19:DG:326:THR:HG22 | 19:DG:329:LEU:H     | 1.85                     | 0.41              |
| 19:DG:392:ARG:CG   | 19:DG:392:ARG:NH1   | 2.81                     | 0.41              |
| 19:DG:405:GLN:HE21 | 19:DG:405:GLN:HB3   | 1.73                     | 0.41              |
| 20:DH:233:MET:HE1  | 20:DH:244:THR:HG21  | 2.02                     | 0.41              |
| 20:DH:247:LEU:HD23 | 20:DH:247:LEU:HA    | 1.92                     | 0.41              |
| 20:DH:327:HIS:CD2  | 20:DH:346:GLU:HG2   | 2.56                     | 0.41              |
| 20:DH:396:VAL:CG2  | 57:CA:420:A:H5"     | 2.50                     | 0.41              |
| 21:DJ:291:ASN:ND2  | 21:DJ:294:MET:HB2   | 2.36                     | 0.41              |
| 24:DV:31:HIS:CD2   | 24:DV:82:VAL:CG1    | 3.00                     | 0.41              |
| 24:DV:51:ASN:HB3   | 47:Cg:373:VAL:HG11  | 2.01                     | 0.41              |
| 25:DW:10:THR:HG23  | 41:CS:132:SER:HB2   | 2.03                     | 0.41              |
| 26:DX:46:ALA:HA    | 41:CS:148:MET:HE1   | 2.03                     | 0.41              |
| 26:DX:107:LEU:HD23 | 26:DX:107:LEU:HA    | 1.94                     | 0.41              |
| 32:CI:99:VAL:O     | 45:Cb:103:ARG:HD2   | 2.21                     | 0.41              |
| 32:CI:295:ASP:OD2  | 33:CJ:100:ARG:NH2   | 2.54                     | 0.41              |
| 32:CI:351:MET:HB2  | 47:Cg:447:LEU:CD2   | 2.51                     | 0.41              |
| 33:CJ:103:PRO:HB2  | 33:CJ:104:PHE:CD1   | 2.55                     | 0.41              |
| 33:CJ:419:ILE:HA   | 33:CJ:422:TRP:NE1   | 2.36                     | 0.41              |
| 33:CJ:457:THR:H    | 33:CJ:460:HIS:HD2   | 1.69                     | 0.41              |
| 33:CJ:731:MET:HE1  | 33:CJ:744:ILE:HD12  | 2.01                     | 0.41              |
| 33:CJ:804:ASN:OD1  | 36:CN:152:TRP:HD1   | 2.04                     | 0.41              |
| 34:CK:109:VAL:HG11 | 42:CU:123:GLN:NE2   | 2.36                     | 0.41              |
| 36:CN:72:THR:HG21  | 41:CS:83:PHE:CE2    | 2.56                     | 0.41              |
| 36:CN:104:THR:HG21 | 41:CS:48:ARG:NH2    | 2.28                     | 0.41              |
| 36:CN:146:GLY:HA3  | 36:CN:150:HIS:HB2   | 2.03                     | 0.41              |
| 37:CO:381:MET:HE2  | 37:CO:385:ARG:NH2   | 2.36                     | 0.41              |
| 40:CR:94:MET:HE2   | 40:CR:94:MET:HB3    | 1.64                     | 0.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:CR:319:LYS:HB3  | 46:Cd:281:MET:HA    | 1.08                     | 0.41              |
| 41:CS:42:LEU:HD13  | 57:CA:411:A:C4      | 2.56                     | 0.41              |
| 42:CU:41:ARG:O     | 42:CU:43:PRO:HD3    | 2.20                     | 0.41              |
| 42:CU:190:TRP:CH2  | 57:CA:614:U:C4      | 3.09                     | 0.41              |
| 44:Ca:82:PRO:HB3   | 56:Cv:1114:ASP:OD2  | 2.21                     | 0.41              |
| 44:Ca:393:GLU:HG3  | 44:Ca:403:TYR:HE1   | 1.85                     | 0.41              |
| 44:Ca:576:TRP:HA   | 44:Ca:577:PRO:C     | 2.46                     | 0.41              |
| 46:Cd:18:LEU:HD12  | 46:Cd:19:PRO:HD2    | 2.02                     | 0.41              |
| 46:Cd:174:PRO:HD3  | 46:Cd:219:HIS:CE1   | 2.56                     | 0.41              |
| 47:Cg:144:GLY:HA3  | 47:Cg:353:PHE:O     | 2.21                     | 0.41              |
| 47:Cg:231:LEU:N    | 47:Cg:239:GLN:HE22  | 2.19                     | 0.41              |
| 47:Cg:356:CYS:SG   | 47:Cg:357:THR:N     | 2.94                     | 0.41              |
| 47:Cg:414:ARG:HD2  | 47:Cg:418:ASN:HD22  | 1.86                     | 0.41              |
| 49:Cj:80:LEU:HD22  | 49:Cj:80:LEU:HA     | 1.97                     | 0.41              |
| 49:Cj:176:VAL:HG12 | 49:Cj:178:GLU:H     | 1.86                     | 0.41              |
| 50:Ck:383:ILE:HG21 | 50:Ck:392:PHE:CE2   | 2.55                     | 0.41              |
| 56:Cv:292:LYS:HG2  | 56:Cv:512:MET:CE    | 2.51                     | 0.41              |
| 56:Cv:407:MET:HA   | 56:Cv:427:TYR:O     | 2.21                     | 0.41              |
| 56:Cv:592:TYR:CE2  | 56:Cv:753:PRO:HB3   | 2.56                     | 0.41              |
| 56:Cv:702:ILE:HD11 | 56:Cv:764:LEU:HD12  | 2.03                     | 0.41              |
| 56:Cv:738:ARG:NH2  | 56:Cv:788:ARG:HD2   | 2.35                     | 0.41              |
| 56:Cv:993:THR:O    | 56:Cv:993:THR:OG1   | 2.39                     | 0.41              |
| 65:A1:85:ARG:HH12  | 102:AA:891:G:C5'    | 2.34                     | 0.41              |
| 65:A1:117:TRP:CE3  | 145:UL:2:UNK:HG1    | 2.56                     | 0.41              |
| 65:A1:140:ILE:HD13 | 65:A1:140:ILE:HA    | 1.93                     | 0.41              |
| 65:A1:167:ILE:HD13 | 112:BJ:289:GLU:OE2  | 2.21                     | 0.41              |
| 66:A2:399:THR:HG22 | 66:A2:400:TYR:CD1   | 2.56                     | 0.41              |
| 66:A2:463:ILE:HD13 | 122:BT:43:ARG:HA    | 2.02                     | 0.41              |
| 67:A3:130:ILE:HG22 | 79:AP:28:ALA:H      | 1.85                     | 0.41              |
| 68:A4:50:ARG:HD3   | 98:Av:188:GLU:CD    | 2.46                     | 0.41              |
| 68:A4:67:GLU:OE2   | 89:Ad:56:LYS:NZ     | 2.53                     | 0.41              |
| 69:A5:78:ILE:H     | 69:A5:78:ILE:HG13   | 1.45                     | 0.41              |
| 73:AE:49:MET:HG3   | 131:Bc:59:ASN:HB3   | 2.01                     | 0.41              |
| 73:AE:71:MET:HE2   | 73:AE:71:MET:HB3    | 1.82                     | 0.41              |
| 73:AE:195:GLU:HB3  | 103:BA:792:SER:HA   | 2.02                     | 0.41              |
| 74:AF:65:ASN:ND2   | 125:BW:174:ILE:HD11 | 2.33                     | 0.41              |
| 75:AI:14:PRO:HA    | 75:AI:15:PRO:HD3    | 1.86                     | 0.41              |
| 77:AK:52:ASN:ND2   | 77:AK:105:GLN:HG3   | 2.36                     | 0.41              |
| 77:AK:156:GLU:HA   | 77:AK:159:LYS:HD2   | 2.03                     | 0.41              |
| 77:AK:213:GLU:O    | 77:AK:216:ARG:HG3   | 2.20                     | 0.41              |
| 77:AK:238:LEU:HD22 | 92:Ag:216:MET:HE2   | 2.02                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 77:AK:239:ILE:O     | 77:AK:242:LEU:HB2   | 2.21                     | 0.41              |
| 78:AN:123:GLU:O     | 96:Ap:61:ASN:ND2    | 2.54                     | 0.41              |
| 78:AN:128:MET:HE1   | 111:BI:29:TRP:CZ2   | 2.56                     | 0.41              |
| 79:AP:106:MET:HE2   | 79:AP:106:MET:HB3   | 1.77                     | 0.41              |
| 79:AP:227:PRO:HG2   | 79:AP:228:TYR:CD2   | 2.56                     | 0.41              |
| 80:AQ:56:GLY:HA3    | 80:AQ:150:LEU:HD13  | 2.02                     | 0.41              |
| 83:AU:36:LEU:HD23   | 83:AU:36:LEU:HA     | 1.82                     | 0.41              |
| 85:AW:194:GLU:H     | 85:AW:194:GLU:HG3   | 1.68                     | 0.41              |
| 86:AX:83:PRO:HA     | 86:AX:84:PRO:HD3    | 1.73                     | 0.41              |
| 88:Ab:62:ASP:OD2    | 88:Ab:69:LYS:HE3    | 2.21                     | 0.41              |
| 88:Ab:97:PRO:HA     | 88:Ab:98:PRO:HD3    | 1.92                     | 0.41              |
| 88:Ab:218:PRO:HA    | 88:Ab:219:PRO:HD3   | 1.81                     | 0.41              |
| 88:Ab:314:VAL:HG12  | 88:Ab:315:ARG:HG2   | 2.03                     | 0.41              |
| 88:Ab:416:ILE:HG13  | 105:BC:76:TYR:CD1   | 2.56                     | 0.41              |
| 89:Ad:85:ARG:CZ     | 93:Aj:266:ARG:HH12  | 2.34                     | 0.41              |
| 89:Ad:220:LEU:HD23  | 89:Ad:220:LEU:HA    | 1.93                     | 0.41              |
| 90:Ae:120:PRO:HG2   | 102:AA:542:U:H4'    | 2.02                     | 0.41              |
| 90:Ae:151:THR:O     | 90:Ae:154:ARG:HG2   | 2.21                     | 0.41              |
| 91:Af:141:GLU:HG2   | 91:Af:142:ASN:N     | 2.36                     | 0.41              |
| 92:Ag:183:ARG:HH12  | 92:Ag:184:HIS:CE1   | 2.37                     | 0.41              |
| 92:Ag:218:GLU:O     | 92:Ag:221:LEU:HB3   | 2.21                     | 0.41              |
| 93:Aj:72:LEU:HD23   | 93:Aj:72:LEU:HA     | 1.86                     | 0.41              |
| 94:Al:109:ALA:HA    | 125:BW:115:TYR:OH   | 2.20                     | 0.41              |
| 95:Ao:47:LEU:HD13   | 95:Ao:47:LEU:HA     | 1.90                     | 0.41              |
| 95:Ao:100:ARG:NH2   | 95:Ao:104:LYS:HE2   | 2.36                     | 0.41              |
| 95:Ao:224:LYS:HB3   | 95:Ao:224:LYS:HZ2   | 1.84                     | 0.41              |
| 96:Ap:67:LEU:N      | 96:Ap:70:GLU:HG3    | 2.36                     | 0.41              |
| 96:Ap:108:LEU:HD23  | 96:Ap:108:LEU:HA    | 1.86                     | 0.41              |
| 98:Av:40:ASN:OD1    | 98:Av:40:ASN:N      | 2.52                     | 0.41              |
| 98:Av:47:ARG:HG3    | 98:Av:51:ARG:HH21   | 1.86                     | 0.41              |
| 98:Av:79:GLU:OE1    | 98:Av:79:GLU:N      | 2.52                     | 0.41              |
| 102:AA:2:U:OP1      | 103:BA:760:TYR:OH   | 2.38                     | 0.41              |
| 102:AA:58:U:C2      | 122:BT:11:PHE:CE2   | 3.09                     | 0.41              |
| 102:AA:380:G:H1     | 147:UU:4:UNK:HB2    | 1.85                     | 0.41              |
| 102:AA:1156:A:H3'   | 103:BA:304:GLY:O    | 2.20                     | 0.41              |
| 103:BA:277:ILE:HG13 | 103:BA:279:VAL:HG13 | 2.03                     | 0.41              |
| 104:BB:230:THR:HG22 | 104:BB:231:GLU:H    | 1.86                     | 0.41              |
| 105:BC:121:GLN:HA   | 105:BC:122:PRO:HD3  | 1.84                     | 0.41              |
| 107:BE:57:PHE:HD2   | 107:BE:62:GLU:HG2   | 1.86                     | 0.41              |
| 107:BE:240:LEU:HA   | 107:BE:240:LEU:HD12 | 1.85                     | 0.41              |
| 108:BF:129:LEU:HD12 | 108:BF:129:LEU:HA   | 1.89                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 109:BG:173:LEU:O   | 109:BG:271:VAL:HA  | 2.20                     | 0.41              |
| 113:BK:227:GLN:HA  | 113:BK:230:GLU:CD  | 2.46                     | 0.41              |
| 114:BL:94:LEU:H    | 114:BL:94:LEU:HD22 | 1.86                     | 0.41              |
| 120:BR:17:LEU:HD12 | 120:BR:17:LEU:HA   | 1.94                     | 0.41              |
| 120:BR:74:THR:HB   | 120:BR:76:LYS:HZ3  | 1.85                     | 0.41              |
| 122:BT:12:THR:O    | 122:BT:13:MET:HB2  | 2.21                     | 0.41              |
| 134:Bf:82:PHE:CE1  | 141:UE:1:UNK:HB2   | 2.56                     | 0.41              |
| 134:Bf:108:THR:HB  | 134:Bf:109:HIS:CD2 | 2.56                     | 0.41              |
| 137:UA:30:UNK:O    | 137:UA:34:UNK:N    | 2.53                     | 0.41              |
| 1:DA:105:PHE:CD1   | 39:CQ:83:LEU:HD13  | 2.56                     | 0.41              |
| 2:DD:425:LYS:HE2   | 2:DD:425:LYS:HB2   | 1.88                     | 0.41              |
| 3:DI:152:LEU:HD12  | 3:DI:152:LEU:HA    | 1.90                     | 0.41              |
| 3:DI:286:GLY:H     | 3:DI:320:GLN:HE22  | 1.69                     | 0.41              |
| 8:DP:133:GLN:HE22  | 49:Cj:66:LEU:HD12  | 1.86                     | 0.41              |
| 9:DQ:101:GLN:OE1   | 9:DQ:101:GLN:N     | 2.52                     | 0.41              |
| 10:DR:182:ARG:NH1  | 12:DU:161:ILE:HG21 | 2.36                     | 0.41              |
| 15:DB:1044:PRO:HG2 | 15:DB:1047:TRP:CD2 | 2.55                     | 0.41              |
| 15:DB:1158:LYS:HE3 | 26:DX:159:ASP:OD2  | 2.21                     | 0.41              |
| 16:DC:780:LEU:HD23 | 16:DC:780:LEU:HA   | 1.90                     | 0.41              |
| 17:DE:220:MET:O    | 17:DE:220:MET:HG3  | 2.21                     | 0.41              |
| 18:DF:540:VAL:HG12 | 18:DF:541:PHE:N    | 2.36                     | 0.41              |
| 19:DG:50:LEU:CD1   | 32:CI:249:GLU:OE1  | 2.69                     | 0.41              |
| 19:DG:80:LEU:HD22  | 19:DG:115:ILE:HD11 | 2.03                     | 0.41              |
| 19:DG:164:LEU:HD12 | 19:DG:164:LEU:HA   | 1.81                     | 0.41              |
| 20:DH:292:ARG:HH12 | 20:DH:330:THR:CG2  | 2.33                     | 0.41              |
| 21:DJ:92:LEU:HD21  | 21:DJ:130:PHE:CD2  | 2.56                     | 0.41              |
| 34:CK:262:ARG:HB3  | 34:CK:267:ARG:O    | 2.21                     | 0.41              |
| 37:CO:105:ASN:O    | 37:CO:240:LEU:HD11 | 2.21                     | 0.41              |
| 39:CQ:56:ARG:HG2   | 57:CA:99:G:OP1     | 2.21                     | 0.41              |
| 42:CU:57:VAL:HA    | 42:CU:60:ARG:HH21  | 1.86                     | 0.41              |
| 44:Ca:17:GLY:HA3   | 62:US:54:UNK:HB2   | 2.02                     | 0.41              |
| 44:Ca:138:LYS:NZ   | 44:Ca:141:THR:HA   | 2.36                     | 0.41              |
| 44:Ca:506:GLN:HE21 | 44:Ca:506:GLN:HB3  | 1.57                     | 0.41              |
| 46:Cd:14:PRO:HD2   | 46:Cd:17:ASN:ND2   | 2.36                     | 0.41              |
| 152:Cg:501:GTP:O2A | 156:Cg:601:HOH:O   | 2.22                     | 0.41              |
| 50:Ck:275:TRP:O    | 50:Ck:278:PHE:HB3  | 2.21                     | 0.41              |
| 56:Cv:53:PRO:O     | 56:Cv:54:ASN:CG    | 2.64                     | 0.41              |
| 57:CA:154:G:H2'    | 57:CA:154:G:N3     | 2.35                     | 0.41              |
| 57:CA:445:C:C2     | 57:CA:480:C:H5     | 2.39                     | 0.41              |
| 64:A0:51:ARG:NH2   | 64:A0:75:ASN:O     | 2.54                     | 0.41              |
| 64:A0:181:ARG:H    | 64:A0:181:ARG:HG2  | 1.70                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 66:A2:167:HIS:HD2   | 66:A2:169:GLY:N     | 2.18                     | 0.41              |
| 66:A2:293:PHE:HD1   | 66:A2:293:PHE:HA    | 1.65                     | 0.41              |
| 68:A4:128:LYS:HE3   | 68:A4:130:ARG:NE    | 2.35                     | 0.41              |
| 74:AF:143:GLU:HB3   | 74:AF:225:MET:HE1   | 2.02                     | 0.41              |
| 74:AF:217:LYS:NZ    | 74:AF:217:LYS:HB3   | 2.36                     | 0.41              |
| 75:AI:189:LEU:HD21  | 127:BY:145:TRP:CZ2  | 2.56                     | 0.41              |
| 77:AK:47:LYS:HD3    | 77:AK:109:ASP:OD2   | 2.21                     | 0.41              |
| 79:AP:190:ASN:HA    | 79:AP:191:PRO:HD3   | 1.99                     | 0.41              |
| 83:AU:87:GLN:HB2    | 83:AU:89:VAL:HG23   | 2.03                     | 0.41              |
| 86:AX:119:PRO:HA    | 86:AX:120:PRO:HD3   | 1.85                     | 0.41              |
| 87:AY:86:GLU:OE2    | 87:AY:88:HIS:CE1    | 2.74                     | 0.41              |
| 88:Ab:470:PRO:HA    | 88:Ab:473:TRP:CD2   | 2.56                     | 0.41              |
| 89:Ad:196:ARG:O     | 89:Ad:200:ILE:HG23  | 2.21                     | 0.41              |
| 92:Ag:156:GLU:HG2   | 111:BI:101:PHE:HD2  | 1.86                     | 0.41              |
| 95:Ao:25:ASN:ND2    | 95:Ao:26:TYR:H      | 2.17                     | 0.41              |
| 102:AA:441:A:OP2    | 124:BV:152:MET:HE2  | 2.21                     | 0.41              |
| 102:AA:490:G:O2'    | 102:AA:492:U:H5''   | 2.21                     | 0.41              |
| 103:BA:375:LEU:HD23 | 103:BA:375:LEU:HA   | 1.80                     | 0.41              |
| 103:BA:491:LEU:HD21 | 103:BA:511:ARG:HH12 | 1.85                     | 0.41              |
| 103:BA:791:PHE:N    | 103:BA:791:PHE:CD1  | 2.89                     | 0.41              |
| 104:BB:176:LEU:HB3  | 104:BB:234:ILE:HD13 | 2.04                     | 0.41              |
| 105:BC:233:LEU:HD11 | 109:BG:197:LYS:CB   | 2.51                     | 0.41              |
| 105:BC:292:ASN:HD22 | 105:BC:292:ASN:HA   | 1.76                     | 0.41              |
| 108:BF:191:ILE:HD12 | 108:BF:191:ILE:HA   | 1.82                     | 0.41              |
| 108:BF:363:GLN:HG3  | 125:BW:175:THR:O    | 2.20                     | 0.41              |
| 110:BH:129:TYR:CD1  | 110:BH:169:GLU:HB3  | 2.56                     | 0.41              |
| 116:BN:183:VAL:HG22 | 140:UD:212:UNK:HB1  | 2.03                     | 0.41              |
| 116:BN:203:TYR:HB3  | 116:BN:213:MET:HE3  | 2.02                     | 0.41              |
| 117:BO:100:ILE:HG13 | 117:BO:220:MET:CE   | 2.50                     | 0.41              |
| 1:DA:985:LYS:HB3    | 1:DA:985:LYS:HZ3    | 1.85                     | 0.40              |
| 1:DA:1483:GLN:O     | 1:DA:1488:GLN:HB2   | 2.21                     | 0.40              |
| 2:DD:26:ARG:NH1     | 57:CA:145:A:C2      | 2.89                     | 0.40              |
| 2:DD:497:ARG:HB3    | 2:DD:497:ARG:NH1    | 2.36                     | 0.40              |
| 2:DD:544:ALA:O      | 2:DD:548:GLN:HG2    | 2.22                     | 0.40              |
| 3:DI:285:GLN:HG3    | 3:DI:313:ARG:O      | 2.21                     | 0.40              |
| 11:DS:31:MET:HB2    | 11:DS:32:PHE:H      | 1.61                     | 0.40              |
| 11:DS:128:SER:OG    | 11:DS:131:ARG:HG3   | 2.20                     | 0.40              |
| 12:DU:80:LEU:HD11   | 12:DU:147:LEU:HD11  | 2.03                     | 0.40              |
| 12:DU:154:GLU:H     | 12:DU:154:GLU:HG3   | 1.59                     | 0.40              |
| 19:DG:261:ARG:HA    | 19:DG:262:PRO:HD3   | 1.77                     | 0.40              |
| 22:DK:238:ILE:HA    | 22:DK:241:VAL:HG23  | 2.03                     | 0.40              |

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| Atom-1              | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 29:CE:153:LYS:NZ    | 57:CA:547:U:OP2      | 2.54                     | 0.40              |
| 33:CJ:528:ARG:O     | 33:CJ:665:ARG:NH2    | 2.52                     | 0.40              |
| 37:CO:113:LYS:HD2   | 37:CO:114:ARG:HH21   | 1.86                     | 0.40              |
| 38:CP:96:ILE:HD13   | 38:CP:96:ILE:HG21    | 1.81                     | 0.40              |
| 39:CQ:69:GLN:HE21   | 39:CQ:69:GLN:HB3     | 1.51                     | 0.40              |
| 40:CR:270:TYR:CD1   | 47:Cg:430:LEU:HD21   | 2.57                     | 0.40              |
| 41:CS:145:LYS:HA    | 41:CS:146:PRO:HD3    | 1.87                     | 0.40              |
| 52:Cn:239:GLY:HA2   | 57:CA:338:U:O2'      | 2.20                     | 0.40              |
| 55:Cr:62:LEU:HD12   | 55:Cr:62:LEU:HA      | 1.87                     | 0.40              |
| 55:Cr:65:LYS:HB2    | 55:Cr:65:LYS:HZ3     | 1.85                     | 0.40              |
| 56:Cv:86:GLU:OE1    | 56:Cv:95:ARG:HG2     | 2.21                     | 0.40              |
| 56:Cv:316:VAL:HG13  | 56:Cv:385:VAL:HG13   | 2.04                     | 0.40              |
| 56:Cv:741:ASP:HB2   | 56:Cv:787:LYS:HB2    | 2.03                     | 0.40              |
| 56:Cv:1012:TRP:HD1  | 56:Cv:1014:ARG:HG3   | 1.83                     | 0.40              |
| 57:CA:320:A:C6      | 57:CA:321:A:C2       | 3.09                     | 0.40              |
| 67:A3:102:ILE:HB    | 67:A3:103:PRO:HD2    | 2.03                     | 0.40              |
| 73:AE:132:MET:HE3   | 73:AE:133:PHE:CZ     | 2.56                     | 0.40              |
| 74:AF:83:HIS:CD2    | 74:AF:85:TYR:HB2     | 2.56                     | 0.40              |
| 76:AJ:41:ARG:HB3    | 76:AJ:42:PRO:HD2     | 2.01                     | 0.40              |
| 85:AW:71:ILE:O      | 85:AW:71:ILE:HG12    | 2.22                     | 0.40              |
| 85:AW:157:LEU:O     | 85:AW:161:MET:HG3    | 2.21                     | 0.40              |
| 88:Ab:366:LYS:NZ    | 88:Ab:427:MET:HG2    | 2.36                     | 0.40              |
| 96:Ap:242:TYR:CG    | 96:Ap:262:GLU:HG2    | 2.56                     | 0.40              |
| 102:AA:40:U:HO2'    | 102:AA:41:U:P        | 2.44                     | 0.40              |
| 102:AA:186:A:H5''   | 102:AA:187:A:OP2     | 2.22                     | 0.40              |
| 102:AA:795:A:H2'    | 102:AA:796:A:H5'     | 2.03                     | 0.40              |
| 105:BC:360:GLU:OE1  | 105:BC:388:HIS:NE2   | 2.54                     | 0.40              |
| 108:BF:263:PHE:O    | 108:BF:267:PHE:HB3   | 2.22                     | 0.40              |
| 109:BG:39:PHE:HZ    | 109:BG:100:LEU:HD12  | 1.85                     | 0.40              |
| 109:BG:79:LEU:O     | 109:BG:149:THR:HG23  | 2.22                     | 0.40              |
| 109:BG:173:LEU:HB3  | 109:BG:271:VAL:HG22  | 2.03                     | 0.40              |
| 111:BI:117:LEU:HD23 | 111:BI:125:ASN:OD1   | 2.21                     | 0.40              |
| 112:BJ:227:ARG:O    | 112:BJ:230:GLU:HG3   | 2.21                     | 0.40              |
| 116:BN:9:TRP:HA     | 116:BN:14:HIS:HD2    | 1.86                     | 0.40              |
| 119:BQ:56:LYS:H     | 119:BQ:56:LYS:HG2    | 1.73                     | 0.40              |
| 121:BS:115:VAL:HG12 | 121:BS:116:THR:HG23  | 2.04                     | 0.40              |
| 122:BT:96:LEU:HB3   | 125:BW:50:ARG:HH21   | 1.86                     | 0.40              |
| 125:BW:168:HIS:CD2  | 125:BW:176:ARG:HB3   | 2.56                     | 0.40              |
| 127:BY:79(C):LYS:H  | 127:BY:79(C):LYS:HD3 | 1.85                     | 0.40              |
| 129:Ba:55:SER:HB3   | 129:Ba:71:TRP:CZ3    | 2.56                     | 0.40              |
| 1:DA:172:GLY:C      | 1:DA:174:HIS:H       | 2.29                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:188:LYS:HE2   | 1:DA:188:LYS:HB2   | 1.88                     | 0.40              |
| 1:DA:387:SER:OG    | 1:DA:388:VAL:N     | 2.53                     | 0.40              |
| 1:DA:602:LEU:HD23  | 1:DA:755:GLY:O     | 2.21                     | 0.40              |
| 1:DA:1098:LEU:HD12 | 1:DA:1098:LEU:HA   | 1.71                     | 0.40              |
| 1:DA:1384:ARG:NH1  | 1:DA:1628:ARG:HG2  | 2.36                     | 0.40              |
| 1:DA:1497:PRO:HG3  | 1:DA:1515:VAL:HG21 | 2.03                     | 0.40              |
| 6:DN:284:PRO:O     | 6:DN:285:GLU:HG2   | 2.21                     | 0.40              |
| 10:DR:87:LEU:HD23  | 10:DR:87:LEU:HA    | 1.85                     | 0.40              |
| 12:DU:87:PHE:HE1   | 12:DU:96:GLN:HB2   | 1.87                     | 0.40              |
| 15:DB:255:LEU:HA   | 15:DB:255:LEU:HD23 | 1.80                     | 0.40              |
| 16:DC:770:LEU:HA   | 16:DC:771:PRO:HD3  | 1.94                     | 0.40              |
| 16:DC:999:GLY:N    | 16:DC:1022:CYS:HB3 | 2.37                     | 0.40              |
| 18:DF:125:TYR:OH   | 18:DF:140:HIS:HE1  | 2.04                     | 0.40              |
| 18:DF:489:ARG:O    | 18:DF:493:MET:HG2  | 2.19                     | 0.40              |
| 20:DH:321:LEU:HD23 | 20:DH:321:LEU:HA   | 1.87                     | 0.40              |
| 20:DH:421:THR:HG22 | 20:DH:422:LYS:N    | 2.36                     | 0.40              |
| 20:DH:462:GLU:H    | 20:DH:462:GLU:HG2  | 1.51                     | 0.40              |
| 21:DJ:119:LEU:HD12 | 21:DJ:119:LEU:HA   | 1.81                     | 0.40              |
| 21:DJ:166:LEU:HD12 | 21:DJ:166:LEU:HA   | 1.81                     | 0.40              |
| 30:CF:78:LYS:HB3   | 30:CF:78:LYS:NZ    | 2.36                     | 0.40              |
| 30:CF:142:LEU:HD23 | 30:CF:142:LEU:HA   | 1.93                     | 0.40              |
| 32:CI:65:MET:HE2   | 32:CI:65:MET:HB3   | 1.78                     | 0.40              |
| 33:CJ:432:HIS:HB3  | 33:CJ:817:PRO:HB3  | 2.03                     | 0.40              |
| 34:CK:196:TYR:O    | 34:CK:206:ALA:HA   | 2.21                     | 0.40              |
| 36:CN:165:ARG:HH11 | 50:Ck:751:ASP:CG   | 2.28                     | 0.40              |
| 37:CO:396:LYS:HE3  | 57:CA:163:G:O6     | 2.21                     | 0.40              |
| 39:CQ:51:PHE:HB3   | 39:CQ:57:HIS:ND1   | 2.36                     | 0.40              |
| 43:CZ:218:VAL:HG13 | 43:CZ:222:PHE:HB3  | 2.03                     | 0.40              |
| 49:Cj:90:ARG:CZ    | 49:Cj:94:ILE:HD11  | 2.51                     | 0.40              |
| 50:Ck:841:LYS:HE2  | 50:Ck:841:LYS:HB3  | 1.73                     | 0.40              |
| 56:Cv:233:LYS:HG3  | 56:Cv:500:TYR:CG   | 2.57                     | 0.40              |
| 57:CA:43:A:H62     | 57:CA:173:A:N6     | 2.19                     | 0.40              |
| 57:CA:259:U:H5'    | 57:CA:260:U:P      | 2.61                     | 0.40              |
| 57:CA:263:A:HO2'   | 57:CA:264:A:H8     | 1.69                     | 0.40              |
| 64:A0:45:LYS:HD3   | 64:A0:78:THR:HG21  | 2.03                     | 0.40              |
| 65:A1:97:ARG:NH1   | 98:Av:30:MET:HA    | 2.35                     | 0.40              |
| 66:A2:413:TYR:CD2  | 66:A2:413:TYR:C    | 3.00                     | 0.40              |
| 68:A4:38:LYS:HG3   | 88:Ab:64:GLN:NE2   | 2.36                     | 0.40              |
| 71:A8:49:ARG:HH22  | 86:AX:80:PHE:HB2   | 1.86                     | 0.40              |
| 73:AE:103:ALA:O    | 73:AE:107:LEU:HB2  | 2.21                     | 0.40              |
| 73:AE:356:GLY:O    | 73:AE:357:LEU:HD23 | 2.22                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 74:AF:366:HIS:O     | 74:AF:370:ILE:HG13  | 2.21                     | 0.40              |
| 76:AJ:86:MET:HA     | 76:AJ:86:MET:HE3    | 2.03                     | 0.40              |
| 79:AP:150:ARG:HG3   | 79:AP:152:MET:H     | 1.86                     | 0.40              |
| 79:AP:364:ALA:O     | 79:AP:367:VAL:HG12  | 2.21                     | 0.40              |
| 85:AW:12:HIS:ND1    | 85:AW:13:MET:HB2    | 2.35                     | 0.40              |
| 87:AY:97:TYR:HB3    | 87:AY:100:PHE:CD1   | 2.57                     | 0.40              |
| 87:AY:106:ILE:HG13  | 87:AY:139:ASN:CG    | 2.46                     | 0.40              |
| 89:Ad:258:ARG:HB2   | 89:Ad:260:MET:HE2   | 2.02                     | 0.40              |
| 91:Af:84:SER:N      | 91:Af:85:PRO:HD2    | 2.37                     | 0.40              |
| 94:Al:177:GLU:HG3   | 94:Al:191:VAL:HG13  | 2.03                     | 0.40              |
| 95:Ao:25:ASN:HD22   | 95:Ao:26:TYR:N      | 2.17                     | 0.40              |
| 96:Ap:140:MET:CG    | 141:UE:4:UNK:HG1    | 2.51                     | 0.40              |
| 96:Ap:201:LEU:HD23  | 96:Ap:201:LEU:HA    | 1.91                     | 0.40              |
| 98:Av:167:ARG:O     | 98:Av:171:ILE:HG13  | 2.21                     | 0.40              |
| 102:AA:1116:U:H2'   | 111:BI:25:LYS:NZ    | 2.36                     | 0.40              |
| 105:BC:348:HIS:HA   | 105:BC:351:ASN:HB3  | 2.02                     | 0.40              |
| 108:BF:184:LEU:HA   | 108:BF:184:LEU:HD23 | 1.77                     | 0.40              |
| 111:BI:196:ARG:HH22 | 111:BI:223:GLN:HE21 | 1.69                     | 0.40              |
| 111:BI:228:GLN:HG3  | 134:Bf:106:SER:O    | 2.21                     | 0.40              |
| 113:BK:382:TYR:CD1  | 135:Bg:69:ARG:HB3   | 2.57                     | 0.40              |
| 117:BO:117:LEU:HD12 | 117:BO:161:MET:HE2  | 2.02                     | 0.40              |
| 118:BP:177:ARG:HA   | 118:BP:178:PRO:HD3  | 1.91                     | 0.40              |
| 119:BQ:71:TYR:HA    | 119:BQ:74:CYS:O     | 2.22                     | 0.40              |
| 120:BR:62:GLU:H     | 120:BR:62:GLU:CD    | 2.29                     | 0.40              |
| 121:BS:47:PRO:O     | 121:BS:74:GLU:HG3   | 2.21                     | 0.40              |
| 133:Be:21:ARG:HH11  | 133:Be:21:ARG:CG    | 2.26                     | 0.40              |
| 136:Bh:44:MET:HE2   | 136:Bh:44:MET:HB3   | 1.49                     | 0.40              |
| 1:DA:71:ASN:HA      | 1:DA:74:LYS:HD2     | 2.03                     | 0.40              |
| 2:DD:297:ARG:O      | 2:DD:301:VAL:HG23   | 2.22                     | 0.40              |
| 4:DL:113:LEU:HD21   | 32:CI:231:LEU:HD22  | 2.03                     | 0.40              |
| 6:DN:12:MET:HE3     | 6:DN:171:LEU:HD22   | 2.03                     | 0.40              |
| 14:Da:40:ARG:HH12   | 57:CA:330:U:H5      | 1.69                     | 0.40              |
| 16:DC:659:LEU:HD23  | 16:DC:659:LEU:HA    | 1.72                     | 0.40              |
| 16:DC:991:LYS:HG2   | 16:DC:1003:ARG:HG2  | 2.04                     | 0.40              |
| 17:DE:720:ASP:OD1   | 17:DE:720:ASP:C     | 2.63                     | 0.40              |
| 18:DF:502:ARG:NH1   | 18:DF:579:GLU:CG    | 2.85                     | 0.40              |
| 22:DK:185:LEU:HD12  | 22:DK:185:LEU:HA    | 1.91                     | 0.40              |
| 22:DK:270:LEU:HD12  | 22:DK:270:LEU:HA    | 1.73                     | 0.40              |
| 27:DY:148:ARG:HD2   | 27:DY:148:ARG:HA    | 1.76                     | 0.40              |
| 28:CC:50:ILE:HG13   | 28:CC:51:HIS:N      | 2.30                     | 0.40              |
| 29:CE:62:ARG:NH1    | 56:Cv:427:TYR:CE1   | 2.89                     | 0.40              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 29:CE:396:LEU:HD21  | 29:CE:418:PRO:HA   | 2.03                     | 0.40              |
| 33:CJ:27:PRO:CG     | 51:Cm:28:GLN:NE2   | 2.85                     | 0.40              |
| 33:CJ:130:ARG:NE    | 50:Ck:712:CYS:SG   | 2.95                     | 0.40              |
| 44:Ca:341:LEU:HB3   | 44:Ca:500:PHE:CE1  | 2.56                     | 0.40              |
| 44:Ca:370:GLU:O     | 56:Cv:951:LYS:NZ   | 2.54                     | 0.40              |
| 44:Ca:443:MET:CE    | 44:Ca:491:TRP:HE1  | 2.34                     | 0.40              |
| 44:Ca:459:LEU:HD23  | 44:Ca:459:LEU:HA   | 1.96                     | 0.40              |
| 45:Cb:193:GLU:H     | 45:Cb:193:GLU:HG3  | 1.59                     | 0.40              |
| 45:Cb:202:LEU:O     | 45:Cb:205:LYS:HG3  | 2.22                     | 0.40              |
| 47:Cg:46:LYS:C      | 47:Cg:48:GLY:H     | 2.29                     | 0.40              |
| 56:Cv:566:MET:HE2   | 56:Cv:566:MET:HB3  | 1.65                     | 0.40              |
| 56:Cv:858:GLY:O     | 56:Cv:861:THR:HB   | 2.22                     | 0.40              |
| 56:Cv:1100:GLY:O    | 56:Cv:1101:TYR:CD1 | 2.74                     | 0.40              |
| 57:CA:43:A:N6       | 57:CA:173:A:H62    | 2.20                     | 0.40              |
| 73:AE:106:ARG:NH1   | 96:Ap:147:TYR:OH   | 2.54                     | 0.40              |
| 74:AF:147:ASN:HD21  | 74:AF:223:ASN:ND2  | 2.19                     | 0.40              |
| 74:AF:428:LYS:HB2   | 74:AF:428:LYS:HE3  | 1.88                     | 0.40              |
| 78:AN:89:LYS:CE     | 96:Ap:62:LYS:HZ1   | 2.34                     | 0.40              |
| 79:AP:209:ARG:H     | 79:AP:209:ARG:HG2  | 1.71                     | 0.40              |
| 79:AP:319:HIS:CD2   | 105:BC:457:ARG:NH1 | 2.90                     | 0.40              |
| 81:AR:188:LEU:HD11  | 81:AR:258:TRP:CE2  | 2.56                     | 0.40              |
| 84:AV:124:THR:OG1   | 91:Af:101:HIS:HE1  | 2.04                     | 0.40              |
| 84:AV:144:LYS:CE    | 84:AV:146:MET:HE3  | 2.51                     | 0.40              |
| 88:Ab:175:ARG:NH1   | 105:BC:91:ALA:HB3  | 2.34                     | 0.40              |
| 89:Ad:85:ARG:CZ     | 93:Aj:266:ARG:NH1  | 2.85                     | 0.40              |
| 92:Ag:204:HIS:CD2   | 92:Ag:209:LEU:HD11 | 2.54                     | 0.40              |
| 93:Aj:62:HIS:HA     | 109:BG:144:TRP:CD1 | 2.54                     | 0.40              |
| 94:Al:50:MET:HA     | 94:Al:51:PRO:HD3   | 1.76                     | 0.40              |
| 97:At:22:LEU:HD22   | 120:BR:116:TRP:HB2 | 2.02                     | 0.40              |
| 102:AA:41:U:H3'     | 102:AA:42:A:H8     | 1.86                     | 0.40              |
| 103:BA:299:TYR:HD1  | 131:Bc:18:ARG:HD3  | 1.86                     | 0.40              |
| 105:BC:239:ARG:HB3  | 105:BC:239:ARG:CZ  | 2.51                     | 0.40              |
| 107:BE:38:PRO:HB3   | 107:BE:43:PRO:HB3  | 2.02                     | 0.40              |
| 109:BG:209:LEU:HD12 | 109:BG:209:LEU:HA  | 1.93                     | 0.40              |
| 119:BQ:224:LEU:HD21 | 119:BQ:230:ARG:HB2 | 2.02                     | 0.40              |
| 120:BR:95:ARG:O     | 120:BR:95:ARG:HD3  | 2.21                     | 0.40              |
| 124:BV:84:SER:HB2   | 124:BV:95:ASP:HB3  | 2.03                     | 0.40              |
| 131:Bc:29:ARG:HA    | 131:Bc:32:ARG:HE   | 1.86                     | 0.40              |
| 131:Bc:33:GLN:HE22  | 131:Bc:37:ARG:NH1  | 2.19                     | 0.40              |
| 133:Be:8:LYS:HB2    | 133:Be:8:LYS:HE2   | 1.67                     | 0.40              |
| 135:Bg:50:ASN:HD22  | 135:Bg:50:ASN:HA   | 1.68                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 136:Bh:12:MET:HE3  | 136:Bh:12:MET:HB3  | 1.92                     | 0.40              |
| 140:UD:140:UNK:HG3 | 140:UD:142:UNK:HG3 | 2.02                     | 0.40              |
| 1:DA:79:LEU:HD21   | 38:CP:53:ARG:HH11  | 1.86                     | 0.40              |
| 1:DA:90:MET:HE3    | 2:DD:125:LEU:HD11  | 2.04                     | 0.40              |
| 1:DA:521:GLU:O     | 1:DA:525:LEU:HG    | 2.22                     | 0.40              |
| 1:DA:681:ILE:HG13  | 1:DA:701:VAL:HG22  | 2.03                     | 0.40              |
| 2:DD:465:PHE:CD2   | 2:DD:479:ARG:HD3   | 2.56                     | 0.40              |
| 2:DD:570:MET:SD    | 10:DR:205:LEU:HD21 | 2.62                     | 0.40              |
| 6:DN:23:VAL:HG12   | 6:DN:116:VAL:HG11  | 2.03                     | 0.40              |
| 6:DN:162:LEU:HD12  | 6:DN:162:LEU:HA    | 1.91                     | 0.40              |
| 6:DN:213:ARG:NH2   | 44:Ca:192:GLN:OE1  | 2.54                     | 0.40              |
| 7:DO:119:ARG:O     | 7:DO:123:LEU:HB2   | 2.22                     | 0.40              |
| 7:DO:123:LEU:HD12  | 7:DO:123:LEU:HA    | 1.78                     | 0.40              |
| 7:DO:198:ARG:HH11  | 7:DO:256:ARG:HH12  | 1.70                     | 0.40              |
| 9:DQ:153:ARG:HB2   | 9:DQ:237:ASP:HA    | 2.03                     | 0.40              |
| 10:DR:105:THR:HG23 | 49:Cj:147:TYR:CE2  | 2.57                     | 0.40              |
| 15:DB:232:ARG:NH1  | 16:DC:953:MET:O    | 2.52                     | 0.40              |
| 15:DB:745:ASP:H    | 15:DB:790:SER:HG   | 1.69                     | 0.40              |
| 15:DB:882:ARG:HA   | 15:DB:883:PRO:HD2  | 1.96                     | 0.40              |
| 16:DC:86:THR:OG1   | 16:DC:959:VAL:HG21 | 2.22                     | 0.40              |
| 16:DC:635:MET:CE   | 16:DC:659:LEU:HD12 | 2.51                     | 0.40              |
| 16:DC:1110:HIS:HD2 | 16:DC:1123:SER:HB2 | 1.85                     | 0.40              |
| 17:DE:229:ARG:NH1  | 17:DE:255:PHE:CZ   | 2.88                     | 0.40              |
| 18:DF:502:ARG:HD3  | 18:DF:577:ALA:O    | 2.22                     | 0.40              |
| 19:DG:124:PHE:CD1  | 19:DG:142:LEU:HD21 | 2.56                     | 0.40              |
| 19:DG:524:PHE:HZ   | 19:DG:582:VAL:HG11 | 1.86                     | 0.40              |
| 21:DJ:21:PRO:HG2   | 33:CJ:74:TRP:CZ2   | 2.56                     | 0.40              |
| 29:CE:221:GLY:H    | 56:Cv:45:PHE:HE1   | 1.70                     | 0.40              |
| 30:CF:15:ARG:HH11  | 30:CF:15:ARG:HG3   | 1.86                     | 0.40              |
| 34:CK:42:PHE:CD1   | 34:CK:42:PHE:C     | 3.00                     | 0.40              |
| 40:CR:259:GLN:OE1  | 47:Cg:480:LYS:NZ   | 2.54                     | 0.40              |
| 42:CU:160:ARG:HH21 | 51:Cm:117:ARG:HH21 | 1.70                     | 0.40              |
| 43:CZ:276:HIS:NE2  | 43:CZ:292:ALA:HB3  | 2.35                     | 0.40              |
| 46:Cd:257:LEU:O    | 46:Cd:260:THR:OG1  | 2.32                     | 0.40              |
| 47:Cg:58:TYR:OH    | 47:Cg:419:SER:HB3  | 2.22                     | 0.40              |
| 47:Cg:209:LYS:O    | 47:Cg:213:VAL:HG13 | 2.21                     | 0.40              |
| 47:Cg:383:ASP:O    | 47:Cg:384:GLU:OE2  | 2.40                     | 0.40              |
| 48:Ci:30:ARG:HH11  | 48:Ci:30:ARG:CG    | 2.34                     | 0.40              |
| 57:CA:79:A:N3      | 57:CA:79:A:H2'     | 2.36                     | 0.40              |
| 65:A1:142:LYS:NZ   | 65:A1:143:ARG:HH11 | 2.19                     | 0.40              |
| 65:A1:180:LEU:HD23 | 65:A1:180:LEU:HA   | 1.88                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 68:A4:33:ARG:HA     | 68:A4:34:PRO:HD2    | 1.93                     | 0.40              |
| 69:A5:78:ILE:HD11   | 107:BE:378:LEU:HD11 | 2.03                     | 0.40              |
| 74:AF:145:SER:O     | 74:AF:149:THR:HG23  | 2.21                     | 0.40              |
| 77:AK:273:HIS:HB3   | 77:AK:285:ARG:NH2   | 2.36                     | 0.40              |
| 79:AP:264:GLN:HG2   | 79:AP:271:TYR:CZ    | 2.57                     | 0.40              |
| 81:AR:250:TRP:CZ2   | 81:AR:255:GLU:HG3   | 2.57                     | 0.40              |
| 83:AU:165:HIS:HD2   | 83:AU:167:ALA:HB3   | 1.86                     | 0.40              |
| 86:AX:173:VAL:O     | 86:AX:177:LYS:HB2   | 2.21                     | 0.40              |
| 88:Ab:253:ILE:HG12  | 88:Ab:280:MET:SD    | 2.62                     | 0.40              |
| 94:Al:178:GLU:O     | 94:Al:182:LYS:HE3   | 2.22                     | 0.40              |
| 95:Ao:73:CYS:HA     | 95:Ao:74:PRO:HD3    | 1.93                     | 0.40              |
| 96:Ap:154:HIS:CD2   | 111:BI:218:LEU:HG   | 2.57                     | 0.40              |
| 97:At:24:VAL:HG22   | 102:AA:383:A:C8     | 2.56                     | 0.40              |
| 98:Av:37:MET:HE3    | 98:Av:43:ARG:HB3    | 2.03                     | 0.40              |
| 102:AA:1166:A:O2'   | 103:BA:775:PRO:HG2  | 2.20                     | 0.40              |
| 105:BC:175:PRO:HB3  | 105:BC:344:PHE:CD1  | 2.57                     | 0.40              |
| 107:BE:287:LEU:HD23 | 107:BE:287:LEU:HA   | 1.86                     | 0.40              |
| 107:BE:310:LYS:HA   | 107:BE:311:PRO:HD3  | 1.89                     | 0.40              |
| 113:BK:110:ALA:O    | 113:BK:114:HIS:HB2  | 2.21                     | 0.40              |
| 116:BN:55:VAL:HG13  | 116:BN:99:VAL:HA    | 2.03                     | 0.40              |
| 121:BS:110:LEU:HD23 | 121:BS:110:LEU:HA   | 1.91                     | 0.40              |
| 126:BX:112:PHE:N    | 126:BX:112:PHE:HD1  | 2.19                     | 0.40              |
| 127:BY:90:LYS:HA    | 127:BY:93:GLU:OE2   | 2.22                     | 0.40              |
| 128:BZ:123:THR:O    | 128:BZ:123:THR:OG1  | 2.38                     | 0.40              |
| 129:Ba:76:TYR:CD2   | 129:Ba:93:LYS:HB2   | 2.57                     | 0.40              |
| 129:Ba:129:GLN:HG3  | 129:Ba:130:ASP:OD2  | 2.21                     | 0.40              |
| 132:Bd:69:LEU:HD13  | 132:Bd:69:LEU:HA    | 1.76                     | 0.40              |
| 134:Bf:38:GLU:HB3   | 134:Bf:39:ALA:H     | 1.76                     | 0.40              |
| 142:UN:19:UNK:HG2   | 142:UN:20:UNK:HG3   | 2.03                     | 0.40              |
| 1:DA:711:ILE:H      | 1:DA:711:ILE:HG13   | 1.64                     | 0.40              |
| 1:DA:904:TRP:HB2    | 44:Ca:401:ASP:OD2   | 2.22                     | 0.40              |
| 1:DA:1255:VAL:HG13  | 1:DA:1258:ASN:HD22  | 1.86                     | 0.40              |
| 1:DA:1417:PHE:C     | 1:DA:1419:GLY:N     | 2.79                     | 0.40              |
| 2:DD:310:ALA:O      | 2:DD:313:HIS:HB3    | 2.21                     | 0.40              |
| 3:DI:344:LEU:HD13   | 3:DI:346:LEU:HD21   | 2.03                     | 0.40              |
| 4:DL:69:GLU:HB2     | 4:DL:73:SER:OG      | 2.22                     | 0.40              |
| 4:DL:203:ARG:HE     | 4:DL:203:ARG:HB3    | 1.71                     | 0.40              |
| 10:DR:126:LEU:HB2   | 10:DR:135:CYS:HB3   | 2.03                     | 0.40              |
| 13:DZ:36:LEU:HD12   | 13:DZ:36:LEU:HA     | 1.94                     | 0.40              |
| 15:DB:383:ARG:HA    | 15:DB:396:ARG:HH12  | 1.85                     | 0.40              |
| 15:DB:1107:THR:HA   | 15:DB:1108:PRO:HD3  | 1.91                     | 0.40              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 16:DC:155:VAL:CG1   | 16:DC:168:PHE:HE1  | 2.23                     | 0.40              |
| 16:DC:496:LYS:CG    | 16:DC:497:PRO:HD2  | 2.51                     | 0.40              |
| 21:DJ:191:TYR:HD1   | 21:DJ:191:TYR:HA   | 1.76                     | 0.40              |
| 21:DJ:251:TYR:CE2   | 21:DJ:255:LYS:HE3  | 2.56                     | 0.40              |
| 24:DV:77:LYS:H      | 24:DV:77:LYS:HG3   | 1.80                     | 0.40              |
| 24:DV:137:ARG:O     | 24:DV:138:ASN:HB2  | 2.22                     | 0.40              |
| 26:DX:68:TYR:HB2    | 26:DX:164:THR:HG23 | 2.02                     | 0.40              |
| 27:DY:84:LYS:HB3    | 27:DY:84:LYS:HE2   | 1.88                     | 0.40              |
| 29:CE:136:PHE:CZ    | 29:CE:201:ILE:HD12 | 2.57                     | 0.40              |
| 30:CF:143:GLU:HA    | 30:CF:146:TRP:HB2  | 2.04                     | 0.40              |
| 32:CI:83:GLY:HA3    | 32:CI:87:TYR:OH    | 2.22                     | 0.40              |
| 33:CJ:723:GLU:HG2   | 33:CJ:724:THR:H    | 1.87                     | 0.40              |
| 35:CL:71:LEU:HB2    | 35:CL:94:VAL:HG13  | 2.04                     | 0.40              |
| 36:CN:30:LEU:HA     | 36:CN:30:LEU:HD12  | 1.75                     | 0.40              |
| 37:CO:267:ARG:NH2   | 39:CQ:168:ASN:OD1  | 2.55                     | 0.40              |
| 40:CR:13:LEU:HA     | 40:CR:16:PHE:CZ    | 2.57                     | 0.40              |
| 43:CZ:311:GLU:H     | 43:CZ:311:GLU:CD   | 2.30                     | 0.40              |
| 44:Ca:153:LYS:HG3   | 44:Ca:154:GLU:N    | 2.36                     | 0.40              |
| 47:Cg:238:ARG:HD2   | 47:Cg:238:ARG:HA   | 1.84                     | 0.40              |
| 48:Ci:121:ASP:HB3   | 48:Ci:127:THR:O    | 2.21                     | 0.40              |
| 52:Cn:231:LYS:HA    | 52:Cn:231:LYS:HD2  | 1.87                     | 0.40              |
| 53:Cp:92:LEU:HD23   | 53:Cp:102:ARG:HB2  | 2.03                     | 0.40              |
| 53:Cp:164:ASP:O     | 53:Cp:168:ILE:HG13 | 2.21                     | 0.40              |
| 55:Cr:282:GLU:O     | 55:Cr:286:VAL:HG23 | 2.20                     | 0.40              |
| 66:A2:84:LEU:O      | 66:A2:87:ILE:HG22  | 2.21                     | 0.40              |
| 73:AE:54:ARG:HB2    | 131:Bc:57:TRP:CZ2  | 2.57                     | 0.40              |
| 73:AE:319:LYS:HB2   | 73:AE:379:CYS:SG   | 2.61                     | 0.40              |
| 78:AN:129:LEU:HA    | 78:AN:129:LEU:HD23 | 1.77                     | 0.40              |
| 80:AQ:39:ASN:OD1    | 80:AQ:39:ASN:N     | 2.43                     | 0.40              |
| 80:AQ:55:PHE:HA     | 80:AQ:115:PHE:O    | 2.22                     | 0.40              |
| 88:Ab:459:ARG:HH11  | 88:Ab:472:PHE:HB3  | 1.87                     | 0.40              |
| 92:Ag:238:MET:HG2   | 115:BM:257:PHE:CG  | 2.55                     | 0.40              |
| 94:Al:137:PHE:HD2   | 94:Al:139:HIS:CD2  | 2.39                     | 0.40              |
| 102:AA:377:A:H2     | 59:UW:7:UNK:HG3    | 1.87                     | 0.40              |
| 102:AA:836:A:O2'    | 131:Bc:10:ASP:N    | 2.45                     | 0.40              |
| 105:BC:301:MET:HE1  | 105:BC:421:PHE:CE1 | 2.56                     | 0.40              |
| 105:BC:340:HIS:HD2  | 105:BC:342:ASP:H   | 1.70                     | 0.40              |
| 107:BE:230:THR:HG23 | 107:BE:271:ASP:HB2 | 2.03                     | 0.40              |
| 108:BF:135:TYR:HD1  | 108:BF:135:TYR:HA  | 1.81                     | 0.40              |
| 112:BJ:291:VAL:HG12 | 112:BJ:297:TRP:CE2 | 2.57                     | 0.40              |
| 117:BO:215:LEU:HD23 | 117:BO:219:ARG:CZ  | 2.51                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 118:BP:215:TRP:CH2 | 118:BP:217:PRO:HG3  | 2.56                     | 0.40              |
| 121:BS:27:VAL:O    | 121:BS:32:ARG:NH2   | 2.52                     | 0.40              |
| 122:BT:11:PHE:CZ   | 122:BT:13:MET:HG2   | 2.56                     | 0.40              |
| 122:BT:61:ARG:HA   | 129:Ba:144:VAL:HG21 | 2.04                     | 0.40              |
| 126:BX:111:PHE:C   | 126:BX:112:PHE:HD1  | 2.30                     | 0.40              |
| 126:BX:112:PHE:N   | 126:BX:112:PHE:CD1  | 2.89                     | 0.40              |
| 135:Bg:97:LEU:HD23 | 135:Bg:97:LEU:HA    | 1.91                     | 0.40              |
| 143:UI:2:UNK:HA    | 143:UI:5:UNK:HG3    | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | DA    | 1551/1788 (87%) | 1498 (97%) | 50 (3%) | 3 (0%)   | 43          | 78  |
| 2   | DD    | 787/812 (97%)   | 747 (95%)  | 38 (5%) | 2 (0%)   | 36          | 72  |
| 3   | DI    | 388/407 (95%)   | 366 (94%)  | 21 (5%) | 1 (0%)   | 36          | 72  |
| 4   | DL    | 279/307 (91%)   | 263 (94%)  | 16 (6%) | 0        | 100         | 100 |
| 5   | DM    | 292/294 (99%)   | 283 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 6   | DN    | 253/293 (86%)   | 242 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 7   | DO    | 220/282 (78%)   | 213 (97%)  | 6 (3%)  | 1 (0%)   | 24          | 63  |
| 8   | DP    | 205/274 (75%)   | 195 (95%)  | 9 (4%)  | 1 (0%)   | 24          | 63  |
| 9   | DQ    | 254/268 (95%)   | 246 (97%)  | 6 (2%)  | 2 (1%)   | 16          | 54  |
| 10  | DR    | 247/270 (92%)   | 239 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 11  | DS    | 234/261 (90%)   | 227 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 12  | DU    | 211/228 (92%)   | 202 (96%)  | 7 (3%)  | 2 (1%)   | 14          | 51  |
| 13  | DZ    | 80/94 (85%)     | 75 (94%)   | 5 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 14  | Da    | 53/64 (83%)     | 52 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 15  | DB    | 1109/1181 (94%) | 1078 (97%) | 29 (3%) | 2 (0%)   | 43          | 78  |
| 16  | DC    | 1087/1165 (93%) | 1052 (97%) | 34 (3%) | 1 (0%)   | 48          | 83  |
| 17  | DE    | 576/746 (77%)   | 564 (98%)  | 11 (2%) | 1 (0%)   | 43          | 78  |
| 18  | DF    | 586/666 (88%)   | 569 (97%)  | 16 (3%) | 1 (0%)   | 43          | 78  |
| 19  | DG    | 558/631 (88%)   | 543 (97%)  | 14 (2%) | 1 (0%)   | 43          | 78  |
| 20  | DH    | 560/581 (96%)   | 540 (96%)  | 20 (4%) | 0        | 100         | 100 |
| 21  | DJ    | 313/396 (79%)   | 304 (97%)  | 8 (3%)  | 1 (0%)   | 36          | 72  |
| 22  | DK    | 249/324 (77%)   | 240 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 23  | DT    | 237/247 (96%)   | 233 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 24  | DV    | 158/183 (86%)   | 151 (96%)  | 6 (4%)  | 1 (1%)   | 21          | 59  |
| 25  | DW    | 159/179 (89%)   | 153 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 26  | DX    | 139/169 (82%)   | 133 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 27  | DY    | 152/163 (93%)   | 148 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 28  | CC    | 72/74 (97%)     | 68 (94%)   | 4 (6%)  | 0        | 100         | 100 |
| 29  | CE    | 413/435 (95%)   | 395 (96%)  | 18 (4%) | 0        | 100         | 100 |
| 30  | CF    | 157/160 (98%)   | 152 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 31  | CH    | 271/282 (96%)   | 265 (98%)  | 5 (2%)  | 1 (0%)   | 30          | 67  |
| 32  | CI    | 418/443 (94%)   | 406 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 33  | CJ    | 796/817 (97%)   | 765 (96%)  | 30 (4%) | 1 (0%)   | 48          | 83  |
| 34  | CK    | 287/326 (88%)   | 272 (95%)  | 15 (5%) | 0        | 100         | 100 |
| 35  | CL    | 85/87 (98%)     | 80 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 36  | CN    | 155/166 (93%)   | 150 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 37  | CO    | 359/429 (84%)   | 343 (96%)  | 14 (4%) | 2 (1%)   | 21          | 59  |
| 38  | CP    | 178/188 (95%)   | 171 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 39  | CQ    | 188/307 (61%)   | 182 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 40  | CR    | 312/320 (98%)   | 301 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 41  | CS    | 140/244 (57%)   | 135 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 42  | CU    | 182/193 (94%)   | 177 (97%)  | 4 (2%)  | 1 (0%)   | 24          | 63  |
| 43  | CZ    | 149/360 (41%)   | 142 (95%)  | 6 (4%)  | 1 (1%)   | 18          | 56  |
| 44  | Ca    | 590/602 (98%)   | 556 (94%)  | 29 (5%) | 5 (1%)   | 16          | 54  |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 45  | Cb    | 248/324 (76%)   | 242 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 46  | Cd    | 289/440 (66%)   | 281 (97%)  | 6 (2%)  | 2 (1%)   | 18          | 56  |
| 47  | Cg    | 480/498 (96%)   | 461 (96%)  | 19 (4%) | 0        | 100         | 100 |
| 48  | Ci    | 163/181 (90%)   | 155 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 49  | Cj    | 224/257 (87%)   | 216 (96%)  | 7 (3%)  | 1 (0%)   | 30          | 67  |
| 50  | Ck    | 699/874 (80%)   | 671 (96%)  | 26 (4%) | 2 (0%)   | 36          | 72  |
| 51  | Cm    | 194/215 (90%)   | 184 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 52  | Cn    | 108/250 (43%)   | 103 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 53  | Cp    | 173/187 (92%)   | 169 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 54  | Cq    | 250/263 (95%)   | 243 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 55  | Cr    | 253/439 (58%)   | 243 (96%)  | 9 (4%)  | 1 (0%)   | 30          | 67  |
| 56  | Cv    | 1051/1211 (87%) | 1011 (96%) | 40 (4%) | 0        | 100         | 100 |
| 64  | A0    | 147/185 (80%)   | 142 (97%)  | 4 (3%)  | 1 (1%)   | 18          | 56  |
| 65  | A1    | 215/241 (89%)   | 209 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 66  | A2    | 445/471 (94%)   | 433 (97%)  | 9 (2%)  | 3 (1%)   | 18          | 56  |
| 67  | A3    | 148/218 (68%)   | 145 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 68  | A4    | 166/183 (91%)   | 156 (94%)  | 10 (6%) | 0        | 100         | 100 |
| 69  | A5    | 53/80 (66%)     | 51 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 70  | A6    | 70/114 (61%)    | 70 (100%)  | 0       | 0        | 100         | 100 |
| 71  | A8    | 139/181 (77%)   | 128 (92%)  | 11 (8%) | 0        | 100         | 100 |
| 72  | A9    | 51/184 (28%)    | 48 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 73  | AE    | 289/473 (61%)   | 278 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 74  | AF    | 440/459 (96%)   | 417 (95%)  | 22 (5%) | 1 (0%)   | 43          | 78  |
| 75  | AI    | 210/263 (80%)   | 199 (95%)  | 11 (5%) | 0        | 100         | 100 |
| 76  | AJ    | 124/177 (70%)   | 117 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 77  | AK    | 319/342 (93%)   | 307 (96%)  | 11 (3%) | 1 (0%)   | 36          | 72  |
| 78  | AN    | 177/202 (88%)   | 172 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 79  | AP    | 348/374 (93%)   | 332 (95%)  | 14 (4%) | 2 (1%)   | 21          | 59  |
| 80  | AQ    | 121/167 (72%)   | 118 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 81  | AR    | 225/301 (75%)   | 212 (94%)  | 12 (5%) | 1 (0%)   | 30          | 67  |
| 82  | AT    | 33/144 (23%)    | 32 (97%)   | 1 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 83  | AU    | 171/213 (80%) | 168 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 84  | AV    | 178/188 (95%) | 174 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 85  | AW    | 274/278 (99%) | 267 (97%) | 6 (2%)  | 1 (0%)   | 30          | 67  |
| 86  | AX    | 166/246 (68%) | 163 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 87  | AY    | 338/378 (89%) | 326 (96%) | 8 (2%)  | 4 (1%)   | 10          | 44  |
| 88  | Ab    | 449/507 (89%) | 425 (95%) | 24 (5%) | 0        | 100         | 100 |
| 89  | Ad    | 255/289 (88%) | 251 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 90  | Ae    | 114/197 (58%) | 109 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 91  | Af    | 124/189 (66%) | 119 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 92  | Ag    | 257/260 (99%) | 249 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 93  | Aj    | 277/296 (94%) | 260 (94%) | 17 (6%) | 0        | 100         | 100 |
| 94  | Al    | 207/218 (95%) | 196 (95%) | 11 (5%) | 0        | 100         | 100 |
| 95  | Ao    | 179/259 (69%) | 170 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 96  | Ap    | 259/309 (84%) | 248 (96%) | 11 (4%) | 0        | 100         | 100 |
| 97  | At    | 136/154 (88%) | 129 (95%) | 6 (4%)  | 1 (1%)   | 18          | 56  |
| 98  | Av    | 211/242 (87%) | 203 (96%) | 6 (3%)  | 2 (1%)   | 14          | 51  |
| 99  | AB    | 54/56 (96%)   | 48 (89%)  | 6 (11%) | 0        | 100         | 100 |
| 100 | AC    | 26/28 (93%)   | 26 (100%) | 0       | 0        | 100         | 100 |
| 100 | AD    | 26/28 (93%)   | 25 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 101 | AG    | 25/27 (93%)   | 25 (100%) | 0       | 0        | 100         | 100 |
| 103 | BA    | 675/831 (81%) | 654 (97%) | 21 (3%) | 0        | 100         | 100 |
| 104 | BB    | 387/541 (72%) | 369 (95%) | 17 (4%) | 1 (0%)   | 36          | 72  |
| 105 | BC    | 476/523 (91%) | 451 (95%) | 23 (5%) | 2 (0%)   | 30          | 67  |
| 106 | BD    | 415/547 (76%) | 385 (93%) | 22 (5%) | 8 (2%)   | 6           | 32  |
| 107 | BE    | 386/449 (86%) | 362 (94%) | 22 (6%) | 2 (0%)   | 24          | 63  |
| 108 | BF    | 341/426 (80%) | 330 (97%) | 10 (3%) | 1 (0%)   | 36          | 72  |
| 109 | BG    | 317/378 (84%) | 292 (92%) | 25 (8%) | 0        | 100         | 100 |
| 110 | BH    | 209/349 (60%) | 203 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 111 | BI    | 317/343 (92%) | 302 (95%) | 14 (4%) | 1 (0%)   | 36          | 72  |
| 112 | BJ    | 164/333 (49%) | 157 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 113 | BK    | 252/386 (65%) | 241 (96%) | 11 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 114 | BL    | 226/312 (72%)     | 221 (98%)   | 5 (2%)    | 0        | 100         | 100 |
| 115 | BM    | 243/283 (86%)     | 227 (93%)   | 15 (6%)   | 1 (0%)   | 30          | 67  |
| 116 | BN    | 212/302 (70%)     | 203 (96%)   | 9 (4%)    | 0        | 100         | 100 |
| 117 | BO    | 143/262 (55%)     | 135 (94%)   | 7 (5%)    | 1 (1%)   | 18          | 56  |
| 118 | BP    | 200/266 (75%)     | 190 (95%)   | 8 (4%)    | 2 (1%)   | 12          | 49  |
| 119 | BQ    | 214/231 (93%)     | 201 (94%)   | 13 (6%)   | 0        | 100         | 100 |
| 120 | BR    | 193/205 (94%)     | 181 (94%)   | 11 (6%)   | 1 (0%)   | 24          | 63  |
| 121 | BS    | 95/160 (59%)      | 92 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 122 | BT    | 166/191 (87%)     | 160 (96%)   | 6 (4%)    | 0        | 100         | 100 |
| 123 | BU    | 80/185 (43%)      | 79 (99%)    | 1 (1%)    | 0        | 100         | 100 |
| 124 | BV    | 153/190 (80%)     | 145 (95%)   | 7 (5%)    | 1 (1%)   | 18          | 56  |
| 125 | BW    | 185/188 (98%)     | 177 (96%)   | 8 (4%)    | 0        | 100         | 100 |
| 126 | BX    | 103/190 (54%)     | 93 (90%)    | 9 (9%)    | 1 (1%)   | 12          | 49  |
| 127 | BY    | 100/172 (58%)     | 91 (91%)    | 8 (8%)    | 1 (1%)   | 12          | 49  |
| 128 | BZ    | 188/190 (99%)     | 180 (96%)   | 8 (4%)    | 0        | 100         | 100 |
| 129 | Ba    | 137/139 (99%)     | 132 (96%)   | 5 (4%)    | 0        | 100         | 100 |
| 130 | Bb    | 97/162 (60%)      | 90 (93%)    | 7 (7%)    | 0        | 100         | 100 |
| 131 | Bc    | 88/146 (60%)      | 85 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 132 | Bd    | 138/144 (96%)     | 133 (96%)   | 5 (4%)    | 0        | 100         | 100 |
| 133 | Be    | 99/113 (88%)      | 99 (100%)   | 0         | 0        | 100         | 100 |
| 134 | Bf    | 46/113 (41%)      | 42 (91%)    | 3 (6%)    | 1 (2%)   | 5           | 29  |
| 135 | Bg    | 80/105 (76%)      | 71 (89%)    | 9 (11%)   | 0        | 100         | 100 |
| 136 | Bh    | 89/92 (97%)       | 84 (94%)    | 4 (4%)    | 1 (1%)   | 11          | 46  |
| All | All   | 34481/41413 (83%) | 33099 (96%) | 1303 (4%) | 79 (0%)  | 44          | 78  |

All (79) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 1188 | GLU  |
| 21  | DJ    | 36   | GLN  |
| 43  | CZ    | 296  | PRO  |
| 44  | Ca    | 32   | PRO  |
| 44  | Ca    | 33   | PRO  |
| 44  | Ca    | 35   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | AW    | 72   | THR  |
| 106 | BD    | 356  | PRO  |
| 106 | BD    | 389  | VAL  |
| 134 | Bf    | 101  | TYR  |
| 24  | DV    | 57   | THR  |
| 44  | Ca    | 34   | LYS  |
| 87  | AY    | 244  | ARG  |
| 98  | Av    | 232  | LYS  |
| 2   | DD    | 256  | PRO  |
| 12  | DU    | 191  | SER  |
| 31  | CH    | 16   | VAL  |
| 33  | CJ    | 799  | ASP  |
| 49  | Cj    | 54   | ALA  |
| 79  | AP    | 159  | ALA  |
| 81  | AR    | 141  | ALA  |
| 87  | AY    | 98   | LYS  |
| 87  | AY    | 107  | SER  |
| 105 | BC    | 268  | LEU  |
| 111 | BI    | 216  | MET  |
| 115 | BM    | 76   | TRP  |
| 124 | BV    | 60   | MET  |
| 1   | DA    | 132  | GLY  |
| 3   | DI    | 190  | PRO  |
| 8   | DP    | 62   | LYS  |
| 15  | DB    | 1033 | TYR  |
| 42  | CU    | 19   | ALA  |
| 46  | Cd    | 224  | ILE  |
| 46  | Cd    | 247  | LYS  |
| 50  | Ck    | 231  | GLY  |
| 50  | Ck    | 653  | LEU  |
| 66  | A2    | 293  | PHE  |
| 79  | AP    | 359  | HIS  |
| 87  | AY    | 108  | PRO  |
| 98  | Av    | 68   | ARG  |
| 106 | BD    | 153  | PRO  |
| 107 | BE    | 348  | VAL  |
| 117 | BO    | 76   | GLY  |
| 118 | BP    | 145  | PRO  |
| 126 | BX    | 88   | ALA  |
| 127 | BY    | 162  | ARG  |
| 2   | DD    | 248  | ASP  |
| 7   | DO    | 115  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | DQ    | 173 | ASP  |
| 12  | DU    | 205 | ALA  |
| 17  | DE    | 71  | LEU  |
| 37  | CO    | 70  | HIS  |
| 66  | A2    | 270 | ASN  |
| 97  | At    | 73  | ARG  |
| 106 | BD    | 162 | PRO  |
| 107 | BE    | 384 | HIS  |
| 118 | BP    | 146 | ALA  |
| 120 | BR    | 172 | PRO  |
| 1   | DA    | 229 | GLU  |
| 16  | DC    | 441 | VAL  |
| 106 | BD    | 449 | PHE  |
| 136 | Bh    | 61  | PRO  |
| 44  | Ca    | 31  | GLU  |
| 64  | A0    | 94  | ILE  |
| 77  | AK    | 17  | VAL  |
| 105 | BC    | 339 | ILE  |
| 106 | BD    | 139 | MET  |
| 55  | Cr    | 29  | PRO  |
| 74  | AF    | 36  | ALA  |
| 104 | BB    | 429 | VAL  |
| 106 | BD    | 450 | PRO  |
| 108 | BF    | 386 | VAL  |
| 9   | DQ    | 254 | SER  |
| 19  | DG    | 48  | VAL  |
| 37  | CO    | 90  | MET  |
| 18  | DF    | 184 | VAL  |
| 66  | A2    | 212 | ALA  |
| 106 | BD    | 175 | GLN  |
| 15  | DB    | 946 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | DA    | 1322/1514 (87%) | 1231 (93%) | 91 (7%)   | 14          | 36 |
| 2   | DD    | 694/711 (98%)   | 651 (94%)  | 43 (6%)   | 16          | 38 |
| 3   | DI    | 350/365 (96%)   | 323 (92%)  | 27 (8%)   | 12          | 32 |
| 4   | DL    | 241/263 (92%)   | 223 (92%)  | 18 (8%)   | 12          | 33 |
| 5   | DM    | 252/252 (100%)  | 232 (92%)  | 20 (8%)   | 11          | 32 |
| 6   | DN    | 229/256 (90%)   | 209 (91%)  | 20 (9%)   | 9           | 29 |
| 7   | DO    | 186/229 (81%)   | 176 (95%)  | 10 (5%)   | 20          | 41 |
| 8   | DP    | 187/239 (78%)   | 179 (96%)  | 8 (4%)    | 26          | 47 |
| 9   | DQ    | 228/239 (95%)   | 218 (96%)  | 10 (4%)   | 25          | 47 |
| 10  | DR    | 220/235 (94%)   | 196 (89%)  | 24 (11%)  | 6           | 21 |
| 11  | DS    | 209/228 (92%)   | 196 (94%)  | 13 (6%)   | 16          | 38 |
| 12  | DU    | 190/201 (94%)   | 171 (90%)  | 19 (10%)  | 7           | 24 |
| 13  | DZ    | 72/84 (86%)     | 68 (94%)   | 4 (6%)    | 19          | 40 |
| 14  | Da    | 50/59 (85%)     | 46 (92%)   | 4 (8%)    | 11          | 31 |
| 15  | DB    | 976/1030 (95%)  | 855 (88%)  | 121 (12%) | 4           | 17 |
| 16  | DC    | 927/985 (94%)   | 803 (87%)  | 124 (13%) | 4           | 14 |
| 17  | DE    | 519/641 (81%)   | 454 (88%)  | 65 (12%)  | 4           | 16 |
| 18  | DF    | 500/560 (89%)   | 433 (87%)  | 67 (13%)  | 4           | 14 |
| 19  | DG    | 490/543 (90%)   | 428 (87%)  | 62 (13%)  | 4           | 16 |
| 20  | DH    | 493/504 (98%)   | 427 (87%)  | 66 (13%)  | 4           | 14 |
| 21  | DJ    | 275/347 (79%)   | 236 (86%)  | 39 (14%)  | 3           | 13 |
| 22  | DK    | 209/261 (80%)   | 184 (88%)  | 25 (12%)  | 5           | 17 |
| 23  | DT    | 220/228 (96%)   | 194 (88%)  | 26 (12%)  | 5           | 18 |
| 24  | DV    | 145/165 (88%)   | 124 (86%)  | 21 (14%)  | 3           | 13 |
| 25  | DW    | 148/163 (91%)   | 136 (92%)  | 12 (8%)   | 11          | 31 |
| 26  | DX    | 124/149 (83%)   | 109 (88%)  | 15 (12%)  | 5           | 17 |
| 27  | DY    | 137/146 (94%)   | 115 (84%)  | 22 (16%)  | 2           | 11 |
| 28  | CC    | 73/73 (100%)    | 58 (80%)   | 15 (20%)  | 1           | 7  |
| 29  | CE    | 358/372 (96%)   | 321 (90%)  | 37 (10%)  | 7           | 23 |
| 30  | CF    | 136/144 (94%)   | 126 (93%)  | 10 (7%)   | 13          | 33 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 31  | CH    | 237/246 (96%)  | 217 (92%) | 20 (8%)  | 10          | 30 |
| 32  | CI    | 357/371 (96%)  | 328 (92%) | 29 (8%)  | 11          | 31 |
| 33  | CJ    | 709/723 (98%)  | 616 (87%) | 93 (13%) | 4           | 15 |
| 34  | CK    | 257/283 (91%)  | 230 (90%) | 27 (10%) | 6           | 21 |
| 35  | CL    | 79/79 (100%)   | 73 (92%)  | 6 (8%)   | 12          | 33 |
| 36  | CN    | 142/150 (95%)  | 122 (86%) | 20 (14%) | 3           | 13 |
| 37  | CO    | 318/377 (84%)  | 290 (91%) | 28 (9%)  | 9           | 28 |
| 38  | CP    | 160/168 (95%)  | 143 (89%) | 17 (11%) | 6           | 21 |
| 39  | CQ    | 171/270 (63%)  | 151 (88%) | 20 (12%) | 5           | 18 |
| 40  | CR    | 275/279 (99%)  | 256 (93%) | 19 (7%)  | 14          | 36 |
| 41  | CS    | 126/220 (57%)  | 108 (86%) | 18 (14%) | 3           | 13 |
| 42  | CU    | 160/169 (95%)  | 149 (93%) | 11 (7%)  | 14          | 36 |
| 43  | CZ    | 121/313 (39%)  | 110 (91%) | 11 (9%)  | 9           | 27 |
| 44  | Ca    | 516/543 (95%)  | 477 (92%) | 39 (8%)  | 12          | 33 |
| 45  | Cb    | 219/277 (79%)  | 207 (94%) | 12 (6%)  | 19          | 41 |
| 46  | Cd    | 240/381 (63%)  | 218 (91%) | 22 (9%)  | 8           | 27 |
| 47  | Cg    | 424/437 (97%)  | 374 (88%) | 50 (12%) | 5           | 18 |
| 48  | Ci    | 144/160 (90%)  | 124 (86%) | 20 (14%) | 3           | 14 |
| 49  | Cj    | 193/219 (88%)  | 180 (93%) | 13 (7%)  | 15          | 36 |
| 50  | Ck    | 608/747 (81%)  | 541 (89%) | 67 (11%) | 6           | 20 |
| 51  | Cm    | 165/184 (90%)  | 141 (86%) | 24 (14%) | 3           | 13 |
| 52  | Cn    | 95/210 (45%)   | 90 (95%)  | 5 (5%)   | 20          | 41 |
| 53  | Cp    | 163/175 (93%)  | 152 (93%) | 11 (7%)  | 15          | 36 |
| 54  | Cq    | 210/221 (95%)  | 193 (92%) | 17 (8%)  | 11          | 31 |
| 55  | Cr    | 211/369 (57%)  | 189 (90%) | 22 (10%) | 7           | 22 |
| 56  | Cv    | 912/1034 (88%) | 830 (91%) | 82 (9%)  | 9           | 27 |
| 64  | A0    | 140/167 (84%)  | 128 (91%) | 12 (9%)  | 10          | 29 |
| 65  | A1    | 195/217 (90%)  | 169 (87%) | 26 (13%) | 4           | 14 |
| 66  | A2    | 394/413 (95%)  | 348 (88%) | 46 (12%) | 5           | 18 |
| 67  | A3    | 131/193 (68%)  | 119 (91%) | 12 (9%)  | 8           | 27 |
| 68  | A4    | 153/164 (93%)  | 138 (90%) | 15 (10%) | 7           | 24 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 69  | A5    | 52/73 (71%)    | 44 (85%)  | 8 (15%)  | 2           | 12 |
| 70  | A6    | 61/99 (62%)    | 53 (87%)  | 8 (13%)  | 4           | 15 |
| 71  | A8    | 126/161 (78%)  | 106 (84%) | 20 (16%) | 2           | 11 |
| 72  | A9    | 51/166 (31%)   | 45 (88%)  | 6 (12%)  | 5           | 18 |
| 73  | AE    | 258/406 (64%)  | 227 (88%) | 31 (12%) | 5           | 17 |
| 74  | AF    | 394/409 (96%)  | 361 (92%) | 33 (8%)  | 10          | 30 |
| 75  | AI    | 192/233 (82%)  | 166 (86%) | 26 (14%) | 4           | 14 |
| 76  | AJ    | 90/151 (60%)   | 80 (89%)  | 10 (11%) | 6           | 20 |
| 77  | AK    | 287/301 (95%)  | 249 (87%) | 38 (13%) | 4           | 15 |
| 78  | AN    | 160/182 (88%)  | 150 (94%) | 10 (6%)  | 16          | 37 |
| 79  | AP    | 310/330 (94%)  | 277 (89%) | 33 (11%) | 6           | 21 |
| 80  | AQ    | 106/141 (75%)  | 99 (93%)  | 7 (7%)   | 15          | 37 |
| 81  | AR    | 198/256 (77%)  | 188 (95%) | 10 (5%)  | 21          | 42 |
| 82  | AT    | 28/124 (23%)   | 24 (86%)  | 4 (14%)  | 3           | 13 |
| 83  | AU    | 151/184 (82%)  | 131 (87%) | 20 (13%) | 4           | 15 |
| 84  | AV    | 153/158 (97%)  | 133 (87%) | 20 (13%) | 4           | 15 |
| 85  | AW    | 244/246 (99%)  | 216 (88%) | 28 (12%) | 5           | 18 |
| 86  | AX    | 156/221 (71%)  | 147 (94%) | 9 (6%)   | 18          | 40 |
| 87  | AY    | 283/337 (84%)  | 257 (91%) | 26 (9%)  | 8           | 27 |
| 88  | Ab    | 373/451 (83%)  | 340 (91%) | 33 (9%)  | 9           | 28 |
| 89  | Ad    | 225/250 (90%)  | 208 (92%) | 17 (8%)  | 12          | 33 |
| 90  | Ae    | 100/172 (58%)  | 88 (88%)  | 12 (12%) | 5           | 17 |
| 91  | Af    | 111/162 (68%)  | 100 (90%) | 11 (10%) | 7           | 24 |
| 92  | Ag    | 238/239 (100%) | 220 (92%) | 18 (8%)  | 12          | 33 |
| 93  | Aj    | 237/260 (91%)  | 225 (95%) | 12 (5%)  | 21          | 42 |
| 94  | Al    | 170/186 (91%)  | 155 (91%) | 15 (9%)  | 9           | 28 |
| 95  | Ao    | 153/216 (71%)  | 134 (88%) | 19 (12%) | 4           | 17 |
| 96  | Ap    | 227/267 (85%)  | 203 (89%) | 24 (11%) | 6           | 21 |
| 97  | At    | 116/140 (83%)  | 101 (87%) | 15 (13%) | 4           | 15 |
| 98  | Av    | 187/210 (89%)  | 173 (92%) | 14 (8%)  | 12          | 33 |
| 103 | BA    | 598/727 (82%)  | 536 (90%) | 62 (10%) | 7           | 22 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 104 | BB    | 351/484 (72%)  | 316 (90%) | 35 (10%) | 7           | 24 |
| 105 | BC    | 406/443 (92%)  | 357 (88%) | 49 (12%) | 5           | 17 |
| 107 | BE    | 334/386 (86%)  | 303 (91%) | 31 (9%)  | 8           | 26 |
| 108 | BF    | 299/368 (81%)  | 271 (91%) | 28 (9%)  | 8           | 26 |
| 109 | BG    | 266/310 (86%)  | 242 (91%) | 24 (9%)  | 9           | 27 |
| 110 | BH    | 182/297 (61%)  | 161 (88%) | 21 (12%) | 5           | 18 |
| 111 | BI    | 268/288 (93%)  | 246 (92%) | 22 (8%)  | 10          | 31 |
| 112 | BJ    | 136/298 (46%)  | 125 (92%) | 11 (8%)  | 11          | 31 |
| 113 | BK    | 196/344 (57%)  | 188 (96%) | 8 (4%)   | 27          | 49 |
| 114 | BL    | 201/262 (77%)  | 177 (88%) | 24 (12%) | 5           | 18 |
| 115 | BM    | 209/240 (87%)  | 191 (91%) | 18 (9%)  | 10          | 29 |
| 116 | BN    | 197/273 (72%)  | 186 (94%) | 11 (6%)  | 19          | 40 |
| 117 | BO    | 129/225 (57%)  | 118 (92%) | 11 (8%)  | 10          | 29 |
| 118 | BP    | 162/219 (74%)  | 149 (92%) | 13 (8%)  | 11          | 31 |
| 119 | BQ    | 182/195 (93%)  | 162 (89%) | 20 (11%) | 6           | 20 |
| 120 | BR    | 171/181 (94%)  | 145 (85%) | 26 (15%) | 3           | 12 |
| 121 | BS    | 85/142 (60%)   | 75 (88%)  | 10 (12%) | 5           | 18 |
| 122 | BT    | 147/163 (90%)  | 135 (92%) | 12 (8%)  | 10          | 31 |
| 123 | BU    | 71/168 (42%)   | 61 (86%)  | 10 (14%) | 3           | 13 |
| 124 | BV    | 138/163 (85%)  | 130 (94%) | 8 (6%)   | 18          | 40 |
| 125 | BW    | 163/164 (99%)  | 147 (90%) | 16 (10%) | 7           | 24 |
| 126 | BX    | 92/170 (54%)   | 81 (88%)  | 11 (12%) | 5           | 17 |
| 127 | BY    | 89/151 (59%)   | 81 (91%)  | 8 (9%)   | 9           | 27 |
| 128 | BZ    | 143/160 (89%)  | 135 (94%) | 8 (6%)   | 19          | 40 |
| 129 | Ba    | 131/131 (100%) | 114 (87%) | 17 (13%) | 4           | 15 |
| 130 | Bb    | 84/135 (62%)   | 69 (82%)  | 15 (18%) | 2           | 9  |
| 131 | Bc    | 82/134 (61%)   | 75 (92%)  | 7 (8%)   | 10          | 29 |
| 132 | Bd    | 117/120 (98%)  | 100 (86%) | 17 (14%) | 3           | 13 |
| 133 | Be    | 89/99 (90%)    | 81 (91%)  | 8 (9%)   | 9           | 27 |
| 134 | Bf    | 45/98 (46%)    | 40 (89%)  | 5 (11%)  | 6           | 20 |
| 135 | Bg    | 65/87 (75%)    | 59 (91%)  | 6 (9%)   | 8           | 27 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers   | Percentiles |    |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 136 | Bh    | 79/80 (99%)       | 70 (89%)    | 9 (11%)    | 5           | 18 |
| All | All   | 29729/35381 (84%) | 26759 (90%) | 2970 (10%) | 9           | 24 |

All (2970) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DA    | 41  | PHE  |
| 1   | DA    | 60  | GLU  |
| 1   | DA    | 74  | LYS  |
| 1   | DA    | 77  | ARG  |
| 1   | DA    | 79  | LEU  |
| 1   | DA    | 85  | LEU  |
| 1   | DA    | 87  | THR  |
| 1   | DA    | 112 | GLN  |
| 1   | DA    | 117 | GLN  |
| 1   | DA    | 131 | ASP  |
| 1   | DA    | 148 | LYS  |
| 1   | DA    | 150 | ILE  |
| 1   | DA    | 158 | LEU  |
| 1   | DA    | 167 | THR  |
| 1   | DA    | 174 | HIS  |
| 1   | DA    | 194 | LEU  |
| 1   | DA    | 200 | ILE  |
| 1   | DA    | 201 | LYS  |
| 1   | DA    | 230 | PHE  |
| 1   | DA    | 254 | PHE  |
| 1   | DA    | 255 | ARG  |
| 1   | DA    | 259 | LEU  |
| 1   | DA    | 274 | LEU  |
| 1   | DA    | 300 | THR  |
| 1   | DA    | 309 | VAL  |
| 1   | DA    | 408 | LEU  |
| 1   | DA    | 419 | THR  |
| 1   | DA    | 436 | ASN  |
| 1   | DA    | 456 | ARG  |
| 1   | DA    | 486 | LYS  |
| 1   | DA    | 493 | TRP  |
| 1   | DA    | 509 | LEU  |
| 1   | DA    | 539 | LEU  |
| 1   | DA    | 540 | GLU  |
| 1   | DA    | 579 | ASP  |
| 1   | DA    | 583 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 602  | LEU  |
| 1   | DA    | 630  | ASP  |
| 1   | DA    | 632  | THR  |
| 1   | DA    | 650  | LEU  |
| 1   | DA    | 653  | LYS  |
| 1   | DA    | 680  | VAL  |
| 1   | DA    | 708  | GLU  |
| 1   | DA    | 711  | ILE  |
| 1   | DA    | 712  | VAL  |
| 1   | DA    | 729  | ARG  |
| 1   | DA    | 781  | ARG  |
| 1   | DA    | 783  | VAL  |
| 1   | DA    | 849  | THR  |
| 1   | DA    | 859  | GLN  |
| 1   | DA    | 870  | GLU  |
| 1   | DA    | 914  | THR  |
| 1   | DA    | 920  | LEU  |
| 1   | DA    | 934  | GLU  |
| 1   | DA    | 958  | SER  |
| 1   | DA    | 963  | LEU  |
| 1   | DA    | 973  | LEU  |
| 1   | DA    | 988  | CYS  |
| 1   | DA    | 1000 | ASN  |
| 1   | DA    | 1045 | ILE  |
| 1   | DA    | 1057 | VAL  |
| 1   | DA    | 1062 | TYR  |
| 1   | DA    | 1077 | ARG  |
| 1   | DA    | 1097 | LEU  |
| 1   | DA    | 1098 | LEU  |
| 1   | DA    | 1145 | THR  |
| 1   | DA    | 1152 | HIS  |
| 1   | DA    | 1191 | ILE  |
| 1   | DA    | 1208 | THR  |
| 1   | DA    | 1220 | VAL  |
| 1   | DA    | 1240 | LEU  |
| 1   | DA    | 1253 | VAL  |
| 1   | DA    | 1263 | VAL  |
| 1   | DA    | 1268 | LEU  |
| 1   | DA    | 1271 | LEU  |
| 1   | DA    | 1278 | THR  |
| 1   | DA    | 1292 | CYS  |
| 1   | DA    | 1381 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 1404 | ARG  |
| 1   | DA    | 1433 | ASP  |
| 1   | DA    | 1440 | ILE  |
| 1   | DA    | 1488 | GLN  |
| 1   | DA    | 1498 | LEU  |
| 1   | DA    | 1517 | ARG  |
| 1   | DA    | 1544 | ASN  |
| 1   | DA    | 1591 | ARG  |
| 1   | DA    | 1597 | GLU  |
| 1   | DA    | 1605 | ARG  |
| 1   | DA    | 1624 | ILE  |
| 1   | DA    | 1662 | ARG  |
| 1   | DA    | 1664 | ILE  |
| 2   | DD    | 12   | SER  |
| 2   | DD    | 27   | MET  |
| 2   | DD    | 48   | MET  |
| 2   | DD    | 79   | GLN  |
| 2   | DD    | 84   | LYS  |
| 2   | DD    | 94   | LYS  |
| 2   | DD    | 108  | THR  |
| 2   | DD    | 122  | GLN  |
| 2   | DD    | 129  | ARG  |
| 2   | DD    | 146  | ARG  |
| 2   | DD    | 149  | SER  |
| 2   | DD    | 151  | SER  |
| 2   | DD    | 173  | GLN  |
| 2   | DD    | 226  | THR  |
| 2   | DD    | 233  | ASN  |
| 2   | DD    | 237  | THR  |
| 2   | DD    | 275  | ASP  |
| 2   | DD    | 298  | MET  |
| 2   | DD    | 350  | LYS  |
| 2   | DD    | 377  | GLU  |
| 2   | DD    | 379  | GLN  |
| 2   | DD    | 439  | GLU  |
| 2   | DD    | 452  | LEU  |
| 2   | DD    | 454  | THR  |
| 2   | DD    | 504  | ASN  |
| 2   | DD    | 521  | ASN  |
| 2   | DD    | 541  | ARG  |
| 2   | DD    | 546  | VAL  |
| 2   | DD    | 577  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | DD    | 592 | TRP  |
| 2   | DD    | 616 | LEU  |
| 2   | DD    | 624 | THR  |
| 2   | DD    | 646 | ILE  |
| 2   | DD    | 651 | ARG  |
| 2   | DD    | 654 | ARG  |
| 2   | DD    | 704 | ASP  |
| 2   | DD    | 741 | ARG  |
| 2   | DD    | 761 | ARG  |
| 2   | DD    | 770 | SER  |
| 2   | DD    | 787 | ARG  |
| 2   | DD    | 794 | ARG  |
| 2   | DD    | 799 | ASP  |
| 2   | DD    | 812 | TYR  |
| 3   | DI    | 79  | ILE  |
| 3   | DI    | 90  | LEU  |
| 3   | DI    | 107 | ILE  |
| 3   | DI    | 113 | VAL  |
| 3   | DI    | 134 | ARG  |
| 3   | DI    | 144 | LEU  |
| 3   | DI    | 161 | MET  |
| 3   | DI    | 164 | GLU  |
| 3   | DI    | 172 | LEU  |
| 3   | DI    | 175 | GLN  |
| 3   | DI    | 178 | PHE  |
| 3   | DI    | 180 | GLU  |
| 3   | DI    | 192 | THR  |
| 3   | DI    | 205 | GLU  |
| 3   | DI    | 232 | TYR  |
| 3   | DI    | 233 | ARG  |
| 3   | DI    | 243 | LEU  |
| 3   | DI    | 258 | VAL  |
| 3   | DI    | 282 | ASP  |
| 3   | DI    | 310 | LEU  |
| 3   | DI    | 313 | ARG  |
| 3   | DI    | 344 | LEU  |
| 3   | DI    | 345 | LEU  |
| 3   | DI    | 353 | LYS  |
| 3   | DI    | 362 | ILE  |
| 3   | DI    | 373 | LEU  |
| 3   | DI    | 399 | THR  |
| 4   | DL    | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | DL    | 39  | THR  |
| 4   | DL    | 68  | LEU  |
| 4   | DL    | 102 | SER  |
| 4   | DL    | 136 | MET  |
| 4   | DL    | 145 | LEU  |
| 4   | DL    | 158 | THR  |
| 4   | DL    | 165 | PHE  |
| 4   | DL    | 183 | LEU  |
| 4   | DL    | 200 | VAL  |
| 4   | DL    | 204 | MET  |
| 4   | DL    | 240 | GLU  |
| 4   | DL    | 243 | LEU  |
| 4   | DL    | 267 | HIS  |
| 4   | DL    | 268 | VAL  |
| 4   | DL    | 269 | MET  |
| 4   | DL    | 270 | THR  |
| 4   | DL    | 286 | THR  |
| 5   | DM    | 1   | MET  |
| 5   | DM    | 15  | LEU  |
| 5   | DM    | 30  | ARG  |
| 5   | DM    | 46  | PHE  |
| 5   | DM    | 56  | TRP  |
| 5   | DM    | 59  | ARG  |
| 5   | DM    | 72  | ARG  |
| 5   | DM    | 75  | VAL  |
| 5   | DM    | 76  | ASN  |
| 5   | DM    | 84  | LEU  |
| 5   | DM    | 90  | LEU  |
| 5   | DM    | 104 | LYS  |
| 5   | DM    | 128 | ILE  |
| 5   | DM    | 129 | ARG  |
| 5   | DM    | 131 | ASN  |
| 5   | DM    | 157 | LEU  |
| 5   | DM    | 179 | ARG  |
| 5   | DM    | 198 | THR  |
| 5   | DM    | 199 | LEU  |
| 5   | DM    | 275 | LEU  |
| 6   | DN    | 17  | MET  |
| 6   | DN    | 23  | VAL  |
| 6   | DN    | 24  | LEU  |
| 6   | DN    | 42  | THR  |
| 6   | DN    | 109 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | DN    | 116 | VAL  |
| 6   | DN    | 118 | LEU  |
| 6   | DN    | 125 | VAL  |
| 6   | DN    | 141 | MET  |
| 6   | DN    | 152 | LEU  |
| 6   | DN    | 162 | LEU  |
| 6   | DN    | 171 | LEU  |
| 6   | DN    | 223 | GLN  |
| 6   | DN    | 224 | ARG  |
| 6   | DN    | 237 | ARG  |
| 6   | DN    | 246 | GLN  |
| 6   | DN    | 261 | ARG  |
| 6   | DN    | 267 | GLU  |
| 6   | DN    | 276 | GLN  |
| 6   | DN    | 288 | PHE  |
| 7   | DO    | 62  | LEU  |
| 7   | DO    | 73  | LEU  |
| 7   | DO    | 115 | ASP  |
| 7   | DO    | 118 | ASP  |
| 7   | DO    | 122 | LEU  |
| 7   | DO    | 125 | LEU  |
| 7   | DO    | 136 | ASP  |
| 7   | DO    | 192 | MET  |
| 7   | DO    | 234 | LEU  |
| 7   | DO    | 255 | ARG  |
| 8   | DP    | 21  | MET  |
| 8   | DP    | 23  | LEU  |
| 8   | DP    | 28  | ASN  |
| 8   | DP    | 34  | VAL  |
| 8   | DP    | 69  | LEU  |
| 8   | DP    | 172 | GLU  |
| 8   | DP    | 195 | THR  |
| 8   | DP    | 208 | PRO  |
| 9   | DQ    | 37  | GLU  |
| 9   | DQ    | 41  | GLN  |
| 9   | DQ    | 61  | ILE  |
| 9   | DQ    | 119 | VAL  |
| 9   | DQ    | 120 | MET  |
| 9   | DQ    | 149 | GLN  |
| 9   | DQ    | 177 | LEU  |
| 9   | DQ    | 192 | LEU  |
| 9   | DQ    | 216 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | DQ    | 250 | ARG  |
| 10  | DR    | 23  | VAL  |
| 10  | DR    | 32  | VAL  |
| 10  | DR    | 39  | GLN  |
| 10  | DR    | 44  | VAL  |
| 10  | DR    | 54  | LEU  |
| 10  | DR    | 60  | VAL  |
| 10  | DR    | 63  | ILE  |
| 10  | DR    | 67  | LYS  |
| 10  | DR    | 68  | HIS  |
| 10  | DR    | 78  | ARG  |
| 10  | DR    | 91  | THR  |
| 10  | DR    | 108 | GLN  |
| 10  | DR    | 117 | ILE  |
| 10  | DR    | 118 | VAL  |
| 10  | DR    | 131 | LEU  |
| 10  | DR    | 133 | LEU  |
| 10  | DR    | 148 | VAL  |
| 10  | DR    | 174 | CYS  |
| 10  | DR    | 188 | LYS  |
| 10  | DR    | 190 | LEU  |
| 10  | DR    | 201 | CYS  |
| 10  | DR    | 245 | MET  |
| 10  | DR    | 261 | ARG  |
| 10  | DR    | 265 | MET  |
| 11  | DS    | 34  | SER  |
| 11  | DS    | 44  | LYS  |
| 11  | DS    | 56  | LEU  |
| 11  | DS    | 61  | ASN  |
| 11  | DS    | 92  | ARG  |
| 11  | DS    | 106 | ARG  |
| 11  | DS    | 108 | ASN  |
| 11  | DS    | 109 | VAL  |
| 11  | DS    | 115 | TYR  |
| 11  | DS    | 119 | CYS  |
| 11  | DS    | 170 | TYR  |
| 11  | DS    | 175 | CYS  |
| 11  | DS    | 205 | VAL  |
| 12  | DU    | 33  | THR  |
| 12  | DU    | 46  | THR  |
| 12  | DU    | 47  | ARG  |
| 12  | DU    | 73  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | DU    | 83  | ARG  |
| 12  | DU    | 86  | ILE  |
| 12  | DU    | 90  | VAL  |
| 12  | DU    | 103 | ILE  |
| 12  | DU    | 107 | LYS  |
| 12  | DU    | 124 | SER  |
| 12  | DU    | 140 | GLU  |
| 12  | DU    | 146 | THR  |
| 12  | DU    | 153 | THR  |
| 12  | DU    | 157 | GLN  |
| 12  | DU    | 165 | ASP  |
| 12  | DU    | 180 | VAL  |
| 12  | DU    | 189 | LYS  |
| 12  | DU    | 207 | ARG  |
| 12  | DU    | 211 | ARG  |
| 13  | DZ    | 17  | LEU  |
| 13  | DZ    | 20  | ARG  |
| 13  | DZ    | 62  | ASP  |
| 13  | DZ    | 63  | LEU  |
| 14  | Da    | 15  | CYS  |
| 14  | Da    | 25  | ARG  |
| 14  | Da    | 38  | ASP  |
| 14  | Da    | 42  | ARG  |
| 15  | DB    | 99  | VAL  |
| 15  | DB    | 118 | VAL  |
| 15  | DB    | 129 | TYR  |
| 15  | DB    | 137 | VAL  |
| 15  | DB    | 146 | MET  |
| 15  | DB    | 173 | ARG  |
| 15  | DB    | 183 | VAL  |
| 15  | DB    | 186 | SER  |
| 15  | DB    | 189 | VAL  |
| 15  | DB    | 192 | ILE  |
| 15  | DB    | 204 | SER  |
| 15  | DB    | 213 | ASP  |
| 15  | DB    | 217 | ILE  |
| 15  | DB    | 221 | HIS  |
| 15  | DB    | 233 | ASP  |
| 15  | DB    | 249 | SER  |
| 15  | DB    | 295 | THR  |
| 15  | DB    | 321 | SER  |
| 15  | DB    | 339 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | DB    | 341 | THR  |
| 15  | DB    | 343 | VAL  |
| 15  | DB    | 357 | ILE  |
| 15  | DB    | 365 | THR  |
| 15  | DB    | 368 | GLU  |
| 15  | DB    | 383 | ARG  |
| 15  | DB    | 388 | VAL  |
| 15  | DB    | 394 | ASP  |
| 15  | DB    | 397 | THR  |
| 15  | DB    | 416 | ASN  |
| 15  | DB    | 424 | ASP  |
| 15  | DB    | 433 | ARG  |
| 15  | DB    | 435 | THR  |
| 15  | DB    | 439 | VAL  |
| 15  | DB    | 445 | ASN  |
| 15  | DB    | 448 | ASP  |
| 15  | DB    | 450 | MET  |
| 15  | DB    | 454 | ASP  |
| 15  | DB    | 479 | VAL  |
| 15  | DB    | 490 | ARG  |
| 15  | DB    | 507 | LEU  |
| 15  | DB    | 511 | ARG  |
| 15  | DB    | 514 | ARG  |
| 15  | DB    | 521 | LEU  |
| 15  | DB    | 522 | MET  |
| 15  | DB    | 532 | GLU  |
| 15  | DB    | 539 | GLN  |
| 15  | DB    | 550 | LEU  |
| 15  | DB    | 553 | LEU  |
| 15  | DB    | 554 | GLU  |
| 15  | DB    | 564 | ARG  |
| 15  | DB    | 572 | ASP  |
| 15  | DB    | 574 | ILE  |
| 15  | DB    | 584 | GLU  |
| 15  | DB    | 585 | MET  |
| 15  | DB    | 587 | VAL  |
| 15  | DB    | 590 | ASP  |
| 15  | DB    | 592 | MET  |
| 15  | DB    | 597 | GLU  |
| 15  | DB    | 637 | THR  |
| 15  | DB    | 671 | VAL  |
| 15  | DB    | 686 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | DB    | 689  | LEU  |
| 15  | DB    | 693  | SER  |
| 15  | DB    | 719  | MET  |
| 15  | DB    | 720  | LYS  |
| 15  | DB    | 743  | VAL  |
| 15  | DB    | 744  | VAL  |
| 15  | DB    | 755  | LEU  |
| 15  | DB    | 756  | THR  |
| 15  | DB    | 757  | VAL  |
| 15  | DB    | 758  | SER  |
| 15  | DB    | 774  | ASN  |
| 15  | DB    | 776  | THR  |
| 15  | DB    | 785  | ASN  |
| 15  | DB    | 790  | SER  |
| 15  | DB    | 793  | ARG  |
| 15  | DB    | 810  | THR  |
| 15  | DB    | 815  | ASP  |
| 15  | DB    | 820  | GLU  |
| 15  | DB    | 830  | LEU  |
| 15  | DB    | 831  | ASN  |
| 15  | DB    | 834  | ILE  |
| 15  | DB    | 849  | ASP  |
| 15  | DB    | 850  | SER  |
| 15  | DB    | 878  | VAL  |
| 15  | DB    | 901  | VAL  |
| 15  | DB    | 908  | GLN  |
| 15  | DB    | 920  | VAL  |
| 15  | DB    | 923  | GLN  |
| 15  | DB    | 937  | MET  |
| 15  | DB    | 941  | ARG  |
| 15  | DB    | 950  | VAL  |
| 15  | DB    | 958  | ASN  |
| 15  | DB    | 964  | ARG  |
| 15  | DB    | 968  | VAL  |
| 15  | DB    | 969  | THR  |
| 15  | DB    | 984  | ASP  |
| 15  | DB    | 995  | VAL  |
| 15  | DB    | 1002 | THR  |
| 15  | DB    | 1009 | ASP  |
| 15  | DB    | 1012 | THR  |
| 15  | DB    | 1013 | ARG  |
| 15  | DB    | 1020 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | DB    | 1026 | SER  |
| 15  | DB    | 1028 | SER  |
| 15  | DB    | 1030 | ARG  |
| 15  | DB    | 1034 | ILE  |
| 15  | DB    | 1067 | ILE  |
| 15  | DB    | 1069 | THR  |
| 15  | DB    | 1080 | ARG  |
| 15  | DB    | 1104 | ASP  |
| 15  | DB    | 1110 | LYS  |
| 15  | DB    | 1117 | THR  |
| 15  | DB    | 1142 | VAL  |
| 15  | DB    | 1153 | ASP  |
| 15  | DB    | 1156 | THR  |
| 15  | DB    | 1165 | SER  |
| 15  | DB    | 1168 | ASP  |
| 15  | DB    | 1172 | LYS  |
| 15  | DB    | 1173 | THR  |
| 15  | DB    | 1181 | LEU  |
| 16  | DC    | 30   | THR  |
| 16  | DC    | 36   | ASP  |
| 16  | DC    | 46   | ARG  |
| 16  | DC    | 57   | GLU  |
| 16  | DC    | 58   | VAL  |
| 16  | DC    | 82   | THR  |
| 16  | DC    | 86   | THR  |
| 16  | DC    | 87   | MET  |
| 16  | DC    | 93   | ARG  |
| 16  | DC    | 106  | SER  |
| 16  | DC    | 108  | SER  |
| 16  | DC    | 114  | GLU  |
| 16  | DC    | 119  | THR  |
| 16  | DC    | 131  | GLU  |
| 16  | DC    | 148  | LEU  |
| 16  | DC    | 154  | THR  |
| 16  | DC    | 155  | VAL  |
| 16  | DC    | 162  | ILE  |
| 16  | DC    | 166  | GLU  |
| 16  | DC    | 227  | GLN  |
| 16  | DC    | 231  | THR  |
| 16  | DC    | 240  | VAL  |
| 16  | DC    | 268  | ASP  |
| 16  | DC    | 271  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | DC    | 279 | GLU  |
| 16  | DC    | 299 | LEU  |
| 16  | DC    | 313 | THR  |
| 16  | DC    | 365 | LYS  |
| 16  | DC    | 371 | ILE  |
| 16  | DC    | 374 | LEU  |
| 16  | DC    | 379 | LEU  |
| 16  | DC    | 386 | MET  |
| 16  | DC    | 423 | ILE  |
| 16  | DC    | 432 | ARG  |
| 16  | DC    | 435 | LEU  |
| 16  | DC    | 437 | LEU  |
| 16  | DC    | 442 | LEU  |
| 16  | DC    | 464 | THR  |
| 16  | DC    | 467 | THR  |
| 16  | DC    | 471 | ARG  |
| 16  | DC    | 474 | LEU  |
| 16  | DC    | 475 | LEU  |
| 16  | DC    | 491 | LEU  |
| 16  | DC    | 498 | LEU  |
| 16  | DC    | 503 | ASP  |
| 16  | DC    | 506 | SER  |
| 16  | DC    | 511 | ARG  |
| 16  | DC    | 513 | SER  |
| 16  | DC    | 519 | SER  |
| 16  | DC    | 525 | THR  |
| 16  | DC    | 533 | LEU  |
| 16  | DC    | 534 | LEU  |
| 16  | DC    | 540 | LEU  |
| 16  | DC    | 544 | GLU  |
| 16  | DC    | 545 | ASP  |
| 16  | DC    | 569 | LEU  |
| 16  | DC    | 595 | SER  |
| 16  | DC    | 604 | VAL  |
| 16  | DC    | 609 | VAL  |
| 16  | DC    | 611 | MET  |
| 16  | DC    | 618 | ARG  |
| 16  | DC    | 620 | VAL  |
| 16  | DC    | 632 | LEU  |
| 16  | DC    | 652 | ARG  |
| 16  | DC    | 659 | LEU  |
| 16  | DC    | 669 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | DC    | 705  | LEU  |
| 16  | DC    | 710  | THR  |
| 16  | DC    | 749  | GLU  |
| 16  | DC    | 752  | VAL  |
| 16  | DC    | 753  | LEU  |
| 16  | DC    | 755  | ASP  |
| 16  | DC    | 756  | ASP  |
| 16  | DC    | 757  | ARG  |
| 16  | DC    | 766  | VAL  |
| 16  | DC    | 774  | ASP  |
| 16  | DC    | 794  | LEU  |
| 16  | DC    | 799  | ASN  |
| 16  | DC    | 807  | VAL  |
| 16  | DC    | 817  | ASP  |
| 16  | DC    | 839  | VAL  |
| 16  | DC    | 865  | CYS  |
| 16  | DC    | 871  | GLN  |
| 16  | DC    | 873  | VAL  |
| 16  | DC    | 881  | MET  |
| 16  | DC    | 885  | LEU  |
| 16  | DC    | 894  | HIS  |
| 16  | DC    | 919  | VAL  |
| 16  | DC    | 928  | GLU  |
| 16  | DC    | 931  | THR  |
| 16  | DC    | 934  | ARG  |
| 16  | DC    | 952  | GLU  |
| 16  | DC    | 953  | MET  |
| 16  | DC    | 954  | LEU  |
| 16  | DC    | 960  | VAL  |
| 16  | DC    | 961  | THR  |
| 16  | DC    | 963  | SER  |
| 16  | DC    | 970  | GLN  |
| 16  | DC    | 984  | THR  |
| 16  | DC    | 985  | VAL  |
| 16  | DC    | 987  | THR  |
| 16  | DC    | 1000 | LEU  |
| 16  | DC    | 1006 | VAL  |
| 16  | DC    | 1009 | THR  |
| 16  | DC    | 1019 | THR  |
| 16  | DC    | 1023 | ASN  |
| 16  | DC    | 1025 | THR  |
| 16  | DC    | 1055 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | DC    | 1062 | GLN  |
| 16  | DC    | 1063 | SER  |
| 16  | DC    | 1071 | VAL  |
| 16  | DC    | 1076 | PHE  |
| 16  | DC    | 1104 | MET  |
| 16  | DC    | 1121 | THR  |
| 16  | DC    | 1125 | SER  |
| 16  | DC    | 1128 | ARG  |
| 16  | DC    | 1132 | THR  |
| 16  | DC    | 1133 | THR  |
| 16  | DC    | 1143 | VAL  |
| 16  | DC    | 1151 | THR  |
| 16  | DC    | 1153 | LEU  |
| 16  | DC    | 1159 | ASP  |
| 16  | DC    | 1161 | LYS  |
| 16  | DC    | 1163 | GLU  |
| 17  | DE    | 46   | SER  |
| 17  | DE    | 51   | ARG  |
| 17  | DE    | 54   | ARG  |
| 17  | DE    | 65   | ILE  |
| 17  | DE    | 80   | LEU  |
| 17  | DE    | 147  | MET  |
| 17  | DE    | 149  | LEU  |
| 17  | DE    | 154  | SER  |
| 17  | DE    | 178  | GLN  |
| 17  | DE    | 196  | ASP  |
| 17  | DE    | 203  | LEU  |
| 17  | DE    | 204  | VAL  |
| 17  | DE    | 212  | LEU  |
| 17  | DE    | 229  | ARG  |
| 17  | DE    | 246  | ILE  |
| 17  | DE    | 280  | LEU  |
| 17  | DE    | 286  | THR  |
| 17  | DE    | 299  | LYS  |
| 17  | DE    | 319  | ASN  |
| 17  | DE    | 333  | ASP  |
| 17  | DE    | 335  | GLU  |
| 17  | DE    | 343  | LEU  |
| 17  | DE    | 398  | LEU  |
| 17  | DE    | 405  | ILE  |
| 17  | DE    | 406  | ASP  |
| 17  | DE    | 408  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | DE    | 418 | LEU  |
| 17  | DE    | 429 | ILE  |
| 17  | DE    | 445 | LEU  |
| 17  | DE    | 451 | THR  |
| 17  | DE    | 466 | VAL  |
| 17  | DE    | 482 | THR  |
| 17  | DE    | 484 | THR  |
| 17  | DE    | 486 | ILE  |
| 17  | DE    | 497 | GLN  |
| 17  | DE    | 503 | ASP  |
| 17  | DE    | 529 | ASP  |
| 17  | DE    | 538 | VAL  |
| 17  | DE    | 545 | ARG  |
| 17  | DE    | 554 | LEU  |
| 17  | DE    | 561 | THR  |
| 17  | DE    | 566 | ARG  |
| 17  | DE    | 570 | GLU  |
| 17  | DE    | 572 | VAL  |
| 17  | DE    | 573 | GLN  |
| 17  | DE    | 575 | CYS  |
| 17  | DE    | 586 | THR  |
| 17  | DE    | 587 | MET  |
| 17  | DE    | 591 | LEU  |
| 17  | DE    | 600 | ILE  |
| 17  | DE    | 601 | ILE  |
| 17  | DE    | 602 | LYS  |
| 17  | DE    | 604 | ASP  |
| 17  | DE    | 607 | ILE  |
| 17  | DE    | 610 | LEU  |
| 17  | DE    | 615 | LEU  |
| 17  | DE    | 651 | ASN  |
| 17  | DE    | 659 | ARG  |
| 17  | DE    | 678 | THR  |
| 17  | DE    | 698 | GLN  |
| 17  | DE    | 704 | LEU  |
| 17  | DE    | 717 | ARG  |
| 17  | DE    | 718 | SER  |
| 17  | DE    | 721 | ASP  |
| 17  | DE    | 726 | THR  |
| 18  | DF    | 8   | SER  |
| 18  | DF    | 13  | ILE  |
| 18  | DF    | 15  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | DF    | 19  | THR  |
| 18  | DF    | 22  | LEU  |
| 18  | DF    | 27  | ARG  |
| 18  | DF    | 33  | GLN  |
| 18  | DF    | 39  | ARG  |
| 18  | DF    | 40  | GLU  |
| 18  | DF    | 50  | LEU  |
| 18  | DF    | 53  | ARG  |
| 18  | DF    | 57  | ARG  |
| 18  | DF    | 69  | THR  |
| 18  | DF    | 72  | THR  |
| 18  | DF    | 85  | ARG  |
| 18  | DF    | 87  | GLU  |
| 18  | DF    | 95  | ILE  |
| 18  | DF    | 110 | ASN  |
| 18  | DF    | 137 | VAL  |
| 18  | DF    | 144 | THR  |
| 18  | DF    | 154 | ASN  |
| 18  | DF    | 157 | THR  |
| 18  | DF    | 170 | ARG  |
| 18  | DF    | 182 | ARG  |
| 18  | DF    | 188 | ARG  |
| 18  | DF    | 189 | ASP  |
| 18  | DF    | 192 | LEU  |
| 18  | DF    | 194 | THR  |
| 18  | DF    | 202 | LEU  |
| 18  | DF    | 238 | THR  |
| 18  | DF    | 246 | LYS  |
| 18  | DF    | 255 | GLU  |
| 18  | DF    | 258 | ASP  |
| 18  | DF    | 259 | SER  |
| 18  | DF    | 264 | VAL  |
| 18  | DF    | 274 | LEU  |
| 18  | DF    | 294 | MET  |
| 18  | DF    | 297 | ARG  |
| 18  | DF    | 307 | GLU  |
| 18  | DF    | 321 | LEU  |
| 18  | DF    | 326 | ASP  |
| 18  | DF    | 331 | GLU  |
| 18  | DF    | 332 | GLU  |
| 18  | DF    | 343 | GLU  |
| 18  | DF    | 362 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | DF    | 370 | LEU  |
| 18  | DF    | 373 | ASP  |
| 18  | DF    | 394 | GLU  |
| 18  | DF    | 395 | LEU  |
| 18  | DF    | 402 | THR  |
| 18  | DF    | 403 | LEU  |
| 18  | DF    | 437 | GLU  |
| 18  | DF    | 439 | THR  |
| 18  | DF    | 450 | VAL  |
| 18  | DF    | 452 | VAL  |
| 18  | DF    | 476 | LEU  |
| 18  | DF    | 491 | ARG  |
| 18  | DF    | 502 | ARG  |
| 18  | DF    | 512 | ASN  |
| 18  | DF    | 516 | ARG  |
| 18  | DF    | 550 | VAL  |
| 18  | DF    | 553 | THR  |
| 18  | DF    | 568 | LEU  |
| 18  | DF    | 573 | THR  |
| 18  | DF    | 575 | VAL  |
| 18  | DF    | 584 | LEU  |
| 18  | DF    | 591 | HIS  |
| 19  | DG    | 36  | THR  |
| 19  | DG    | 56  | ARG  |
| 19  | DG    | 57  | GLU  |
| 19  | DG    | 62  | SER  |
| 19  | DG    | 74  | LEU  |
| 19  | DG    | 78  | HIS  |
| 19  | DG    | 84  | LEU  |
| 19  | DG    | 93  | ARG  |
| 19  | DG    | 95  | VAL  |
| 19  | DG    | 115 | ILE  |
| 19  | DG    | 125 | ASP  |
| 19  | DG    | 127 | LEU  |
| 19  | DG    | 130 | LEU  |
| 19  | DG    | 141 | THR  |
| 19  | DG    | 142 | LEU  |
| 19  | DG    | 147 | SER  |
| 19  | DG    | 149 | SER  |
| 19  | DG    | 155 | GLU  |
| 19  | DG    | 162 | LEU  |
| 19  | DG    | 165 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | DG    | 176 | VAL  |
| 19  | DG    | 179 | LEU  |
| 19  | DG    | 186 | ARG  |
| 19  | DG    | 200 | GLN  |
| 19  | DG    | 206 | LEU  |
| 19  | DG    | 210 | VAL  |
| 19  | DG    | 220 | THR  |
| 19  | DG    | 236 | VAL  |
| 19  | DG    | 296 | ASP  |
| 19  | DG    | 305 | VAL  |
| 19  | DG    | 318 | ILE  |
| 19  | DG    | 326 | THR  |
| 19  | DG    | 332 | GLN  |
| 19  | DG    | 334 | MET  |
| 19  | DG    | 336 | MET  |
| 19  | DG    | 365 | GLN  |
| 19  | DG    | 366 | ASP  |
| 19  | DG    | 367 | SER  |
| 19  | DG    | 370 | ARG  |
| 19  | DG    | 377 | GLU  |
| 19  | DG    | 384 | VAL  |
| 19  | DG    | 392 | ARG  |
| 19  | DG    | 405 | GLN  |
| 19  | DG    | 444 | THR  |
| 19  | DG    | 448 | LEU  |
| 19  | DG    | 457 | ARG  |
| 19  | DG    | 466 | VAL  |
| 19  | DG    | 472 | ARG  |
| 19  | DG    | 473 | CYS  |
| 19  | DG    | 494 | THR  |
| 19  | DG    | 496 | ARG  |
| 19  | DG    | 497 | ARG  |
| 19  | DG    | 529 | ASP  |
| 19  | DG    | 547 | MET  |
| 19  | DG    | 557 | GLN  |
| 19  | DG    | 577 | LEU  |
| 19  | DG    | 582 | VAL  |
| 19  | DG    | 608 | ARG  |
| 19  | DG    | 615 | SER  |
| 19  | DG    | 616 | ARG  |
| 19  | DG    | 623 | MET  |
| 19  | DG    | 626 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | DH    | 1   | MET  |
| 20  | DH    | 4   | GLN  |
| 20  | DH    | 6   | VAL  |
| 20  | DH    | 9   | THR  |
| 20  | DH    | 40  | THR  |
| 20  | DH    | 46  | LEU  |
| 20  | DH    | 47  | ILE  |
| 20  | DH    | 51  | ARG  |
| 20  | DH    | 74  | GLU  |
| 20  | DH    | 76  | LEU  |
| 20  | DH    | 79  | ASP  |
| 20  | DH    | 81  | LYS  |
| 20  | DH    | 82  | GLN  |
| 20  | DH    | 83  | GLU  |
| 20  | DH    | 84  | SER  |
| 20  | DH    | 85  | LEU  |
| 20  | DH    | 102 | LEU  |
| 20  | DH    | 105 | GLN  |
| 20  | DH    | 135 | ARG  |
| 20  | DH    | 167 | GLU  |
| 20  | DH    | 174 | LEU  |
| 20  | DH    | 181 | VAL  |
| 20  | DH    | 195 | TYR  |
| 20  | DH    | 206 | ILE  |
| 20  | DH    | 236 | MET  |
| 20  | DH    | 257 | ASN  |
| 20  | DH    | 258 | MET  |
| 20  | DH    | 268 | LEU  |
| 20  | DH    | 273 | SER  |
| 20  | DH    | 297 | CYS  |
| 20  | DH    | 311 | ARG  |
| 20  | DH    | 318 | GLU  |
| 20  | DH    | 323 | SER  |
| 20  | DH    | 344 | VAL  |
| 20  | DH    | 345 | VAL  |
| 20  | DH    | 346 | GLU  |
| 20  | DH    | 348 | LYS  |
| 20  | DH    | 350 | VAL  |
| 20  | DH    | 354 | LEU  |
| 20  | DH    | 359 | GLU  |
| 20  | DH    | 360 | LEU  |
| 20  | DH    | 364 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | DH    | 369 | ARG  |
| 20  | DH    | 375 | VAL  |
| 20  | DH    | 380 | ARG  |
| 20  | DH    | 382 | PHE  |
| 20  | DH    | 386 | ARG  |
| 20  | DH    | 396 | VAL  |
| 20  | DH    | 411 | LEU  |
| 20  | DH    | 414 | LEU  |
| 20  | DH    | 421 | THR  |
| 20  | DH    | 428 | ARG  |
| 20  | DH    | 450 | ASN  |
| 20  | DH    | 452 | ARG  |
| 20  | DH    | 460 | LEU  |
| 20  | DH    | 474 | ASP  |
| 20  | DH    | 476 | VAL  |
| 20  | DH    | 486 | THR  |
| 20  | DH    | 495 | THR  |
| 20  | DH    | 499 | GLU  |
| 20  | DH    | 503 | THR  |
| 20  | DH    | 515 | ASP  |
| 20  | DH    | 523 | ARG  |
| 20  | DH    | 554 | ARG  |
| 20  | DH    | 557 | VAL  |
| 20  | DH    | 562 | THR  |
| 21  | DJ    | 16  | ASN  |
| 21  | DJ    | 19  | THR  |
| 21  | DJ    | 38  | MET  |
| 21  | DJ    | 46  | ARG  |
| 21  | DJ    | 54  | SER  |
| 21  | DJ    | 55  | ASN  |
| 21  | DJ    | 59  | VAL  |
| 21  | DJ    | 71  | MET  |
| 21  | DJ    | 76  | SER  |
| 21  | DJ    | 91  | THR  |
| 21  | DJ    | 92  | LEU  |
| 21  | DJ    | 100 | VAL  |
| 21  | DJ    | 107 | LEU  |
| 21  | DJ    | 110 | LEU  |
| 21  | DJ    | 119 | LEU  |
| 21  | DJ    | 123 | LYS  |
| 21  | DJ    | 137 | MET  |
| 21  | DJ    | 149 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | DJ    | 151 | GLU  |
| 21  | DJ    | 164 | SER  |
| 21  | DJ    | 166 | LEU  |
| 21  | DJ    | 178 | ARG  |
| 21  | DJ    | 180 | LEU  |
| 21  | DJ    | 182 | ASP  |
| 21  | DJ    | 206 | SER  |
| 21  | DJ    | 210 | MET  |
| 21  | DJ    | 212 | ASP  |
| 21  | DJ    | 226 | VAL  |
| 21  | DJ    | 234 | GLU  |
| 21  | DJ    | 236 | ARG  |
| 21  | DJ    | 246 | THR  |
| 21  | DJ    | 258 | LEU  |
| 21  | DJ    | 266 | VAL  |
| 21  | DJ    | 271 | THR  |
| 21  | DJ    | 291 | ASN  |
| 21  | DJ    | 302 | SER  |
| 21  | DJ    | 305 | ARG  |
| 21  | DJ    | 308 | ARG  |
| 21  | DJ    | 323 | THR  |
| 22  | DK    | 2   | SER  |
| 22  | DK    | 6   | THR  |
| 22  | DK    | 18  | LEU  |
| 22  | DK    | 34  | ASN  |
| 22  | DK    | 36  | ARG  |
| 22  | DK    | 54  | THR  |
| 22  | DK    | 111 | LEU  |
| 22  | DK    | 115 | THR  |
| 22  | DK    | 116 | ARG  |
| 22  | DK    | 134 | THR  |
| 22  | DK    | 167 | THR  |
| 22  | DK    | 172 | LEU  |
| 22  | DK    | 173 | VAL  |
| 22  | DK    | 225 | THR  |
| 22  | DK    | 226 | LEU  |
| 22  | DK    | 238 | ILE  |
| 22  | DK    | 240 | SER  |
| 22  | DK    | 250 | VAL  |
| 22  | DK    | 263 | GLU  |
| 22  | DK    | 265 | VAL  |
| 22  | DK    | 270 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DK    | 273 | LEU  |
| 22  | DK    | 275 | ARG  |
| 22  | DK    | 282 | GLU  |
| 22  | DK    | 294 | SER  |
| 23  | DT    | 12  | ARG  |
| 23  | DT    | 14  | THR  |
| 23  | DT    | 35  | LYS  |
| 23  | DT    | 52  | ARG  |
| 23  | DT    | 88  | THR  |
| 23  | DT    | 90  | THR  |
| 23  | DT    | 91  | GLN  |
| 23  | DT    | 103 | LEU  |
| 23  | DT    | 105 | ARG  |
| 23  | DT    | 106 | ASP  |
| 23  | DT    | 114 | LEU  |
| 23  | DT    | 122 | MET  |
| 23  | DT    | 131 | SER  |
| 23  | DT    | 137 | LEU  |
| 23  | DT    | 163 | ARG  |
| 23  | DT    | 166 | THR  |
| 23  | DT    | 168 | GLU  |
| 23  | DT    | 176 | ASP  |
| 23  | DT    | 177 | MET  |
| 23  | DT    | 179 | VAL  |
| 23  | DT    | 181 | ASP  |
| 23  | DT    | 195 | VAL  |
| 23  | DT    | 202 | LYS  |
| 23  | DT    | 205 | VAL  |
| 23  | DT    | 209 | THR  |
| 23  | DT    | 241 | ASN  |
| 24  | DV    | 26  | THR  |
| 24  | DV    | 39  | ARG  |
| 24  | DV    | 41  | THR  |
| 24  | DV    | 43  | ASN  |
| 24  | DV    | 56  | ARG  |
| 24  | DV    | 63  | ILE  |
| 24  | DV    | 68  | ILE  |
| 24  | DV    | 71  | GLN  |
| 24  | DV    | 77  | LYS  |
| 24  | DV    | 114 | VAL  |
| 24  | DV    | 118 | GLN  |
| 24  | DV    | 127 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DV    | 131 | GLN  |
| 24  | DV    | 134 | ASP  |
| 24  | DV    | 140 | PHE  |
| 24  | DV    | 143 | ILE  |
| 24  | DV    | 151 | GLU  |
| 24  | DV    | 178 | THR  |
| 24  | DV    | 179 | LEU  |
| 24  | DV    | 180 | ASP  |
| 24  | DV    | 183 | LEU  |
| 25  | DW    | 10  | THR  |
| 25  | DW    | 12  | THR  |
| 25  | DW    | 22  | THR  |
| 25  | DW    | 37  | MET  |
| 25  | DW    | 58  | ARG  |
| 25  | DW    | 60  | VAL  |
| 25  | DW    | 70  | LEU  |
| 25  | DW    | 74  | THR  |
| 25  | DW    | 83  | THR  |
| 25  | DW    | 128 | LEU  |
| 25  | DW    | 133 | LYS  |
| 25  | DW    | 163 | GLU  |
| 26  | DX    | 34  | LYS  |
| 26  | DX    | 57  | ARG  |
| 26  | DX    | 72  | SER  |
| 26  | DX    | 76  | ARG  |
| 26  | DX    | 78  | GLU  |
| 26  | DX    | 89  | ARG  |
| 26  | DX    | 90  | ILE  |
| 26  | DX    | 98  | LEU  |
| 26  | DX    | 124 | ILE  |
| 26  | DX    | 131 | ILE  |
| 26  | DX    | 132 | THR  |
| 26  | DX    | 136 | ARG  |
| 26  | DX    | 162 | VAL  |
| 26  | DX    | 164 | THR  |
| 26  | DX    | 168 | ASN  |
| 27  | DY    | 11  | THR  |
| 27  | DY    | 14  | THR  |
| 27  | DY    | 15  | SER  |
| 27  | DY    | 23  | SER  |
| 27  | DY    | 39  | VAL  |
| 27  | DY    | 43  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DY    | 47  | THR  |
| 27  | DY    | 50  | VAL  |
| 27  | DY    | 52  | GLN  |
| 27  | DY    | 64  | ASP  |
| 27  | DY    | 65  | LEU  |
| 27  | DY    | 77  | VAL  |
| 27  | DY    | 79  | ASP  |
| 27  | DY    | 81  | THR  |
| 27  | DY    | 84  | LYS  |
| 27  | DY    | 87  | ARG  |
| 27  | DY    | 93  | THR  |
| 27  | DY    | 113 | VAL  |
| 27  | DY    | 124 | THR  |
| 27  | DY    | 128 | GLN  |
| 27  | DY    | 141 | VAL  |
| 27  | DY    | 163 | LYS  |
| 28  | CC    | 4   | MET  |
| 28  | CC    | 7   | ILE  |
| 28  | CC    | 10  | VAL  |
| 28  | CC    | 14  | THR  |
| 28  | CC    | 20  | THR  |
| 28  | CC    | 21  | PHE  |
| 28  | CC    | 22  | LYS  |
| 28  | CC    | 45  | ILE  |
| 28  | CC    | 46  | TRP  |
| 28  | CC    | 47  | LEU  |
| 28  | CC    | 50  | ILE  |
| 28  | CC    | 55  | ILE  |
| 28  | CC    | 69  | GLU  |
| 28  | CC    | 72  | ILE  |
| 28  | CC    | 76  | SER  |
| 29  | CE    | 13  | ASN  |
| 29  | CE    | 17  | THR  |
| 29  | CE    | 27  | ARG  |
| 29  | CE    | 41  | ARG  |
| 29  | CE    | 48  | ASN  |
| 29  | CE    | 58  | SER  |
| 29  | CE    | 64  | THR  |
| 29  | CE    | 65  | ARG  |
| 29  | CE    | 80  | ILE  |
| 29  | CE    | 83  | MET  |
| 29  | CE    | 87  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | CE    | 112 | THR  |
| 29  | CE    | 121 | THR  |
| 29  | CE    | 124 | THR  |
| 29  | CE    | 137 | LEU  |
| 29  | CE    | 163 | ILE  |
| 29  | CE    | 165 | CYS  |
| 29  | CE    | 188 | GLU  |
| 29  | CE    | 201 | ILE  |
| 29  | CE    | 217 | VAL  |
| 29  | CE    | 232 | ILE  |
| 29  | CE    | 233 | VAL  |
| 29  | CE    | 279 | LEU  |
| 29  | CE    | 285 | ILE  |
| 29  | CE    | 313 | MET  |
| 29  | CE    | 314 | MET  |
| 29  | CE    | 332 | ASP  |
| 29  | CE    | 364 | ARG  |
| 29  | CE    | 365 | MET  |
| 29  | CE    | 370 | ASP  |
| 29  | CE    | 391 | THR  |
| 29  | CE    | 395 | THR  |
| 29  | CE    | 396 | LEU  |
| 29  | CE    | 405 | LYS  |
| 29  | CE    | 410 | LEU  |
| 29  | CE    | 420 | VAL  |
| 29  | CE    | 422 | VAL  |
| 30  | CF    | 2   | VAL  |
| 30  | CF    | 39  | ILE  |
| 30  | CF    | 42  | GLU  |
| 30  | CF    | 71  | MET  |
| 30  | CF    | 93  | LEU  |
| 30  | CF    | 124 | LEU  |
| 30  | CF    | 133 | GLN  |
| 30  | CF    | 138 | ILE  |
| 30  | CF    | 141 | GLN  |
| 30  | CF    | 152 | THR  |
| 31  | CH    | 26  | ARG  |
| 31  | CH    | 29  | HIS  |
| 31  | CH    | 88  | LEU  |
| 31  | CH    | 89  | VAL  |
| 31  | CH    | 108 | LEU  |
| 31  | CH    | 118 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | CH    | 128 | VAL  |
| 31  | CH    | 131 | ASP  |
| 31  | CH    | 132 | ASP  |
| 31  | CH    | 138 | LYS  |
| 31  | CH    | 150 | THR  |
| 31  | CH    | 152 | ILE  |
| 31  | CH    | 163 | THR  |
| 31  | CH    | 170 | VAL  |
| 31  | CH    | 172 | VAL  |
| 31  | CH    | 229 | GLU  |
| 31  | CH    | 248 | ASN  |
| 31  | CH    | 276 | ARG  |
| 31  | CH    | 279 | MET  |
| 31  | CH    | 280 | MET  |
| 32  | CI    | 2   | GLN  |
| 32  | CI    | 9   | THR  |
| 32  | CI    | 18  | LEU  |
| 32  | CI    | 33  | SER  |
| 32  | CI    | 34  | ASP  |
| 32  | CI    | 38  | LEU  |
| 32  | CI    | 43  | SER  |
| 32  | CI    | 57  | GLU  |
| 32  | CI    | 59  | ARG  |
| 32  | CI    | 65  | MET  |
| 32  | CI    | 139 | ASP  |
| 32  | CI    | 179 | CYS  |
| 32  | CI    | 218 | ARG  |
| 32  | CI    | 219 | LEU  |
| 32  | CI    | 290 | ILE  |
| 32  | CI    | 303 | THR  |
| 32  | CI    | 309 | ARG  |
| 32  | CI    | 311 | CYS  |
| 32  | CI    | 324 | ARG  |
| 32  | CI    | 330 | ASN  |
| 32  | CI    | 332 | ILE  |
| 32  | CI    | 338 | LYS  |
| 32  | CI    | 343 | VAL  |
| 32  | CI    | 356 | MET  |
| 32  | CI    | 372 | ILE  |
| 32  | CI    | 406 | THR  |
| 32  | CI    | 415 | LEU  |
| 32  | CI    | 420 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | CI    | 439 | ARG  |
| 33  | CJ    | 17  | MET  |
| 33  | CJ    | 20  | GLN  |
| 33  | CJ    | 23  | LYS  |
| 33  | CJ    | 34  | GLN  |
| 33  | CJ    | 43  | GLU  |
| 33  | CJ    | 50  | ASP  |
| 33  | CJ    | 65  | VAL  |
| 33  | CJ    | 68  | ASP  |
| 33  | CJ    | 77  | CYS  |
| 33  | CJ    | 78  | THR  |
| 33  | CJ    | 84  | MET  |
| 33  | CJ    | 93  | SER  |
| 33  | CJ    | 105 | ASN  |
| 33  | CJ    | 106 | GLU  |
| 33  | CJ    | 110 | LYS  |
| 33  | CJ    | 118 | MET  |
| 33  | CJ    | 141 | ASP  |
| 33  | CJ    | 149 | GLU  |
| 33  | CJ    | 158 | THR  |
| 33  | CJ    | 162 | ILE  |
| 33  | CJ    | 186 | VAL  |
| 33  | CJ    | 202 | ASP  |
| 33  | CJ    | 204 | SER  |
| 33  | CJ    | 212 | THR  |
| 33  | CJ    | 257 | VAL  |
| 33  | CJ    | 273 | ARG  |
| 33  | CJ    | 279 | LYS  |
| 33  | CJ    | 286 | LEU  |
| 33  | CJ    | 287 | LEU  |
| 33  | CJ    | 293 | ASP  |
| 33  | CJ    | 311 | LEU  |
| 33  | CJ    | 313 | GLU  |
| 33  | CJ    | 325 | SER  |
| 33  | CJ    | 328 | ARG  |
| 33  | CJ    | 330 | LEU  |
| 33  | CJ    | 345 | VAL  |
| 33  | CJ    | 346 | PRO  |
| 33  | CJ    | 370 | MET  |
| 33  | CJ    | 372 | GLU  |
| 33  | CJ    | 380 | THR  |
| 33  | CJ    | 396 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | CJ    | 399 | ARG  |
| 33  | CJ    | 401 | ILE  |
| 33  | CJ    | 403 | CYS  |
| 33  | CJ    | 409 | SER  |
| 33  | CJ    | 413 | GLU  |
| 33  | CJ    | 434 | ILE  |
| 33  | CJ    | 456 | THR  |
| 33  | CJ    | 457 | THR  |
| 33  | CJ    | 480 | THR  |
| 33  | CJ    | 481 | ASP  |
| 33  | CJ    | 490 | ASP  |
| 33  | CJ    | 498 | CYS  |
| 33  | CJ    | 500 | VAL  |
| 33  | CJ    | 517 | VAL  |
| 33  | CJ    | 519 | ILE  |
| 33  | CJ    | 523 | VAL  |
| 33  | CJ    | 526 | THR  |
| 33  | CJ    | 530 | THR  |
| 33  | CJ    | 542 | LYS  |
| 33  | CJ    | 543 | THR  |
| 33  | CJ    | 547 | LYS  |
| 33  | CJ    | 552 | ILE  |
| 33  | CJ    | 556 | GLU  |
| 33  | CJ    | 565 | THR  |
| 33  | CJ    | 569 | LEU  |
| 33  | CJ    | 585 | SER  |
| 33  | CJ    | 605 | THR  |
| 33  | CJ    | 618 | VAL  |
| 33  | CJ    | 629 | ARG  |
| 33  | CJ    | 633 | CYS  |
| 33  | CJ    | 648 | VAL  |
| 33  | CJ    | 654 | VAL  |
| 33  | CJ    | 667 | VAL  |
| 33  | CJ    | 671 | LEU  |
| 33  | CJ    | 684 | THR  |
| 33  | CJ    | 687 | GLU  |
| 33  | CJ    | 704 | GLU  |
| 33  | CJ    | 714 | THR  |
| 33  | CJ    | 720 | THR  |
| 33  | CJ    | 724 | THR  |
| 33  | CJ    | 727 | THR  |
| 33  | CJ    | 731 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | CJ    | 757 | LEU  |
| 33  | CJ    | 762 | GLN  |
| 33  | CJ    | 769 | GLN  |
| 33  | CJ    | 770 | THR  |
| 33  | CJ    | 773 | GLU  |
| 33  | CJ    | 781 | HIS  |
| 33  | CJ    | 796 | ASP  |
| 33  | CJ    | 797 | LEU  |
| 33  | CJ    | 798 | GLN  |
| 33  | CJ    | 803 | ILE  |
| 34  | CK    | 15  | ARG  |
| 34  | CK    | 23  | ASP  |
| 34  | CK    | 32  | LEU  |
| 34  | CK    | 33  | LYS  |
| 34  | CK    | 40  | GLN  |
| 34  | CK    | 47  | ILE  |
| 34  | CK    | 48  | ARG  |
| 34  | CK    | 56  | GLN  |
| 34  | CK    | 70  | ILE  |
| 34  | CK    | 73  | GLN  |
| 34  | CK    | 98  | LEU  |
| 34  | CK    | 107 | GLN  |
| 34  | CK    | 109 | VAL  |
| 34  | CK    | 112 | GLU  |
| 34  | CK    | 113 | ARG  |
| 34  | CK    | 149 | VAL  |
| 34  | CK    | 156 | LYS  |
| 34  | CK    | 174 | VAL  |
| 34  | CK    | 192 | MET  |
| 34  | CK    | 205 | TYR  |
| 34  | CK    | 207 | VAL  |
| 34  | CK    | 232 | ARG  |
| 34  | CK    | 264 | SER  |
| 34  | CK    | 311 | THR  |
| 34  | CK    | 315 | LEU  |
| 34  | CK    | 324 | VAL  |
| 34  | CK    | 326 | LYS  |
| 35  | CL    | 59  | MET  |
| 35  | CL    | 91  | LEU  |
| 35  | CL    | 97  | LEU  |
| 35  | CL    | 118 | LEU  |
| 35  | CL    | 121 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | CL    | 122 | GLU  |
| 36  | CN    | 22  | THR  |
| 36  | CN    | 27  | GLU  |
| 36  | CN    | 30  | LEU  |
| 36  | CN    | 41  | LEU  |
| 36  | CN    | 43  | SER  |
| 36  | CN    | 49  | SER  |
| 36  | CN    | 57  | LYS  |
| 36  | CN    | 60  | VAL  |
| 36  | CN    | 66  | MET  |
| 36  | CN    | 70  | LYS  |
| 36  | CN    | 72  | THR  |
| 36  | CN    | 77  | ASN  |
| 36  | CN    | 81  | LEU  |
| 36  | CN    | 83  | LYS  |
| 36  | CN    | 105 | ARG  |
| 36  | CN    | 111 | VAL  |
| 36  | CN    | 118 | MET  |
| 36  | CN    | 127 | LEU  |
| 36  | CN    | 135 | THR  |
| 36  | CN    | 158 | ARG  |
| 37  | CO    | 69  | GLU  |
| 37  | CO    | 75  | LEU  |
| 37  | CO    | 82  | ASN  |
| 37  | CO    | 87  | THR  |
| 37  | CO    | 108 | THR  |
| 37  | CO    | 112 | LYS  |
| 37  | CO    | 190 | SER  |
| 37  | CO    | 209 | GLU  |
| 37  | CO    | 210 | ARG  |
| 37  | CO    | 220 | SER  |
| 37  | CO    | 224 | LEU  |
| 37  | CO    | 237 | ASN  |
| 37  | CO    | 240 | LEU  |
| 37  | CO    | 242 | ASN  |
| 37  | CO    | 245 | ASN  |
| 37  | CO    | 247 | ILE  |
| 37  | CO    | 266 | LEU  |
| 37  | CO    | 285 | ASP  |
| 37  | CO    | 304 | ASP  |
| 37  | CO    | 329 | GLU  |
| 37  | CO    | 336 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | CO    | 353 | GLU  |
| 37  | CO    | 362 | VAL  |
| 37  | CO    | 395 | VAL  |
| 37  | CO    | 399 | ILE  |
| 37  | CO    | 400 | ARG  |
| 37  | CO    | 412 | ARG  |
| 37  | CO    | 419 | VAL  |
| 38  | CP    | 13  | ILE  |
| 38  | CP    | 14  | LYS  |
| 38  | CP    | 15  | ARG  |
| 38  | CP    | 28  | ILE  |
| 38  | CP    | 36  | VAL  |
| 38  | CP    | 37  | VAL  |
| 38  | CP    | 40  | PHE  |
| 38  | CP    | 59  | ARG  |
| 38  | CP    | 68  | CYS  |
| 38  | CP    | 90  | MET  |
| 38  | CP    | 93  | THR  |
| 38  | CP    | 123 | LEU  |
| 38  | CP    | 129 | THR  |
| 38  | CP    | 152 | ASN  |
| 38  | CP    | 163 | LYS  |
| 38  | CP    | 170 | SER  |
| 38  | CP    | 188 | LEU  |
| 39  | CQ    | 16  | THR  |
| 39  | CQ    | 21  | ARG  |
| 39  | CQ    | 31  | THR  |
| 39  | CQ    | 34  | THR  |
| 39  | CQ    | 56  | ARG  |
| 39  | CQ    | 66  | VAL  |
| 39  | CQ    | 67  | LEU  |
| 39  | CQ    | 69  | GLN  |
| 39  | CQ    | 73  | ARG  |
| 39  | CQ    | 83  | LEU  |
| 39  | CQ    | 103 | MET  |
| 39  | CQ    | 108 | VAL  |
| 39  | CQ    | 114 | MET  |
| 39  | CQ    | 136 | ASP  |
| 39  | CQ    | 147 | ILE  |
| 39  | CQ    | 158 | HIS  |
| 39  | CQ    | 169 | VAL  |
| 39  | CQ    | 173 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | CQ    | 182 | VAL  |
| 39  | CQ    | 199 | ASN  |
| 40  | CR    | 15  | GLN  |
| 40  | CR    | 30  | LEU  |
| 40  | CR    | 44  | GLU  |
| 40  | CR    | 59  | LEU  |
| 40  | CR    | 80  | LEU  |
| 40  | CR    | 92  | ILE  |
| 40  | CR    | 96  | GLN  |
| 40  | CR    | 167 | ARG  |
| 40  | CR    | 184 | LYS  |
| 40  | CR    | 198 | THR  |
| 40  | CR    | 202 | LYS  |
| 40  | CR    | 228 | VAL  |
| 40  | CR    | 233 | SER  |
| 40  | CR    | 235 | SER  |
| 40  | CR    | 259 | GLN  |
| 40  | CR    | 278 | VAL  |
| 40  | CR    | 305 | THR  |
| 40  | CR    | 315 | LEU  |
| 40  | CR    | 320 | VAL  |
| 41  | CS    | 32  | LYS  |
| 41  | CS    | 33  | ILE  |
| 41  | CS    | 45  | ARG  |
| 41  | CS    | 47  | GLN  |
| 41  | CS    | 48  | ARG  |
| 41  | CS    | 59  | LYS  |
| 41  | CS    | 64  | MET  |
| 41  | CS    | 75  | MET  |
| 41  | CS    | 76  | THR  |
| 41  | CS    | 86  | GLU  |
| 41  | CS    | 95  | THR  |
| 41  | CS    | 105 | VAL  |
| 41  | CS    | 107 | THR  |
| 41  | CS    | 119 | VAL  |
| 41  | CS    | 121 | SER  |
| 41  | CS    | 125 | ILE  |
| 41  | CS    | 140 | MET  |
| 41  | CS    | 152 | ASP  |
| 42  | CU    | 13  | MET  |
| 42  | CU    | 32  | HIS  |
| 42  | CU    | 35  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | CU    | 44  | MET  |
| 42  | CU    | 74  | GLN  |
| 42  | CU    | 148 | ASN  |
| 42  | CU    | 161 | GLN  |
| 42  | CU    | 168 | VAL  |
| 42  | CU    | 169 | ASN  |
| 42  | CU    | 170 | VAL  |
| 42  | CU    | 171 | VAL  |
| 43  | CZ    | 218 | VAL  |
| 43  | CZ    | 236 | ARG  |
| 43  | CZ    | 240 | VAL  |
| 43  | CZ    | 244 | ILE  |
| 43  | CZ    | 260 | MET  |
| 43  | CZ    | 265 | GLN  |
| 43  | CZ    | 273 | ILE  |
| 43  | CZ    | 277 | PHE  |
| 43  | CZ    | 318 | LEU  |
| 43  | CZ    | 321 | MET  |
| 43  | CZ    | 360 | ASP  |
| 44  | Ca    | 14  | ASN  |
| 44  | Ca    | 15  | LYS  |
| 44  | Ca    | 39  | ARG  |
| 44  | Ca    | 67  | ARG  |
| 44  | Ca    | 71  | MET  |
| 44  | Ca    | 160 | GLU  |
| 44  | Ca    | 168 | TYR  |
| 44  | Ca    | 179 | LEU  |
| 44  | Ca    | 181 | GLU  |
| 44  | Ca    | 194 | LEU  |
| 44  | Ca    | 201 | ARG  |
| 44  | Ca    | 221 | THR  |
| 44  | Ca    | 227 | ASN  |
| 44  | Ca    | 240 | SER  |
| 44  | Ca    | 297 | LEU  |
| 44  | Ca    | 299 | ARG  |
| 44  | Ca    | 314 | CYS  |
| 44  | Ca    | 338 | LYS  |
| 44  | Ca    | 350 | GLU  |
| 44  | Ca    | 365 | LEU  |
| 44  | Ca    | 376 | VAL  |
| 44  | Ca    | 380 | ASP  |
| 44  | Ca    | 384 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | Ca    | 398 | ASP  |
| 44  | Ca    | 399 | ASN  |
| 44  | Ca    | 410 | MET  |
| 44  | Ca    | 433 | GLN  |
| 44  | Ca    | 447 | ILE  |
| 44  | Ca    | 451 | VAL  |
| 44  | Ca    | 479 | THR  |
| 44  | Ca    | 480 | LEU  |
| 44  | Ca    | 506 | GLN  |
| 44  | Ca    | 520 | TYR  |
| 44  | Ca    | 538 | ILE  |
| 44  | Ca    | 541 | ARG  |
| 44  | Ca    | 552 | THR  |
| 44  | Ca    | 569 | ARG  |
| 44  | Ca    | 585 | GLN  |
| 44  | Ca    | 599 | ILE  |
| 45  | Cb    | 40  | LEU  |
| 45  | Cb    | 57  | MET  |
| 45  | Cb    | 71  | LEU  |
| 45  | Cb    | 108 | GLU  |
| 45  | Cb    | 110 | MET  |
| 45  | Cb    | 144 | ARG  |
| 45  | Cb    | 171 | THR  |
| 45  | Cb    | 193 | GLU  |
| 45  | Cb    | 195 | LEU  |
| 45  | Cb    | 288 | GLU  |
| 45  | Cb    | 291 | GLU  |
| 45  | Cb    | 306 | THR  |
| 46  | Cd    | 44  | GLU  |
| 46  | Cd    | 74  | ASP  |
| 46  | Cd    | 102 | ARG  |
| 46  | Cd    | 106 | ARG  |
| 46  | Cd    | 108 | MET  |
| 46  | Cd    | 112 | ARG  |
| 46  | Cd    | 120 | LEU  |
| 46  | Cd    | 122 | LEU  |
| 46  | Cd    | 125 | GLU  |
| 46  | Cd    | 164 | LEU  |
| 46  | Cd    | 168 | VAL  |
| 46  | Cd    | 180 | VAL  |
| 46  | Cd    | 182 | GLN  |
| 46  | Cd    | 193 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | Cd    | 208 | HIS  |
| 46  | Cd    | 210 | ASP  |
| 46  | Cd    | 216 | HIS  |
| 46  | Cd    | 217 | GLU  |
| 46  | Cd    | 219 | HIS  |
| 46  | Cd    | 259 | GLU  |
| 46  | Cd    | 267 | GLU  |
| 46  | Cd    | 284 | THR  |
| 47  | Cg    | 20  | THR  |
| 47  | Cg    | 27  | GLU  |
| 47  | Cg    | 56  | ARG  |
| 47  | Cg    | 57  | THR  |
| 47  | Cg    | 73  | ASP  |
| 47  | Cg    | 76  | SER  |
| 47  | Cg    | 77  | MET  |
| 47  | Cg    | 87  | GLN  |
| 47  | Cg    | 107 | ARG  |
| 47  | Cg    | 112 | ARG  |
| 47  | Cg    | 114 | GLU  |
| 47  | Cg    | 117 | LEU  |
| 47  | Cg    | 120 | LEU  |
| 47  | Cg    | 127 | HIS  |
| 47  | Cg    | 143 | THR  |
| 47  | Cg    | 153 | CYS  |
| 47  | Cg    | 170 | ASN  |
| 47  | Cg    | 173 | THR  |
| 47  | Cg    | 194 | LEU  |
| 47  | Cg    | 213 | VAL  |
| 47  | Cg    | 221 | SER  |
| 47  | Cg    | 224 | LEU  |
| 47  | Cg    | 225 | ARG  |
| 47  | Cg    | 226 | CYS  |
| 47  | Cg    | 227 | THR  |
| 47  | Cg    | 230 | ASP  |
| 47  | Cg    | 233 | THR  |
| 47  | Cg    | 254 | VAL  |
| 47  | Cg    | 262 | GLN  |
| 47  | Cg    | 290 | LEU  |
| 47  | Cg    | 296 | HIS  |
| 47  | Cg    | 308 | LEU  |
| 47  | Cg    | 310 | SER  |
| 47  | Cg    | 316 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | Cg    | 318 | ILE  |
| 47  | Cg    | 319 | ASP  |
| 47  | Cg    | 325 | LEU  |
| 47  | Cg    | 337 | ARG  |
| 47  | Cg    | 344 | LEU  |
| 47  | Cg    | 355 | THR  |
| 47  | Cg    | 357 | THR  |
| 47  | Cg    | 373 | VAL  |
| 47  | Cg    | 391 | GLU  |
| 47  | Cg    | 401 | ILE  |
| 47  | Cg    | 421 | GLU  |
| 47  | Cg    | 422 | LEU  |
| 47  | Cg    | 436 | ASP  |
| 47  | Cg    | 464 | VAL  |
| 47  | Cg    | 468 | ASP  |
| 47  | Cg    | 480 | LYS  |
| 48  | Ci    | 18  | THR  |
| 48  | Ci    | 27  | CYS  |
| 48  | Ci    | 30  | ARG  |
| 48  | Ci    | 32  | ASP  |
| 48  | Ci    | 54  | GLN  |
| 48  | Ci    | 58  | GLU  |
| 48  | Ci    | 76  | MET  |
| 48  | Ci    | 82  | GLN  |
| 48  | Ci    | 105 | ARG  |
| 48  | Ci    | 114 | MET  |
| 48  | Ci    | 119 | LEU  |
| 48  | Ci    | 122 | MET  |
| 48  | Ci    | 136 | HIS  |
| 48  | Ci    | 138 | ASP  |
| 48  | Ci    | 144 | ARG  |
| 48  | Ci    | 145 | ASN  |
| 48  | Ci    | 146 | ASP  |
| 48  | Ci    | 157 | LEU  |
| 48  | Ci    | 164 | ASN  |
| 48  | Ci    | 174 | ASP  |
| 49  | Cj    | 10  | ARG  |
| 49  | Cj    | 66  | LEU  |
| 49  | Cj    | 71  | ILE  |
| 49  | Cj    | 77  | LEU  |
| 49  | Cj    | 80  | LEU  |
| 49  | Cj    | 135 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | Cj    | 138 | ASP  |
| 49  | Cj    | 145 | THR  |
| 49  | Cj    | 155 | GLU  |
| 49  | Cj    | 161 | VAL  |
| 49  | Cj    | 173 | MET  |
| 49  | Cj    | 206 | LEU  |
| 49  | Cj    | 210 | PRO  |
| 50  | Ck    | 41  | THR  |
| 50  | Ck    | 57  | ASP  |
| 50  | Ck    | 86  | GLU  |
| 50  | Ck    | 87  | ARG  |
| 50  | Ck    | 93  | THR  |
| 50  | Ck    | 97  | GLN  |
| 50  | Ck    | 99  | SER  |
| 50  | Ck    | 103 | GLU  |
| 50  | Ck    | 108 | GLN  |
| 50  | Ck    | 111 | THR  |
| 50  | Ck    | 136 | ASP  |
| 50  | Ck    | 137 | THR  |
| 50  | Ck    | 161 | GLU  |
| 50  | Ck    | 176 | THR  |
| 50  | Ck    | 185 | LEU  |
| 50  | Ck    | 188 | LEU  |
| 50  | Ck    | 207 | ARG  |
| 50  | Ck    | 214 | LEU  |
| 50  | Ck    | 219 | THR  |
| 50  | Ck    | 237 | LEU  |
| 50  | Ck    | 242 | LEU  |
| 50  | Ck    | 254 | ILE  |
| 50  | Ck    | 283 | GLU  |
| 50  | Ck    | 290 | LEU  |
| 50  | Ck    | 316 | ASP  |
| 50  | Ck    | 317 | VAL  |
| 50  | Ck    | 320 | VAL  |
| 50  | Ck    | 337 | VAL  |
| 50  | Ck    | 341 | LEU  |
| 50  | Ck    | 350 | ASP  |
| 50  | Ck    | 353 | ARG  |
| 50  | Ck    | 370 | THR  |
| 50  | Ck    | 373 | ARG  |
| 50  | Ck    | 376 | VAL  |
| 50  | Ck    | 380 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Ck    | 401 | LEU  |
| 50  | Ck    | 568 | LEU  |
| 50  | Ck    | 573 | THR  |
| 50  | Ck    | 574 | GLU  |
| 50  | Ck    | 575 | LEU  |
| 50  | Ck    | 597 | LEU  |
| 50  | Ck    | 606 | THR  |
| 50  | Ck    | 607 | LYS  |
| 50  | Ck    | 611 | ASN  |
| 50  | Ck    | 618 | ILE  |
| 50  | Ck    | 620 | THR  |
| 50  | Ck    | 629 | LEU  |
| 50  | Ck    | 633 | MET  |
| 50  | Ck    | 642 | VAL  |
| 50  | Ck    | 652 | ARG  |
| 50  | Ck    | 654 | SER  |
| 50  | Ck    | 661 | ILE  |
| 50  | Ck    | 682 | ASN  |
| 50  | Ck    | 691 | GLN  |
| 50  | Ck    | 695 | GLN  |
| 50  | Ck    | 703 | ARG  |
| 50  | Ck    | 706 | SER  |
| 50  | Ck    | 707 | LEU  |
| 50  | Ck    | 733 | LEU  |
| 50  | Ck    | 755 | ASP  |
| 50  | Ck    | 760 | VAL  |
| 50  | Ck    | 766 | LYS  |
| 50  | Ck    | 775 | ARG  |
| 50  | Ck    | 782 | GLU  |
| 50  | Ck    | 806 | ASP  |
| 50  | Ck    | 838 | LEU  |
| 50  | Ck    | 841 | LYS  |
| 51  | Cm    | 21  | GLN  |
| 51  | Cm    | 35  | ASN  |
| 51  | Cm    | 50  | ARG  |
| 51  | Cm    | 60  | ARG  |
| 51  | Cm    | 61  | ARG  |
| 51  | Cm    | 80  | THR  |
| 51  | Cm    | 85  | ILE  |
| 51  | Cm    | 92  | GLN  |
| 51  | Cm    | 93  | LEU  |
| 51  | Cm    | 94  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | Cm    | 95  | MET  |
| 51  | Cm    | 98  | SER  |
| 51  | Cm    | 106 | CYS  |
| 51  | Cm    | 124 | SER  |
| 51  | Cm    | 125 | CYS  |
| 51  | Cm    | 126 | LEU  |
| 51  | Cm    | 128 | ARG  |
| 51  | Cm    | 153 | ASP  |
| 51  | Cm    | 160 | GLN  |
| 51  | Cm    | 162 | ARG  |
| 51  | Cm    | 168 | HIS  |
| 51  | Cm    | 173 | GLU  |
| 51  | Cm    | 178 | GLU  |
| 51  | Cm    | 202 | THR  |
| 52  | Cn    | 165 | LEU  |
| 52  | Cn    | 172 | LYS  |
| 52  | Cn    | 195 | PHE  |
| 52  | Cn    | 203 | MET  |
| 52  | Cn    | 214 | ARG  |
| 53  | Cp    | 30  | LEU  |
| 53  | Cp    | 50  | THR  |
| 53  | Cp    | 67  | ARG  |
| 53  | Cp    | 84  | LEU  |
| 53  | Cp    | 87  | CYS  |
| 53  | Cp    | 105 | ILE  |
| 53  | Cp    | 107 | THR  |
| 53  | Cp    | 123 | THR  |
| 53  | Cp    | 137 | ASP  |
| 53  | Cp    | 166 | ARG  |
| 53  | Cp    | 168 | ILE  |
| 54  | Cq    | 19  | VAL  |
| 54  | Cq    | 24  | THR  |
| 54  | Cq    | 30  | ILE  |
| 54  | Cq    | 52  | THR  |
| 54  | Cq    | 64  | VAL  |
| 54  | Cq    | 65  | SER  |
| 54  | Cq    | 78  | ASP  |
| 54  | Cq    | 79  | MET  |
| 54  | Cq    | 96  | THR  |
| 54  | Cq    | 106 | LEU  |
| 54  | Cq    | 107 | GLU  |
| 54  | Cq    | 144 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | Cq    | 185 | CYS  |
| 54  | Cq    | 207 | CYS  |
| 54  | Cq    | 227 | ILE  |
| 54  | Cq    | 235 | LEU  |
| 54  | Cq    | 250 | LEU  |
| 55  | Cr    | 18  | LEU  |
| 55  | Cr    | 25  | LEU  |
| 55  | Cr    | 26  | LEU  |
| 55  | Cr    | 36  | VAL  |
| 55  | Cr    | 37  | CYS  |
| 55  | Cr    | 45  | THR  |
| 55  | Cr    | 58  | ASN  |
| 55  | Cr    | 61  | VAL  |
| 55  | Cr    | 65  | LYS  |
| 55  | Cr    | 74  | ASP  |
| 55  | Cr    | 96  | GLU  |
| 55  | Cr    | 103 | VAL  |
| 55  | Cr    | 122 | VAL  |
| 55  | Cr    | 161 | ARG  |
| 55  | Cr    | 163 | LEU  |
| 55  | Cr    | 171 | GLN  |
| 55  | Cr    | 176 | LEU  |
| 55  | Cr    | 247 | ILE  |
| 55  | Cr    | 248 | ARG  |
| 55  | Cr    | 250 | LYS  |
| 55  | Cr    | 265 | LEU  |
| 55  | Cr    | 282 | GLU  |
| 56  | Cv    | 27  | LYS  |
| 56  | Cv    | 28  | THR  |
| 56  | Cv    | 32  | ARG  |
| 56  | Cv    | 35  | ARG  |
| 56  | Cv    | 60  | GLN  |
| 56  | Cv    | 87  | GLN  |
| 56  | Cv    | 98  | ARG  |
| 56  | Cv    | 151 | SER  |
| 56  | Cv    | 162 | SER  |
| 56  | Cv    | 172 | THR  |
| 56  | Cv    | 192 | LEU  |
| 56  | Cv    | 195 | LEU  |
| 56  | Cv    | 201 | THR  |
| 56  | Cv    | 204 | ILE  |
| 56  | Cv    | 209 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | Cv    | 235 | MET  |
| 56  | Cv    | 261 | ILE  |
| 56  | Cv    | 266 | CYS  |
| 56  | Cv    | 278 | LEU  |
| 56  | Cv    | 283 | ASP  |
| 56  | Cv    | 284 | LYS  |
| 56  | Cv    | 301 | SER  |
| 56  | Cv    | 305 | ASP  |
| 56  | Cv    | 312 | ASN  |
| 56  | Cv    | 367 | ASP  |
| 56  | Cv    | 382 | GLU  |
| 56  | Cv    | 399 | VAL  |
| 56  | Cv    | 401 | THR  |
| 56  | Cv    | 407 | MET  |
| 56  | Cv    | 411 | ASN  |
| 56  | Cv    | 417 | THR  |
| 56  | Cv    | 437 | ILE  |
| 56  | Cv    | 446 | THR  |
| 56  | Cv    | 462 | LEU  |
| 56  | Cv    | 512 | MET  |
| 56  | Cv    | 531 | MET  |
| 56  | Cv    | 562 | VAL  |
| 56  | Cv    | 566 | MET  |
| 56  | Cv    | 569 | LEU  |
| 56  | Cv    | 594 | LEU  |
| 56  | Cv    | 612 | THR  |
| 56  | Cv    | 613 | LEU  |
| 56  | Cv    | 617 | ASP  |
| 56  | Cv    | 618 | ILE  |
| 56  | Cv    | 638 | VAL  |
| 56  | Cv    | 647 | VAL  |
| 56  | Cv    | 649 | THR  |
| 56  | Cv    | 673 | LEU  |
| 56  | Cv    | 678 | HIS  |
| 56  | Cv    | 689 | CYS  |
| 56  | Cv    | 739 | ASN  |
| 56  | Cv    | 754 | ILE  |
| 56  | Cv    | 782 | ILE  |
| 56  | Cv    | 795 | GLU  |
| 56  | Cv    | 813 | ARG  |
| 56  | Cv    | 818 | LEU  |
| 56  | Cv    | 838 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 56  | Cv    | 861  | THR  |
| 56  | Cv    | 916  | ARG  |
| 56  | Cv    | 918  | LEU  |
| 56  | Cv    | 921  | VAL  |
| 56  | Cv    | 927  | LEU  |
| 56  | Cv    | 938  | ASP  |
| 56  | Cv    | 945  | VAL  |
| 56  | Cv    | 959  | LEU  |
| 56  | Cv    | 967  | VAL  |
| 56  | Cv    | 969  | ASP  |
| 56  | Cv    | 987  | SER  |
| 56  | Cv    | 993  | THR  |
| 56  | Cv    | 995  | VAL  |
| 56  | Cv    | 996  | SER  |
| 56  | Cv    | 1002 | ARG  |
| 56  | Cv    | 1018 | THR  |
| 56  | Cv    | 1030 | ARG  |
| 56  | Cv    | 1034 | ARG  |
| 56  | Cv    | 1039 | GLU  |
| 56  | Cv    | 1040 | GLU  |
| 56  | Cv    | 1069 | GLN  |
| 56  | Cv    | 1070 | GLU  |
| 56  | Cv    | 1077 | GLU  |
| 56  | Cv    | 1108 | GLN  |
| 56  | Cv    | 1136 | ASN  |
| 64  | A0    | 31   | LEU  |
| 64  | A0    | 71   | ARG  |
| 64  | A0    | 75   | ASN  |
| 64  | A0    | 76   | THR  |
| 64  | A0    | 82   | THR  |
| 64  | A0    | 116  | LEU  |
| 64  | A0    | 130  | VAL  |
| 64  | A0    | 139  | GLU  |
| 64  | A0    | 143  | LEU  |
| 64  | A0    | 155  | VAL  |
| 64  | A0    | 163  | LYS  |
| 64  | A0    | 166  | ASN  |
| 65  | A1    | 15   | LEU  |
| 65  | A1    | 46   | CYS  |
| 65  | A1    | 49   | VAL  |
| 65  | A1    | 60   | VAL  |
| 65  | A1    | 61   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | A1    | 71  | GLN  |
| 65  | A1    | 75  | VAL  |
| 65  | A1    | 77  | TRP  |
| 65  | A1    | 78  | LEU  |
| 65  | A1    | 104 | VAL  |
| 65  | A1    | 106 | THR  |
| 65  | A1    | 114 | LEU  |
| 65  | A1    | 120 | VAL  |
| 65  | A1    | 130 | VAL  |
| 65  | A1    | 133 | ASP  |
| 65  | A1    | 142 | LYS  |
| 65  | A1    | 154 | GLU  |
| 65  | A1    | 156 | ILE  |
| 65  | A1    | 174 | GLN  |
| 65  | A1    | 178 | GLN  |
| 65  | A1    | 191 | MET  |
| 65  | A1    | 192 | GLU  |
| 65  | A1    | 201 | LEU  |
| 65  | A1    | 215 | ILE  |
| 65  | A1    | 223 | LYS  |
| 65  | A1    | 225 | GLN  |
| 66  | A2    | 17  | VAL  |
| 66  | A2    | 22  | LEU  |
| 66  | A2    | 25  | LYS  |
| 66  | A2    | 26  | ARG  |
| 66  | A2    | 36  | VAL  |
| 66  | A2    | 37  | GLU  |
| 66  | A2    | 44  | LEU  |
| 66  | A2    | 50  | ILE  |
| 66  | A2    | 69  | LEU  |
| 66  | A2    | 72  | GLN  |
| 66  | A2    | 84  | LEU  |
| 66  | A2    | 88  | ASP  |
| 66  | A2    | 90  | SER  |
| 66  | A2    | 94  | ILE  |
| 66  | A2    | 114 | LYS  |
| 66  | A2    | 138 | THR  |
| 66  | A2    | 157 | LEU  |
| 66  | A2    | 165 | GLU  |
| 66  | A2    | 170 | ILE  |
| 66  | A2    | 182 | LEU  |
| 66  | A2    | 186 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | A2    | 189 | GLU  |
| 66  | A2    | 194 | GLN  |
| 66  | A2    | 207 | GLN  |
| 66  | A2    | 255 | ARG  |
| 66  | A2    | 270 | ASN  |
| 66  | A2    | 272 | LEU  |
| 66  | A2    | 296 | VAL  |
| 66  | A2    | 298 | LEU  |
| 66  | A2    | 305 | THR  |
| 66  | A2    | 318 | ILE  |
| 66  | A2    | 345 | ILE  |
| 66  | A2    | 347 | VAL  |
| 66  | A2    | 350 | VAL  |
| 66  | A2    | 366 | VAL  |
| 66  | A2    | 374 | LEU  |
| 66  | A2    | 381 | GLU  |
| 66  | A2    | 384 | LEU  |
| 66  | A2    | 390 | VAL  |
| 66  | A2    | 399 | THR  |
| 66  | A2    | 415 | ASN  |
| 66  | A2    | 417 | VAL  |
| 66  | A2    | 420 | VAL  |
| 66  | A2    | 436 | ILE  |
| 66  | A2    | 463 | ILE  |
| 66  | A2    | 468 | VAL  |
| 67  | A3    | 61  | ARG  |
| 67  | A3    | 62  | VAL  |
| 67  | A3    | 97  | THR  |
| 67  | A3    | 104 | GLN  |
| 67  | A3    | 118 | VAL  |
| 67  | A3    | 122 | ASP  |
| 67  | A3    | 130 | ILE  |
| 67  | A3    | 134 | GLU  |
| 67  | A3    | 140 | ASP  |
| 67  | A3    | 152 | VAL  |
| 67  | A3    | 171 | ARG  |
| 67  | A3    | 178 | LEU  |
| 68  | A4    | 8   | VAL  |
| 68  | A4    | 9   | VAL  |
| 68  | A4    | 11  | ARG  |
| 68  | A4    | 19  | LEU  |
| 68  | A4    | 39  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | A4    | 42  | VAL  |
| 68  | A4    | 61  | ARG  |
| 68  | A4    | 90  | LEU  |
| 68  | A4    | 99  | VAL  |
| 68  | A4    | 110 | LEU  |
| 68  | A4    | 119 | GLU  |
| 68  | A4    | 126 | LEU  |
| 68  | A4    | 130 | ARG  |
| 68  | A4    | 142 | VAL  |
| 68  | A4    | 165 | VAL  |
| 69  | A5    | 34  | GLN  |
| 69  | A5    | 39  | VAL  |
| 69  | A5    | 49  | LEU  |
| 69  | A5    | 50  | LYS  |
| 69  | A5    | 51  | MET  |
| 69  | A5    | 73  | GLU  |
| 69  | A5    | 76  | ARG  |
| 69  | A5    | 78  | ILE  |
| 70  | A6    | 41  | ARG  |
| 70  | A6    | 70  | VAL  |
| 70  | A6    | 80  | CYS  |
| 70  | A6    | 81  | LEU  |
| 70  | A6    | 86  | LYS  |
| 70  | A6    | 87  | ILE  |
| 70  | A6    | 88  | LYS  |
| 70  | A6    | 92  | MET  |
| 71  | A8    | 44  | CYS  |
| 71  | A8    | 54  | VAL  |
| 71  | A8    | 67  | MET  |
| 71  | A8    | 76  | GLU  |
| 71  | A8    | 83  | ARG  |
| 71  | A8    | 84  | VAL  |
| 71  | A8    | 91  | LYS  |
| 71  | A8    | 92  | MET  |
| 71  | A8    | 96  | ARG  |
| 71  | A8    | 104 | LYS  |
| 71  | A8    | 113 | ILE  |
| 71  | A8    | 136 | GLN  |
| 71  | A8    | 140 | LEU  |
| 71  | A8    | 143 | THR  |
| 71  | A8    | 147 | ILE  |
| 71  | A8    | 151 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71  | A8    | 154 | ILE  |
| 71  | A8    | 155 | GLU  |
| 71  | A8    | 173 | ARG  |
| 71  | A8    | 175 | ASP  |
| 72  | A9    | 68  | LEU  |
| 72  | A9    | 82  | ASP  |
| 72  | A9    | 88  | CYS  |
| 72  | A9    | 98  | GLU  |
| 72  | A9    | 99  | MET  |
| 72  | A9    | 110 | GLN  |
| 73  | AE    | 47  | SER  |
| 73  | AE    | 70  | LYS  |
| 73  | AE    | 71  | MET  |
| 73  | AE    | 73  | LEU  |
| 73  | AE    | 83  | GLU  |
| 73  | AE    | 98  | GLU  |
| 73  | AE    | 102 | ASP  |
| 73  | AE    | 106 | ARG  |
| 73  | AE    | 107 | LEU  |
| 73  | AE    | 117 | ASP  |
| 73  | AE    | 137 | ARG  |
| 73  | AE    | 158 | PHE  |
| 73  | AE    | 175 | THR  |
| 73  | AE    | 190 | MET  |
| 73  | AE    | 192 | VAL  |
| 73  | AE    | 195 | GLU  |
| 73  | AE    | 210 | VAL  |
| 73  | AE    | 215 | VAL  |
| 73  | AE    | 221 | ILE  |
| 73  | AE    | 236 | ARG  |
| 73  | AE    | 244 | VAL  |
| 73  | AE    | 246 | ILE  |
| 73  | AE    | 340 | SER  |
| 73  | AE    | 343 | ILE  |
| 73  | AE    | 345 | THR  |
| 73  | AE    | 362 | THR  |
| 73  | AE    | 364 | ILE  |
| 73  | AE    | 370 | ASP  |
| 73  | AE    | 371 | LEU  |
| 73  | AE    | 379 | CYS  |
| 73  | AE    | 380 | GLN  |
| 74  | AF    | 20  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74  | AF    | 26  | ASP  |
| 74  | AF    | 72  | ILE  |
| 74  | AF    | 73  | SER  |
| 74  | AF    | 90  | LEU  |
| 74  | AF    | 92  | GLU  |
| 74  | AF    | 98  | THR  |
| 74  | AF    | 105 | THR  |
| 74  | AF    | 165 | GLU  |
| 74  | AF    | 167 | ARG  |
| 74  | AF    | 205 | LYS  |
| 74  | AF    | 211 | MET  |
| 74  | AF    | 235 | ARG  |
| 74  | AF    | 241 | ARG  |
| 74  | AF    | 248 | THR  |
| 74  | AF    | 259 | MET  |
| 74  | AF    | 263 | VAL  |
| 74  | AF    | 270 | VAL  |
| 74  | AF    | 280 | THR  |
| 74  | AF    | 296 | ASN  |
| 74  | AF    | 317 | THR  |
| 74  | AF    | 352 | THR  |
| 74  | AF    | 367 | LYS  |
| 74  | AF    | 368 | LEU  |
| 74  | AF    | 369 | GLN  |
| 74  | AF    | 388 | GLU  |
| 74  | AF    | 394 | VAL  |
| 74  | AF    | 409 | GLU  |
| 74  | AF    | 416 | TYR  |
| 74  | AF    | 420 | ILE  |
| 74  | AF    | 430 | ASN  |
| 74  | AF    | 443 | THR  |
| 74  | AF    | 456 | SER  |
| 75  | AI    | 20  | ILE  |
| 75  | AI    | 22  | VAL  |
| 75  | AI    | 32  | VAL  |
| 75  | AI    | 44  | ASP  |
| 75  | AI    | 45  | ARG  |
| 75  | AI    | 48  | ARG  |
| 75  | AI    | 49  | THR  |
| 75  | AI    | 61  | LYS  |
| 75  | AI    | 70  | ARG  |
| 75  | AI    | 77  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | AI    | 97  | ARG  |
| 75  | AI    | 100 | LEU  |
| 75  | AI    | 115 | VAL  |
| 75  | AI    | 130 | PHE  |
| 75  | AI    | 158 | THR  |
| 75  | AI    | 165 | LEU  |
| 75  | AI    | 169 | VAL  |
| 75  | AI    | 170 | VAL  |
| 75  | AI    | 178 | ILE  |
| 75  | AI    | 181 | THR  |
| 75  | AI    | 183 | ARG  |
| 75  | AI    | 196 | GLU  |
| 75  | AI    | 197 | GLU  |
| 75  | AI    | 200 | LYS  |
| 75  | AI    | 210 | TYR  |
| 75  | AI    | 211 | GLU  |
| 76  | AJ    | 14  | ARG  |
| 76  | AJ    | 20  | ARG  |
| 76  | AJ    | 25  | ARG  |
| 76  | AJ    | 31  | VAL  |
| 76  | AJ    | 38  | VAL  |
| 76  | AJ    | 61  | VAL  |
| 76  | AJ    | 75  | THR  |
| 76  | AJ    | 88  | ASP  |
| 76  | AJ    | 94  | LEU  |
| 76  | AJ    | 98  | THR  |
| 77  | AK    | 19  | VAL  |
| 77  | AK    | 20  | GLU  |
| 77  | AK    | 31  | VAL  |
| 77  | AK    | 33  | GLU  |
| 77  | AK    | 37  | ASP  |
| 77  | AK    | 49  | VAL  |
| 77  | AK    | 68  | VAL  |
| 77  | AK    | 71  | GLU  |
| 77  | AK    | 90  | THR  |
| 77  | AK    | 148 | LEU  |
| 77  | AK    | 150 | THR  |
| 77  | AK    | 172 | LEU  |
| 77  | AK    | 173 | LEU  |
| 77  | AK    | 174 | GLU  |
| 77  | AK    | 177 | VAL  |
| 77  | AK    | 196 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 77  | AK    | 207 | GLU  |
| 77  | AK    | 208 | GLN  |
| 77  | AK    | 209 | GLN  |
| 77  | AK    | 218 | ARG  |
| 77  | AK    | 230 | GLN  |
| 77  | AK    | 231 | ARG  |
| 77  | AK    | 232 | GLU  |
| 77  | AK    | 239 | ILE  |
| 77  | AK    | 257 | GLU  |
| 77  | AK    | 284 | GLU  |
| 77  | AK    | 286 | GLU  |
| 77  | AK    | 295 | ARG  |
| 77  | AK    | 298 | VAL  |
| 77  | AK    | 300 | ASP  |
| 77  | AK    | 301 | MET  |
| 77  | AK    | 311 | MET  |
| 77  | AK    | 314 | ARG  |
| 77  | AK    | 320 | LYS  |
| 77  | AK    | 326 | GLU  |
| 77  | AK    | 329 | MET  |
| 77  | AK    | 332 | GLU  |
| 77  | AK    | 336 | THR  |
| 78  | AN    | 26  | LEU  |
| 78  | AN    | 31  | ASP  |
| 78  | AN    | 35  | GLN  |
| 78  | AN    | 54  | LEU  |
| 78  | AN    | 70  | ARG  |
| 78  | AN    | 88  | ILE  |
| 78  | AN    | 121 | MET  |
| 78  | AN    | 127 | CYS  |
| 78  | AN    | 143 | VAL  |
| 78  | AN    | 148 | THR  |
| 79  | AP    | 29  | LYS  |
| 79  | AP    | 31  | ILE  |
| 79  | AP    | 34  | LEU  |
| 79  | AP    | 45  | ARG  |
| 79  | AP    | 46  | ASN  |
| 79  | AP    | 50  | ASP  |
| 79  | AP    | 52  | THR  |
| 79  | AP    | 55  | LYS  |
| 79  | AP    | 58  | ASP  |
| 79  | AP    | 63  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | AP    | 65  | VAL  |
| 79  | AP    | 86  | LEU  |
| 79  | AP    | 93  | SER  |
| 79  | AP    | 98  | THR  |
| 79  | AP    | 100 | THR  |
| 79  | AP    | 136 | VAL  |
| 79  | AP    | 157 | VAL  |
| 79  | AP    | 163 | ARG  |
| 79  | AP    | 173 | SER  |
| 79  | AP    | 186 | THR  |
| 79  | AP    | 189 | ILE  |
| 79  | AP    | 196 | THR  |
| 79  | AP    | 205 | VAL  |
| 79  | AP    | 217 | VAL  |
| 79  | AP    | 225 | ARG  |
| 79  | AP    | 235 | GLN  |
| 79  | AP    | 255 | VAL  |
| 79  | AP    | 257 | MET  |
| 79  | AP    | 262 | LEU  |
| 79  | AP    | 281 | GLU  |
| 79  | AP    | 283 | ARG  |
| 79  | AP    | 358 | TRP  |
| 79  | AP    | 373 | ARG  |
| 80  | AQ    | 25  | ILE  |
| 80  | AQ    | 26  | ARG  |
| 80  | AQ    | 30  | ARG  |
| 80  | AQ    | 55  | PHE  |
| 80  | AQ    | 71  | LEU  |
| 80  | AQ    | 116 | THR  |
| 80  | AQ    | 138 | GLU  |
| 81  | AR    | 55  | LEU  |
| 81  | AR    | 67  | GLN  |
| 81  | AR    | 85  | VAL  |
| 81  | AR    | 93  | LEU  |
| 81  | AR    | 94  | ARG  |
| 81  | AR    | 139 | MET  |
| 81  | AR    | 167 | ASN  |
| 81  | AR    | 186 | PHE  |
| 81  | AR    | 219 | GLU  |
| 81  | AR    | 237 | VAL  |
| 82  | AT    | 24  | LEU  |
| 82  | AT    | 29  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | AT    | 35  | MET  |
| 82  | AT    | 40  | GLU  |
| 83  | AU    | 14  | LYS  |
| 83  | AU    | 15  | LEU  |
| 83  | AU    | 20  | ILE  |
| 83  | AU    | 25  | ARG  |
| 83  | AU    | 29  | ARG  |
| 83  | AU    | 50  | ARG  |
| 83  | AU    | 68  | SER  |
| 83  | AU    | 75  | THR  |
| 83  | AU    | 90  | MET  |
| 83  | AU    | 103 | GLU  |
| 83  | AU    | 117 | ARG  |
| 83  | AU    | 132 | GLU  |
| 83  | AU    | 136 | LEU  |
| 83  | AU    | 163 | LEU  |
| 83  | AU    | 170 | VAL  |
| 83  | AU    | 173 | ARG  |
| 83  | AU    | 178 | ARG  |
| 83  | AU    | 185 | SER  |
| 83  | AU    | 189 | ASN  |
| 83  | AU    | 195 | ILE  |
| 84  | AV    | 59  | LEU  |
| 84  | AV    | 82  | ILE  |
| 84  | AV    | 86  | ASN  |
| 84  | AV    | 90  | LYS  |
| 84  | AV    | 91  | VAL  |
| 84  | AV    | 97  | ILE  |
| 84  | AV    | 106 | ILE  |
| 84  | AV    | 109 | HIS  |
| 84  | AV    | 110 | ILE  |
| 84  | AV    | 147 | ARG  |
| 84  | AV    | 151 | SER  |
| 84  | AV    | 175 | ILE  |
| 84  | AV    | 177 | GLU  |
| 84  | AV    | 196 | LEU  |
| 84  | AV    | 203 | GLN  |
| 84  | AV    | 211 | VAL  |
| 84  | AV    | 222 | ASP  |
| 84  | AV    | 226 | MET  |
| 84  | AV    | 228 | ASN  |
| 84  | AV    | 231 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | AW    | 7   | ARG  |
| 85  | AW    | 14  | LEU  |
| 85  | AW    | 35  | THR  |
| 85  | AW    | 61  | LEU  |
| 85  | AW    | 69  | LEU  |
| 85  | AW    | 75  | GLN  |
| 85  | AW    | 76  | LEU  |
| 85  | AW    | 82  | TRP  |
| 85  | AW    | 92  | THR  |
| 85  | AW    | 99  | VAL  |
| 85  | AW    | 102 | GLU  |
| 85  | AW    | 105 | MET  |
| 85  | AW    | 119 | THR  |
| 85  | AW    | 120 | GLU  |
| 85  | AW    | 128 | LEU  |
| 85  | AW    | 138 | VAL  |
| 85  | AW    | 149 | ILE  |
| 85  | AW    | 158 | ARG  |
| 85  | AW    | 167 | SER  |
| 85  | AW    | 181 | MET  |
| 85  | AW    | 197 | ARG  |
| 85  | AW    | 203 | CYS  |
| 85  | AW    | 208 | THR  |
| 85  | AW    | 212 | ILE  |
| 85  | AW    | 246 | THR  |
| 85  | AW    | 247 | CYS  |
| 85  | AW    | 251 | SER  |
| 85  | AW    | 273 | ILE  |
| 86  | AX    | 62  | HIS  |
| 86  | AX    | 63  | LYS  |
| 86  | AX    | 78  | ARG  |
| 86  | AX    | 137 | ARG  |
| 86  | AX    | 148 | LEU  |
| 86  | AX    | 155 | GLU  |
| 86  | AX    | 165 | CYS  |
| 86  | AX    | 197 | ARG  |
| 86  | AX    | 219 | ASP  |
| 87  | AY    | 1   | MET  |
| 87  | AY    | 14  | ARG  |
| 87  | AY    | 56  | LEU  |
| 87  | AY    | 58  | LEU  |
| 87  | AY    | 83  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | AY    | 90  | LYS  |
| 87  | AY    | 146 | ILE  |
| 87  | AY    | 182 | THR  |
| 87  | AY    | 186 | CYS  |
| 87  | AY    | 188 | ILE  |
| 87  | AY    | 205 | ARG  |
| 87  | AY    | 212 | ILE  |
| 87  | AY    | 214 | MET  |
| 87  | AY    | 219 | VAL  |
| 87  | AY    | 222 | GLU  |
| 87  | AY    | 224 | GLU  |
| 87  | AY    | 225 | VAL  |
| 87  | AY    | 241 | THR  |
| 87  | AY    | 247 | GLU  |
| 87  | AY    | 256 | LEU  |
| 87  | AY    | 264 | VAL  |
| 87  | AY    | 278 | ARG  |
| 87  | AY    | 283 | GLU  |
| 87  | AY    | 299 | MET  |
| 87  | AY    | 300 | LEU  |
| 87  | AY    | 302 | GLU  |
| 88  | Ab    | 70  | THR  |
| 88  | Ab    | 74  | ASP  |
| 88  | Ab    | 102 | VAL  |
| 88  | Ab    | 105 | ASN  |
| 88  | Ab    | 110 | GLU  |
| 88  | Ab    | 129 | SER  |
| 88  | Ab    | 155 | LEU  |
| 88  | Ab    | 167 | VAL  |
| 88  | Ab    | 171 | VAL  |
| 88  | Ab    | 175 | ARG  |
| 88  | Ab    | 182 | THR  |
| 88  | Ab    | 192 | VAL  |
| 88  | Ab    | 196 | THR  |
| 88  | Ab    | 203 | THR  |
| 88  | Ab    | 206 | CYS  |
| 88  | Ab    | 258 | ASP  |
| 88  | Ab    | 263 | VAL  |
| 88  | Ab    | 284 | LEU  |
| 88  | Ab    | 325 | ASP  |
| 88  | Ab    | 337 | GLU  |
| 88  | Ab    | 341 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 88  | Ab    | 355 | VAL  |
| 88  | Ab    | 365 | SER  |
| 88  | Ab    | 372 | ARG  |
| 88  | Ab    | 385 | ILE  |
| 88  | Ab    | 408 | THR  |
| 88  | Ab    | 412 | THR  |
| 88  | Ab    | 416 | ILE  |
| 88  | Ab    | 428 | LEU  |
| 88  | Ab    | 454 | VAL  |
| 88  | Ab    | 457 | ARG  |
| 88  | Ab    | 482 | MET  |
| 88  | Ab    | 491 | SER  |
| 89  | Ad    | 45  | LEU  |
| 89  | Ad    | 58  | GLN  |
| 89  | Ad    | 66  | ARG  |
| 89  | Ad    | 67  | MET  |
| 89  | Ad    | 77  | VAL  |
| 89  | Ad    | 80  | LYS  |
| 89  | Ad    | 100 | ILE  |
| 89  | Ad    | 111 | GLU  |
| 89  | Ad    | 151 | GLN  |
| 89  | Ad    | 159 | ARG  |
| 89  | Ad    | 170 | LYS  |
| 89  | Ad    | 173 | SER  |
| 89  | Ad    | 189 | CYS  |
| 89  | Ad    | 192 | GLU  |
| 89  | Ad    | 200 | ILE  |
| 89  | Ad    | 227 | ARG  |
| 89  | Ad    | 261 | LEU  |
| 90  | Ae    | 74  | SER  |
| 90  | Ae    | 75  | ARG  |
| 90  | Ae    | 80  | LEU  |
| 90  | Ae    | 87  | VAL  |
| 90  | Ae    | 89  | ARG  |
| 90  | Ae    | 98  | VAL  |
| 90  | Ae    | 104 | VAL  |
| 90  | Ae    | 106 | LEU  |
| 90  | Ae    | 123 | THR  |
| 90  | Ae    | 127 | CYS  |
| 90  | Ae    | 133 | LYS  |
| 90  | Ae    | 148 | ILE  |
| 91  | Af    | 60  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 91  | Af    | 65  | LEU  |
| 91  | Af    | 72  | ASP  |
| 91  | Af    | 73  | ASP  |
| 91  | Af    | 81  | ARG  |
| 91  | Af    | 97  | VAL  |
| 91  | Af    | 100 | THR  |
| 91  | Af    | 118 | GLU  |
| 91  | Af    | 127 | MET  |
| 91  | Af    | 128 | ASP  |
| 91  | Af    | 129 | THR  |
| 92  | Ag    | 14  | ILE  |
| 92  | Ag    | 27  | GLN  |
| 92  | Ag    | 42  | SER  |
| 92  | Ag    | 44  | SER  |
| 92  | Ag    | 50  | ARG  |
| 92  | Ag    | 55  | MET  |
| 92  | Ag    | 82  | ARG  |
| 92  | Ag    | 83  | LEU  |
| 92  | Ag    | 117 | LEU  |
| 92  | Ag    | 122 | THR  |
| 92  | Ag    | 127 | THR  |
| 92  | Ag    | 134 | ARG  |
| 92  | Ag    | 158 | GLU  |
| 92  | Ag    | 168 | CYS  |
| 92  | Ag    | 189 | MET  |
| 92  | Ag    | 214 | VAL  |
| 92  | Ag    | 224 | VAL  |
| 92  | Ag    | 235 | VAL  |
| 93  | Aj    | 27  | VAL  |
| 93  | Aj    | 53  | ARG  |
| 93  | Aj    | 68  | MET  |
| 93  | Aj    | 80  | SER  |
| 93  | Aj    | 95  | ARG  |
| 93  | Aj    | 137 | VAL  |
| 93  | Aj    | 168 | ARG  |
| 93  | Aj    | 180 | ASP  |
| 93  | Aj    | 188 | VAL  |
| 93  | Aj    | 215 | LEU  |
| 93  | Aj    | 217 | CYS  |
| 93  | Aj    | 276 | PHE  |
| 94  | Al    | 15  | THR  |
| 94  | Al    | 23  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 94  | Al    | 25  | VAL  |
| 94  | Al    | 45  | ILE  |
| 94  | Al    | 81  | GLU  |
| 94  | Al    | 85  | LEU  |
| 94  | Al    | 87  | LEU  |
| 94  | Al    | 88  | ARG  |
| 94  | Al    | 146 | LEU  |
| 94  | Al    | 170 | GLU  |
| 94  | Al    | 177 | GLU  |
| 94  | Al    | 191 | VAL  |
| 94  | Al    | 201 | VAL  |
| 94  | Al    | 206 | ARG  |
| 94  | Al    | 208 | VAL  |
| 95  | Ao    | 25  | ASN  |
| 95  | Ao    | 54  | GLN  |
| 95  | Ao    | 57  | MET  |
| 95  | Ao    | 61  | ARG  |
| 95  | Ao    | 73  | CYS  |
| 95  | Ao    | 87  | GLU  |
| 95  | Ao    | 113 | GLN  |
| 95  | Ao    | 125 | ASP  |
| 95  | Ao    | 136 | THR  |
| 95  | Ao    | 141 | ASN  |
| 95  | Ao    | 150 | LEU  |
| 95  | Ao    | 158 | ARG  |
| 95  | Ao    | 221 | ASP  |
| 95  | Ao    | 223 | VAL  |
| 95  | Ao    | 224 | LYS  |
| 95  | Ao    | 243 | LYS  |
| 95  | Ao    | 244 | PHE  |
| 95  | Ao    | 245 | LEU  |
| 95  | Ao    | 246 | VAL  |
| 96  | Ap    | 38  | LEU  |
| 96  | Ap    | 52  | ARG  |
| 96  | Ap    | 56  | ASN  |
| 96  | Ap    | 74  | ARG  |
| 96  | Ap    | 79  | GLN  |
| 96  | Ap    | 108 | LEU  |
| 96  | Ap    | 118 | VAL  |
| 96  | Ap    | 127 | LEU  |
| 96  | Ap    | 145 | VAL  |
| 96  | Ap    | 151 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 96  | Ap    | 154 | HIS  |
| 96  | Ap    | 155 | ILE  |
| 96  | Ap    | 173 | LEU  |
| 96  | Ap    | 186 | SER  |
| 96  | Ap    | 196 | ILE  |
| 96  | Ap    | 234 | VAL  |
| 96  | Ap    | 243 | VAL  |
| 96  | Ap    | 246 | VAL  |
| 96  | Ap    | 253 | GLN  |
| 96  | Ap    | 278 | ASN  |
| 96  | Ap    | 280 | LEU  |
| 96  | Ap    | 284 | ASP  |
| 96  | Ap    | 285 | TYR  |
| 96  | Ap    | 294 | LYS  |
| 97  | At    | 24  | VAL  |
| 97  | At    | 25  | ARG  |
| 97  | At    | 43  | ILE  |
| 97  | At    | 44  | LEU  |
| 97  | At    | 50  | THR  |
| 97  | At    | 78  | SER  |
| 97  | At    | 84  | LEU  |
| 97  | At    | 94  | THR  |
| 97  | At    | 105 | LEU  |
| 97  | At    | 119 | SER  |
| 97  | At    | 124 | SER  |
| 97  | At    | 136 | ARG  |
| 97  | At    | 143 | THR  |
| 97  | At    | 144 | VAL  |
| 97  | At    | 153 | LEU  |
| 98  | Av    | 45  | LEU  |
| 98  | Av    | 47  | ARG  |
| 98  | Av    | 52  | GLU  |
| 98  | Av    | 71  | VAL  |
| 98  | Av    | 103 | ARG  |
| 98  | Av    | 107 | GLN  |
| 98  | Av    | 146 | THR  |
| 98  | Av    | 166 | TYR  |
| 98  | Av    | 167 | ARG  |
| 98  | Av    | 181 | THR  |
| 98  | Av    | 182 | LYS  |
| 98  | Av    | 185 | LYS  |
| 98  | Av    | 200 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 98  | Av    | 233 | THR  |
| 103 | BA    | 129 | PHE  |
| 103 | BA    | 133 | THR  |
| 103 | BA    | 142 | GLU  |
| 103 | BA    | 143 | MET  |
| 103 | BA    | 151 | ASP  |
| 103 | BA    | 160 | CYS  |
| 103 | BA    | 190 | THR  |
| 103 | BA    | 194 | ARG  |
| 103 | BA    | 200 | LEU  |
| 103 | BA    | 206 | ILE  |
| 103 | BA    | 212 | VAL  |
| 103 | BA    | 217 | LEU  |
| 103 | BA    | 221 | THR  |
| 103 | BA    | 236 | SER  |
| 103 | BA    | 254 | ARG  |
| 103 | BA    | 266 | LEU  |
| 103 | BA    | 305 | VAL  |
| 103 | BA    | 307 | HIS  |
| 103 | BA    | 318 | LEU  |
| 103 | BA    | 327 | ARG  |
| 103 | BA    | 328 | VAL  |
| 103 | BA    | 336 | THR  |
| 103 | BA    | 339 | ASP  |
| 103 | BA    | 340 | LEU  |
| 103 | BA    | 349 | LEU  |
| 103 | BA    | 359 | CYS  |
| 103 | BA    | 368 | LYS  |
| 103 | BA    | 396 | ARG  |
| 103 | BA    | 401 | THR  |
| 103 | BA    | 419 | THR  |
| 103 | BA    | 466 | LEU  |
| 103 | BA    | 495 | ARG  |
| 103 | BA    | 510 | LEU  |
| 103 | BA    | 519 | SER  |
| 103 | BA    | 542 | ASN  |
| 103 | BA    | 567 | THR  |
| 103 | BA    | 569 | LEU  |
| 103 | BA    | 573 | GLU  |
| 103 | BA    | 588 | LEU  |
| 103 | BA    | 593 | THR  |
| 103 | BA    | 625 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 103 | BA    | 631 | LYS  |
| 103 | BA    | 638 | ARG  |
| 103 | BA    | 655 | LEU  |
| 103 | BA    | 660 | GLU  |
| 103 | BA    | 663 | LEU  |
| 103 | BA    | 664 | HIS  |
| 103 | BA    | 665 | ASP  |
| 103 | BA    | 672 | GLU  |
| 103 | BA    | 714 | ASN  |
| 103 | BA    | 720 | ARG  |
| 103 | BA    | 733 | LEU  |
| 103 | BA    | 747 | LEU  |
| 103 | BA    | 753 | ASP  |
| 103 | BA    | 757 | THR  |
| 103 | BA    | 767 | ARG  |
| 103 | BA    | 779 | LYS  |
| 103 | BA    | 782 | VAL  |
| 103 | BA    | 793 | ARG  |
| 103 | BA    | 799 | ASP  |
| 103 | BA    | 809 | ASP  |
| 103 | BA    | 820 | THR  |
| 104 | BB    | 66  | GLU  |
| 104 | BB    | 75  | MET  |
| 104 | BB    | 91  | LEU  |
| 104 | BB    | 94  | THR  |
| 104 | BB    | 100 | GLU  |
| 104 | BB    | 105 | LEU  |
| 104 | BB    | 106 | LEU  |
| 104 | BB    | 111 | ILE  |
| 104 | BB    | 132 | GLU  |
| 104 | BB    | 138 | CYS  |
| 104 | BB    | 148 | LYS  |
| 104 | BB    | 169 | SER  |
| 104 | BB    | 180 | GLU  |
| 104 | BB    | 188 | LEU  |
| 104 | BB    | 206 | ASP  |
| 104 | BB    | 213 | LEU  |
| 104 | BB    | 230 | THR  |
| 104 | BB    | 234 | ILE  |
| 104 | BB    | 240 | HIS  |
| 104 | BB    | 243 | ILE  |
| 104 | BB    | 244 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 104 | BB    | 251 | ILE  |
| 104 | BB    | 255 | LEU  |
| 104 | BB    | 259 | GLU  |
| 104 | BB    | 261 | VAL  |
| 104 | BB    | 281 | SER  |
| 104 | BB    | 307 | SER  |
| 104 | BB    | 344 | CYS  |
| 104 | BB    | 356 | ASN  |
| 104 | BB    | 357 | THR  |
| 104 | BB    | 364 | VAL  |
| 104 | BB    | 390 | LEU  |
| 104 | BB    | 395 | GLU  |
| 104 | BB    | 413 | LEU  |
| 104 | BB    | 422 | MET  |
| 105 | BC    | 49  | SER  |
| 105 | BC    | 71  | GLN  |
| 105 | BC    | 75  | MET  |
| 105 | BC    | 81  | LEU  |
| 105 | BC    | 109 | THR  |
| 105 | BC    | 115 | GLN  |
| 105 | BC    | 120 | ILE  |
| 105 | BC    | 125 | CYS  |
| 105 | BC    | 126 | GLU  |
| 105 | BC    | 155 | ARG  |
| 105 | BC    | 188 | HIS  |
| 105 | BC    | 191 | ASP  |
| 105 | BC    | 203 | SER  |
| 105 | BC    | 207 | GLN  |
| 105 | BC    | 210 | GLN  |
| 105 | BC    | 212 | VAL  |
| 105 | BC    | 216 | GLU  |
| 105 | BC    | 220 | LEU  |
| 105 | BC    | 235 | VAL  |
| 105 | BC    | 240 | LYS  |
| 105 | BC    | 243 | VAL  |
| 105 | BC    | 252 | GLN  |
| 105 | BC    | 255 | ARG  |
| 105 | BC    | 267 | ILE  |
| 105 | BC    | 268 | LEU  |
| 105 | BC    | 278 | GLU  |
| 105 | BC    | 283 | ILE  |
| 105 | BC    | 288 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 105 | BC    | 296 | LEU  |
| 105 | BC    | 303 | LEU  |
| 105 | BC    | 306 | GLU  |
| 105 | BC    | 309 | PHE  |
| 105 | BC    | 336 | LEU  |
| 105 | BC    | 339 | ILE  |
| 105 | BC    | 343 | MET  |
| 105 | BC    | 356 | LEU  |
| 105 | BC    | 362 | VAL  |
| 105 | BC    | 392 | VAL  |
| 105 | BC    | 394 | LEU  |
| 105 | BC    | 410 | LYS  |
| 105 | BC    | 427 | LEU  |
| 105 | BC    | 461 | ASP  |
| 105 | BC    | 465 | LEU  |
| 105 | BC    | 470 | ARG  |
| 105 | BC    | 475 | LEU  |
| 105 | BC    | 490 | LEU  |
| 105 | BC    | 512 | ARG  |
| 105 | BC    | 522 | LEU  |
| 105 | BC    | 523 | TYR  |
| 107 | BE    | 32  | LEU  |
| 107 | BE    | 34  | LEU  |
| 107 | BE    | 37  | PHE  |
| 107 | BE    | 61  | MET  |
| 107 | BE    | 63  | VAL  |
| 107 | BE    | 66  | ARG  |
| 107 | BE    | 71  | LEU  |
| 107 | BE    | 81  | VAL  |
| 107 | BE    | 137 | LYS  |
| 107 | BE    | 142 | LEU  |
| 107 | BE    | 144 | VAL  |
| 107 | BE    | 152 | ARG  |
| 107 | BE    | 153 | SER  |
| 107 | BE    | 154 | VAL  |
| 107 | BE    | 186 | LEU  |
| 107 | BE    | 239 | ILE  |
| 107 | BE    | 244 | THR  |
| 107 | BE    | 245 | ILE  |
| 107 | BE    | 250 | ILE  |
| 107 | BE    | 257 | ASP  |
| 107 | BE    | 266 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 107 | BE    | 271 | ASP  |
| 107 | BE    | 301 | GLU  |
| 107 | BE    | 348 | VAL  |
| 107 | BE    | 354 | GLU  |
| 107 | BE    | 359 | LYS  |
| 107 | BE    | 380 | GLU  |
| 107 | BE    | 395 | SER  |
| 107 | BE    | 419 | MET  |
| 107 | BE    | 422 | ARG  |
| 107 | BE    | 442 | THR  |
| 108 | BF    | 31  | THR  |
| 108 | BF    | 50  | LEU  |
| 108 | BF    | 60  | LEU  |
| 108 | BF    | 131 | LEU  |
| 108 | BF    | 166 | GLN  |
| 108 | BF    | 167 | ARG  |
| 108 | BF    | 168 | ILE  |
| 108 | BF    | 170 | ILE  |
| 108 | BF    | 181 | THR  |
| 108 | BF    | 192 | GLU  |
| 108 | BF    | 199 | ASP  |
| 108 | BF    | 208 | LEU  |
| 108 | BF    | 216 | LEU  |
| 108 | BF    | 221 | GLU  |
| 108 | BF    | 225 | MET  |
| 108 | BF    | 230 | THR  |
| 108 | BF    | 237 | LEU  |
| 108 | BF    | 264 | ASN  |
| 108 | BF    | 289 | CYS  |
| 108 | BF    | 309 | VAL  |
| 108 | BF    | 345 | LEU  |
| 108 | BF    | 354 | LEU  |
| 108 | BF    | 355 | LEU  |
| 108 | BF    | 360 | THR  |
| 108 | BF    | 386 | VAL  |
| 108 | BF    | 398 | ARG  |
| 108 | BF    | 419 | VAL  |
| 108 | BF    | 420 | ARG  |
| 109 | BG    | 40  | THR  |
| 109 | BG    | 57  | ARG  |
| 109 | BG    | 65  | MET  |
| 109 | BG    | 74  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 109 | BG    | 78  | ILE  |
| 109 | BG    | 102 | GLN  |
| 109 | BG    | 103 | LEU  |
| 109 | BG    | 106 | ASP  |
| 109 | BG    | 124 | ASP  |
| 109 | BG    | 125 | LEU  |
| 109 | BG    | 148 | LEU  |
| 109 | BG    | 149 | THR  |
| 109 | BG    | 158 | VAL  |
| 109 | BG    | 164 | GLN  |
| 109 | BG    | 177 | ASP  |
| 109 | BG    | 178 | THR  |
| 109 | BG    | 183 | ARG  |
| 109 | BG    | 186 | LEU  |
| 109 | BG    | 195 | ILE  |
| 109 | BG    | 216 | LEU  |
| 109 | BG    | 265 | LEU  |
| 109 | BG    | 295 | ARG  |
| 109 | BG    | 339 | GLU  |
| 109 | BG    | 350 | LEU  |
| 110 | BH    | 74  | ARG  |
| 110 | BH    | 87  | LEU  |
| 110 | BH    | 93  | LEU  |
| 110 | BH    | 113 | LEU  |
| 110 | BH    | 119 | VAL  |
| 110 | BH    | 135 | ARG  |
| 110 | BH    | 146 | GLU  |
| 110 | BH    | 149 | ARG  |
| 110 | BH    | 156 | LEU  |
| 110 | BH    | 168 | THR  |
| 110 | BH    | 171 | GLU  |
| 110 | BH    | 173 | LEU  |
| 110 | BH    | 178 | GLU  |
| 110 | BH    | 187 | LEU  |
| 110 | BH    | 236 | ARG  |
| 110 | BH    | 239 | ASN  |
| 110 | BH    | 250 | VAL  |
| 110 | BH    | 255 | PHE  |
| 110 | BH    | 257 | ASP  |
| 110 | BH    | 258 | THR  |
| 110 | BH    | 267 | VAL  |
| 111 | BI    | 60  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 111 | BI    | 71  | LYS  |
| 111 | BI    | 84  | LEU  |
| 111 | BI    | 103 | THR  |
| 111 | BI    | 139 | ARG  |
| 111 | BI    | 140 | PHE  |
| 111 | BI    | 151 | MET  |
| 111 | BI    | 159 | ASP  |
| 111 | BI    | 160 | PHE  |
| 111 | BI    | 166 | LEU  |
| 111 | BI    | 173 | LEU  |
| 111 | BI    | 219 | ASP  |
| 111 | BI    | 239 | VAL  |
| 111 | BI    | 247 | GLU  |
| 111 | BI    | 250 | SER  |
| 111 | BI    | 252 | MET  |
| 111 | BI    | 254 | ARG  |
| 111 | BI    | 270 | ILE  |
| 111 | BI    | 293 | THR  |
| 111 | BI    | 294 | VAL  |
| 111 | BI    | 338 | CYS  |
| 111 | BI    | 342 | TYR  |
| 112 | BJ    | 182 | VAL  |
| 112 | BJ    | 203 | LEU  |
| 112 | BJ    | 223 | THR  |
| 112 | BJ    | 234 | THR  |
| 112 | BJ    | 250 | LEU  |
| 112 | BJ    | 270 | ARG  |
| 112 | BJ    | 292 | ARG  |
| 112 | BJ    | 300 | GLU  |
| 112 | BJ    | 301 | ASP  |
| 112 | BJ    | 307 | ARG  |
| 112 | BJ    | 309 | LYS  |
| 113 | BK    | 98  | THR  |
| 113 | BK    | 140 | LEU  |
| 113 | BK    | 193 | VAL  |
| 113 | BK    | 285 | GLN  |
| 113 | BK    | 300 | TRP  |
| 113 | BK    | 302 | VAL  |
| 113 | BK    | 328 | LEU  |
| 113 | BK    | 349 | VAL  |
| 114 | BL    | 41  | LEU  |
| 114 | BL    | 48  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 114 | BL    | 59  | ASN  |
| 114 | BL    | 61  | VAL  |
| 114 | BL    | 62  | ARG  |
| 114 | BL    | 78  | ARG  |
| 114 | BL    | 85  | ARG  |
| 114 | BL    | 100 | ASP  |
| 114 | BL    | 102 | CYS  |
| 114 | BL    | 108 | ILE  |
| 114 | BL    | 123 | LEU  |
| 114 | BL    | 125 | GLU  |
| 114 | BL    | 141 | ASN  |
| 114 | BL    | 161 | VAL  |
| 114 | BL    | 165 | LEU  |
| 114 | BL    | 172 | ILE  |
| 114 | BL    | 180 | LEU  |
| 114 | BL    | 237 | ASN  |
| 114 | BL    | 242 | THR  |
| 114 | BL    | 246 | VAL  |
| 114 | BL    | 256 | ARG  |
| 114 | BL    | 291 | LEU  |
| 114 | BL    | 294 | CYS  |
| 114 | BL    | 304 | VAL  |
| 115 | BM    | 67  | LEU  |
| 115 | BM    | 68  | ARG  |
| 115 | BM    | 94  | CYS  |
| 115 | BM    | 99  | SER  |
| 115 | BM    | 102 | VAL  |
| 115 | BM    | 106 | ASN  |
| 115 | BM    | 113 | ASN  |
| 115 | BM    | 117 | GLU  |
| 115 | BM    | 133 | MET  |
| 115 | BM    | 151 | GLU  |
| 115 | BM    | 160 | ARG  |
| 115 | BM    | 163 | LEU  |
| 115 | BM    | 178 | GLU  |
| 115 | BM    | 184 | MET  |
| 115 | BM    | 224 | THR  |
| 115 | BM    | 236 | ARG  |
| 115 | BM    | 241 | MET  |
| 115 | BM    | 249 | SER  |
| 116 | BN    | 13  | VAL  |
| 116 | BN    | 36  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 116 | BN    | 48  | THR  |
| 116 | BN    | 55  | VAL  |
| 116 | BN    | 60  | ARG  |
| 116 | BN    | 70  | HIS  |
| 116 | BN    | 71  | GLN  |
| 116 | BN    | 90  | LEU  |
| 116 | BN    | 180 | GLU  |
| 116 | BN    | 182 | GLU  |
| 116 | BN    | 219 | ARG  |
| 117 | BO    | 79  | VAL  |
| 117 | BO    | 84  | VAL  |
| 117 | BO    | 97  | LYS  |
| 117 | BO    | 100 | ILE  |
| 117 | BO    | 124 | ARG  |
| 117 | BO    | 135 | LEU  |
| 117 | BO    | 139 | LEU  |
| 117 | BO    | 142 | GLU  |
| 117 | BO    | 144 | GLN  |
| 117 | BO    | 227 | ILE  |
| 117 | BO    | 232 | GLU  |
| 118 | BP    | 39  | LEU  |
| 118 | BP    | 72  | GLN  |
| 118 | BP    | 91  | GLU  |
| 118 | BP    | 93  | LYS  |
| 118 | BP    | 107 | VAL  |
| 118 | BP    | 121 | ARG  |
| 118 | BP    | 152 | ASN  |
| 118 | BP    | 176 | THR  |
| 118 | BP    | 186 | VAL  |
| 118 | BP    | 211 | MET  |
| 118 | BP    | 214 | ASN  |
| 118 | BP    | 222 | SER  |
| 118 | BP    | 234 | GLU  |
| 119 | BQ    | 16  | LEU  |
| 119 | BQ    | 23  | GLU  |
| 119 | BQ    | 38  | GLU  |
| 119 | BQ    | 53  | ILE  |
| 119 | BQ    | 97  | ILE  |
| 119 | BQ    | 98  | LEU  |
| 119 | BQ    | 99  | LEU  |
| 119 | BQ    | 100 | LYS  |
| 119 | BQ    | 101 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 119 | BQ    | 115 | ASP  |
| 119 | BQ    | 116 | GLU  |
| 119 | BQ    | 152 | ASP  |
| 119 | BQ    | 163 | GLN  |
| 119 | BQ    | 182 | CYS  |
| 119 | BQ    | 193 | GLU  |
| 119 | BQ    | 202 | LEU  |
| 119 | BQ    | 212 | GLU  |
| 119 | BQ    | 215 | LEU  |
| 119 | BQ    | 222 | GLU  |
| 119 | BQ    | 227 | LEU  |
| 120 | BR    | 11  | MET  |
| 120 | BR    | 19  | TYR  |
| 120 | BR    | 22  | VAL  |
| 120 | BR    | 38  | GLU  |
| 120 | BR    | 41  | LEU  |
| 120 | BR    | 48  | ARG  |
| 120 | BR    | 58  | THR  |
| 120 | BR    | 70  | TYR  |
| 120 | BR    | 73  | ASP  |
| 120 | BR    | 81  | ILE  |
| 120 | BR    | 82  | GLU  |
| 120 | BR    | 88  | LEU  |
| 120 | BR    | 89  | ASP  |
| 120 | BR    | 96  | GLN  |
| 120 | BR    | 105 | ASN  |
| 120 | BR    | 110 | LEU  |
| 120 | BR    | 111 | PHE  |
| 120 | BR    | 114 | GLN  |
| 120 | BR    | 121 | LEU  |
| 120 | BR    | 127 | ARG  |
| 120 | BR    | 143 | ILE  |
| 120 | BR    | 159 | ILE  |
| 120 | BR    | 160 | GLN  |
| 120 | BR    | 179 | ILE  |
| 120 | BR    | 189 | VAL  |
| 120 | BR    | 193 | ILE  |
| 121 | BS    | 26  | ARG  |
| 121 | BS    | 29  | ASN  |
| 121 | BS    | 30  | GLU  |
| 121 | BS    | 37  | VAL  |
| 121 | BS    | 40  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 121 | BS    | 57  | CYS  |
| 121 | BS    | 87  | LEU  |
| 121 | BS    | 99  | VAL  |
| 121 | BS    | 106 | ILE  |
| 121 | BS    | 107 | ILE  |
| 122 | BT    | 13  | MET  |
| 122 | BT    | 17  | LYS  |
| 122 | BT    | 31  | LYS  |
| 122 | BT    | 33  | ASN  |
| 122 | BT    | 46  | GLN  |
| 122 | BT    | 72  | LEU  |
| 122 | BT    | 100 | THR  |
| 122 | BT    | 105 | VAL  |
| 122 | BT    | 118 | LYS  |
| 122 | BT    | 163 | VAL  |
| 122 | BT    | 171 | THR  |
| 122 | BT    | 174 | ILE  |
| 123 | BU    | 108 | LEU  |
| 123 | BU    | 114 | THR  |
| 123 | BU    | 117 | ILE  |
| 123 | BU    | 120 | GLU  |
| 123 | BU    | 129 | THR  |
| 123 | BU    | 131 | LYS  |
| 123 | BU    | 137 | ARG  |
| 123 | BU    | 140 | ILE  |
| 123 | BU    | 145 | THR  |
| 123 | BU    | 147 | GLU  |
| 124 | BV    | 20  | THR  |
| 124 | BV    | 43  | ARG  |
| 124 | BV    | 60  | MET  |
| 124 | BV    | 61  | GLU  |
| 124 | BV    | 65  | LEU  |
| 124 | BV    | 144 | VAL  |
| 124 | BV    | 154 | ARG  |
| 124 | BV    | 167 | GLN  |
| 125 | BW    | 11  | ARG  |
| 125 | BW    | 12  | SER  |
| 125 | BW    | 17  | THR  |
| 125 | BW    | 49  | VAL  |
| 125 | BW    | 50  | ARG  |
| 125 | BW    | 53  | ILE  |
| 125 | BW    | 65  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 125 | BW    | 75  | ARG  |
| 125 | BW    | 81  | ARG  |
| 125 | BW    | 84  | MET  |
| 125 | BW    | 128 | THR  |
| 125 | BW    | 149 | ASN  |
| 125 | BW    | 156 | VAL  |
| 125 | BW    | 159 | VAL  |
| 125 | BW    | 169 | ARG  |
| 125 | BW    | 174 | ILE  |
| 126 | BX    | 64  | ASN  |
| 126 | BX    | 67  | VAL  |
| 126 | BX    | 68  | ASP  |
| 126 | BX    | 71  | MET  |
| 126 | BX    | 91  | VAL  |
| 126 | BX    | 112 | PHE  |
| 126 | BX    | 120 | ASN  |
| 126 | BX    | 145 | LEU  |
| 126 | BX    | 155 | ARG  |
| 126 | BX    | 170 | LEU  |
| 126 | BX    | 173 | HIS  |
| 127 | BY    | 80  | GLN  |
| 127 | BY    | 87  | GLU  |
| 127 | BY    | 89  | MET  |
| 127 | BY    | 94  | GLU  |
| 127 | BY    | 95  | ILE  |
| 127 | BY    | 116 | LEU  |
| 127 | BY    | 123 | MET  |
| 127 | BY    | 141 | GLU  |
| 128 | BZ    | 5   | GLU  |
| 128 | BZ    | 21  | ILE  |
| 128 | BZ    | 97  | LEU  |
| 128 | BZ    | 139 | THR  |
| 128 | BZ    | 146 | LEU  |
| 128 | BZ    | 151 | ILE  |
| 128 | BZ    | 162 | VAL  |
| 128 | BZ    | 188 | VAL  |
| 129 | Ba    | 15  | PHE  |
| 129 | Ba    | 23  | SER  |
| 129 | Ba    | 25  | GLN  |
| 129 | Ba    | 26  | LEU  |
| 129 | Ba    | 32  | LYS  |
| 129 | Ba    | 35  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 129 | Ba    | 36  | HIS  |
| 129 | Ba    | 37  | ARG  |
| 129 | Ba    | 72  | ASP  |
| 129 | Ba    | 73  | GLU  |
| 129 | Ba    | 82  | MET  |
| 129 | Ba    | 101 | LEU  |
| 129 | Ba    | 104 | ARG  |
| 129 | Ba    | 113 | VAL  |
| 129 | Ba    | 116 | ARG  |
| 129 | Ba    | 141 | TYR  |
| 129 | Ba    | 147 | ASN  |
| 130 | Bb    | 47  | ARG  |
| 130 | Bb    | 50  | LEU  |
| 130 | Bb    | 53  | ARG  |
| 130 | Bb    | 62  | ARG  |
| 130 | Bb    | 66  | GLU  |
| 130 | Bb    | 76  | VAL  |
| 130 | Bb    | 78  | LEU  |
| 130 | Bb    | 82  | ASP  |
| 130 | Bb    | 83  | LEU  |
| 130 | Bb    | 85  | SER  |
| 130 | Bb    | 92  | LEU  |
| 130 | Bb    | 97  | SER  |
| 130 | Bb    | 110 | ARG  |
| 130 | Bb    | 134 | LEU  |
| 130 | Bb    | 140 | VAL  |
| 131 | Bc    | 11  | SER  |
| 131 | Bc    | 14  | GLU  |
| 131 | Bc    | 32  | ARG  |
| 131 | Bc    | 49  | VAL  |
| 131 | Bc    | 54  | ASN  |
| 131 | Bc    | 82  | GLU  |
| 131 | Bc    | 93  | TRP  |
| 132 | Bd    | 7   | ARG  |
| 132 | Bd    | 9   | LEU  |
| 132 | Bd    | 30  | GLN  |
| 132 | Bd    | 32  | THR  |
| 132 | Bd    | 42  | ARG  |
| 132 | Bd    | 54  | MET  |
| 132 | Bd    | 58  | LEU  |
| 132 | Bd    | 69  | LEU  |
| 132 | Bd    | 75  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 132 | Bd    | 83  | SER  |
| 132 | Bd    | 93  | THR  |
| 132 | Bd    | 102 | LEU  |
| 132 | Bd    | 124 | GLU  |
| 132 | Bd    | 126 | ILE  |
| 132 | Bd    | 135 | PHE  |
| 132 | Bd    | 136 | GLU  |
| 132 | Bd    | 140 | LEU  |
| 133 | Be    | 11  | ILE  |
| 133 | Be    | 34  | LEU  |
| 133 | Be    | 49  | ARG  |
| 133 | Be    | 54  | LEU  |
| 133 | Be    | 71  | SER  |
| 133 | Be    | 77  | ASP  |
| 133 | Be    | 79  | GLN  |
| 133 | Be    | 94  | THR  |
| 134 | Bf    | 79  | GLU  |
| 134 | Bf    | 93  | HIS  |
| 134 | Bf    | 98  | TYR  |
| 134 | Bf    | 99  | ILE  |
| 134 | Bf    | 105 | VAL  |
| 135 | Bg    | 35  | LEU  |
| 135 | Bg    | 37  | LEU  |
| 135 | Bg    | 50  | ASN  |
| 135 | Bg    | 64  | LYS  |
| 135 | Bg    | 102 | LEU  |
| 135 | Bg    | 104 | THR  |
| 136 | Bh    | 17  | VAL  |
| 136 | Bh    | 37  | GLN  |
| 136 | Bh    | 44  | MET  |
| 136 | Bh    | 46  | VAL  |
| 136 | Bh    | 53  | MET  |
| 136 | Bh    | 56  | LYS  |
| 136 | Bh    | 83  | LEU  |
| 136 | Bh    | 87  | CYS  |
| 136 | Bh    | 88  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (799) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DA    | 49  | HIS  |
| 1   | DA    | 59  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 91   | ASN  |
| 1   | DA    | 112  | GLN  |
| 1   | DA    | 123  | HIS  |
| 1   | DA    | 134  | ASN  |
| 1   | DA    | 237  | HIS  |
| 1   | DA    | 287  | HIS  |
| 1   | DA    | 402  | GLN  |
| 1   | DA    | 414  | HIS  |
| 1   | DA    | 436  | ASN  |
| 1   | DA    | 457  | GLN  |
| 1   | DA    | 565  | ASN  |
| 1   | DA    | 623  | HIS  |
| 1   | DA    | 626  | GLN  |
| 1   | DA    | 644  | HIS  |
| 1   | DA    | 746  | GLN  |
| 1   | DA    | 907  | GLN  |
| 1   | DA    | 910  | HIS  |
| 1   | DA    | 940  | GLN  |
| 1   | DA    | 979  | GLN  |
| 1   | DA    | 984  | GLN  |
| 1   | DA    | 993  | GLN  |
| 1   | DA    | 1038 | HIS  |
| 1   | DA    | 1046 | HIS  |
| 1   | DA    | 1048 | ASN  |
| 1   | DA    | 1117 | ASN  |
| 1   | DA    | 1175 | HIS  |
| 1   | DA    | 1179 | GLN  |
| 1   | DA    | 1225 | HIS  |
| 1   | DA    | 1258 | ASN  |
| 1   | DA    | 1376 | HIS  |
| 1   | DA    | 1399 | ASN  |
| 1   | DA    | 1488 | GLN  |
| 1   | DA    | 1513 | GLN  |
| 1   | DA    | 1550 | GLN  |
| 1   | DA    | 1570 | ASN  |
| 1   | DA    | 1614 | GLN  |
| 1   | DA    | 1619 | HIS  |
| 1   | DA    | 1629 | GLN  |
| 2   | DD    | 64   | HIS  |
| 2   | DD    | 76   | ASN  |
| 2   | DD    | 82   | ASN  |
| 2   | DD    | 137  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | DD    | 156 | GLN  |
| 2   | DD    | 176 | HIS  |
| 2   | DD    | 300 | GLN  |
| 2   | DD    | 312 | GLN  |
| 2   | DD    | 313 | HIS  |
| 2   | DD    | 348 | HIS  |
| 2   | DD    | 353 | HIS  |
| 2   | DD    | 379 | GLN  |
| 2   | DD    | 387 | GLN  |
| 2   | DD    | 404 | HIS  |
| 2   | DD    | 408 | HIS  |
| 2   | DD    | 453 | ASN  |
| 2   | DD    | 499 | ASN  |
| 2   | DD    | 507 | GLN  |
| 2   | DD    | 521 | ASN  |
| 2   | DD    | 542 | HIS  |
| 2   | DD    | 649 | GLN  |
| 2   | DD    | 679 | ASN  |
| 2   | DD    | 687 | HIS  |
| 3   | DI    | 30  | GLN  |
| 3   | DI    | 61  | ASN  |
| 3   | DI    | 140 | ASN  |
| 3   | DI    | 320 | GLN  |
| 3   | DI    | 370 | GLN  |
| 4   | DL    | 125 | HIS  |
| 5   | DM    | 27  | GLN  |
| 5   | DM    | 43  | GLN  |
| 5   | DM    | 76  | ASN  |
| 5   | DM    | 89  | GLN  |
| 5   | DM    | 112 | ASN  |
| 5   | DM    | 131 | ASN  |
| 5   | DM    | 159 | HIS  |
| 5   | DM    | 188 | ASN  |
| 5   | DM    | 193 | GLN  |
| 6   | DN    | 28  | HIS  |
| 6   | DN    | 74  | HIS  |
| 6   | DN    | 79  | ASN  |
| 6   | DN    | 179 | ASN  |
| 6   | DN    | 223 | GLN  |
| 6   | DN    | 234 | HIS  |
| 6   | DN    | 235 | ASN  |
| 6   | DN    | 238 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | DN    | 246 | GLN  |
| 6   | DN    | 266 | ASN  |
| 6   | DN    | 272 | HIS  |
| 7   | DO    | 181 | HIS  |
| 8   | DP    | 28  | ASN  |
| 8   | DP    | 66  | ASN  |
| 8   | DP    | 98  | HIS  |
| 8   | DP    | 116 | HIS  |
| 8   | DP    | 186 | HIS  |
| 8   | DP    | 194 | GLN  |
| 8   | DP    | 204 | ASN  |
| 9   | DQ    | 27  | HIS  |
| 9   | DQ    | 41  | GLN  |
| 9   | DQ    | 73  | HIS  |
| 9   | DQ    | 95  | HIS  |
| 9   | DQ    | 219 | GLN  |
| 9   | DQ    | 235 | HIS  |
| 10  | DR    | 26  | ASN  |
| 10  | DR    | 62  | HIS  |
| 10  | DR    | 108 | GLN  |
| 10  | DR    | 145 | HIS  |
| 10  | DR    | 191 | GLN  |
| 11  | DS    | 47  | ASN  |
| 11  | DS    | 134 | GLN  |
| 11  | DS    | 150 | GLN  |
| 11  | DS    | 197 | GLN  |
| 11  | DS    | 201 | HIS  |
| 12  | DU    | 63  | HIS  |
| 12  | DU    | 96  | GLN  |
| 12  | DU    | 133 | HIS  |
| 12  | DU    | 199 | GLN  |
| 14  | Da    | 41  | ASN  |
| 14  | Da    | 48  | HIS  |
| 15  | DB    | 90  | GLN  |
| 15  | DB    | 92  | HIS  |
| 15  | DB    | 106 | GLN  |
| 15  | DB    | 114 | ASN  |
| 15  | DB    | 122 | HIS  |
| 15  | DB    | 134 | HIS  |
| 15  | DB    | 194 | GLN  |
| 15  | DB    | 209 | GLN  |
| 15  | DB    | 292 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | DB    | 395  | GLN  |
| 15  | DB    | 401  | HIS  |
| 15  | DB    | 414  | GLN  |
| 15  | DB    | 461  | GLN  |
| 15  | DB    | 486  | HIS  |
| 15  | DB    | 539  | GLN  |
| 15  | DB    | 551  | HIS  |
| 15  | DB    | 562  | GLN  |
| 15  | DB    | 569  | HIS  |
| 15  | DB    | 630  | HIS  |
| 15  | DB    | 682  | HIS  |
| 15  | DB    | 684  | GLN  |
| 15  | DB    | 686  | GLN  |
| 15  | DB    | 691  | HIS  |
| 15  | DB    | 703  | HIS  |
| 15  | DB    | 737  | HIS  |
| 15  | DB    | 748  | HIS  |
| 15  | DB    | 774  | ASN  |
| 15  | DB    | 785  | ASN  |
| 15  | DB    | 800  | GLN  |
| 15  | DB    | 828  | HIS  |
| 15  | DB    | 836  | ASN  |
| 15  | DB    | 908  | GLN  |
| 15  | DB    | 923  | GLN  |
| 15  | DB    | 958  | ASN  |
| 15  | DB    | 981  | HIS  |
| 15  | DB    | 1051 | GLN  |
| 15  | DB    | 1055 | GLN  |
| 15  | DB    | 1113 | GLN  |
| 15  | DB    | 1124 | HIS  |
| 16  | DC    | 81   | HIS  |
| 16  | DC    | 128  | HIS  |
| 16  | DC    | 242  | HIS  |
| 16  | DC    | 263  | GLN  |
| 16  | DC    | 360  | HIS  |
| 16  | DC    | 368  | ASN  |
| 16  | DC    | 445  | HIS  |
| 16  | DC    | 574  | GLN  |
| 16  | DC    | 797  | ASN  |
| 16  | DC    | 801  | HIS  |
| 16  | DC    | 920  | HIS  |
| 16  | DC    | 943  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | DC    | 970  | GLN  |
| 16  | DC    | 1110 | HIS  |
| 16  | DC    | 1141 | GLN  |
| 16  | DC    | 1160 | GLN  |
| 17  | DE    | 38   | GLN  |
| 17  | DE    | 40   | ASN  |
| 17  | DE    | 67   | ASN  |
| 17  | DE    | 84   | HIS  |
| 17  | DE    | 105  | ASN  |
| 17  | DE    | 202  | HIS  |
| 17  | DE    | 327  | ASN  |
| 17  | DE    | 414  | ASN  |
| 17  | DE    | 442  | HIS  |
| 17  | DE    | 465  | ASN  |
| 17  | DE    | 501  | HIS  |
| 17  | DE    | 628  | HIS  |
| 17  | DE    | 658  | ASN  |
| 17  | DE    | 660  | GLN  |
| 17  | DE    | 671  | ASN  |
| 17  | DE    | 698  | GLN  |
| 17  | DE    | 699  | ASN  |
| 18  | DF    | 41   | ASN  |
| 18  | DF    | 62   | ASN  |
| 18  | DF    | 140  | HIS  |
| 18  | DF    | 175  | GLN  |
| 18  | DF    | 187  | ASN  |
| 18  | DF    | 198  | HIS  |
| 18  | DF    | 214  | HIS  |
| 18  | DF    | 283  | HIS  |
| 18  | DF    | 474  | GLN  |
| 18  | DF    | 520  | GLN  |
| 18  | DF    | 543  | HIS  |
| 18  | DF    | 556  | HIS  |
| 18  | DF    | 572  | HIS  |
| 19  | DG    | 23   | HIS  |
| 19  | DG    | 65   | ASN  |
| 19  | DG    | 71   | ASN  |
| 19  | DG    | 92   | GLN  |
| 19  | DG    | 143  | HIS  |
| 19  | DG    | 170  | ASN  |
| 19  | DG    | 191  | GLN  |
| 19  | DG    | 200  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | DG    | 201 | GLN  |
| 19  | DG    | 229 | HIS  |
| 19  | DG    | 230 | ASN  |
| 19  | DG    | 240 | HIS  |
| 19  | DG    | 365 | GLN  |
| 19  | DG    | 405 | GLN  |
| 19  | DG    | 476 | GLN  |
| 19  | DG    | 477 | GLN  |
| 19  | DG    | 554 | HIS  |
| 20  | DH    | 4   | GLN  |
| 20  | DH    | 28  | ASN  |
| 20  | DH    | 45  | HIS  |
| 20  | DH    | 100 | HIS  |
| 20  | DH    | 105 | GLN  |
| 20  | DH    | 123 | HIS  |
| 20  | DH    | 138 | GLN  |
| 20  | DH    | 142 | HIS  |
| 20  | DH    | 146 | GLN  |
| 20  | DH    | 166 | GLN  |
| 20  | DH    | 257 | ASN  |
| 20  | DH    | 302 | GLN  |
| 20  | DH    | 437 | GLN  |
| 20  | DH    | 469 | ASN  |
| 20  | DH    | 490 | HIS  |
| 20  | DH    | 498 | ASN  |
| 20  | DH    | 526 | ASN  |
| 21  | DJ    | 27  | GLN  |
| 21  | DJ    | 31  | HIS  |
| 21  | DJ    | 33  | ASN  |
| 21  | DJ    | 42  | HIS  |
| 21  | DJ    | 55  | ASN  |
| 21  | DJ    | 82  | GLN  |
| 21  | DJ    | 190 | ASN  |
| 21  | DJ    | 199 | GLN  |
| 21  | DJ    | 227 | GLN  |
| 21  | DJ    | 247 | ASN  |
| 21  | DJ    | 291 | ASN  |
| 21  | DJ    | 293 | ASN  |
| 21  | DJ    | 301 | HIS  |
| 21  | DJ    | 314 | GLN  |
| 22  | DK    | 132 | HIS  |
| 22  | DK    | 171 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DK    | 175 | HIS  |
| 23  | DT    | 45  | HIS  |
| 23  | DT    | 58  | HIS  |
| 23  | DT    | 64  | GLN  |
| 23  | DT    | 72  | HIS  |
| 23  | DT    | 82  | HIS  |
| 23  | DT    | 91  | GLN  |
| 23  | DT    | 139 | HIS  |
| 23  | DT    | 140 | ASN  |
| 23  | DT    | 161 | ASN  |
| 23  | DT    | 219 | GLN  |
| 24  | DV    | 31  | HIS  |
| 24  | DV    | 40  | HIS  |
| 24  | DV    | 48  | HIS  |
| 24  | DV    | 71  | GLN  |
| 24  | DV    | 83  | GLN  |
| 24  | DV    | 131 | GLN  |
| 24  | DV    | 145 | ASN  |
| 25  | DW    | 87  | ASN  |
| 25  | DW    | 99  | HIS  |
| 25  | DW    | 121 | HIS  |
| 25  | DW    | 132 | HIS  |
| 25  | DW    | 135 | ASN  |
| 25  | DW    | 154 | HIS  |
| 26  | DX    | 43  | HIS  |
| 26  | DX    | 58  | HIS  |
| 26  | DX    | 130 | GLN  |
| 26  | DX    | 167 | HIS  |
| 26  | DX    | 168 | ASN  |
| 27  | DY    | 41  | GLN  |
| 27  | DY    | 99  | GLN  |
| 27  | DY    | 106 | GLN  |
| 28  | CC    | 25  | HIS  |
| 28  | CC    | 48  | ASN  |
| 28  | CC    | 51  | HIS  |
| 29  | CE    | 85  | ASN  |
| 29  | CE    | 105 | GLN  |
| 29  | CE    | 132 | HIS  |
| 29  | CE    | 187 | GLN  |
| 29  | CE    | 235 | ASN  |
| 29  | CE    | 260 | ASN  |
| 29  | CE    | 317 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | CE    | 417 | ASN  |
| 31  | CH    | 80  | HIS  |
| 31  | CH    | 116 | HIS  |
| 31  | CH    | 242 | ASN  |
| 31  | CH    | 247 | HIS  |
| 31  | CH    | 260 | ASN  |
| 31  | CH    | 267 | HIS  |
| 31  | CH    | 272 | ASN  |
| 31  | CH    | 282 | HIS  |
| 32  | CI    | 84  | ASN  |
| 32  | CI    | 104 | ASN  |
| 32  | CI    | 165 | ASN  |
| 32  | CI    | 211 | ASN  |
| 32  | CI    | 229 | HIS  |
| 32  | CI    | 269 | HIS  |
| 32  | CI    | 397 | ASN  |
| 33  | CJ    | 82  | HIS  |
| 33  | CJ    | 134 | GLN  |
| 33  | CJ    | 171 | HIS  |
| 33  | CJ    | 232 | ASN  |
| 33  | CJ    | 441 | HIS  |
| 33  | CJ    | 450 | HIS  |
| 33  | CJ    | 460 | HIS  |
| 33  | CJ    | 476 | ASN  |
| 33  | CJ    | 484 | HIS  |
| 33  | CJ    | 619 | HIS  |
| 33  | CJ    | 621 | ASN  |
| 33  | CJ    | 711 | HIS  |
| 33  | CJ    | 755 | ASN  |
| 33  | CJ    | 761 | GLN  |
| 33  | CJ    | 769 | GLN  |
| 33  | CJ    | 781 | HIS  |
| 33  | CJ    | 792 | HIS  |
| 33  | CJ    | 793 | HIS  |
| 33  | CJ    | 815 | ASN  |
| 34  | CK    | 73  | GLN  |
| 34  | CK    | 105 | GLN  |
| 34  | CK    | 107 | GLN  |
| 34  | CK    | 111 | ASN  |
| 34  | CK    | 166 | ASN  |
| 34  | CK    | 244 | HIS  |
| 36  | CN    | 50  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | CN    | 142 | HIS  |
| 36  | CN    | 150 | HIS  |
| 36  | CN    | 153 | ASN  |
| 37  | CO    | 82  | ASN  |
| 37  | CO    | 92  | GLN  |
| 37  | CO    | 111 | GLN  |
| 37  | CO    | 117 | GLN  |
| 37  | CO    | 129 | GLN  |
| 37  | CO    | 214 | HIS  |
| 37  | CO    | 281 | HIS  |
| 37  | CO    | 359 | HIS  |
| 37  | CO    | 426 | HIS  |
| 38  | CP    | 41  | GLN  |
| 38  | CP    | 87  | HIS  |
| 39  | CQ    | 13  | ASN  |
| 40  | CR    | 24  | ASN  |
| 40  | CR    | 96  | GLN  |
| 40  | CR    | 214 | GLN  |
| 40  | CR    | 249 | GLN  |
| 40  | CR    | 250 | GLN  |
| 41  | CS    | 110 | HIS  |
| 41  | CS    | 135 | ASN  |
| 42  | CU    | 16  | HIS  |
| 42  | CU    | 32  | HIS  |
| 42  | CU    | 72  | HIS  |
| 42  | CU    | 123 | GLN  |
| 42  | CU    | 148 | ASN  |
| 42  | CU    | 174 | HIS  |
| 43  | CZ    | 283 | ASN  |
| 43  | CZ    | 305 | HIS  |
| 44  | Ca    | 14  | ASN  |
| 44  | Ca    | 63  | GLN  |
| 44  | Ca    | 105 | GLN  |
| 44  | Ca    | 150 | ASN  |
| 44  | Ca    | 177 | GLN  |
| 44  | Ca    | 227 | ASN  |
| 44  | Ca    | 423 | GLN  |
| 44  | Ca    | 440 | HIS  |
| 44  | Ca    | 506 | GLN  |
| 44  | Ca    | 519 | GLN  |
| 45  | Cb    | 63  | HIS  |
| 45  | Cb    | 64  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | Cb    | 67  | GLN  |
| 45  | Cb    | 81  | GLN  |
| 45  | Cb    | 191 | HIS  |
| 45  | Cb    | 198 | HIS  |
| 45  | Cb    | 207 | GLN  |
| 45  | Cb    | 280 | ASN  |
| 46  | Cd    | 48  | ASN  |
| 46  | Cd    | 72  | ASN  |
| 46  | Cd    | 155 | GLN  |
| 46  | Cd    | 159 | HIS  |
| 46  | Cd    | 182 | GLN  |
| 47  | Cg    | 164 | HIS  |
| 47  | Cg    | 170 | ASN  |
| 47  | Cg    | 184 | HIS  |
| 47  | Cg    | 239 | GLN  |
| 47  | Cg    | 289 | ASN  |
| 47  | Cg    | 296 | HIS  |
| 47  | Cg    | 301 | HIS  |
| 47  | Cg    | 323 | GLN  |
| 47  | Cg    | 458 | HIS  |
| 48  | Ci    | 19  | HIS  |
| 48  | Ci    | 29  | GLN  |
| 48  | Ci    | 83  | ASN  |
| 48  | Ci    | 95  | ASN  |
| 48  | Ci    | 96  | ASN  |
| 48  | Ci    | 109 | ASN  |
| 48  | Ci    | 112 | ASN  |
| 48  | Ci    | 125 | HIS  |
| 48  | Ci    | 136 | HIS  |
| 48  | Ci    | 143 | GLN  |
| 48  | Ci    | 145 | ASN  |
| 49  | Cj    | 34  | HIS  |
| 49  | Cj    | 153 | HIS  |
| 50  | Ck    | 49  | HIS  |
| 50  | Ck    | 95  | HIS  |
| 50  | Ck    | 97  | GLN  |
| 50  | Ck    | 110 | HIS  |
| 50  | Ck    | 113 | ASN  |
| 50  | Ck    | 134 | HIS  |
| 50  | Ck    | 236 | ASN  |
| 50  | Ck    | 264 | ASN  |
| 50  | Ck    | 589 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Ck    | 611 | ASN  |
| 50  | Ck    | 634 | HIS  |
| 50  | Ck    | 644 | HIS  |
| 50  | Ck    | 679 | GLN  |
| 50  | Ck    | 682 | ASN  |
| 50  | Ck    | 691 | GLN  |
| 50  | Ck    | 695 | GLN  |
| 50  | Ck    | 723 | GLN  |
| 50  | Ck    | 728 | GLN  |
| 51  | Cm    | 28  | GLN  |
| 51  | Cm    | 56  | ASN  |
| 51  | Cm    | 73  | HIS  |
| 51  | Cm    | 155 | HIS  |
| 51  | Cm    | 168 | HIS  |
| 51  | Cm    | 182 | ASN  |
| 51  | Cm    | 184 | HIS  |
| 52  | Cn    | 149 | GLN  |
| 52  | Cn    | 170 | GLN  |
| 52  | Cn    | 192 | ASN  |
| 52  | Cn    | 232 | ASN  |
| 52  | Cn    | 240 | GLN  |
| 53  | Cp    | 82  | ASN  |
| 53  | Cp    | 91  | GLN  |
| 53  | Cp    | 154 | GLN  |
| 53  | Cp    | 182 | GLN  |
| 54  | Cq    | 20  | GLN  |
| 54  | Cq    | 29  | ASN  |
| 54  | Cq    | 61  | ASN  |
| 54  | Cq    | 93  | ASN  |
| 54  | Cq    | 104 | HIS  |
| 54  | Cq    | 129 | HIS  |
| 54  | Cq    | 196 | HIS  |
| 54  | Cq    | 237 | GLN  |
| 55  | Cr    | 80  | HIS  |
| 55  | Cr    | 125 | GLN  |
| 55  | Cr    | 142 | ASN  |
| 55  | Cr    | 157 | GLN  |
| 55  | Cr    | 287 | HIS  |
| 56  | Cv    | 147 | HIS  |
| 56  | Cv    | 166 | HIS  |
| 56  | Cv    | 245 | ASN  |
| 56  | Cv    | 312 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 56  | Cv    | 321  | HIS  |
| 56  | Cv    | 411  | ASN  |
| 56  | Cv    | 511  | HIS  |
| 56  | Cv    | 523  | HIS  |
| 56  | Cv    | 535  | HIS  |
| 56  | Cv    | 559  | GLN  |
| 56  | Cv    | 581  | HIS  |
| 56  | Cv    | 678  | HIS  |
| 56  | Cv    | 739  | ASN  |
| 56  | Cv    | 755  | HIS  |
| 56  | Cv    | 830  | ASN  |
| 56  | Cv    | 878  | ASN  |
| 56  | Cv    | 948  | HIS  |
| 56  | Cv    | 960  | GLN  |
| 56  | Cv    | 1066 | GLN  |
| 56  | Cv    | 1108 | GLN  |
| 56  | Cv    | 1129 | ASN  |
| 65  | A1    | 16   | ASN  |
| 65  | A1    | 116  | HIS  |
| 66  | A2    | 41   | ASN  |
| 66  | A2    | 67   | HIS  |
| 66  | A2    | 167  | HIS  |
| 66  | A2    | 206  | HIS  |
| 66  | A2    | 207  | GLN  |
| 66  | A2    | 270  | ASN  |
| 66  | A2    | 295  | ASN  |
| 66  | A2    | 389  | HIS  |
| 66  | A2    | 440  | HIS  |
| 67  | A3    | 77   | HIS  |
| 67  | A3    | 104  | GLN  |
| 68  | A4    | 29   | HIS  |
| 68  | A4    | 51   | HIS  |
| 68  | A4    | 85   | GLN  |
| 68  | A4    | 113  | HIS  |
| 69  | A5    | 77   | GLN  |
| 70  | A6    | 48   | HIS  |
| 70  | A6    | 77   | GLN  |
| 70  | A6    | 79   | HIS  |
| 71  | A8    | 55   | GLN  |
| 72  | A9    | 81   | HIS  |
| 72  | A9    | 102  | HIS  |
| 73  | AE    | 88   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 73  | AE    | 168 | ASN  |
| 73  | AE    | 169 | GLN  |
| 73  | AE    | 191 | ASN  |
| 73  | AE    | 214 | HIS  |
| 74  | AF    | 33  | HIS  |
| 74  | AF    | 46  | GLN  |
| 74  | AF    | 56  | HIS  |
| 74  | AF    | 62  | HIS  |
| 74  | AF    | 64  | HIS  |
| 74  | AF    | 83  | HIS  |
| 74  | AF    | 193 | HIS  |
| 74  | AF    | 223 | ASN  |
| 74  | AF    | 321 | GLN  |
| 74  | AF    | 331 | ASN  |
| 74  | AF    | 346 | HIS  |
| 74  | AF    | 430 | ASN  |
| 75  | AI    | 76  | HIS  |
| 75  | AI    | 96  | ASN  |
| 75  | AI    | 120 | ASN  |
| 76  | AJ    | 81  | ASN  |
| 77  | AK    | 24  | ASN  |
| 77  | AK    | 52  | ASN  |
| 77  | AK    | 144 | HIS  |
| 77  | AK    | 230 | GLN  |
| 77  | AK    | 279 | HIS  |
| 78  | AN    | 19  | HIS  |
| 78  | AN    | 30  | ASN  |
| 78  | AN    | 82  | HIS  |
| 78  | AN    | 97  | GLN  |
| 78  | AN    | 141 | HIS  |
| 78  | AN    | 164 | HIS  |
| 78  | AN    | 166 | HIS  |
| 79  | AP    | 89  | GLN  |
| 79  | AP    | 111 | ASN  |
| 79  | AP    | 199 | HIS  |
| 79  | AP    | 259 | HIS  |
| 79  | AP    | 310 | HIS  |
| 79  | AP    | 346 | HIS  |
| 79  | AP    | 348 | ASN  |
| 80  | AQ    | 47  | GLN  |
| 80  | AQ    | 164 | HIS  |
| 81  | AR    | 65  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | AR    | 99  | HIS  |
| 81  | AR    | 113 | GLN  |
| 81  | AR    | 120 | HIS  |
| 81  | AR    | 167 | ASN  |
| 81  | AR    | 223 | HIS  |
| 81  | AR    | 229 | HIS  |
| 81  | AR    | 242 | HIS  |
| 83  | AU    | 56  | HIS  |
| 83  | AU    | 65  | ASN  |
| 83  | AU    | 165 | HIS  |
| 83  | AU    | 192 | ASN  |
| 84  | AV    | 75  | ASN  |
| 84  | AV    | 87  | HIS  |
| 84  | AV    | 100 | GLN  |
| 84  | AV    | 168 | HIS  |
| 84  | AV    | 183 | ASN  |
| 84  | AV    | 206 | ASN  |
| 85  | AW    | 26  | HIS  |
| 85  | AW    | 40  | HIS  |
| 85  | AW    | 50  | GLN  |
| 85  | AW    | 109 | ASN  |
| 85  | AW    | 172 | HIS  |
| 85  | AW    | 183 | GLN  |
| 85  | AW    | 195 | HIS  |
| 86  | AX    | 72  | HIS  |
| 87  | AY    | 64  | HIS  |
| 87  | AY    | 72  | GLN  |
| 87  | AY    | 74  | HIS  |
| 87  | AY    | 91  | GLN  |
| 87  | AY    | 168 | HIS  |
| 87  | AY    | 262 | HIS  |
| 87  | AY    | 269 | GLN  |
| 88  | Ab    | 61  | HIS  |
| 88  | Ab    | 78  | GLN  |
| 88  | Ab    | 93  | ASN  |
| 88  | Ab    | 122 | HIS  |
| 88  | Ab    | 205 | HIS  |
| 88  | Ab    | 278 | ASN  |
| 88  | Ab    | 351 | GLN  |
| 88  | Ab    | 374 | ASN  |
| 88  | Ab    | 419 | GLN  |
| 88  | Ab    | 471 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 89  | Ad    | 78  | ASN  |
| 89  | Ad    | 146 | GLN  |
| 89  | Ad    | 151 | GLN  |
| 89  | Ad    | 221 | GLN  |
| 89  | Ad    | 271 | HIS  |
| 89  | Ad    | 276 | HIS  |
| 89  | Ad    | 279 | GLN  |
| 89  | Ad    | 284 | HIS  |
| 90  | Ae    | 96  | GLN  |
| 90  | Ae    | 100 | HIS  |
| 90  | Ae    | 115 | ASN  |
| 91  | Af    | 60  | GLN  |
| 91  | Af    | 86  | ASN  |
| 91  | Af    | 101 | HIS  |
| 91  | Af    | 106 | GLN  |
| 91  | Af    | 146 | ASN  |
| 91  | Af    | 156 | HIS  |
| 91  | Af    | 164 | HIS  |
| 92  | Ag    | 32  | HIS  |
| 92  | Ag    | 73  | ASN  |
| 92  | Ag    | 84  | ASN  |
| 92  | Ag    | 95  | GLN  |
| 92  | Ag    | 101 | HIS  |
| 92  | Ag    | 170 | GLN  |
| 92  | Ag    | 196 | ASN  |
| 92  | Ag    | 204 | HIS  |
| 92  | Ag    | 244 | HIS  |
| 93  | Aj    | 22  | GLN  |
| 93  | Aj    | 37  | GLN  |
| 93  | Aj    | 54  | GLN  |
| 93  | Aj    | 82  | HIS  |
| 93  | Aj    | 90  | HIS  |
| 93  | Aj    | 103 | ASN  |
| 93  | Aj    | 121 | GLN  |
| 93  | Aj    | 211 | ASN  |
| 93  | Aj    | 225 | GLN  |
| 94  | Al    | 34  | ASN  |
| 95  | Ao    | 25  | ASN  |
| 95  | Ao    | 54  | GLN  |
| 95  | Ao    | 107 | GLN  |
| 95  | Ao    | 141 | ASN  |
| 96  | Ap    | 55  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 96  | Ap    | 78  | HIS  |
| 96  | Ap    | 83  | HIS  |
| 96  | Ap    | 150 | HIS  |
| 96  | Ap    | 154 | HIS  |
| 96  | Ap    | 194 | HIS  |
| 96  | Ap    | 253 | GLN  |
| 96  | Ap    | 278 | ASN  |
| 97  | At    | 116 | GLN  |
| 97  | At    | 148 | GLN  |
| 98  | Av    | 195 | GLN  |
| 98  | Av    | 206 | ASN  |
| 98  | Av    | 212 | ASN  |
| 103 | BA    | 139 | HIS  |
| 103 | BA    | 159 | HIS  |
| 103 | BA    | 272 | GLN  |
| 103 | BA    | 291 | HIS  |
| 103 | BA    | 301 | HIS  |
| 103 | BA    | 307 | HIS  |
| 103 | BA    | 408 | ASN  |
| 103 | BA    | 502 | HIS  |
| 103 | BA    | 585 | HIS  |
| 103 | BA    | 693 | HIS  |
| 103 | BA    | 699 | ASN  |
| 103 | BA    | 734 | HIS  |
| 103 | BA    | 798 | HIS  |
| 104 | BB    | 82  | HIS  |
| 104 | BB    | 128 | HIS  |
| 104 | BB    | 162 | GLN  |
| 104 | BB    | 170 | GLN  |
| 104 | BB    | 218 | HIS  |
| 104 | BB    | 240 | HIS  |
| 104 | BB    | 242 | GLN  |
| 104 | BB    | 359 | HIS  |
| 104 | BB    | 420 | ASN  |
| 104 | BB    | 432 | HIS  |
| 105 | BC    | 71  | GLN  |
| 105 | BC    | 108 | GLN  |
| 105 | BC    | 115 | GLN  |
| 105 | BC    | 165 | HIS  |
| 105 | BC    | 210 | GLN  |
| 105 | BC    | 282 | HIS  |
| 105 | BC    | 289 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 105 | BC    | 292 | ASN  |
| 105 | BC    | 340 | HIS  |
| 105 | BC    | 351 | ASN  |
| 107 | BE    | 23  | GLN  |
| 107 | BE    | 25  | HIS  |
| 107 | BE    | 29  | ASN  |
| 107 | BE    | 41  | HIS  |
| 107 | BE    | 76  | GLN  |
| 107 | BE    | 100 | ASN  |
| 107 | BE    | 352 | HIS  |
| 107 | BE    | 361 | GLN  |
| 108 | BF    | 132 | GLN  |
| 108 | BF    | 143 | GLN  |
| 108 | BF    | 148 | HIS  |
| 108 | BF    | 164 | HIS  |
| 108 | BF    | 180 | GLN  |
| 108 | BF    | 245 | ASN  |
| 108 | BF    | 250 | HIS  |
| 108 | BF    | 298 | ASN  |
| 108 | BF    | 311 | GLN  |
| 108 | BF    | 332 | HIS  |
| 108 | BF    | 343 | GLN  |
| 108 | BF    | 362 | HIS  |
| 108 | BF    | 413 | HIS  |
| 109 | BG    | 81  | HIS  |
| 109 | BG    | 269 | HIS  |
| 109 | BG    | 287 | HIS  |
| 109 | BG    | 340 | GLN  |
| 110 | BH    | 102 | ASN  |
| 110 | BH    | 122 | HIS  |
| 110 | BH    | 134 | GLN  |
| 110 | BH    | 239 | ASN  |
| 111 | BI    | 45  | HIS  |
| 111 | BI    | 52  | HIS  |
| 111 | BI    | 60  | GLN  |
| 111 | BI    | 144 | HIS  |
| 111 | BI    | 152 | GLN  |
| 111 | BI    | 223 | GLN  |
| 111 | BI    | 228 | GLN  |
| 111 | BI    | 245 | ASN  |
| 111 | BI    | 274 | GLN  |
| 111 | BI    | 307 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 112 | BJ    | 249 | GLN  |
| 113 | BK    | 200 | ASN  |
| 113 | BK    | 227 | GLN  |
| 113 | BK    | 285 | GLN  |
| 113 | BK    | 383 | HIS  |
| 114 | BL    | 83  | HIS  |
| 114 | BL    | 99  | HIS  |
| 114 | BL    | 141 | ASN  |
| 114 | BL    | 144 | GLN  |
| 114 | BL    | 226 | HIS  |
| 114 | BL    | 238 | GLN  |
| 115 | BM    | 88  | GLN  |
| 115 | BM    | 89  | HIS  |
| 115 | BM    | 138 | HIS  |
| 115 | BM    | 189 | HIS  |
| 115 | BM    | 193 | GLN  |
| 115 | BM    | 279 | ASN  |
| 116 | BN    | 14  | HIS  |
| 116 | BN    | 28  | ASN  |
| 116 | BN    | 81  | HIS  |
| 116 | BN    | 95  | HIS  |
| 117 | BO    | 101 | GLN  |
| 118 | BP    | 82  | GLN  |
| 118 | BP    | 213 | HIS  |
| 119 | BQ    | 147 | ASN  |
| 119 | BQ    | 163 | GLN  |
| 120 | BR    | 96  | GLN  |
| 120 | BR    | 118 | GLN  |
| 120 | BR    | 133 | GLN  |
| 120 | BR    | 138 | GLN  |
| 120 | BR    | 164 | HIS  |
| 122 | BT    | 33  | ASN  |
| 122 | BT    | 66  | HIS  |
| 122 | BT    | 69  | ASN  |
| 122 | BT    | 73  | HIS  |
| 122 | BT    | 152 | ASN  |
| 124 | BV    | 54  | GLN  |
| 124 | BV    | 57  | HIS  |
| 124 | BV    | 74  | ASN  |
| 124 | BV    | 167 | GLN  |
| 125 | BW    | 35  | GLN  |
| 125 | BW    | 46  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 125 | BW    | 61  | ASN  |
| 125 | BW    | 65  | ASN  |
| 125 | BW    | 79  | HIS  |
| 125 | BW    | 95  | HIS  |
| 125 | BW    | 149 | ASN  |
| 125 | BW    | 168 | HIS  |
| 127 | BY    | 100 | HIS  |
| 127 | BY    | 102 | GLN  |
| 127 | BY    | 103 | HIS  |
| 127 | BY    | 150 | GLN  |
| 128 | BZ    | 66  | GLN  |
| 128 | BZ    | 96  | GLN  |
| 128 | BZ    | 129 | ASN  |
| 128 | BZ    | 144 | ASN  |
| 129 | Ba    | 19  | GLN  |
| 129 | Ba    | 24  | HIS  |
| 129 | Ba    | 31  | GLN  |
| 129 | Ba    | 36  | HIS  |
| 129 | Ba    | 39  | ASN  |
| 129 | Ba    | 147 | ASN  |
| 130 | Bb    | 79  | HIS  |
| 130 | Bb    | 80  | HIS  |
| 131 | Bc    | 17  | HIS  |
| 131 | Bc    | 33  | GLN  |
| 131 | Bc    | 34  | GLN  |
| 131 | Bc    | 38  | ASN  |
| 131 | Bc    | 66  | HIS  |
| 131 | Bc    | 67  | GLN  |
| 132 | Bd    | 11  | GLN  |
| 132 | Bd    | 77  | HIS  |
| 132 | Bd    | 90  | GLN  |
| 132 | Bd    | 97  | GLN  |
| 133 | Be    | 15  | ASN  |
| 133 | Be    | 70  | HIS  |
| 133 | Be    | 72  | HIS  |
| 134 | Bf    | 92  | HIS  |
| 134 | Bf    | 104 | ASN  |
| 135 | Bg    | 27  | ASN  |
| 135 | Bg    | 58  | GLN  |
| 135 | Bg    | 85  | GLN  |
| 135 | Bg    | 87  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 102 | AA    | 581/1179 (49%)  | 289 (49%)         | 17 (2%)         |
| 57  | CA    | 620/621 (99%)   | 300 (48%)         | 8 (1%)          |
| All | All   | 1201/1800 (66%) | 589 (49%)         | 25 (2%)         |

All (589) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 2   | A    |
| 57  | CA    | 3   | A    |
| 57  | CA    | 4   | A    |
| 57  | CA    | 5   | U    |
| 57  | CA    | 6   | U    |
| 57  | CA    | 8   | U    |
| 57  | CA    | 10  | G    |
| 57  | CA    | 11  | U    |
| 57  | CA    | 15  | U    |
| 57  | CA    | 16  | U    |
| 57  | CA    | 19  | U    |
| 57  | CA    | 20  | A    |
| 57  | CA    | 25  | U    |
| 57  | CA    | 26  | C    |
| 57  | CA    | 27  | A    |
| 57  | CA    | 33  | A    |
| 57  | CA    | 36  | U    |
| 57  | CA    | 37  | U    |
| 57  | CA    | 38  | U    |
| 57  | CA    | 39  | U    |
| 57  | CA    | 42  | A    |
| 57  | CA    | 44  | U    |
| 57  | CA    | 45  | G    |
| 57  | CA    | 46  | U    |
| 57  | CA    | 50  | A    |
| 57  | CA    | 52  | C    |
| 57  | CA    | 53  | A    |
| 57  | CA    | 56  | U    |
| 57  | CA    | 57  | U    |
| 57  | CA    | 58  | A    |
| 57  | CA    | 59  | U    |
| 57  | CA    | 60  | A    |
| 57  | CA    | 61  | A    |
| 57  | CA    | 64  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 67  | U    |
| 57  | CA    | 68  | A    |
| 57  | CA    | 70  | U    |
| 57  | CA    | 74  | G    |
| 57  | CA    | 78  | G    |
| 57  | CA    | 79  | A    |
| 57  | CA    | 81  | U    |
| 57  | CA    | 84  | U    |
| 57  | CA    | 85  | U    |
| 57  | CA    | 86  | G    |
| 57  | CA    | 87  | U    |
| 57  | CA    | 88  | A    |
| 57  | CA    | 89  | U    |
| 57  | CA    | 91  | A    |
| 57  | CA    | 94  | U    |
| 57  | CA    | 95  | U    |
| 57  | CA    | 97  | U    |
| 57  | CA    | 100 | G    |
| 57  | CA    | 102 | A    |
| 57  | CA    | 103 | U    |
| 57  | CA    | 104 | A    |
| 57  | CA    | 105 | G    |
| 57  | CA    | 107 | U    |
| 57  | CA    | 108 | A    |
| 57  | CA    | 109 | A    |
| 57  | CA    | 110 | U    |
| 57  | CA    | 111 | A    |
| 57  | CA    | 112 | A    |
| 57  | CA    | 113 | U    |
| 57  | CA    | 114 | A    |
| 57  | CA    | 115 | A    |
| 57  | CA    | 116 | U    |
| 57  | CA    | 117 | U    |
| 57  | CA    | 124 | U    |
| 57  | CA    | 127 | G    |
| 57  | CA    | 132 | G    |
| 57  | CA    | 135 | U    |
| 57  | CA    | 136 | G    |
| 57  | CA    | 138 | U    |
| 57  | CA    | 139 | U    |
| 57  | CA    | 146 | U    |
| 57  | CA    | 152 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 156 | U    |
| 57  | CA    | 159 | G    |
| 57  | CA    | 160 | U    |
| 57  | CA    | 167 | A    |
| 57  | CA    | 170 | U    |
| 57  | CA    | 171 | A    |
| 57  | CA    | 172 | A    |
| 57  | CA    | 173 | A    |
| 57  | CA    | 174 | A    |
| 57  | CA    | 175 | A    |
| 57  | CA    | 178 | A    |
| 57  | CA    | 179 | U    |
| 57  | CA    | 183 | U    |
| 57  | CA    | 188 | U    |
| 57  | CA    | 189 | A    |
| 57  | CA    | 191 | A    |
| 57  | CA    | 193 | C    |
| 57  | CA    | 194 | A    |
| 57  | CA    | 197 | A    |
| 57  | CA    | 198 | A    |
| 57  | CA    | 199 | U    |
| 57  | CA    | 200 | A    |
| 57  | CA    | 202 | A    |
| 57  | CA    | 203 | U    |
| 57  | CA    | 204 | U    |
| 57  | CA    | 205 | A    |
| 57  | CA    | 206 | A    |
| 57  | CA    | 208 | U    |
| 57  | CA    | 209 | U    |
| 57  | CA    | 210 | A    |
| 57  | CA    | 211 | A    |
| 57  | CA    | 214 | U    |
| 57  | CA    | 216 | U    |
| 57  | CA    | 217 | U    |
| 57  | CA    | 218 | A    |
| 57  | CA    | 219 | G    |
| 57  | CA    | 221 | C    |
| 57  | CA    | 223 | G    |
| 57  | CA    | 230 | A    |
| 57  | CA    | 236 | G    |
| 57  | CA    | 242 | G    |
| 57  | CA    | 246 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 247 | A    |
| 57  | CA    | 250 | U    |
| 57  | CA    | 256 | G    |
| 57  | CA    | 258 | U    |
| 57  | CA    | 259 | U    |
| 57  | CA    | 261 | U    |
| 57  | CA    | 262 | A    |
| 57  | CA    | 263 | A    |
| 57  | CA    | 272 | C    |
| 57  | CA    | 275 | U    |
| 57  | CA    | 276 | U    |
| 57  | CA    | 279 | C    |
| 57  | CA    | 280 | A    |
| 57  | CA    | 281 | U    |
| 57  | CA    | 282 | A    |
| 57  | CA    | 283 | U    |
| 57  | CA    | 286 | A    |
| 57  | CA    | 296 | U    |
| 57  | CA    | 297 | G    |
| 57  | CA    | 299 | U    |
| 57  | CA    | 300 | G    |
| 57  | CA    | 301 | A    |
| 57  | CA    | 305 | A    |
| 57  | CA    | 311 | U    |
| 57  | CA    | 315 | A    |
| 57  | CA    | 316 | A    |
| 57  | CA    | 321 | A    |
| 57  | CA    | 323 | U    |
| 57  | CA    | 325 | A    |
| 57  | CA    | 326 | U    |
| 57  | CA    | 327 | U    |
| 57  | CA    | 328 | U    |
| 57  | CA    | 330 | U    |
| 57  | CA    | 334 | U    |
| 57  | CA    | 335 | G    |
| 57  | CA    | 337 | U    |
| 57  | CA    | 338 | U    |
| 57  | CA    | 340 | U    |
| 57  | CA    | 341 | A    |
| 57  | CA    | 342 | A    |
| 57  | CA    | 343 | A    |
| 57  | CA    | 350 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 351 | A    |
| 57  | CA    | 352 | G    |
| 57  | CA    | 356 | U    |
| 57  | CA    | 357 | A    |
| 57  | CA    | 358 | U    |
| 57  | CA    | 359 | G    |
| 57  | CA    | 360 | C    |
| 57  | CA    | 361 | A    |
| 57  | CA    | 364 | U    |
| 57  | CA    | 367 | A    |
| 57  | CA    | 368 | A    |
| 57  | CA    | 369 | A    |
| 57  | CA    | 371 | U    |
| 57  | CA    | 374 | U    |
| 57  | CA    | 378 | A    |
| 57  | CA    | 380 | U    |
| 57  | CA    | 384 | A    |
| 57  | CA    | 385 | A    |
| 57  | CA    | 386 | A    |
| 57  | CA    | 389 | A    |
| 57  | CA    | 394 | A    |
| 57  | CA    | 395 | U    |
| 57  | CA    | 397 | U    |
| 57  | CA    | 398 | U    |
| 57  | CA    | 399 | A    |
| 57  | CA    | 400 | U    |
| 57  | CA    | 401 | A    |
| 57  | CA    | 406 | U    |
| 57  | CA    | 407 | U    |
| 57  | CA    | 408 | C    |
| 57  | CA    | 410 | U    |
| 57  | CA    | 411 | A    |
| 57  | CA    | 413 | A    |
| 57  | CA    | 414 | A    |
| 57  | CA    | 415 | U    |
| 57  | CA    | 418 | A    |
| 57  | CA    | 419 | U    |
| 57  | CA    | 421 | G    |
| 57  | CA    | 423 | A    |
| 57  | CA    | 426 | A    |
| 57  | CA    | 427 | U    |
| 57  | CA    | 428 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 430 | U    |
| 57  | CA    | 431 | U    |
| 57  | CA    | 433 | U    |
| 57  | CA    | 434 | A    |
| 57  | CA    | 435 | G    |
| 57  | CA    | 438 | U    |
| 57  | CA    | 441 | G    |
| 57  | CA    | 442 | A    |
| 57  | CA    | 444 | A    |
| 57  | CA    | 445 | C    |
| 57  | CA    | 446 | C    |
| 57  | CA    | 448 | U    |
| 57  | CA    | 449 | G    |
| 57  | CA    | 450 | A    |
| 57  | CA    | 451 | U    |
| 57  | CA    | 452 | A    |
| 57  | CA    | 453 | A    |
| 57  | CA    | 455 | G    |
| 57  | CA    | 457 | U    |
| 57  | CA    | 458 | U    |
| 57  | CA    | 459 | A    |
| 57  | CA    | 460 | U    |
| 57  | CA    | 461 | A    |
| 57  | CA    | 462 | A    |
| 57  | CA    | 463 | A    |
| 57  | CA    | 464 | U    |
| 57  | CA    | 467 | A    |
| 57  | CA    | 468 | A    |
| 57  | CA    | 469 | A    |
| 57  | CA    | 470 | G    |
| 57  | CA    | 471 | U    |
| 57  | CA    | 472 | G    |
| 57  | CA    | 476 | A    |
| 57  | CA    | 478 | A    |
| 57  | CA    | 480 | C    |
| 57  | CA    | 481 | A    |
| 57  | CA    | 482 | U    |
| 57  | CA    | 483 | A    |
| 57  | CA    | 484 | A    |
| 57  | CA    | 485 | U    |
| 57  | CA    | 486 | C    |
| 57  | CA    | 487 | A    |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 489 | A    |
| 57  | CA    | 491 | U    |
| 57  | CA    | 494 | A    |
| 57  | CA    | 495 | U    |
| 57  | CA    | 496 | U    |
| 57  | CA    | 497 | A    |
| 57  | CA    | 498 | U    |
| 57  | CA    | 500 | U    |
| 57  | CA    | 502 | U    |
| 57  | CA    | 505 | U    |
| 57  | CA    | 507 | A    |
| 57  | CA    | 509 | U    |
| 57  | CA    | 510 | A    |
| 57  | CA    | 513 | U    |
| 57  | CA    | 514 | A    |
| 57  | CA    | 517 | U    |
| 57  | CA    | 518 | G    |
| 57  | CA    | 519 | U    |
| 57  | CA    | 520 | A    |
| 57  | CA    | 532 | A    |
| 57  | CA    | 535 | U    |
| 57  | CA    | 536 | U    |
| 57  | CA    | 537 | A    |
| 57  | CA    | 538 | A    |
| 57  | CA    | 539 | A    |
| 57  | CA    | 540 | A    |
| 57  | CA    | 544 | U    |
| 57  | CA    | 546 | U    |
| 57  | CA    | 547 | U    |
| 57  | CA    | 548 | G    |
| 57  | CA    | 555 | A    |
| 57  | CA    | 556 | C    |
| 57  | CA    | 558 | A    |
| 57  | CA    | 560 | U    |
| 57  | CA    | 564 | U    |
| 57  | CA    | 565 | A    |
| 57  | CA    | 566 | U    |
| 57  | CA    | 567 | A    |
| 57  | CA    | 570 | A    |
| 57  | CA    | 576 | A    |
| 57  | CA    | 581 | G    |
| 57  | CA    | 586 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 587 | A    |
| 57  | CA    | 588 | U    |
| 57  | CA    | 590 | A    |
| 57  | CA    | 602 | A    |
| 57  | CA    | 603 | A    |
| 57  | CA    | 611 | U    |
| 57  | CA    | 613 | U    |
| 57  | CA    | 614 | U    |
| 57  | CA    | 615 | U    |
| 57  | CA    | 616 | U    |
| 57  | CA    | 617 | U    |
| 57  | CA    | 618 | U    |
| 57  | CA    | 619 | U    |
| 57  | CA    | 620 | U    |
| 102 | AA    | 2   | U    |
| 102 | AA    | 3   | U    |
| 102 | AA    | 4   | U    |
| 102 | AA    | 5   | U    |
| 102 | AA    | 10  | A    |
| 102 | AA    | 11  | U    |
| 102 | AA    | 12  | U    |
| 102 | AA    | 13  | A    |
| 102 | AA    | 16  | A    |
| 102 | AA    | 17  | A    |
| 102 | AA    | 18  | G    |
| 102 | AA    | 19  | A    |
| 102 | AA    | 20  | A    |
| 102 | AA    | 21  | U    |
| 102 | AA    | 27  | A    |
| 102 | AA    | 28  | A    |
| 102 | AA    | 29  | U    |
| 102 | AA    | 32  | U    |
| 102 | AA    | 33  | G    |
| 102 | AA    | 34  | G    |
| 102 | AA    | 38  | U    |
| 102 | AA    | 40  | U    |
| 102 | AA    | 41  | U    |
| 102 | AA    | 42  | A    |
| 102 | AA    | 43  | U    |
| 102 | AA    | 44  | A    |
| 102 | AA    | 50  | A    |
| 102 | AA    | 53  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 102 | AA    | 54  | A    |
| 102 | AA    | 57  | A    |
| 102 | AA    | 58  | U    |
| 102 | AA    | 59  | U    |
| 102 | AA    | 60  | U    |
| 102 | AA    | 64  | U    |
| 102 | AA    | 65  | U    |
| 102 | AA    | 66  | C    |
| 102 | AA    | 68  | G    |
| 102 | AA    | 69  | U    |
| 102 | AA    | 70  | G    |
| 102 | AA    | 71  | U    |
| 102 | AA    | 72  | A    |
| 102 | AA    | 73  | G    |
| 102 | AA    | 74  | U    |
| 102 | AA    | 75  | A    |
| 102 | AA    | 77  | A    |
| 102 | AA    | 78  | U    |
| 102 | AA    | 79  | U    |
| 102 | AA    | 80  | U    |
| 102 | AA    | 81  | A    |
| 102 | AA    | 82  | U    |
| 102 | AA    | 84  | A    |
| 102 | AA    | 85  | U    |
| 102 | AA    | 86  | U    |
| 102 | AA    | 88  | G    |
| 102 | AA    | 89  | U    |
| 102 | AA    | 98  | U    |
| 102 | AA    | 101 | A    |
| 102 | AA    | 104 | A    |
| 102 | AA    | 105 | G    |
| 102 | AA    | 106 | G    |
| 102 | AA    | 107 | U    |
| 102 | AA    | 111 | U    |
| 102 | AA    | 112 | U    |
| 102 | AA    | 113 | A    |
| 102 | AA    | 114 | U    |
| 102 | AA    | 115 | A    |
| 102 | AA    | 116 | U    |
| 102 | AA    | 119 | A    |
| 102 | AA    | 120 | A    |
| 102 | AA    | 123 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 102 | AA    | 124 | U    |
| 102 | AA    | 125 | U    |
| 102 | AA    | 126 | A    |
| 102 | AA    | 127 | A    |
| 102 | AA    | 130 | U    |
| 102 | AA    | 131 | U    |
| 102 | AA    | 133 | U    |
| 102 | AA    | 134 | U    |
| 102 | AA    | 135 | G    |
| 102 | AA    | 136 | U    |
| 102 | AA    | 137 | U    |
| 102 | AA    | 146 | A    |
| 102 | AA    | 148 | A    |
| 102 | AA    | 149 | U    |
| 102 | AA    | 152 | A    |
| 102 | AA    | 154 | A    |
| 102 | AA    | 159 | U    |
| 102 | AA    | 162 | A    |
| 102 | AA    | 164 | U    |
| 102 | AA    | 168 | A    |
| 102 | AA    | 170 | A    |
| 102 | AA    | 171 | U    |
| 102 | AA    | 172 | U    |
| 102 | AA    | 174 | A    |
| 102 | AA    | 176 | A    |
| 102 | AA    | 177 | U    |
| 102 | AA    | 178 | A    |
| 102 | AA    | 179 | A    |
| 102 | AA    | 183 | U    |
| 102 | AA    | 186 | A    |
| 102 | AA    | 187 | A    |
| 102 | AA    | 189 | A    |
| 102 | AA    | 282 | A    |
| 102 | AA    | 283 | A    |
| 102 | AA    | 284 | U    |
| 102 | AA    | 285 | A    |
| 102 | AA    | 288 | G    |
| 102 | AA    | 289 | U    |
| 102 | AA    | 290 | A    |
| 102 | AA    | 296 | A    |
| 102 | AA    | 297 | U    |
| 102 | AA    | 299 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 102 | AA    | 301 | A    |
| 102 | AA    | 319 | A    |
| 102 | AA    | 327 | U    |
| 102 | AA    | 328 | U    |
| 102 | AA    | 330 | U    |
| 102 | AA    | 331 | C    |
| 102 | AA    | 336 | U    |
| 102 | AA    | 342 | U    |
| 102 | AA    | 344 | A    |
| 102 | AA    | 370 | U    |
| 102 | AA    | 371 | A    |
| 102 | AA    | 375 | A    |
| 102 | AA    | 378 | A    |
| 102 | AA    | 380 | G    |
| 102 | AA    | 381 | U    |
| 102 | AA    | 383 | A    |
| 102 | AA    | 384 | U    |
| 102 | AA    | 385 | A    |
| 102 | AA    | 387 | A    |
| 102 | AA    | 388 | U    |
| 102 | AA    | 393 | A    |
| 102 | AA    | 394 | U    |
| 102 | AA    | 397 | A    |
| 102 | AA    | 411 | A    |
| 102 | AA    | 414 | A    |
| 102 | AA    | 418 | G    |
| 102 | AA    | 419 | U    |
| 102 | AA    | 420 | A    |
| 102 | AA    | 423 | A    |
| 102 | AA    | 424 | G    |
| 102 | AA    | 425 | U    |
| 102 | AA    | 426 | A    |
| 102 | AA    | 427 | U    |
| 102 | AA    | 428 | A    |
| 102 | AA    | 438 | U    |
| 102 | AA    | 440 | U    |
| 102 | AA    | 441 | A    |
| 102 | AA    | 446 | A    |
| 102 | AA    | 447 | U    |
| 102 | AA    | 448 | A    |
| 102 | AA    | 455 | U    |
| 102 | AA    | 456 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 102 | AA    | 458 | U    |
| 102 | AA    | 460 | U    |
| 102 | AA    | 461 | U    |
| 102 | AA    | 462 | U    |
| 102 | AA    | 463 | U    |
| 102 | AA    | 468 | A    |
| 102 | AA    | 470 | G    |
| 102 | AA    | 472 | A    |
| 102 | AA    | 473 | A    |
| 102 | AA    | 474 | A    |
| 102 | AA    | 475 | U    |
| 102 | AA    | 476 | G    |
| 102 | AA    | 477 | A    |
| 102 | AA    | 481 | G    |
| 102 | AA    | 483 | A    |
| 102 | AA    | 484 | U    |
| 102 | AA    | 485 | A    |
| 102 | AA    | 486 | A    |
| 102 | AA    | 488 | U    |
| 102 | AA    | 489 | G    |
| 102 | AA    | 490 | G    |
| 102 | AA    | 491 | A    |
| 102 | AA    | 492 | U    |
| 102 | AA    | 493 | A    |
| 102 | AA    | 494 | U    |
| 102 | AA    | 495 | A    |
| 102 | AA    | 496 | A    |
| 102 | AA    | 497 | C    |
| 102 | AA    | 498 | U    |
| 102 | AA    | 499 | U    |
| 102 | AA    | 503 | A    |
| 102 | AA    | 504 | U    |
| 102 | AA    | 509 | U    |
| 102 | AA    | 513 | U    |
| 102 | AA    | 514 | G    |
| 102 | AA    | 515 | U    |
| 102 | AA    | 516 | U    |
| 102 | AA    | 518 | A    |
| 102 | AA    | 519 | A    |
| 102 | AA    | 520 | U    |
| 102 | AA    | 523 | A    |
| 102 | AA    | 524 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 102 | AA    | 525 | A    |
| 102 | AA    | 526 | G    |
| 102 | AA    | 527 | U    |
| 102 | AA    | 529 | U    |
| 102 | AA    | 530 | U    |
| 102 | AA    | 531 | U    |
| 102 | AA    | 532 | U    |
| 102 | AA    | 533 | A    |
| 102 | AA    | 535 | U    |
| 102 | AA    | 536 | A    |
| 102 | AA    | 537 | U    |
| 102 | AA    | 538 | U    |
| 102 | AA    | 540 | U    |
| 102 | AA    | 545 | U    |
| 102 | AA    | 546 | A    |
| 102 | AA    | 548 | A    |
| 102 | AA    | 549 | G    |
| 102 | AA    | 551 | A    |
| 102 | AA    | 554 | A    |
| 102 | AA    | 555 | U    |
| 102 | AA    | 556 | U    |
| 102 | AA    | 557 | A    |
| 102 | AA    | 559 | A    |
| 102 | AA    | 560 | G    |
| 102 | AA    | 562 | G    |
| 102 | AA    | 563 | U    |
| 102 | AA    | 564 | A    |
| 102 | AA    | 565 | U    |
| 102 | AA    | 566 | A    |
| 102 | AA    | 567 | G    |
| 102 | AA    | 568 | U    |
| 102 | AA    | 570 | U    |
| 102 | AA    | 571 | U    |
| 102 | AA    | 572 | U    |
| 102 | AA    | 573 | U    |
| 102 | AA    | 574 | A    |
| 102 | AA    | 575 | A    |
| 102 | AA    | 583 | A    |
| 102 | AA    | 800 | A    |
| 102 | AA    | 801 | A    |
| 102 | AA    | 802 | G    |
| 102 | AA    | 803 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 102 | AA    | 814  | A    |
| 102 | AA    | 815  | U    |
| 102 | AA    | 816  | C    |
| 102 | AA    | 818  | A    |
| 102 | AA    | 819  | A    |
| 102 | AA    | 825  | A    |
| 102 | AA    | 826  | A    |
| 102 | AA    | 827  | U    |
| 102 | AA    | 828  | A    |
| 102 | AA    | 830  | A    |
| 102 | AA    | 836  | A    |
| 102 | AA    | 837  | A    |
| 102 | AA    | 838  | A    |
| 102 | AA    | 845  | A    |
| 102 | AA    | 883  | U    |
| 102 | AA    | 884  | A    |
| 102 | AA    | 885  | U    |
| 102 | AA    | 886  | G    |
| 102 | AA    | 887  | A    |
| 102 | AA    | 891  | G    |
| 102 | AA    | 892  | U    |
| 102 | AA    | 893  | A    |
| 102 | AA    | 948  | A    |
| 102 | AA    | 949  | U    |
| 102 | AA    | 950  | U    |
| 102 | AA    | 951  | C    |
| 102 | AA    | 952  | U    |
| 102 | AA    | 953  | U    |
| 102 | AA    | 954  | U    |
| 102 | AA    | 955  | G    |
| 102 | AA    | 1100 | U    |
| 102 | AA    | 1106 | U    |
| 102 | AA    | 1107 | U    |
| 102 | AA    | 1111 | A    |
| 102 | AA    | 1112 | U    |
| 102 | AA    | 1113 | U    |
| 102 | AA    | 1157 | A    |
| 102 | AA    | 1158 | G    |
| 102 | AA    | 1159 | A    |
| 102 | AA    | 1160 | A    |
| 102 | AA    | 1163 | A    |
| 102 | AA    | 1164 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 102 | AA    | 1165 | G    |
| 102 | AA    | 1166 | A    |
| 102 | AA    | 1168 | U    |
| 102 | AA    | 1169 | A    |
| 102 | AA    | 1171 | A    |
| 102 | AA    | 1172 | A    |
| 102 | AA    | 1173 | U    |
| 102 | AA    | 1174 | U    |
| 102 | AA    | 1175 | U    |

All (25) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 57  | CA    | 14   | A    |
| 57  | CA    | 38   | U    |
| 57  | CA    | 80   | U    |
| 57  | CA    | 84   | U    |
| 57  | CA    | 198  | A    |
| 57  | CA    | 350  | U    |
| 57  | CA    | 512  | G    |
| 57  | CA    | 527  | A    |
| 102 | AA    | 40   | U    |
| 102 | AA    | 69   | U    |
| 102 | AA    | 171  | U    |
| 102 | AA    | 335  | G    |
| 102 | AA    | 379  | U    |
| 102 | AA    | 384  | U    |
| 102 | AA    | 387  | A    |
| 102 | AA    | 392  | A    |
| 102 | AA    | 418  | G    |
| 102 | AA    | 422  | A    |
| 102 | AA    | 425  | U    |
| 102 | AA    | 440  | U    |
| 102 | AA    | 485  | A    |
| 102 | AA    | 528  | A    |
| 102 | AA    | 534  | U    |
| 102 | AA    | 1162 | G    |
| 102 | AA    | 1164 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 56 are monoatomic and 1 is modelled with single atom - leaving 8 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 | $\# Z  > 2$ |
| 153 | SPM  | CA    | 738 | -    | 13,13,13     | 0.33 | 0           | 12,12,12    | 0.84 | 0           |
| 152 | GTP  | Cg    | 501 | 151  | 33,34,34     | 0.94 | 1 (3%)      | 50,54,54    | 1.93 | 15 (30%)    |
| 149 | SPD  | CA    | 737 | -    | 9,9,9        | 0.35 | 0           | 8,8,8       | 0.67 | 0           |
| 149 | SPD  | CA    | 735 | -    | 9,9,9        | 0.39 | 0           | 8,8,8       | 0.58 | 0           |
| 154 | NAD  | Av    | 301 | -    | 46,48,48     | 2.09 | 12 (26%)    | 64,73,73    | 2.03 | 13 (20%)    |
| 149 | SPD  | CA    | 736 | -    | 9,9,9        | 0.48 | 0           | 8,8,8       | 0.48 | 0           |
| 149 | SPD  | DL    | 401 | -    | 9,9,9        | 0.39 | 0           | 8,8,8       | 1.03 | 0           |
| 150 | UTP  | DJ    | 401 | -    | 29,30,30     | 1.72 | 7 (24%)     | 43,47,47    | 1.78 | 8 (18%)     |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 153 | SPM  | CA    | 738 | -    | -       | 8/11/11/11  | -       |
| 152 | GTP  | Cg    | 501 | 151  | -       | 4/22/38/38  | 0/3/3/3 |
| 149 | SPD  | CA    | 737 | -    | -       | 3/7/7/7     | -       |
| 149 | SPD  | CA    | 735 | -    | -       | 5/7/7/7     | -       |
| 154 | NAD  | Av    | 301 | -    | -       | 8/30/62/62  | 0/5/5/5 |
| 149 | SPD  | CA    | 736 | -    | -       | 5/7/7/7     | -       |
| 149 | SPD  | DL    | 401 | -    | -       | 2/7/7/7     | -       |
| 150 | UTP  | DJ    | 401 | -    | -       | 10/22/38/38 | 0/2/2/2 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 154 | Av    | 301 | NAD  | C3N-C7N | -7.66 | 1.39        | 1.50     |
| 150 | DJ    | 401 | UTP  | PB-O3A  | 5.28  | 1.65        | 1.59     |
| 154 | Av    | 301 | NAD  | C2N-N1N | 4.49  | 1.39        | 1.35     |
| 154 | Av    | 301 | NAD  | PA-O3   | 4.40  | 1.64        | 1.59     |
| 154 | Av    | 301 | NAD  | PN-O3   | 4.29  | 1.64        | 1.59     |
| 154 | Av    | 301 | NAD  | C2A-N1A | 3.24  | 1.39        | 1.33     |
| 154 | Av    | 301 | NAD  | C5A-C4A | -3.12 | 1.33        | 1.39     |
| 154 | Av    | 301 | NAD  | C5A-N7A | -3.11 | 1.33        | 1.39     |
| 154 | Av    | 301 | NAD  | C2A-N3A | 3.09  | 1.39        | 1.33     |
| 154 | Av    | 301 | NAD  | C5A-C6A | -2.93 | 1.32        | 1.41     |
| 154 | Av    | 301 | NAD  | C4A-N9A | -2.68 | 1.32        | 1.37     |
| 154 | Av    | 301 | NAD  | C8A-N9A | -2.45 | 1.33        | 1.37     |
| 150 | DJ    | 401 | UTP  | PA-O3A  | 2.44  | 1.62        | 1.59     |
| 150 | DJ    | 401 | UTP  | PB-O3B  | 2.23  | 1.61        | 1.59     |
| 150 | DJ    | 401 | UTP  | PA-O5'  | 2.17  | 1.67        | 1.59     |
| 150 | DJ    | 401 | UTP  | C6-C5   | 2.16  | 1.40        | 1.35     |
| 150 | DJ    | 401 | UTP  | C1'-N1  | 2.15  | 1.53        | 1.47     |
| 154 | Av    | 301 | NAD  | C6N-N1N | 2.14  | 1.40        | 1.35     |
| 150 | DJ    | 401 | UTP  | PG-O3G  | -2.11 | 1.47        | 1.54     |
| 152 | Cg    | 501 | GTP  | O4'-C4' | -2.07 | 1.40        | 1.45     |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 154 | Av    | 301 | NAD  | C4D-O4D-C1D | -7.24 | 103.29      | 109.92   |
| 154 | Av    | 301 | NAD  | N3A-C2A-N1A | -6.68 | 118.48      | 128.58   |
| 152 | Cg    | 501 | GTP  | C5-C4-N3    | -5.02 | 120.40      | 128.39   |
| 152 | Cg    | 501 | GTP  | O2G-PG-O3B  | 4.60  | 120.05      | 104.64   |
| 152 | Cg    | 501 | GTP  | C2-N1-C6    | -4.31 | 117.29      | 125.11   |
| 154 | Av    | 301 | NAD  | N9A-C8A-N7A | -4.28 | 107.87      | 113.94   |
| 150 | DJ    | 401 | UTP  | C4-N3-C2    | -4.26 | 121.32      | 126.61   |
| 150 | DJ    | 401 | UTP  | N3-C2-N1    | 4.18  | 120.33      | 114.89   |
| 150 | DJ    | 401 | UTP  | C1'-N1-C2   | 4.07  | 124.91      | 117.59   |
| 154 | Av    | 301 | NAD  | C5A-C4A-N3A | -4.04 | 121.16      | 126.72   |
| 152 | Cg    | 501 | GTP  | C2-N3-C4    | 3.74  | 118.74      | 112.30   |
| 150 | DJ    | 401 | UTP  | O4-C4-C5    | -3.42 | 119.26      | 125.16   |
| 150 | DJ    | 401 | UTP  | C5-C4-N3    | 3.40  | 119.56      | 114.80   |
| 154 | Av    | 301 | NAD  | C2B-C3B-C4B | -3.31 | 96.21       | 102.61   |
| 154 | Av    | 301 | NAD  | C2A-N3A-C4A | 3.07  | 119.34      | 111.83   |
| 154 | Av    | 301 | NAD  | C5A-C6A-N6A | -3.07 | 115.68      | 123.29   |
| 154 | Av    | 301 | NAD  | C4A-N9A-C8A | 2.95  | 108.84      | 105.74   |
| 152 | Cg    | 501 | GTP  | C2'-C1'-N9  | -2.86 | 105.29      | 113.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 152 | Cg    | 501 | GTP  | O2A-PA-O3A  | 2.83  | 114.92      | 107.27   |
| 150 | DJ    | 401 | UTP  | C2'-C1'-N1  | 2.75  | 120.90      | 113.25   |
| 152 | Cg    | 501 | GTP  | O6-C6-C5    | -2.70 | 119.40      | 126.53   |
| 152 | Cg    | 501 | GTP  | N9-C4-N3    | 2.67  | 131.29      | 125.95   |
| 152 | Cg    | 501 | GTP  | O3B-PB-O1B  | -2.64 | 102.75      | 110.70   |
| 152 | Cg    | 501 | GTP  | N2-C2-N3    | -2.63 | 114.53      | 119.67   |
| 154 | Av    | 301 | NAD  | N3A-C4A-N9A | 2.62  | 131.63      | 127.17   |
| 154 | Av    | 301 | NAD  | C3N-C7N-N7N | -2.58 | 114.56      | 117.74   |
| 154 | Av    | 301 | NAD  | C6A-C5A-C4A | 2.55  | 120.67      | 117.18   |
| 152 | Cg    | 501 | GTP  | O2B-PB-O3B  | 2.53  | 114.11      | 107.27   |
| 154 | Av    | 301 | NAD  | C5A-N7A-C8A | 2.53  | 107.42      | 103.45   |
| 150 | DJ    | 401 | UTP  | O4'-C4'-C3' | -2.48 | 100.23      | 105.15   |
| 150 | DJ    | 401 | UTP  | C6-N1-C2    | -2.46 | 118.00      | 121.00   |
| 152 | Cg    | 501 | GTP  | O2G-PG-O1G  | -2.41 | 101.43      | 110.83   |
| 154 | Av    | 301 | NAD  | C2D-C3D-C4D | -2.39 | 98.00       | 102.61   |
| 152 | Cg    | 501 | GTP  | C4-C5-N7    | -2.32 | 106.99      | 110.67   |
| 152 | Cg    | 501 | GTP  | N2-C2-N1    | 2.23  | 121.46      | 116.76   |
| 152 | Cg    | 501 | GTP  | C8-N7-C5    | 2.09  | 107.99      | 104.26   |

There are no chirality outliers.

All (45) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 150 | DJ    | 401 | UTP  | C5'-O5'-PA-O1A  |
| 150 | DJ    | 401 | UTP  | C5'-O5'-PA-O2A  |
| 150 | DJ    | 401 | UTP  | O4'-C4'-C5'-O5' |
| 152 | Cg    | 501 | GTP  | PB-O3B-PG-O2G   |
| 154 | Av    | 301 | NAD  | O4D-C4D-C5D-O5D |
| 149 | CA    | 735 | SPD  | N6-C7-C8-C9     |
| 153 | CA    | 738 | SPM  | C2-C3-C4-N5     |
| 149 | CA    | 735 | SPD  | C3-C4-C5-N6     |
| 153 | CA    | 738 | SPM  | N10-C11-C12-C13 |
| 149 | CA    | 736 | SPD  | C3-C4-C5-N6     |
| 150 | DJ    | 401 | UTP  | C3'-C4'-C5'-O5' |
| 149 | CA    | 735 | SPD  | C2-C3-C4-C5     |
| 154 | Av    | 301 | NAD  | C3D-C4D-C5D-O5D |
| 153 | CA    | 738 | SPM  | C6-C7-C8-C9     |
| 153 | CA    | 738 | SPM  | C7-C8-C9-N10    |
| 149 | DL    | 401 | SPD  | C4-C5-N6-C7     |
| 149 | CA    | 735 | SPD  | C4-C5-N6-C7     |
| 154 | Av    | 301 | NAD  | C2B-C1B-N9A-C8A |
| 149 | DL    | 401 | SPD  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 150 | DJ    | 401 | UTP  | C5'-O5'-PA-O3A  |
| 154 | Av    | 301 | NAD  | C5D-O5D-PN-O3   |
| 149 | CA    | 736 | SPD  | N1-C2-C3-C4     |
| 150 | DJ    | 401 | UTP  | O4'-C1'-N1-C2   |
| 149 | CA    | 736 | SPD  | C7-C8-C9-N10    |
| 149 | CA    | 737 | SPD  | C7-C8-C9-N10    |
| 150 | DJ    | 401 | UTP  | O4'-C1'-N1-C6   |
| 153 | CA    | 738 | SPM  | C11-C12-C13-N14 |
| 152 | Cg    | 501 | GTP  | PG-O3B-PB-O2B   |
| 153 | CA    | 738 | SPM  | C12-C11-N10-C9  |
| 150 | DJ    | 401 | UTP  | C2'-C1'-N1-C6   |
| 149 | CA    | 737 | SPD  | C3-C4-C5-N6     |
| 150 | DJ    | 401 | UTP  | C2'-C1'-N1-C2   |
| 153 | CA    | 738 | SPM  | C7-C6-N5-C4     |
| 154 | Av    | 301 | NAD  | PA-O3-PN-O1N    |
| 149 | CA    | 736 | SPD  | C4-C5-N6-C7     |
| 152 | Cg    | 501 | GTP  | PB-O3B-PG-O1G   |
| 149 | CA    | 736 | SPD  | C8-C7-N6-C5     |
| 152 | Cg    | 501 | GTP  | PG-O3B-PB-O1B   |
| 154 | Av    | 301 | NAD  | PA-O3-PN-O2N    |
| 150 | DJ    | 401 | UTP  | C4'-C5'-O5'-PA  |
| 154 | Av    | 301 | NAD  | C2B-C1B-N9A-C4A |
| 149 | CA    | 737 | SPD  | C2-C3-C4-C5     |
| 149 | CA    | 735 | SPD  | C7-C8-C9-N10    |
| 153 | CA    | 738 | SPM  | N1-C2-C3-C4     |
| 154 | Av    | 301 | NAD  | O4B-C1B-N9A-C8A |

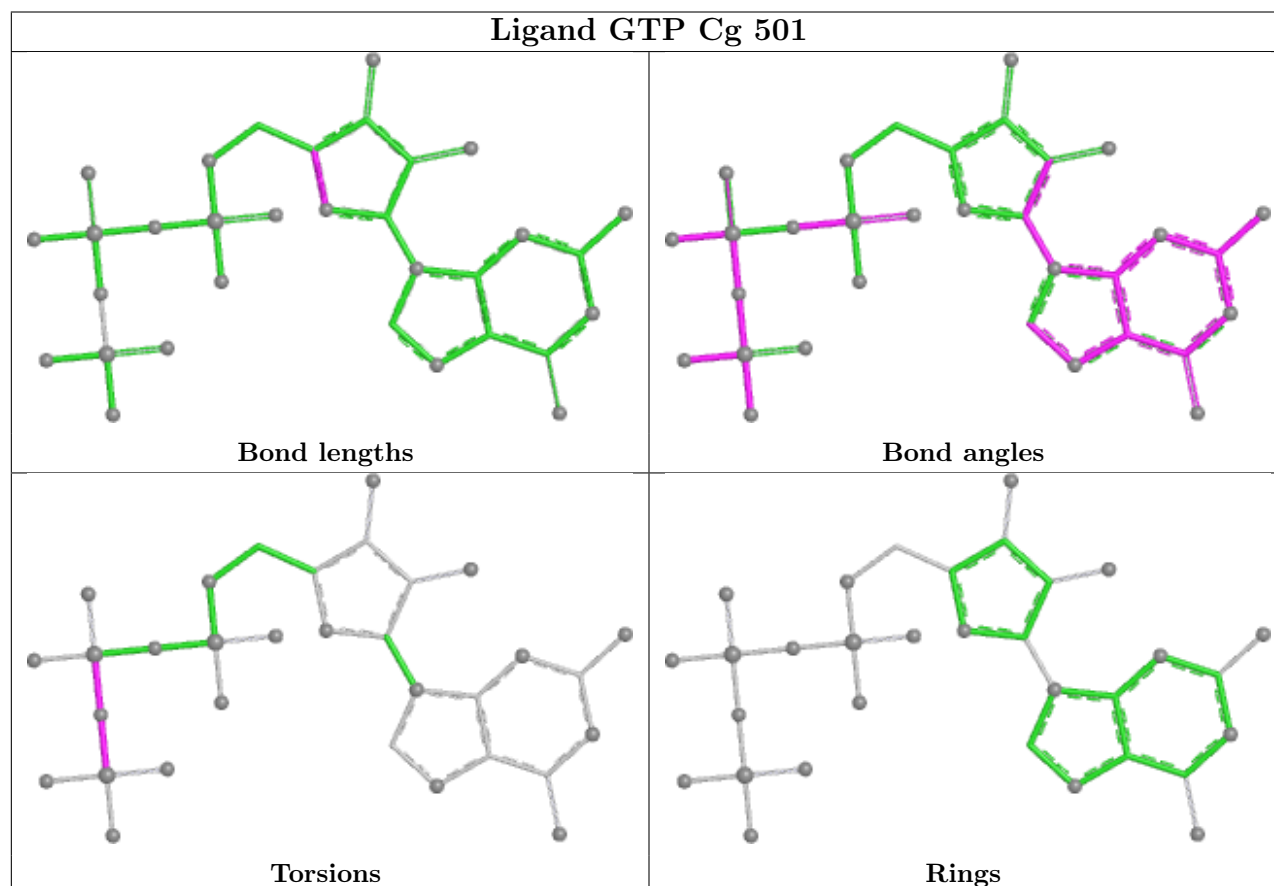
There are no ring outliers.

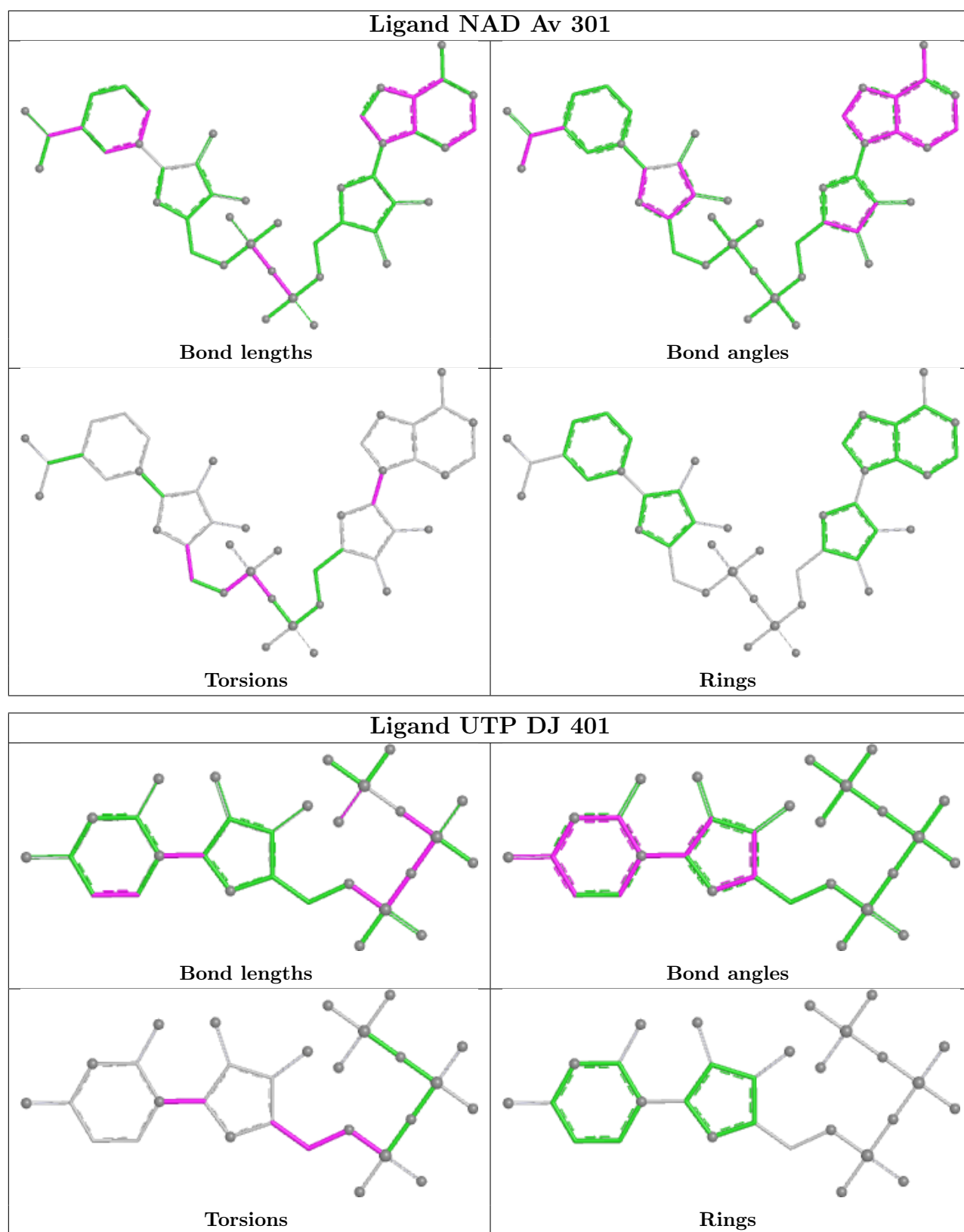
6 monomers are involved in 20 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 153 | CA    | 738 | SPM  | 1       | 0            |
| 152 | Cg    | 501 | GTP  | 7       | 0            |
| 149 | CA    | 735 | SPD  | 2       | 0            |
| 154 | Av    | 301 | NAD  | 4       | 0            |
| 149 | CA    | 736 | SPD  | 1       | 0            |
| 150 | DJ    | 401 | UTP  | 5       | 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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 140 | UD    | 3                |
| 77  | AK    | 1                |
| 71  | A8    | 1                |
| 84  | AV    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | UD    | 90:UNK    | C      | 136:UNK   | N      | 14.38        |
| 1     | UD    | 158:UNK   | C      | 159:UNK   | N      | 11.27        |
| 1     | UD    | 68:UNK    | C      | 69:UNK    | N      | 10.02        |
| 1     | AK    | 250:LEU   | C      | 251:THR   | N      | 5.50         |
| 1     | A8    | 40:PRO    | C      | 41:LYS    | N      | 5.26         |
| 1     | AV    | 56:ALA    | C      | 57:ASN    | N      | 5.01         |

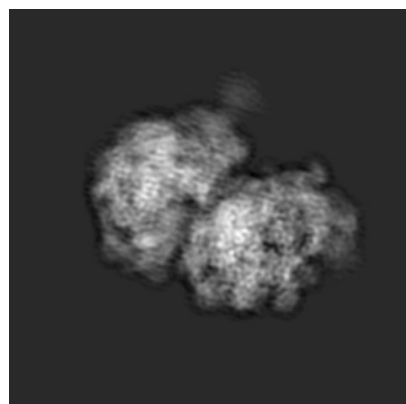
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0229. These allow visual inspection of the internal detail of the map and identification of artifacts.

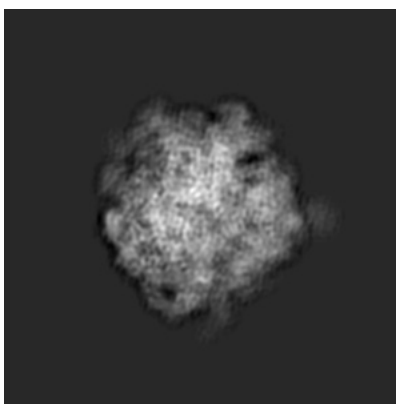
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

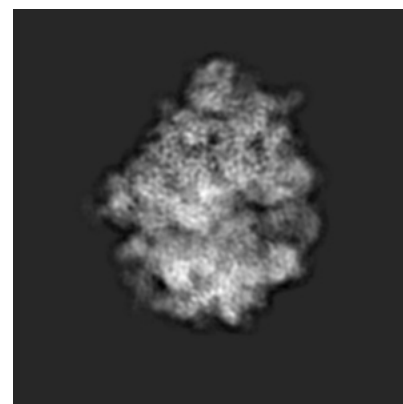
#### 6.1.1 Primary map



X

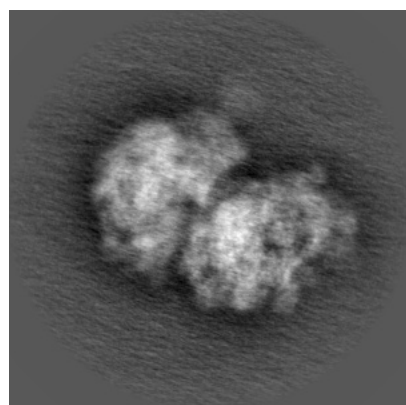


Y

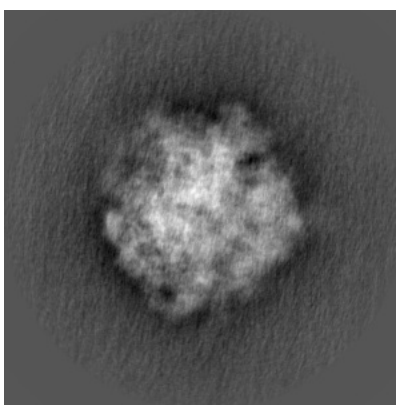


Z

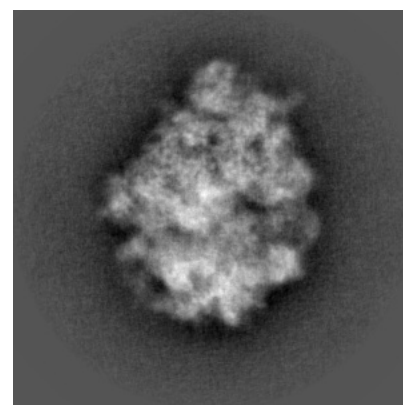
#### 6.1.2 Raw map



X



Y

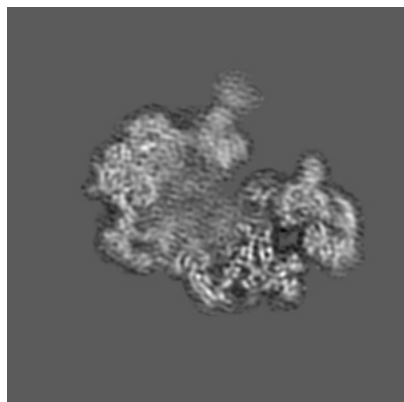


Z

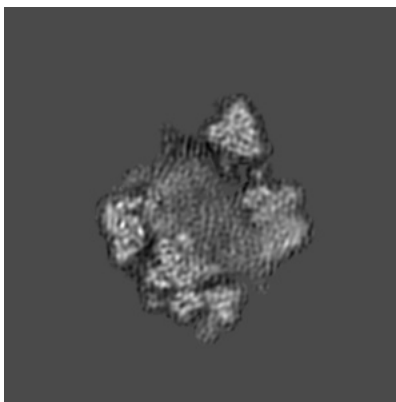
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

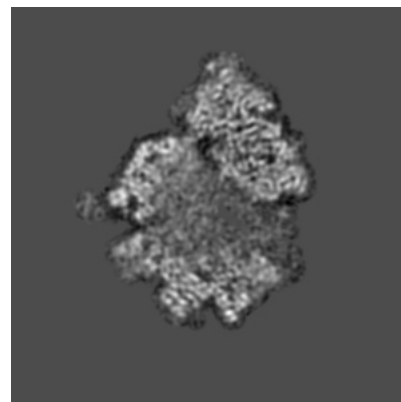
### 6.2.1 Primary map



X Index: 200

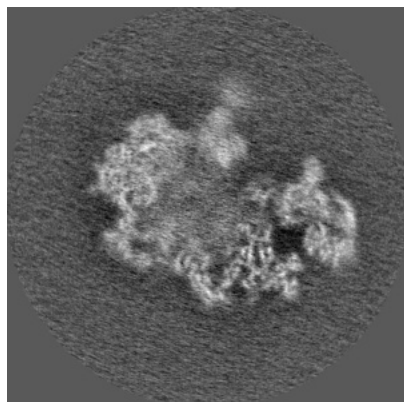


Y Index: 200

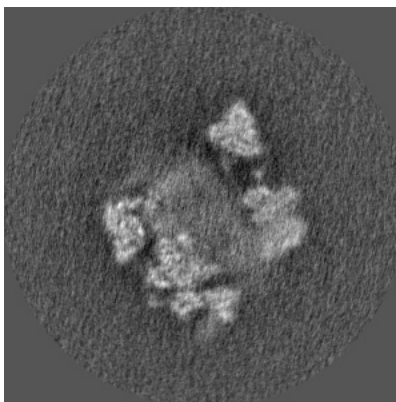


Z Index: 200

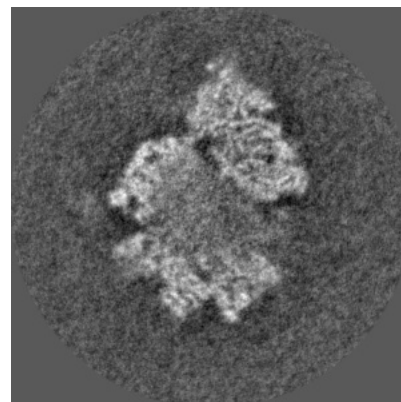
### 6.2.2 Raw map



X Index: 200



Y Index: 200

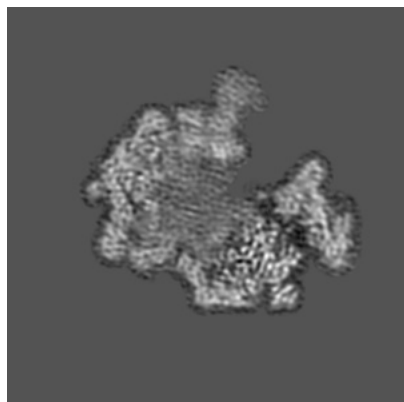


Z Index: 200

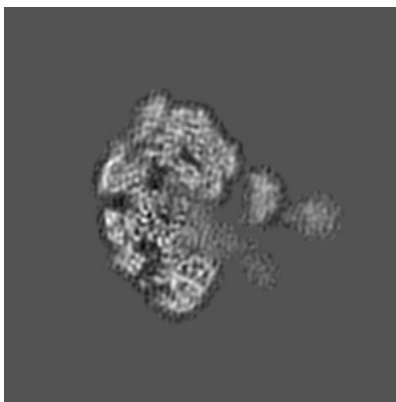
The images above show central slices of the map in three orthogonal directions.

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

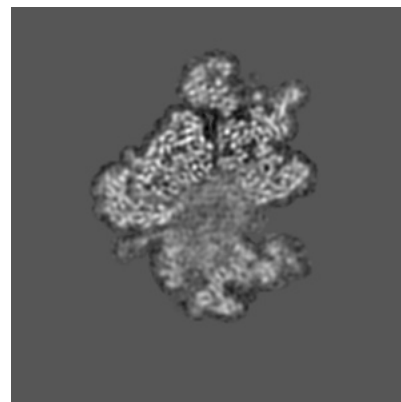
### 6.3.1 Primary map



X Index: 192

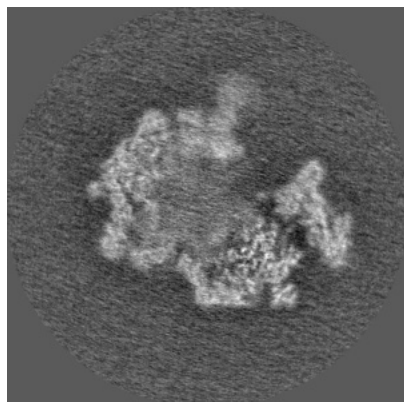


Y Index: 231

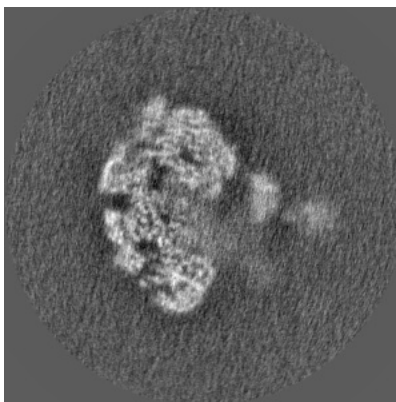


Z Index: 174

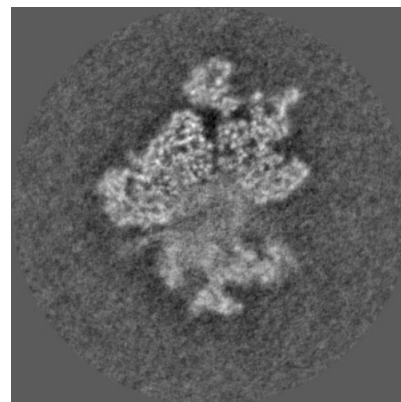
### 6.3.2 Raw map



X Index: 192



Y Index: 230

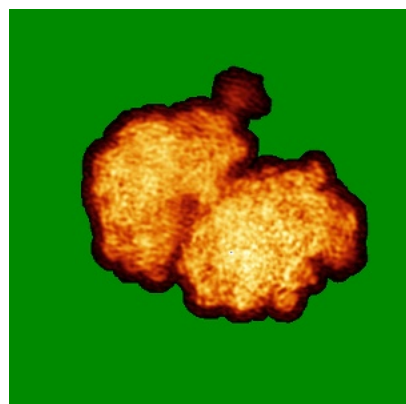


Z Index: 173

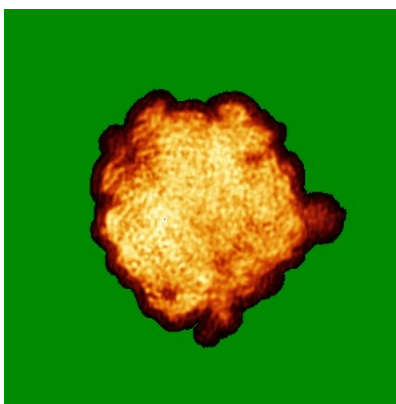
The images above show the largest variance slices of the map in three orthogonal directions.

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

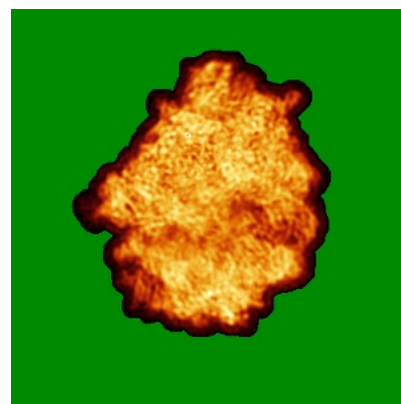
### 6.4.1 Primary map



X

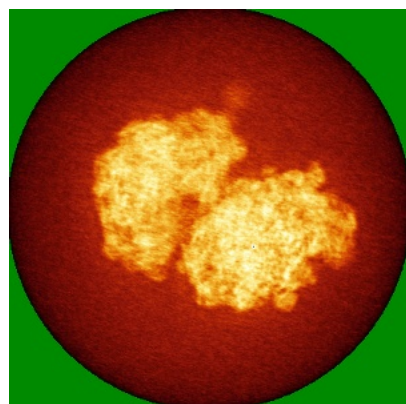


Y

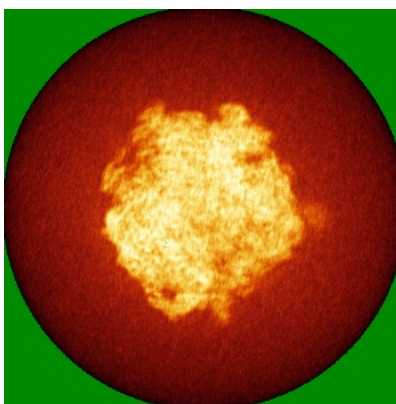


Z

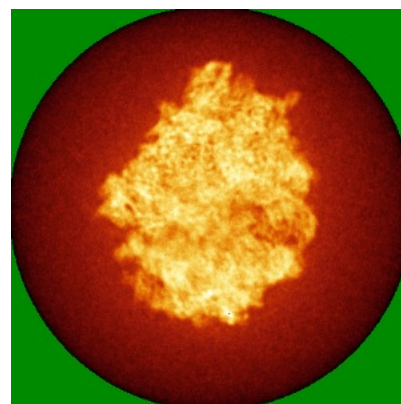
### 6.4.2 Raw map



X



Y

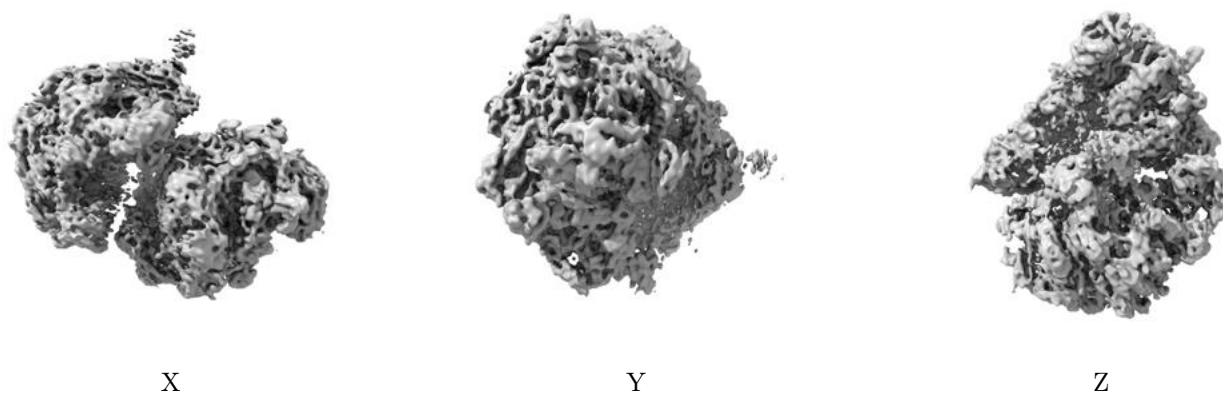


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

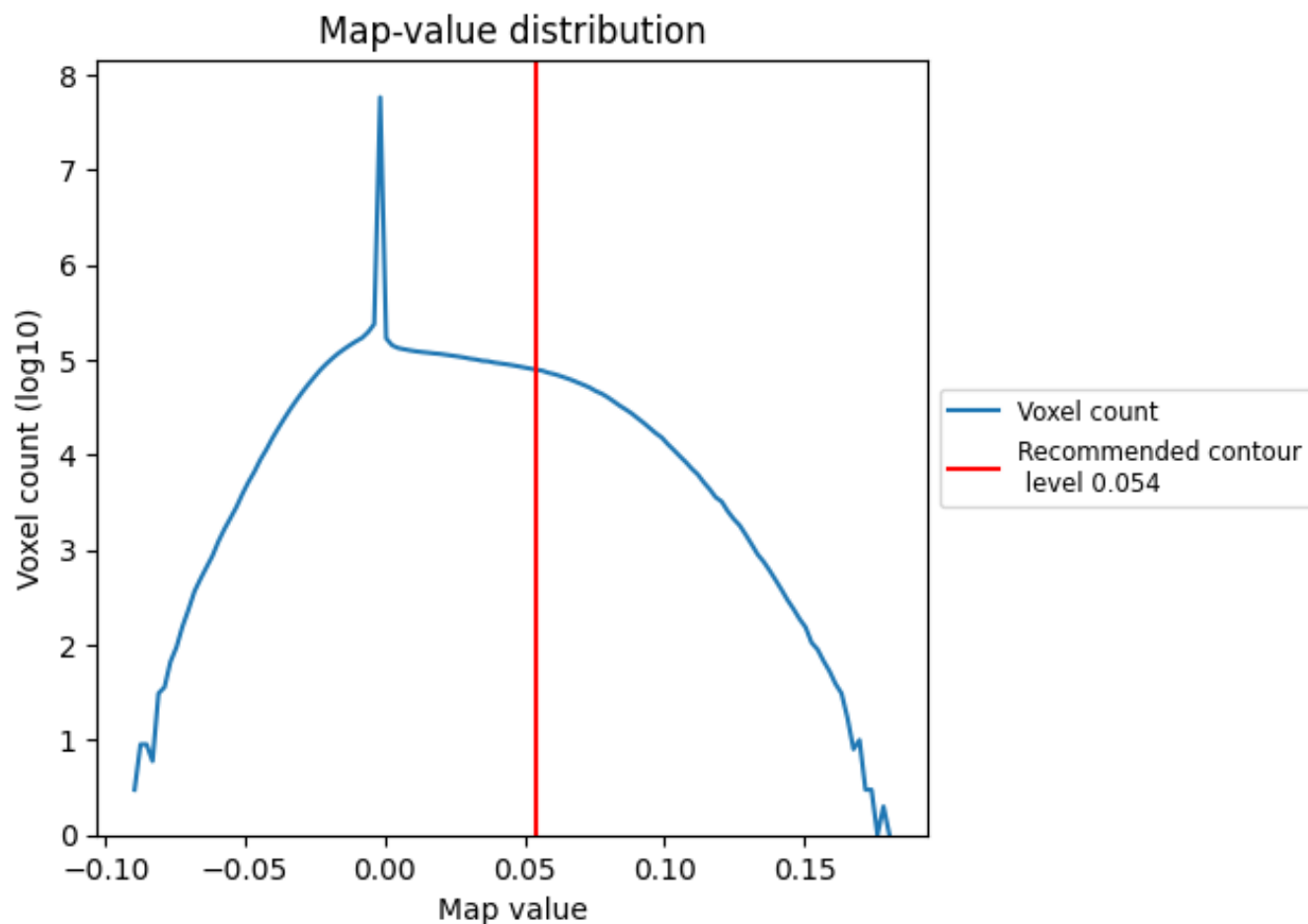
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

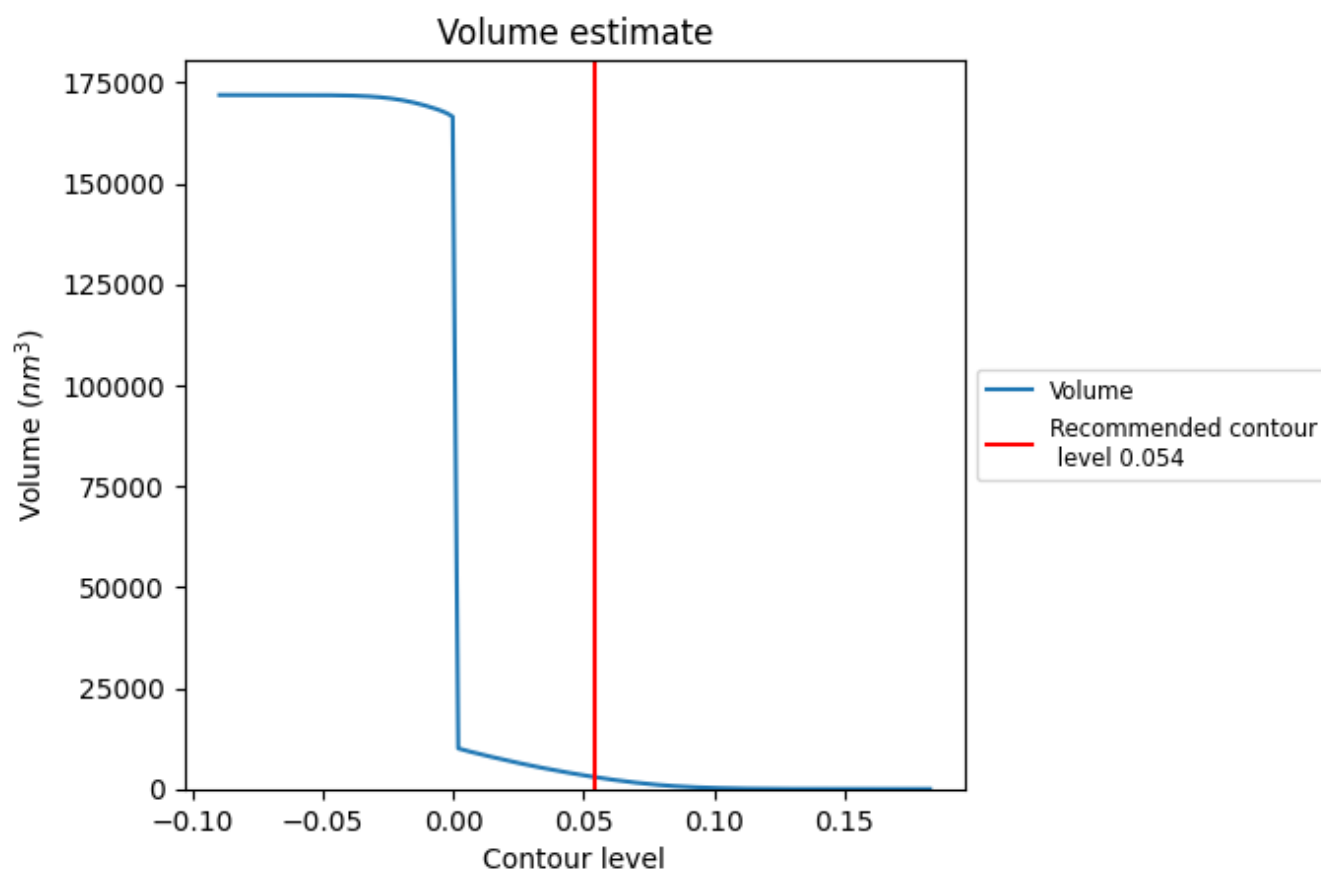
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

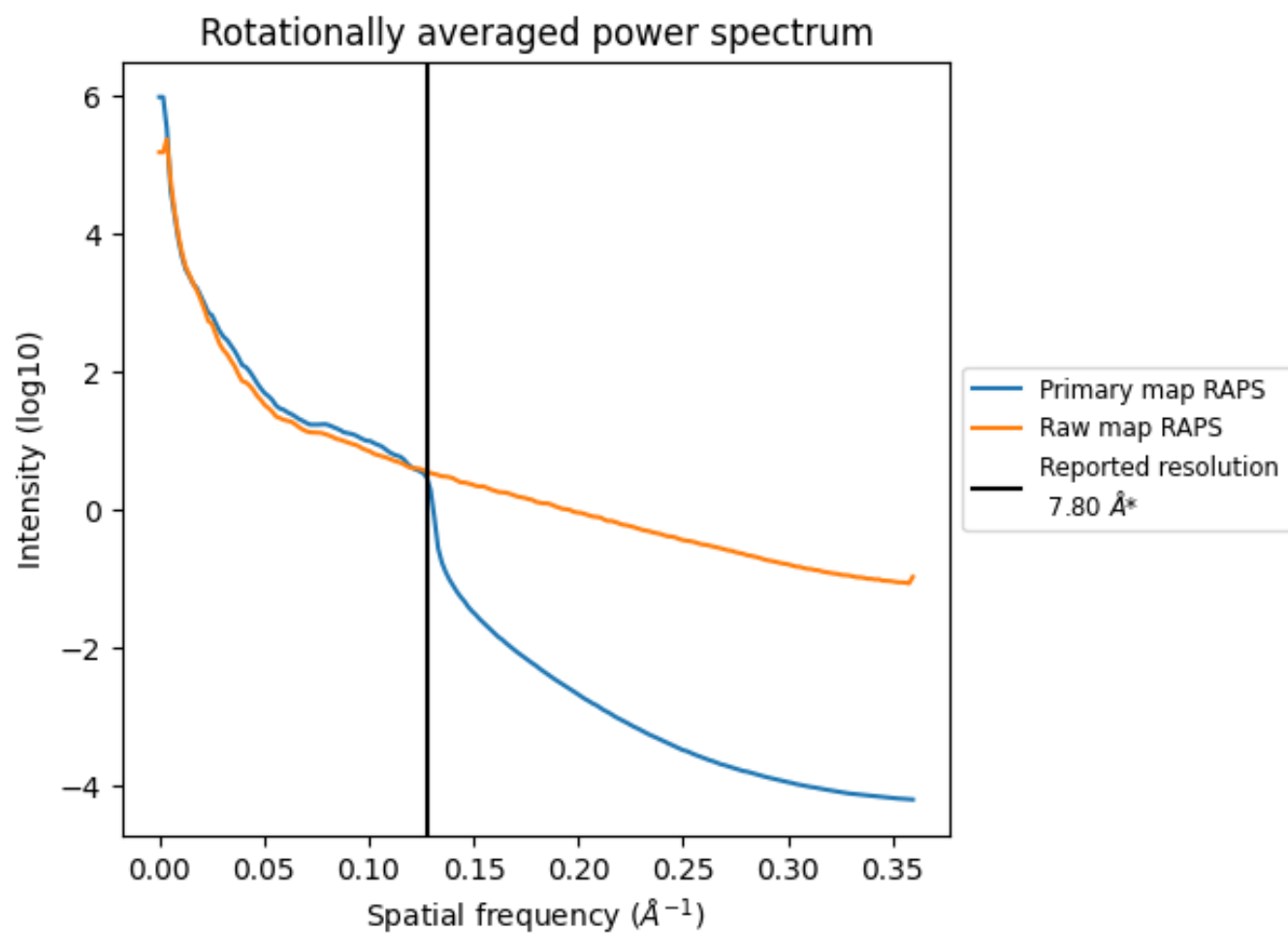


The volume at the recommended contour level is 2967  $\text{nm}^3$ ; this corresponds to an approximate mass of 2680 kDa.

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 ⓘ

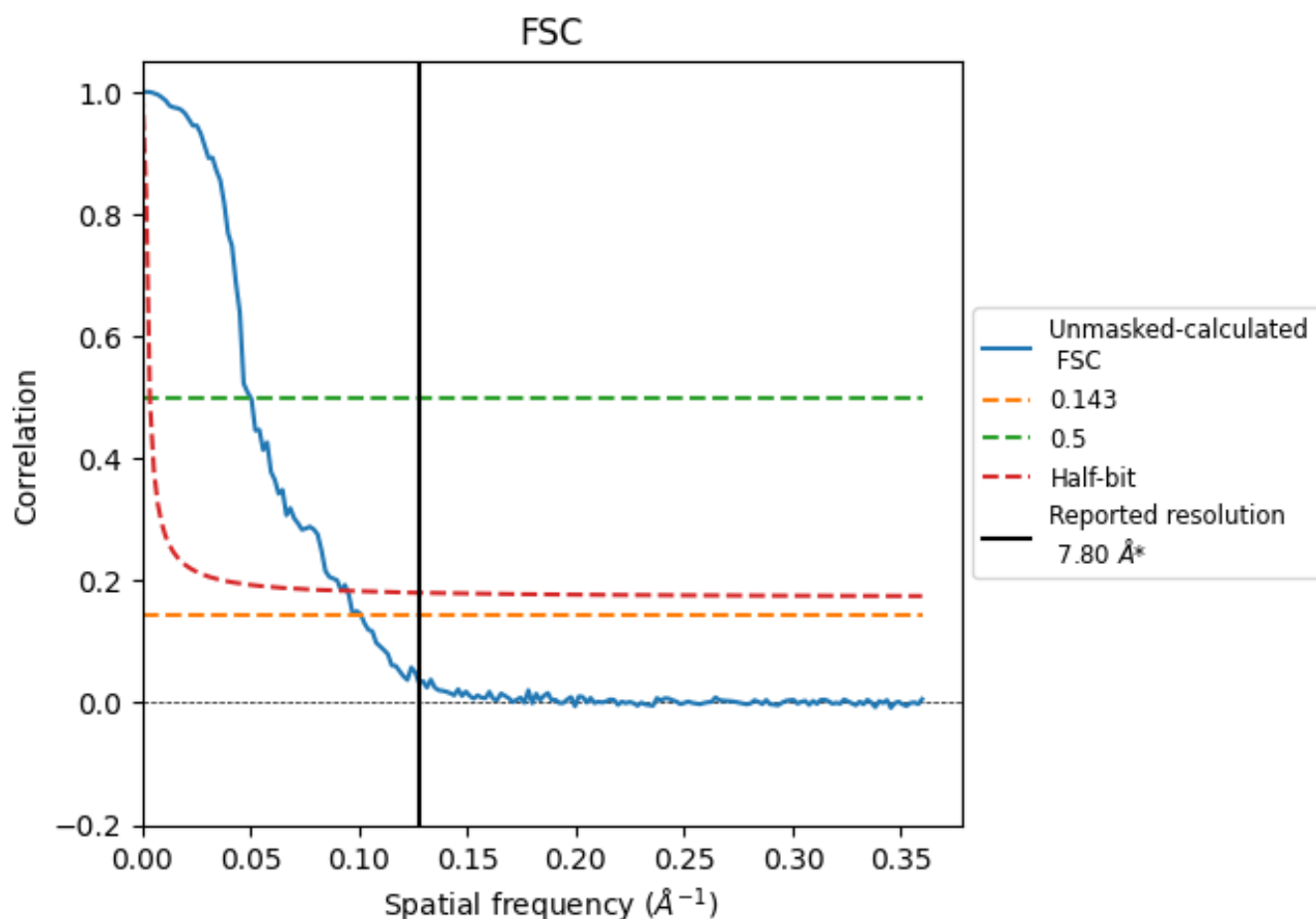


\*Reported resolution corresponds to spatial frequency of 0.128 Å<sup>-1</sup>

## 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 0.128  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

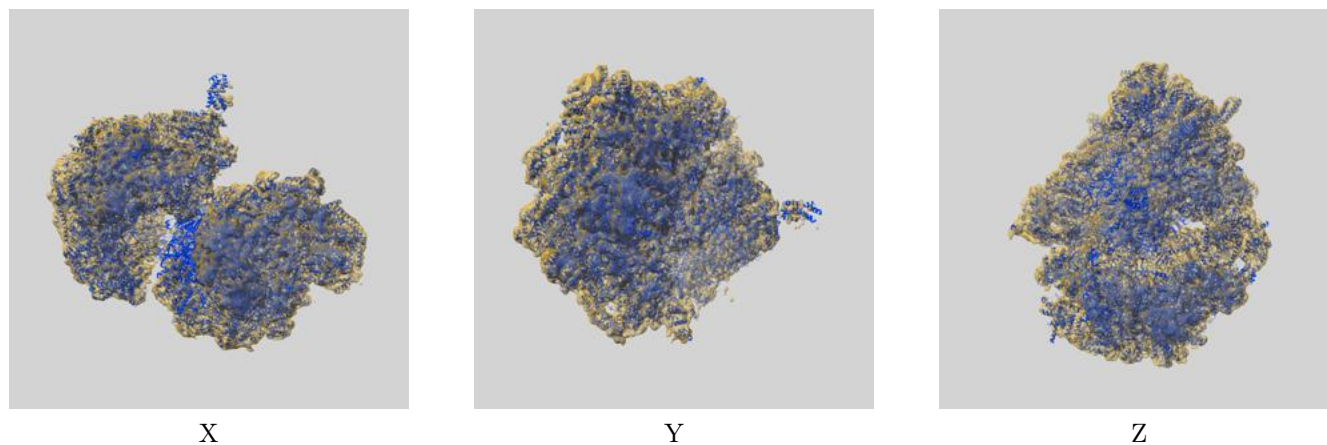
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 7.80                               | -     | -        |
| Author-provided FSC curve | -                                  | -     | -        |
| Unmasked-calculated*      | 9.90                               | 20.04 | 10.57    |

\*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 9.90 differs from the reported value 7.8 by more than 10 %

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

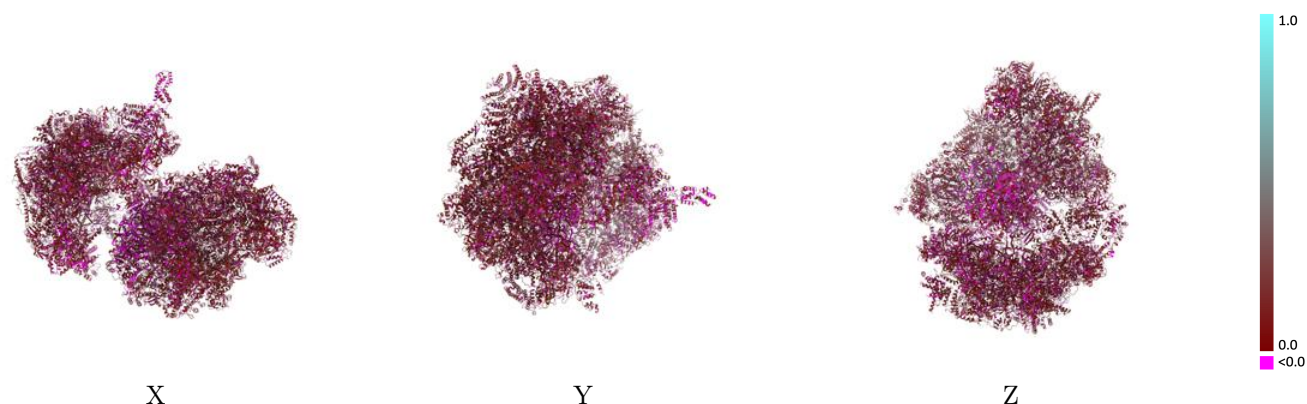
This section contains information regarding the fit between EMDB map EMD-0229 and PDB model 6HIV. Per-residue inclusion information can be found in section [3](#) on page [51](#).

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



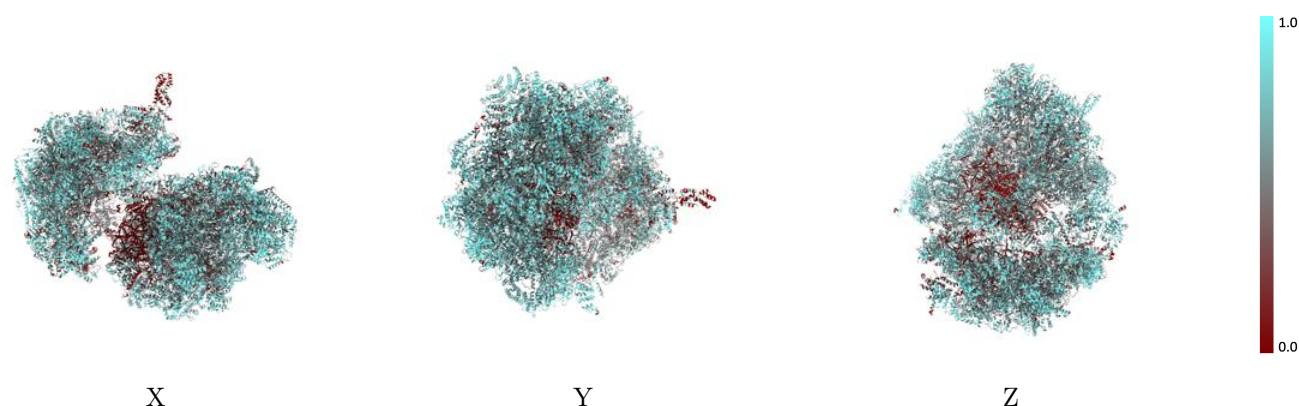
The images above show the 3D surface view of the map at the recommended contour level 0.054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



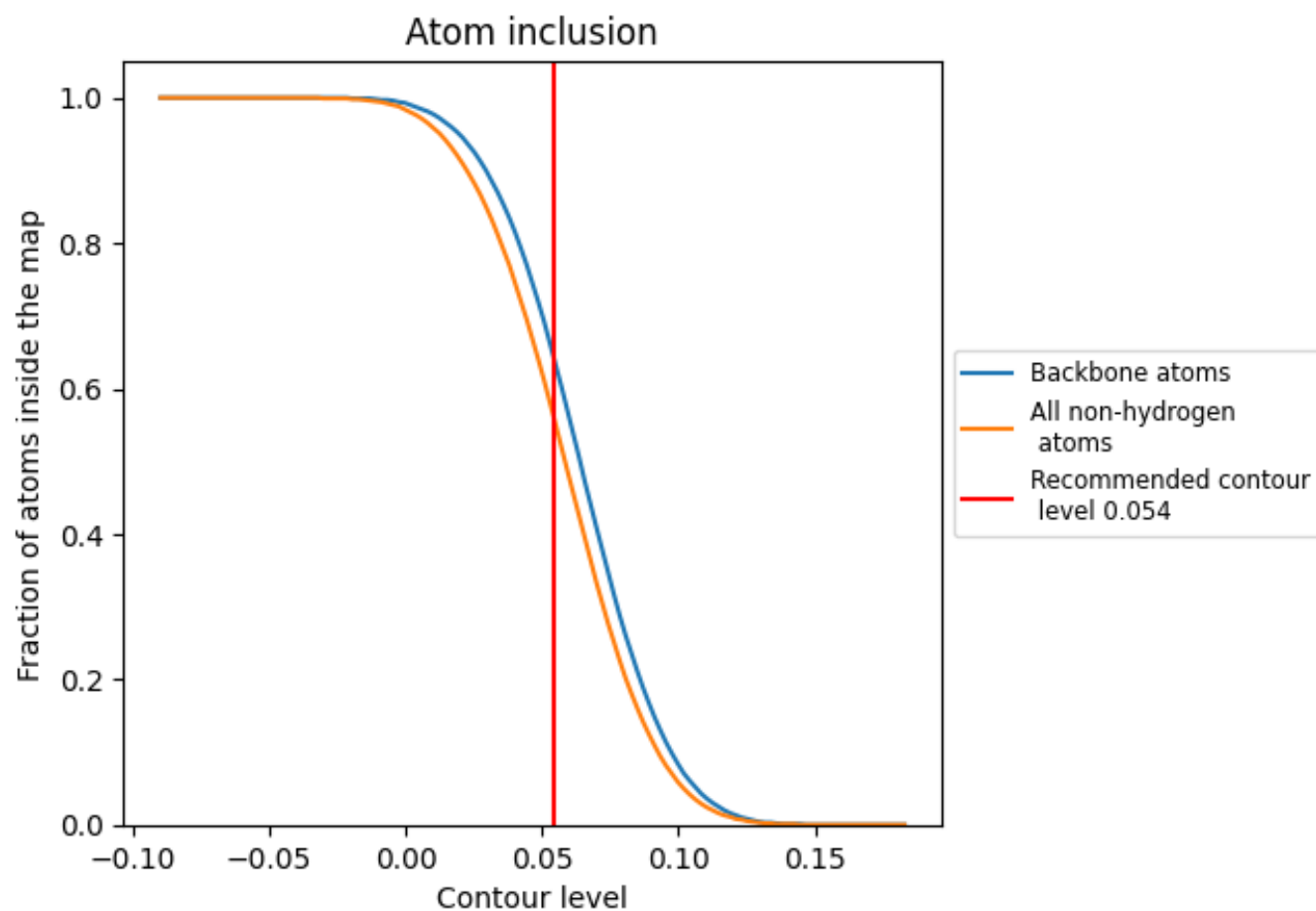
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.054).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (0.054) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5660   |  0.1160   |
| A0    |  0.5420   |  0.1260   |
| A1    |  0.4980   |  0.1090   |
| A2    |  0.7340   |  0.1440   |
| A3    |  0.5540   |  0.1270   |
| A4    |  0.4820   |  0.1320   |
| A5    |  0.5620   |  0.0700   |
| A6    |  0.3140   |  0.1280   |
| A8    |  0.3560   |  0.1060   |
| A9    |  0.2450   |  0.0770   |
| AA    |  0.6590   |  0.1450   |
| AB    |  0.2040   |  0.0370   |
| AC    |  0.2140   |  0.1210   |
| AD    |  0.0640   |  0.0040   |
| AE    |  0.5220  |  0.0880  |
| AF    |  0.6060 |  0.1060 |
| AG    |  0.0370 |  0.0440 |
| AI    |  0.6170 |  0.1130 |
| AJ    |  0.4960 |  0.0700 |
| AK    |  0.6040 |  0.0940 |
| AN    |  0.4240 |  0.0880 |
| AP    |  0.5230 |  0.0920 |
| AQ    |  0.4830 |  0.1010 |
| AR    |  0.5570 |  0.1100 |
| AT    |  0.3660 |  0.0830 |
| AU    |  0.5740 |  0.1090 |
| AV    |  0.5840 |  0.0980 |
| AW    |  0.5430 |  0.1180 |
| AX    |  0.5900 |  0.1150 |
| AY    |  0.6000 |  0.1320 |
| Ab    |  0.6640 |  0.1270 |
| Ad    |  0.6080 |  0.1340 |
| Ae    |  0.6080 |  0.1130 |
| Af    |  0.5990 |  0.1290 |
| Ag    |  0.5790 |  0.1100 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Aj    |  0.7350   |  0.1160   |
| Al    |  0.5230   |  0.1230   |
| Ao    |  0.5200   |  0.1080   |
| Ap    |  0.5030   |  0.0730   |
| At    |  0.5650   |  0.1310   |
| Av    |  0.5980   |  0.1430   |
| BA    |  0.5790   |  0.1110   |
| BB    |  0.6650   |  0.1170   |
| BC    |  0.6660   |  0.1150   |
| BD    |  0.5600   |  0.1170   |
| BE    |  0.6100   |  0.1310   |
| BF    |  0.6480   |  0.1140   |
| BG    |  0.7310   |  0.1240   |
| BH    |  0.6260   |  0.1080   |
| BI    |  0.5810   |  0.0910   |
| BJ    |  0.6030   |  0.1280   |
| BK    |  0.3890   |  0.1030   |
| BL    |  0.5740   |  0.1290   |
| BM    |  0.6190   |  0.1250   |
| BN    |  0.5290  |  0.1070  |
| BO    |  0.5530 |  0.1050 |
| BP    |  0.5210 |  0.1280 |
| BQ    |  0.6600 |  0.1280 |
| BR    |  0.5920 |  0.1280 |
| BS    |  0.5660 |  0.1060 |
| BT    |  0.7240 |  0.1300 |
| BU    |  0.6410 |  0.1230 |
| BV    |  0.5610 |  0.0840 |
| BW    |  0.7220 |  0.1420 |
| BX    |  0.2220 |  0.0500 |
| BY    |  0.4920 |  0.1180 |
| BZ    |  0.6760 |  0.1050 |
| Ba    |  0.6570 |  0.1170 |
| Bb    |  0.6710 |  0.1280 |
| Bc    |  0.4770 |  0.1130 |
| Bd    |  0.6380 |  0.1270 |
| Be    |  0.4140 |  0.1240 |
| Bf    |  0.5700 |  0.0380 |
| Bg    |  0.5530 |  0.1120 |
| Bh    |  0.2680 |  0.0620 |
| CA    |  0.3200 |  0.0570 |
| CC    |  0.3480 |  0.0990 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| CE    |  0.5330   |  0.1260    |
| CF    |  0.5460   |  0.1060    |
| CH    |  0.5320   |  0.1480    |
| CI    |  0.5220   |  0.1190    |
| CJ    |  0.5830   |  0.1300    |
| CK    |  0.3840   |  0.0780    |
| CL    |  0.0040   |  0.0000    |
| CN    |  0.5190   |  0.1030    |
| CO    |  0.4830   |  0.1020    |
| CP    |  0.6340   |  0.1170    |
| CQ    |  0.3600   |  0.0700    |
| CR    |  0.4340   |  0.1130    |
| CS    |  0.5010   |  0.0870    |
| CU    |  0.2200   |  0.0410    |
| CZ    |  0.0000   |  0.0060    |
| Ca    |  0.5430   |  0.1220    |
| Cb    |  0.5640   |  0.1400    |
| Cd    |  0.5260   |  0.0810    |
| Cg    |  0.6680  |  0.1090   |
| Ci    |  0.5280 |  0.1080  |
| Cj    |  0.7420 |  0.1290  |
| Ck    |  0.6130 |  0.1340  |
| Cm    |  0.1540 |  0.0260  |
| Cn    |  0.0090 |  -0.0110 |
| Cp    |  0.6070 |  0.1290  |
| Cq    |  0.6400 |  0.1420  |
| Cr    |  0.7050 |  0.1400  |
| Cv    |  0.5840 |  0.1210  |
| DA    |  0.6830 |  0.1390  |
| DB    |  0.6110 |  0.1430  |
| DC    |  0.6740 |  0.1160  |
| DD    |  0.6320 |  0.1340  |
| DE    |  0.6960 |  0.1280  |
| DF    |  0.6430 |  0.1270  |
| DG    |  0.6740 |  0.1300  |
| DH    |  0.5390 |  0.1280  |
| DI    |  0.7140 |  0.1380  |
| DJ    |  0.6640 |  0.1200  |
| DK    |  0.6240 |  0.1310  |
| DL    |  0.3870 |  0.1200  |
| DM    |  0.6530 |  0.1280  |
| DN    |  0.6360 |  0.1350  |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| DO    |  0.7250   |  0.1350    |
| DP    |  0.7300   |  0.1320    |
| DQ    |  0.6990   |  0.1410    |
| DR    |  0.7140   |  0.1300    |
| DS    |  0.7080   |  0.1260    |
| DT    |  0.5890   |  0.1170    |
| DU    |  0.5920   |  0.1340    |
| DV    |  0.5520   |  0.1030    |
| DW    |  0.5560   |  0.1060    |
| DX    |  0.6310   |  0.1080    |
| DY    |  0.6290   |  0.1110    |
| DZ    |  0.5340   |  0.1430    |
| Da    |  0.0130   |  -0.0220   |
| UA    |  0.6300   |  0.1420    |
| UB    |  0.6430   |  0.1370    |
| UC    |  0.1810   |  0.0290    |
| UD    |  0.3370   |  0.1450    |
| UE    |  0.1510   |  0.0250    |
| UF    |  0.4720   |  0.1480    |
| UG    |  0.3680   |  0.1280    |
| UH    |  0.5690  |  0.2180   |
| UI    |  0.2160 |  0.1470  |
| UK    |  0.7500 |  0.2190  |
| UL    |  0.3670 |  0.1000  |
| UM    |  0.0560 |  0.0120  |
| UN    |  0.0760 |  0.0010  |
| UO    |  0.2670 |  0.1750  |
| UP    |  0.9050 |  0.2410  |
| UQ    |  0.0000 |  -0.0030 |
| UR    |  0.9790 |  0.2030  |
| US    |  0.0000 |  -0.0250 |
| UT    |  0.0230 |  0.0160  |
| UU    |  0.2880 |  0.0830  |
| UV    |  0.5420 |  0.1600  |
| UW    |  0.2620 |  0.0490  |
| UX    |  0.6670 |  0.2630  |