



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:57 PM UTC

PDB ID : 6HIW / pdb\_00006hiw  
EMDB ID : EMD-0230  
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the complete small mitoribosomal subunit in complex with mt-IF-3  
Authors : Ramrath, D.; 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 : 3.37 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

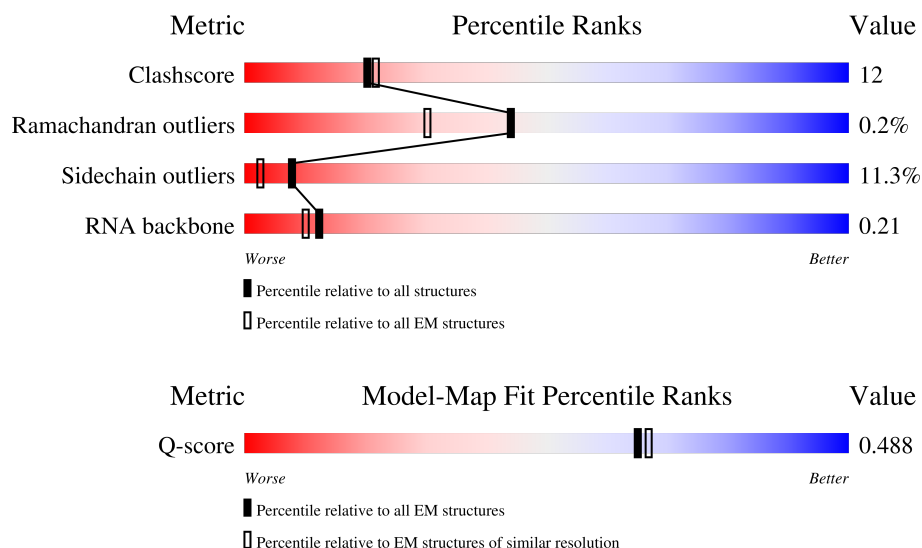
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.37 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.



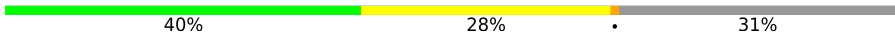
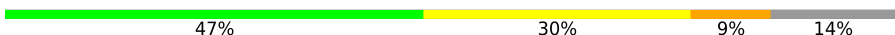
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14287 ( 2.87 - 3.87 )                                    |

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   |                  |
| 2   | DD    | 812    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | DI    | 407    |    |
| 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    | 747    |  |
| 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    |  |

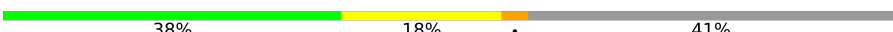
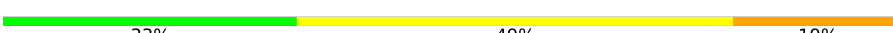
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | CC    | 74     |                  |
| 29  | CE    | 435    |                  |
| 30  | CF    | 160    |                  |
| 31  | CH    | 282    |                  |
| 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    | 325    |                  |
| 46  | Cd    | 440    |                  |
| 47  | Cg    | 498    |                  |
| 48  | Ci    | 181    |                  |
| 49  | Cj    | 257    |                  |
| 50  | Ck    | 874    |                  |
| 51  | Cm    | 215    |                  |
| 52  | Cn    | 250    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 53  | Cp    | 187    |  |
| 54  | Cq    | 263    |  |
| 55  | Cr    | 439    |  |
| 56  | Cv    | 1211   |  |
| 57  | CA    | 621    |  |
| 58  | UO    | 5      |  |
| 59  | UP    | 7      |  |
| 60  | UQ    | 32     |  |
| 61  | UR    | 8      |  |
| 62  | US    | 54     |  |
| 63  | UT    | 44     |  |

## 2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 177122 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 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DM    | 69      | PHE      | TYR    | conflict | UNP Q57XL2 |
| DM    | 97      | ASN      | SER    | conflict | UNP Q57XL2 |
| DM    | 138     | SER      | PRO    | conflict | UNP Q57XL2 |
| DM    | 173     | ALA      | THR    | conflict | UNP Q57XL2 |
| DM    | 206     | ALA      | THR    | conflict | UNP Q57XL2 |

- 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    | 189      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1613  | 1037 | 290 | 277 | 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 are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DR    | 65      | GLY      | SER    | conflict | UNP Q57UA2 |
| DR    | 94      | GLY      | GLU    | conflict | UNP Q57UA2 |
| DR    | 128     | PRO      | SER    | conflict | UNP Q57UA2 |
| DR    | 229     | ARG      | GLN    | conflict | UNP Q57UA2 |

- 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 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DU    | 119     | ILE      | LEU    | conflict | UNP Q582T9 |
| DU    | 152     | ILE      | VAL    | conflict | UNP Q582T9 |

- 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 are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DB    | 23      | VAL      | ALA    | conflict | UNP Q586P5 |
| DB    | 359     | ILE      | THR    | conflict | UNP Q586P5 |
| DB    | 384     | GLN      | HIS    | conflict | UNP Q586P5 |
| DB    | 402     | THR      | ILE    | conflict | UNP Q586P5 |
| DB    | 423     | THR      | ALA    | conflict | UNP Q586P5 |
| DB    | 586     | ARG      | HIS    | conflict | UNP Q586P5 |
| DB    | 593     | ARG      | LYS    | conflict | UNP Q586P5 |
| DB    | 647     | SER      | GLY    | conflict | UNP Q586P5 |

- 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 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DC    | 53      | ALA      | THR    | conflict | UNP Q57YB5 |
| DC    | 365     | LYS      | GLU    | conflict | UNP Q57YB5 |
| DC    | 385     | THR      | ALA    | conflict | UNP Q57YB5 |
| DC    | 405     | ILE      | VAL    | conflict | UNP Q57YB5 |
| DC    | 641     | SER      | PRO    | conflict | UNP Q57YB5 |
| DC    | 651     | LYS      | GLU    | conflict | UNP Q57YB5 |
| DC    | 731     | GLU      | ASP    | conflict | UNP Q57YB5 |
| DC    | 814     | GLN      | HIS    | conflict | UNP Q57YB5 |
| DC    | 1097    | ALA      | VAL    | conflict | UNP Q57YB5 |
| DC    | 1113    | THR      | ILE    | conflict | UNP Q57YB5 |

- 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 is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DE    | 514     | THR      | SER    | conflict | 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 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 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 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DW    | 74      | THR      | MET    | conflict | UNP Q383N9 |

- 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 |         |       |

- Molecule 29 is a protein called uS5m.

| 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 uS12m.

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

- 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 |
| 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 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 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 |
| 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 bS21m.

| 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 are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CZ    | 6       | SER      | GLY    | conflict | UNP Q57WU2 |
| CZ    | 30      | THR      | ILE    | conflict | UNP Q57WU2 |
| CZ    | 172     | THR      | ALA    | conflict | UNP Q57WU2 |

- 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 16 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     | ALA      | -      | expression tag | UNP Q57VB2 |
| Cb    | 313     | CYS      | -      | expression tag | UNP Q57VB2 |
| Cb    | 314     | SER      | -      | expression tag | UNP Q57VB2 |
| Cb    | 315     | ARG      | -      | expression tag | UNP Q57VB2 |
| Cb    | 316     | ASP      | -      | expression tag | UNP Q57VB2 |
| Cb    | 317     | GLY      | -      | expression tag | UNP Q57VB2 |
| Cb    | 318     | PHE      | -      | expression tag | UNP Q57VB2 |
| Cb    | 319     | ALA      | -      | expression tag | UNP Q57VB2 |
| Cb    | 320     | LEU      | -      | expression tag | UNP Q57VB2 |
| Cb    | 321     | MET      | -      | expression tag | UNP Q57VB2 |
| Cb    | 322     | LYS      | -      | expression tag | UNP Q57VB2 |
| Cb    | 323     | ALA      | -      | expression tag | UNP Q57VB2 |
| Cb    | 324     | ASN      | -      | expression tag | UNP Q57VB2 |
| Cb    | 325     | 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     |
|     |       |          | 2386  | 1491 | 442 | 443 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Cd    | 299     | UNK      | GLY    | conflict | UNP Q38DK6 |

- 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 mS41.

| 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 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Cq    | 48      | THR      | ALA    | conflict | UNP Q586A1 |
| Cq    | 167     | MET      | VAL    | conflict | UNP Q586A1 |

- 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 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 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        | -      | insertion | GB 343546 |
| CA    | 615     | U        | -      | insertion | GB 343546 |
| CA    | 616     | U        | -      | insertion | GB 343546 |
| CA    | 617     | U        | -      | insertion | GB 343546 |
| CA    | 618     | U        | -      | insertion | GB 343546 |
| CA    | 619     | U        | -      | insertion | GB 343546 |
| CA    | 620     | U        | -      | insertion | GB 343546 |
| CA    | 621     | U        | -      | insertion | GB 343546 |

- Molecule 58 is a protein called Unknown Protein.

| 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 Unknown Protein.

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

- Molecule 60 is a protein called Unknown Protein.

| 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 Unknown Protein.

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

- Molecule 62 is a protein called Unknown Protein.

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

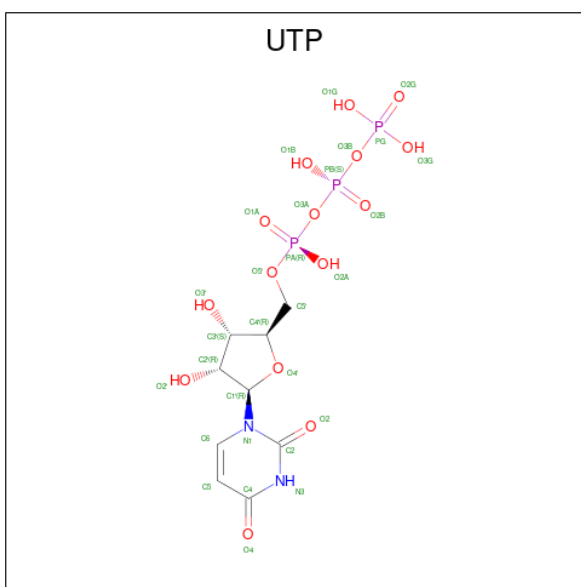
- Molecule 63 is a protein called Unknown Protein.

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

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 64  | DA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 64  | DS    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 64  | Cr    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 65 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>2</sub>O<sub>15</sub>P<sub>3</sub>).

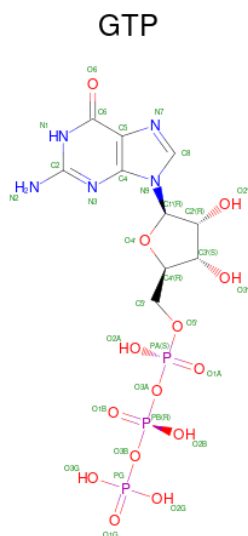


| Mol | Chain | Residues | Atoms |   |   |    |   | AltConf |
|-----|-------|----------|-------|---|---|----|---|---------|
| 65  | DJ    | 1        | Total | C | N | O  | P | 0       |
|     |       |          | 29    | 9 | 2 | 15 | 3 |         |

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

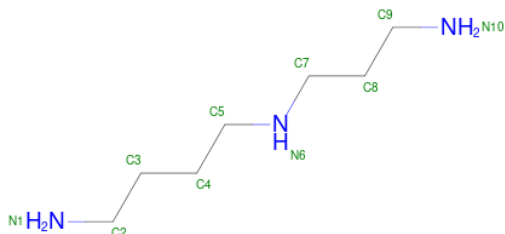
| Mol | Chain | Residues | Atoms             | AltConf |
|-----|-------|----------|-------------------|---------|
| 66  | CQ    | 1        | Total Mg<br>1 1   | 0       |
| 66  | Ca    | 1        | Total Mg<br>1 1   | 0       |
| 66  | Cg    | 1        | Total Mg<br>1 1   | 0       |
| 66  | Cv    | 1        | Total Mg<br>1 1   | 0       |
| 66  | CA    | 35       | Total Mg<br>35 35 | 0       |

- Molecule 67 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 67  | Cg    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 68 is SPERMIDINE (CCD ID: SPD) (formula:  $\text{C}_7\text{H}_{19}\text{N}_3$ ).



| Mol | Chain | Residues | Atoms       |        |        | AltConf |
|-----|-------|----------|-------------|--------|--------|---------|
| 68  | CA    | 1        | Total<br>10 | C<br>7 | N<br>3 | 0       |
| 68  | CA    | 1        | Total<br>10 | C<br>7 | N<br>3 | 0       |
| 68  | CA    | 1        | Total<br>10 | C<br>7 | N<br>3 | 0       |

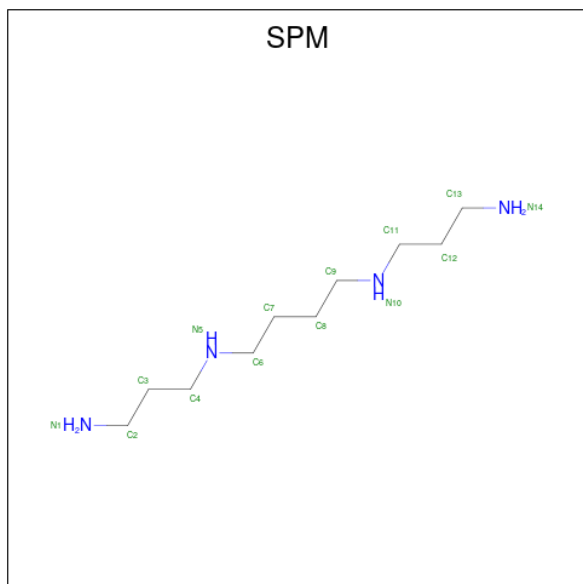
*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 68  | CA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 69 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 69  | CA    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

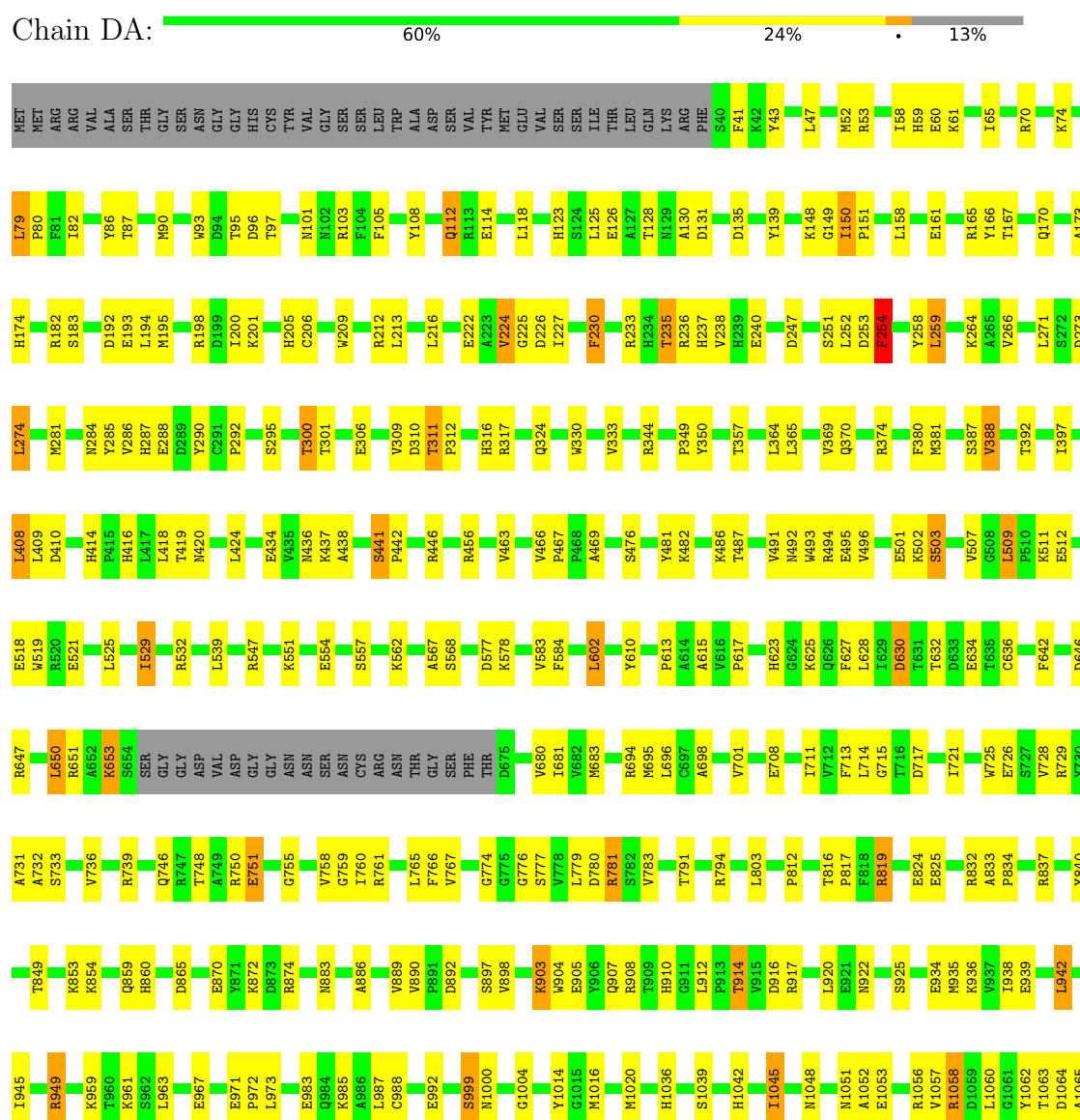
- Molecule 70 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 70  | Cg    | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |

### 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

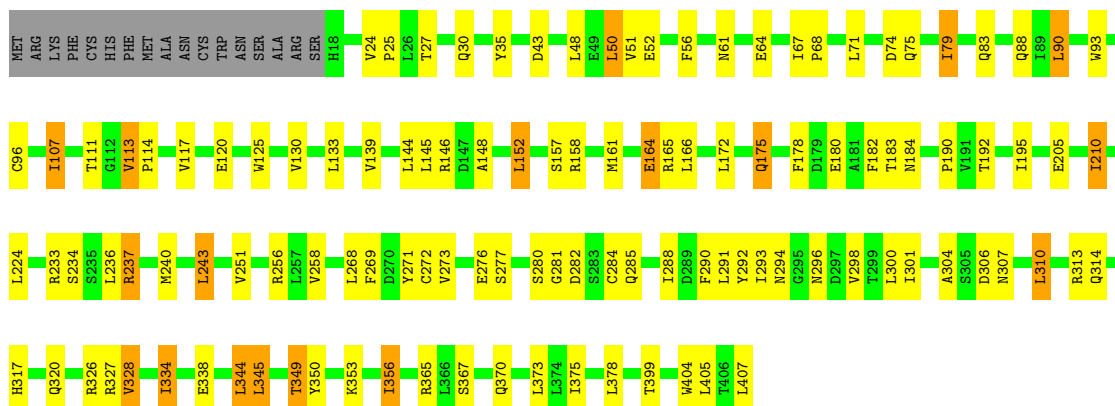






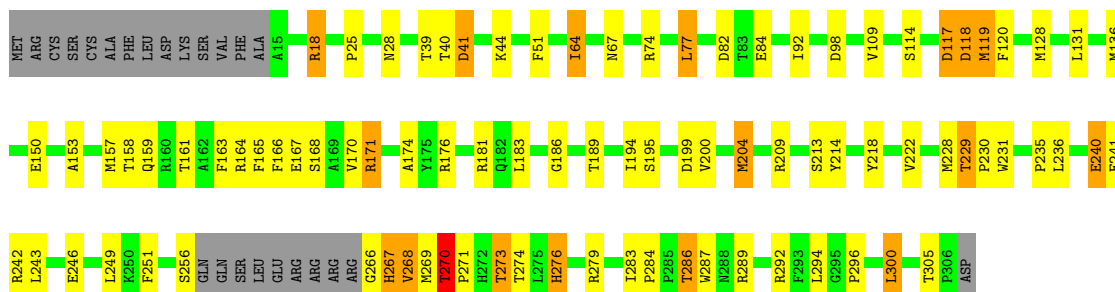
• Molecule 3: mS56

Chain DI: 67% 25%



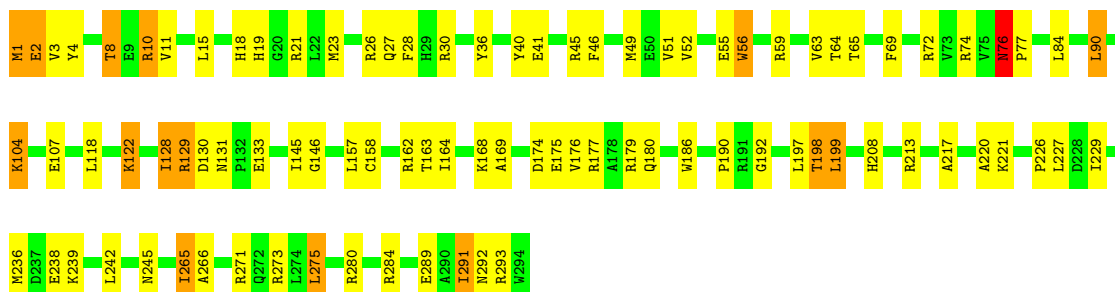
• Molecule 4: mS59

Chain DL: 63% 23% 6% 8%



• Molecule 5: mS60

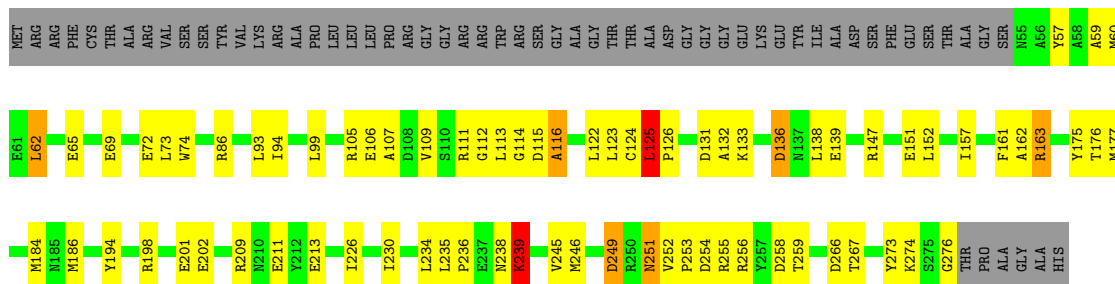
Chain DM: 69% 26% 5%



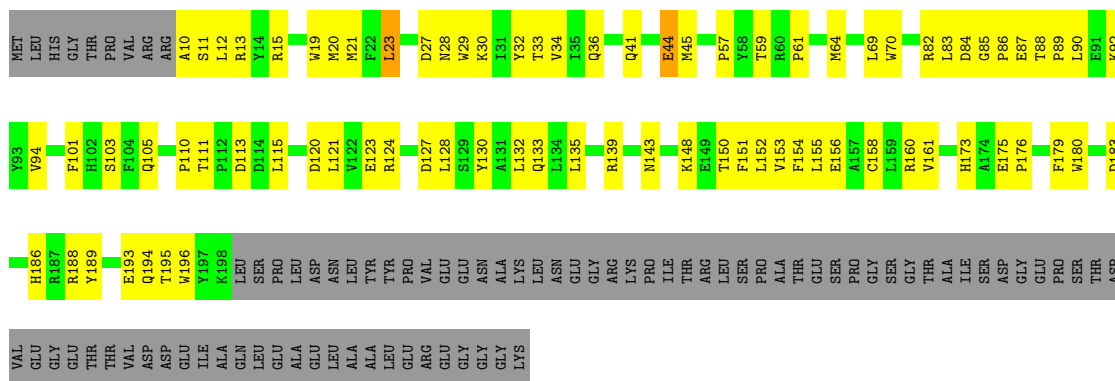
• Molecule 6: mS61

Chain DN: 55% 26% 6% 12%

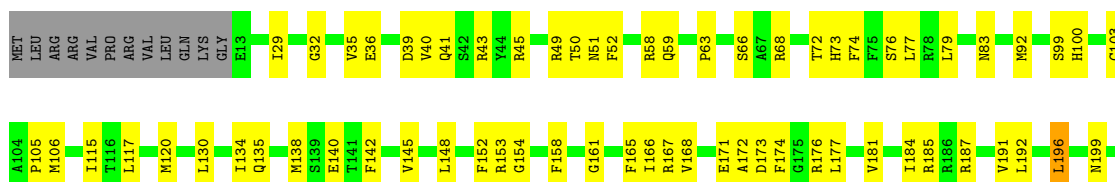
- Molecule 7: mS62

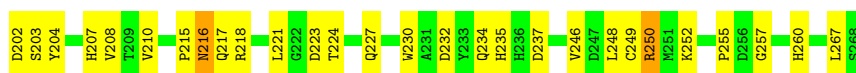


- Molecule 8: mS63



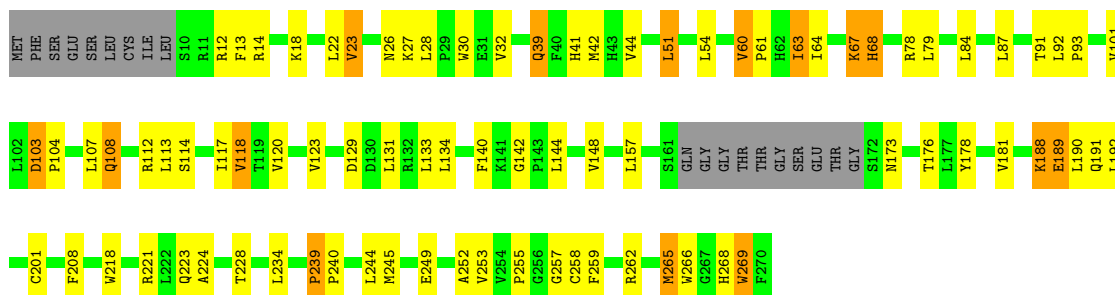
- Molecule 9: mS64





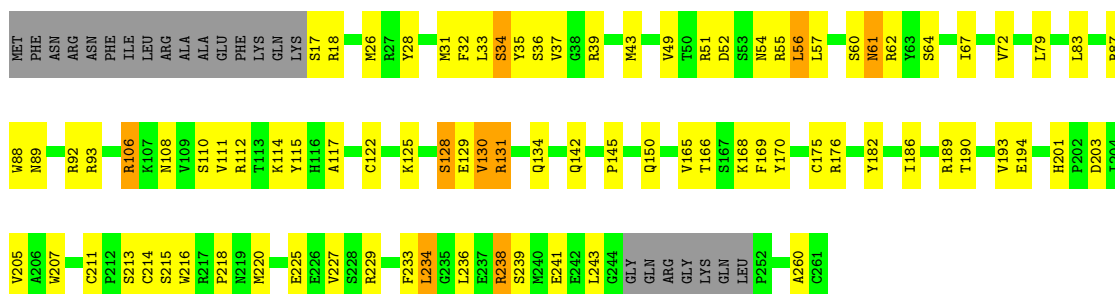
• Molecule 10: mS65

Chain DR: 62% 26% 6% 7%



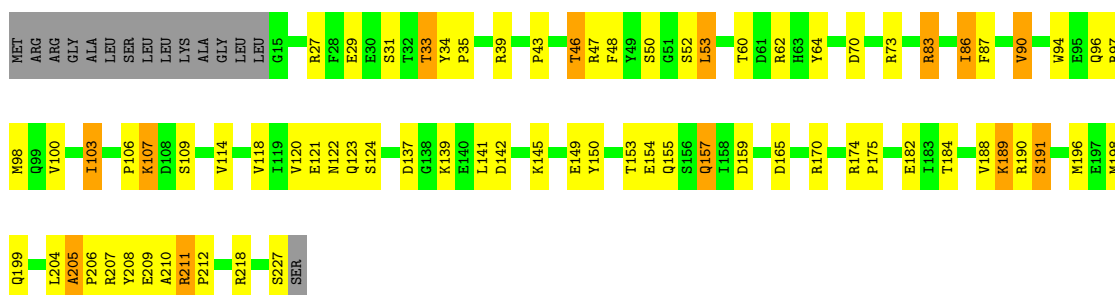
• Molecule 11: mS66

Chain DS: 58% 30% 9%



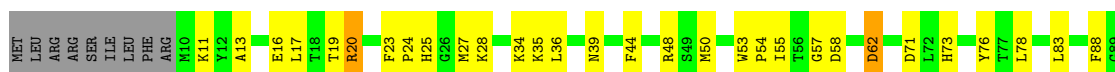
• Molecule 12: mS68

Chain DU: 61% 27% 6% 7%



• Molecule 13: mS73

Chain DZ: 54% 31% 13%

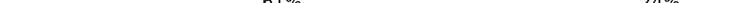






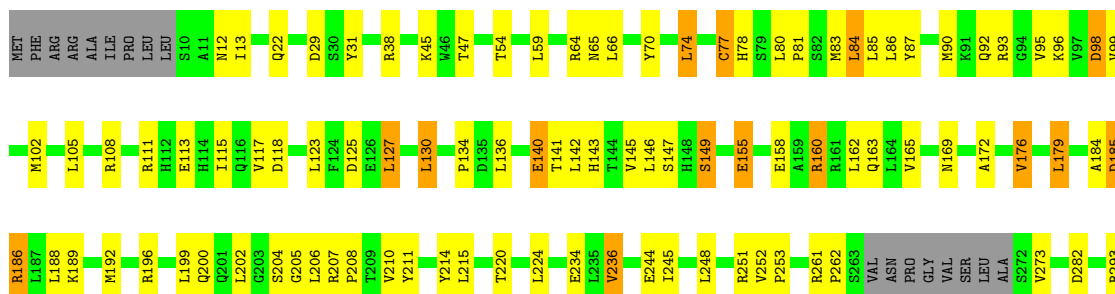


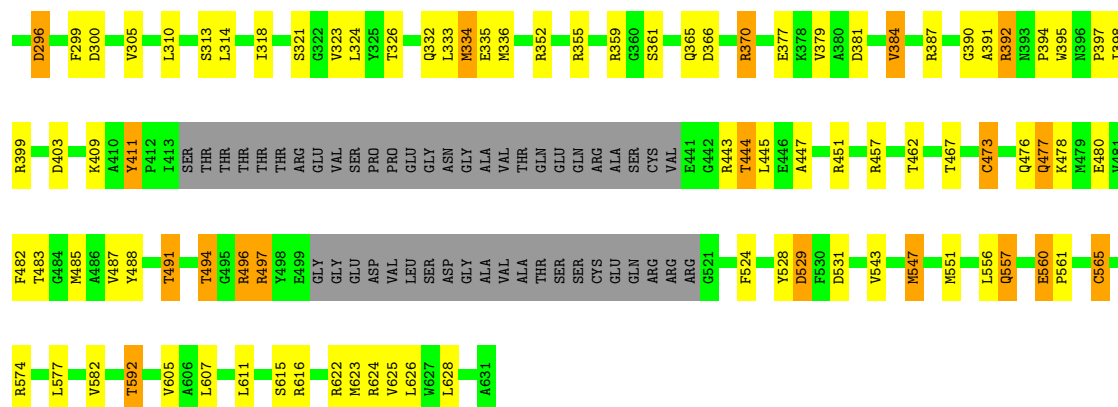
- Molecule 18: mS53

Chain DF: 

- Molecule 19: mS54

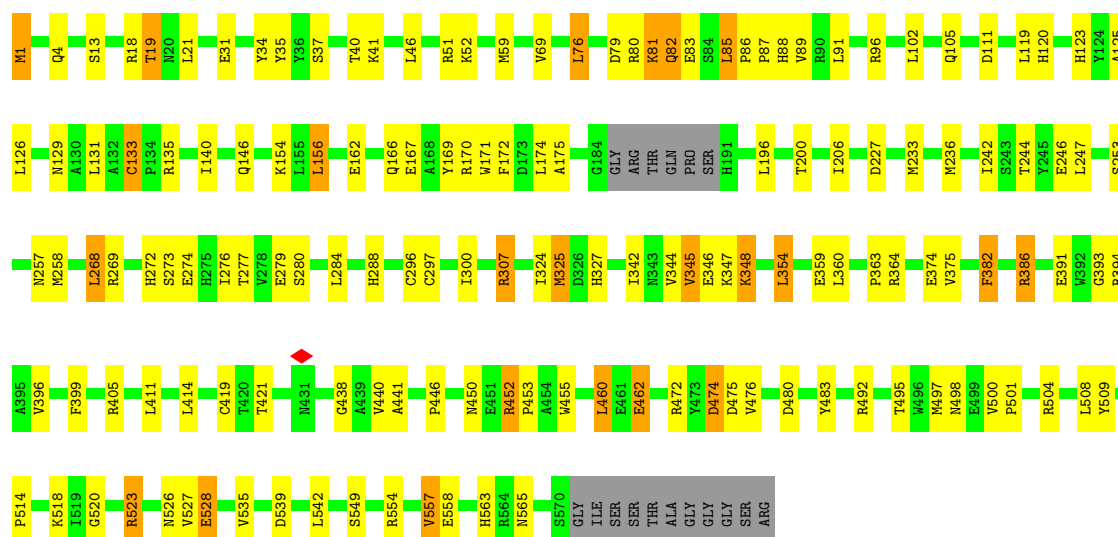
Chain DG: 





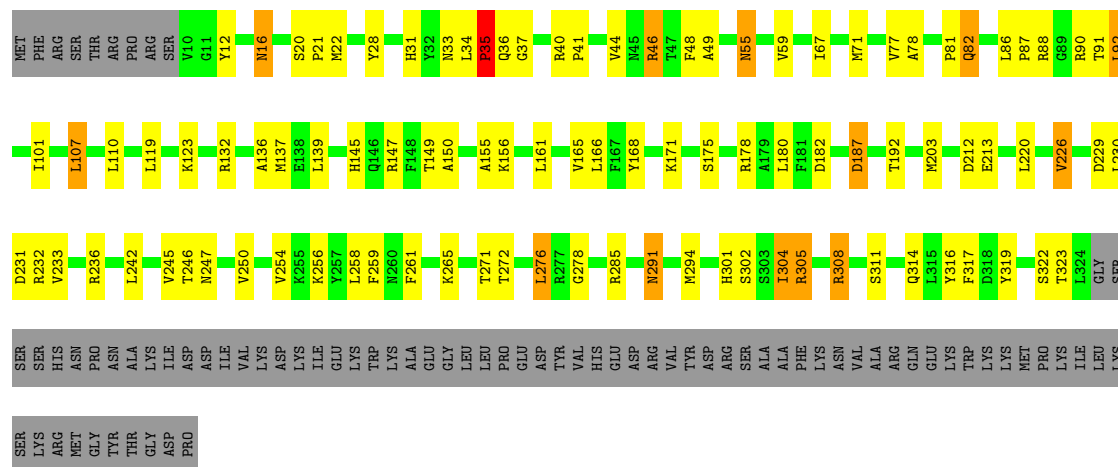
• Molecule 20: mS55

Chain DH: 71% 22%



• Molecule 21: mS57

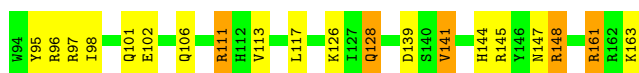
Chain DJ: 55% 21% 20%







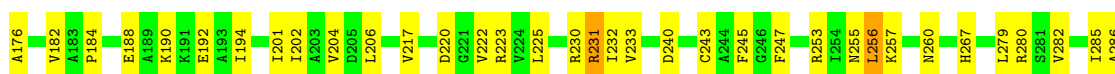
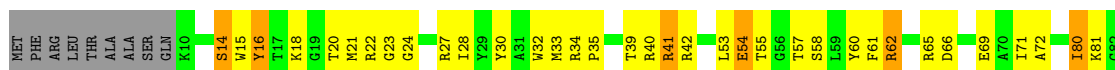
• Molecule 27: mS72



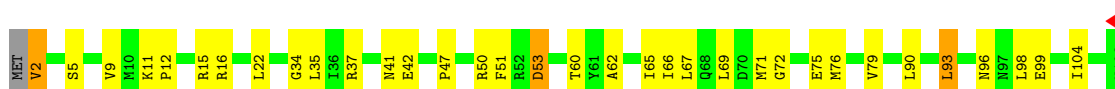
• Molecule 28: uS3m



• Molecule 29: uS5m



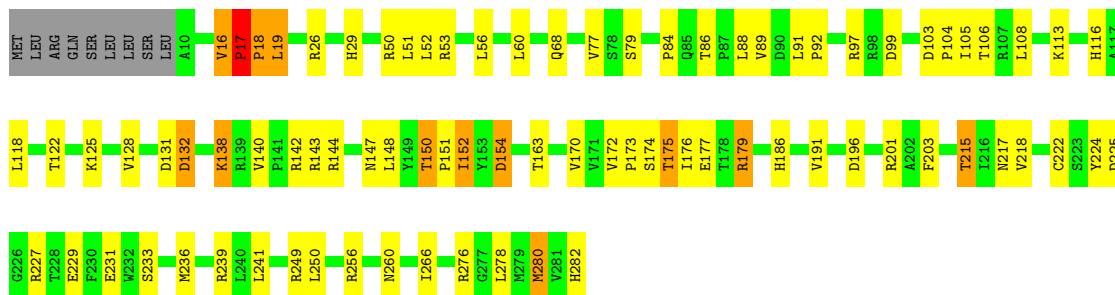
• Molecule 30: bS6m





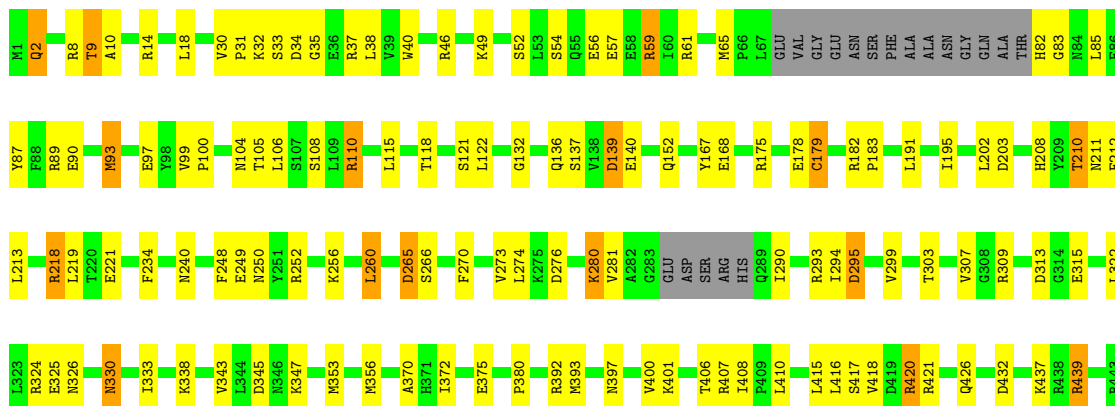
## • Molecule 31: uS8m

Chain CH: 67% 25%



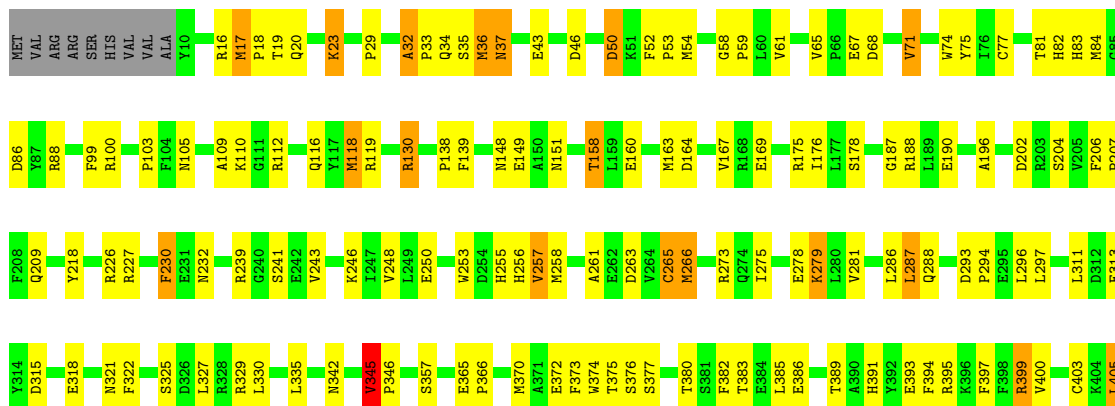
## • Molecule 32: uS9m

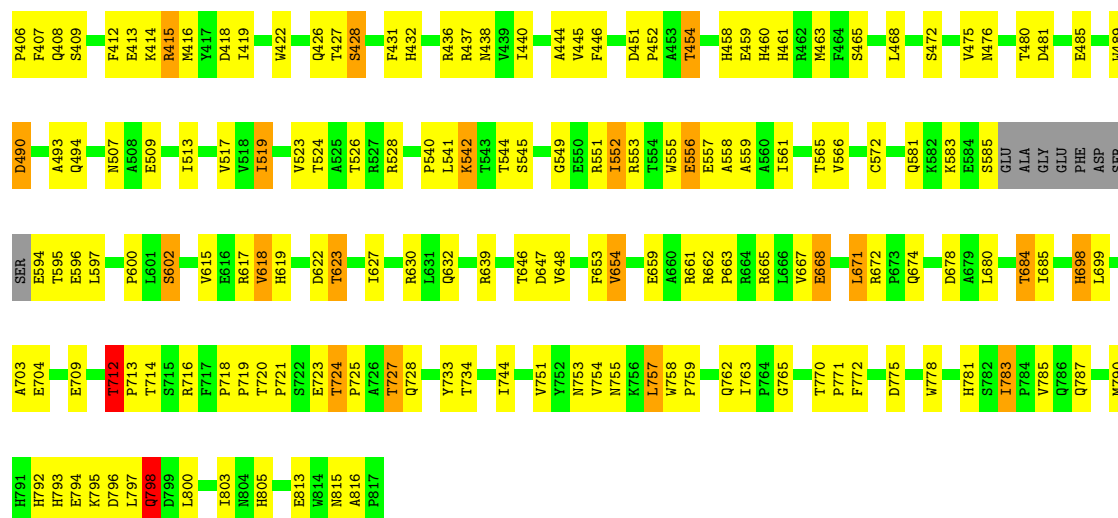
Chain CI: 67% 26%



## • Molecule 33: uS10m

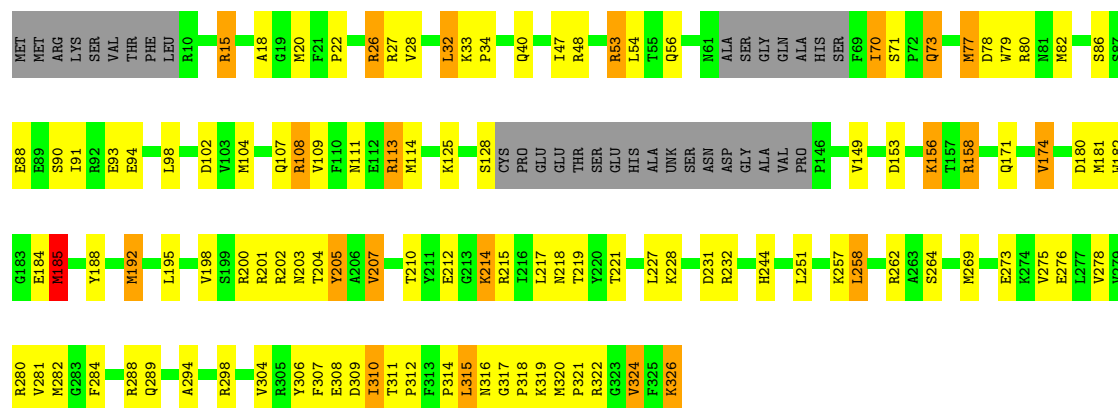
Chain CJ: 61% 32% 5%





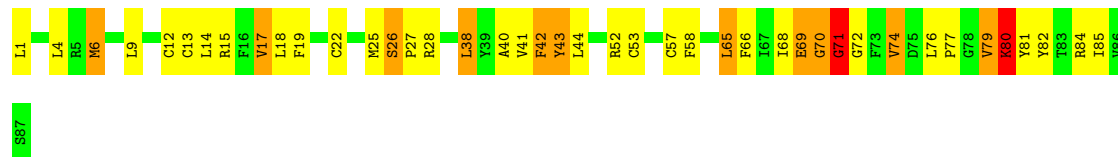
• Molecule 34: uS11m

Chain CK: 55% 28% 6% 10%



• Molecule 35: uS12m

Chain CL: 52% 33% 13% .



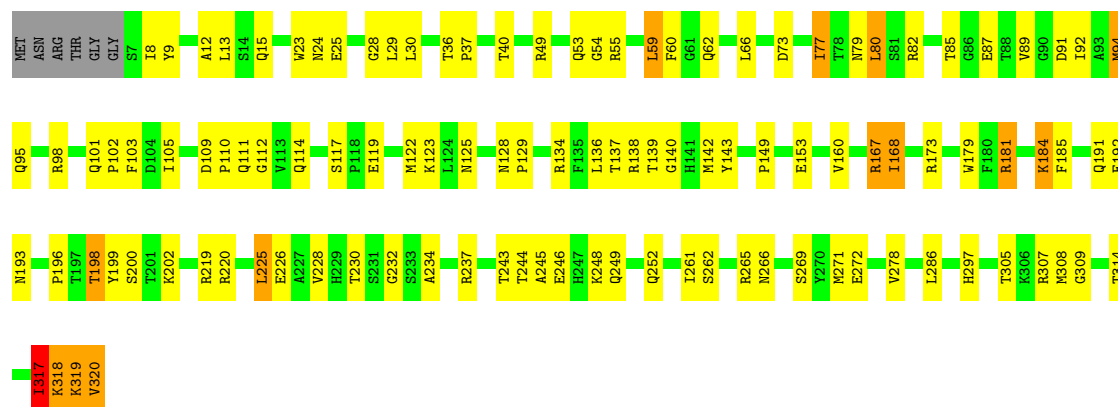
• Molecule 36: uS14m

Chain CN: 58% 29% 8% 5%

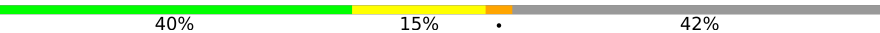
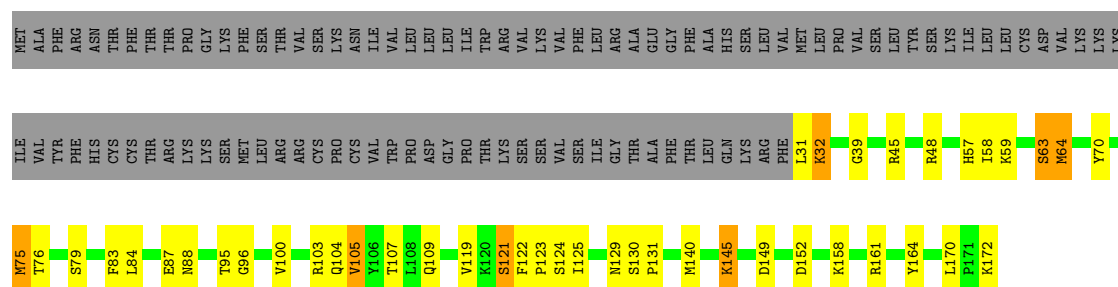




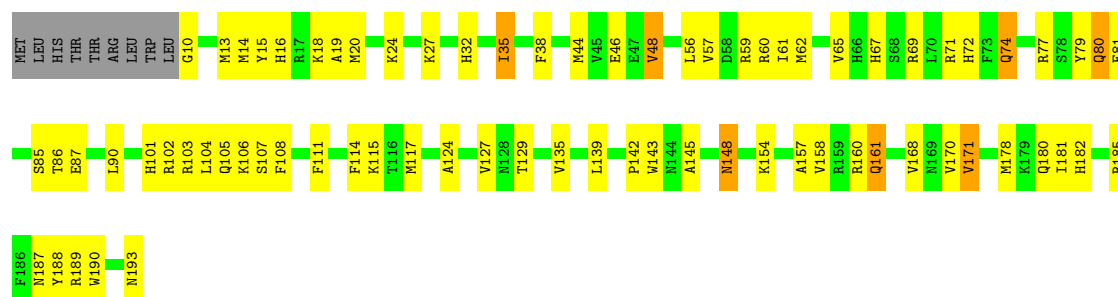
## ● Molecule 40: bS18m

Chain CR:  63% 31% . .

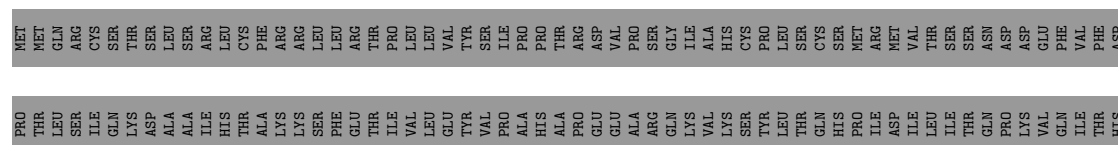
## ● Molecule 41: uS19m

Chain CS:  40% 15% . 42%

## ● Molecule 42: bS21m

Chain CU:  56% 35% . 5%

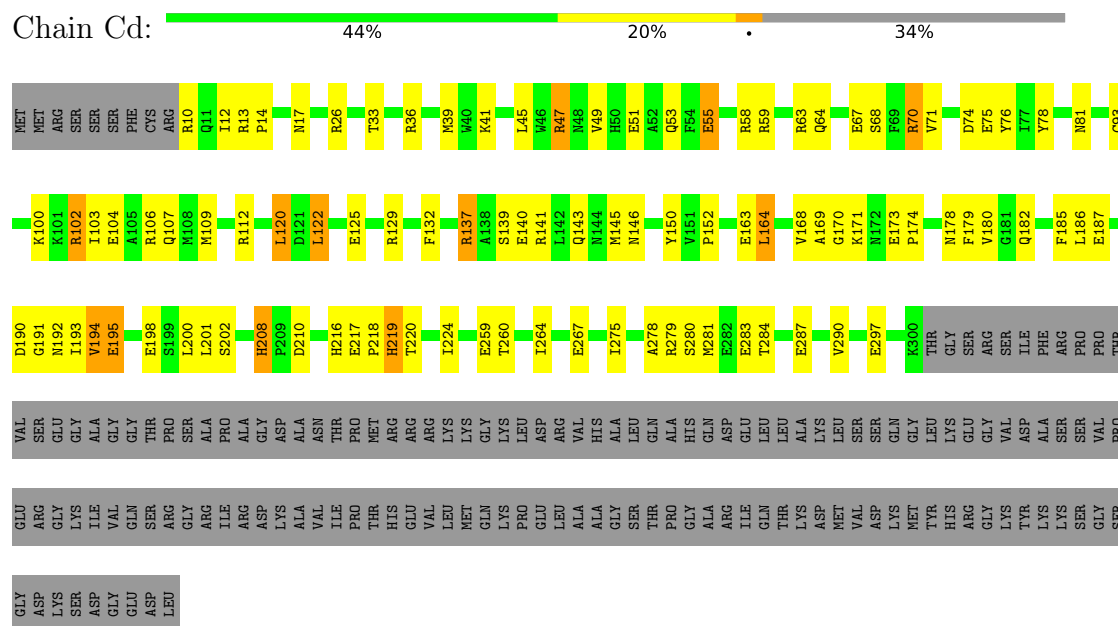
## ● Molecule 43: mt-IF-3

Chain CZ:  31% 9% . 58%

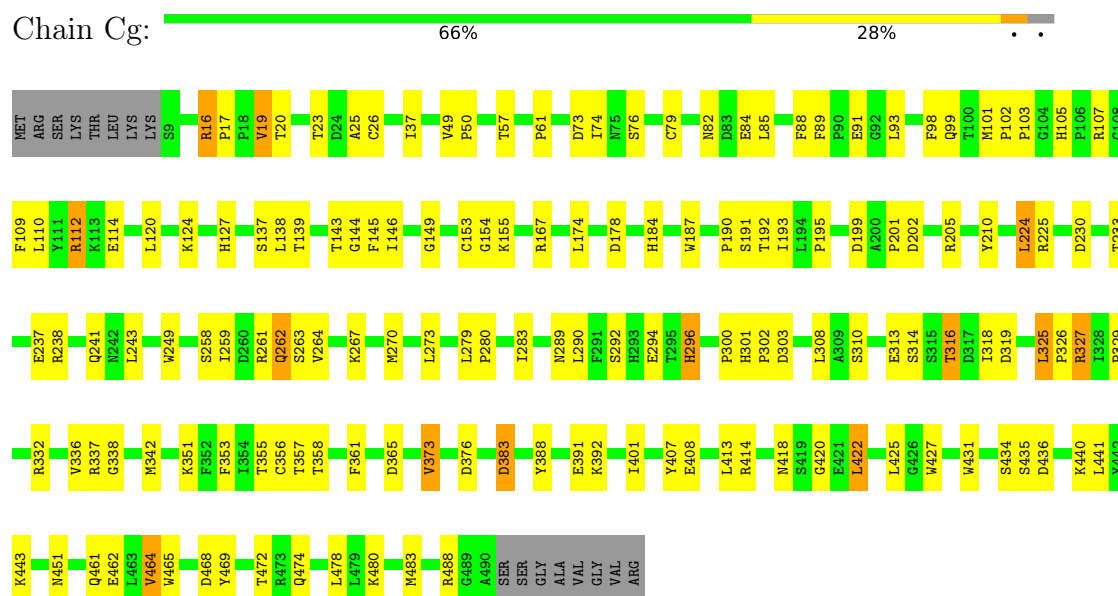




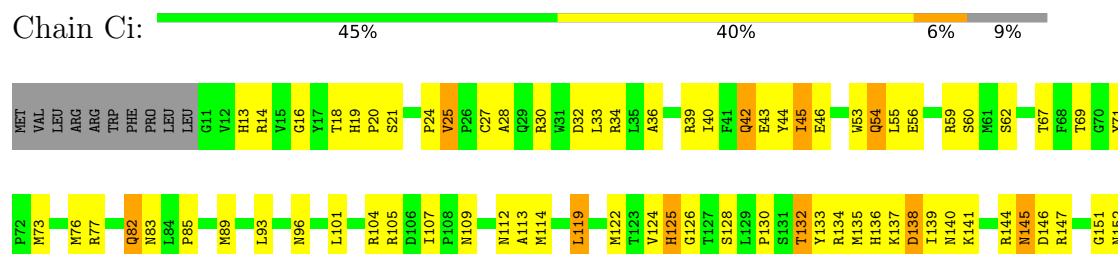
- Molecule 46: mS26



- Molecule 47: mS29

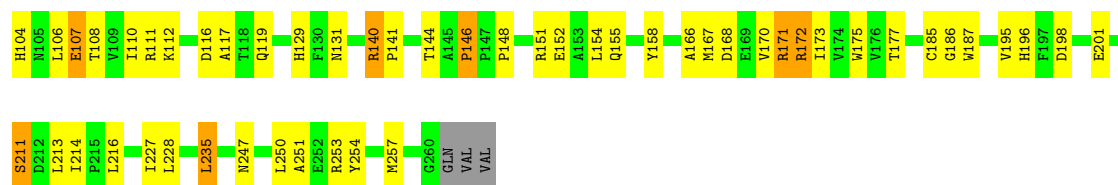


- Molecule 48: mS33

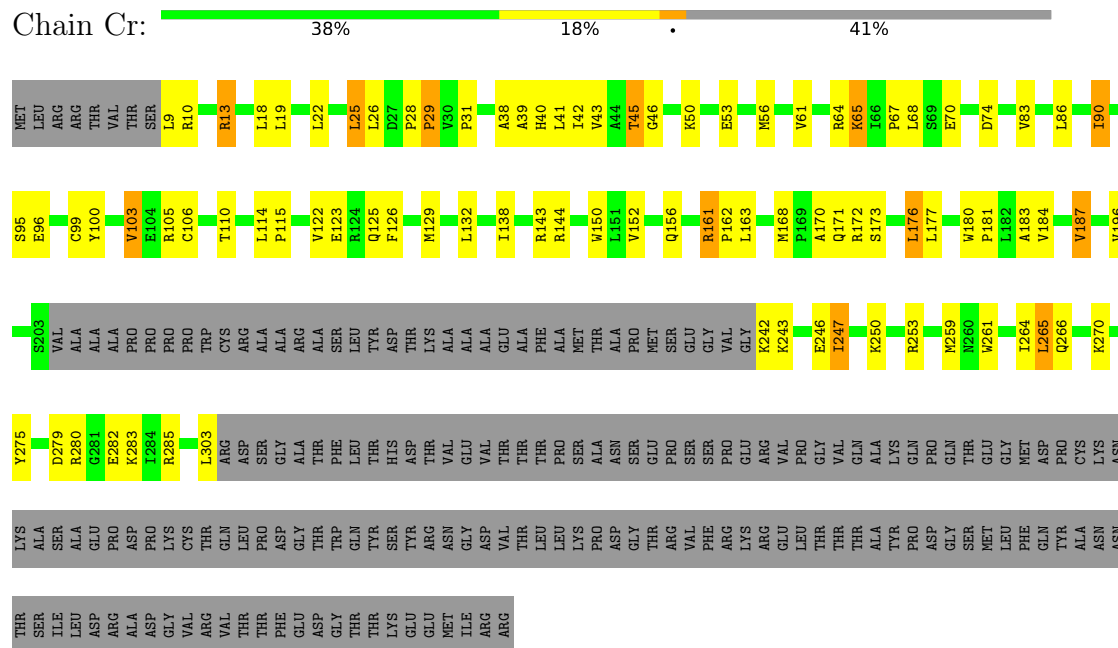




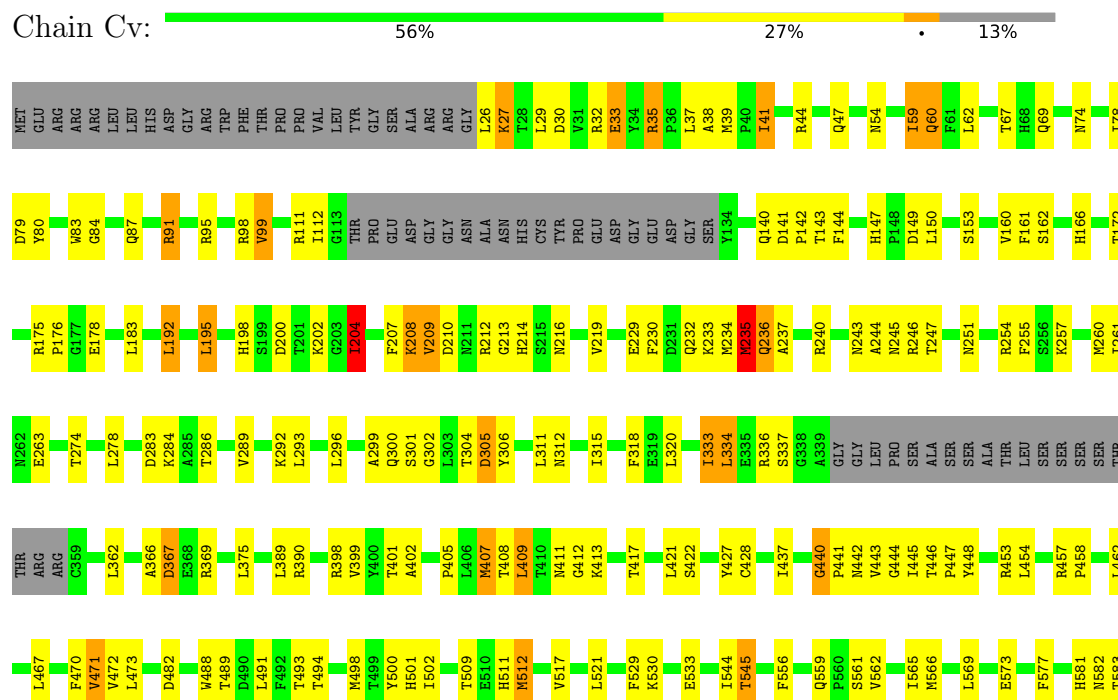
|     |     |     |     |     |     |     |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|
| Met | Arg | Leu | Cys | Arg | Leu | Ser | Y9 | V19 | Q20 | M21 | T24 | F25 | M26 | P27 | I30 | R36 | T52 | F55 | S56 | P57 | P58 | R59 | L60 | M61 | Y62 | P63 | V64 | S65 | Q76 | F77 | D78 | M79 | G80 | Y81 | S82 | L83 | F84 | H85 | R86 | L92 | N93 | R94 | H95 | T96 | L97 | G98 | T99 | P100 | L101 |
|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|



### • Molecule 55: mS43



### • Molecule 56: mS47







- Molecule 58: Unknown Protein



- Molecule 59: Unknown Protein



- Molecule 60: Unknown Protein



There are no outlier residues recorded for this chain.

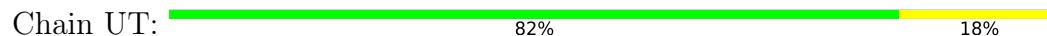
- Molecule 61: Unknown Protein



- Molecule 62: Unknown Protein



- Molecule 63: Unknown Protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 31911                                   | 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                    | 0.538                                   | Depositor |
| Minimum map value                    | -0.316                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.023                                   | Depositor |
| Recommended contour level            | 0.0114                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 444.8, 444.8, 444.8                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 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: SPD, MG, SPM, UTP, ZN, GTP

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$     |
| 1   | DA    | 0.47         | 1/12780 (0.0%) | 0.89        | 34/17297 (0.2%) |
| 2   | DD    | 0.48         | 0/6710         | 0.94        | 24/9087 (0.3%)  |
| 3   | DI    | 0.47         | 0/3248         | 0.86        | 1/4401 (0.0%)   |
| 4   | DL    | 0.54         | 0/2346         | 0.97        | 8/3164 (0.3%)   |
| 5   | DM    | 0.51         | 0/2488         | 0.92        | 6/3362 (0.2%)   |
| 6   | DN    | 0.50         | 0/2148         | 1.01        | 14/2916 (0.5%)  |
| 7   | DO    | 0.47         | 0/1840         | 0.95        | 7/2482 (0.3%)   |
| 8   | DP    | 0.43         | 0/1662         | 0.81        | 1/2249 (0.0%)   |
| 9   | DQ    | 0.48         | 0/2111         | 0.93        | 4/2863 (0.1%)   |
| 10  | DR    | 0.46         | 0/2090         | 0.96        | 8/2849 (0.3%)   |
| 11  | DS    | 0.45         | 0/1950         | 0.87        | 1/2633 (0.0%)   |
| 12  | DU    | 0.45         | 0/1799         | 0.85        | 2/2438 (0.1%)   |
| 13  | DZ    | 0.46         | 0/725          | 0.89        | 2/984 (0.2%)    |
| 14  | Da    | 0.46         | 0/520          | 0.87        | 0/694           |
| 15  | DB    | 0.45         | 0/9369         | 0.88        | 17/12692 (0.1%) |
| 16  | DC    | 0.44         | 0/8952         | 0.88        | 19/12145 (0.2%) |
| 17  | DE    | 0.41         | 0/4955         | 0.92        | 20/6708 (0.3%)  |
| 18  | DF    | 0.46         | 0/4856         | 0.88        | 12/6581 (0.2%)  |
| 19  | DG    | 0.43         | 0/4674         | 0.88        | 12/6333 (0.2%)  |
| 20  | DH    | 0.46         | 0/4684         | 0.88        | 6/6347 (0.1%)   |
| 21  | DJ    | 0.47         | 0/2649         | 0.89        | 9/3598 (0.3%)   |
| 22  | DK    | 0.41         | 0/2045         | 0.84        | 2/2759 (0.1%)   |
| 23  | DT    | 0.42         | 0/2133         | 0.89        | 7/2889 (0.2%)   |
| 24  | DV    | 0.47         | 0/1382         | 0.95        | 7/1871 (0.4%)   |
| 25  | DW    | 0.45         | 0/1407         | 0.93        | 2/1916 (0.1%)   |
| 26  | DX    | 0.43         | 0/1231         | 0.88        | 5/1654 (0.3%)   |
| 27  | DY    | 0.54         | 0/1334         | 0.96        | 5/1810 (0.3%)   |
| 28  | CC    | 0.49         | 0/666          | 0.95        | 4/900 (0.4%)    |
| 29  | CE    | 0.54         | 0/3484         | 0.96        | 7/4708 (0.1%)   |
| 30  | CF    | 0.48         | 0/1319         | 0.87        | 1/1783 (0.1%)   |
| 31  | CH    | 0.56         | 0/2276         | 0.97        | 7/3071 (0.2%)   |
| 32  | CI    | 0.51         | 0/3453         | 0.88        | 2/4655 (0.0%)   |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 33  | CJ    | 0.52         | 0/6705          | 0.97        | 32/9124 (0.4%)    |
| 34  | CK    | 0.47         | 0/2472          | 0.89        | 2/3315 (0.1%)     |
| 35  | CL    | 0.48         | 0/759           | 0.96        | 4/1026 (0.4%)     |
| 36  | CN    | 0.50         | 0/1361          | 0.90        | 2/1840 (0.1%)     |
| 37  | CO    | 0.51         | 0/3085          | 0.94        | 11/4165 (0.3%)    |
| 38  | CP    | 0.54         | 0/1533          | 1.02        | 8/2074 (0.4%)     |
| 39  | CQ    | 0.58         | 0/1631          | 1.07        | 5/2203 (0.2%)     |
| 40  | CR    | 0.52         | 0/2640          | 0.97        | 2/3572 (0.1%)     |
| 41  | CS    | 0.47         | 0/1209          | 0.95        | 5/1626 (0.3%)     |
| 42  | CU    | 0.48         | 0/1576          | 0.85        | 0/2115            |
| 43  | CZ    | 0.46         | 0/1237          | 0.90        | 3/1659 (0.2%)     |
| 44  | Ca    | 0.51         | 0/5159          | 0.94        | 19/6980 (0.3%)    |
| 45  | Cb    | 0.53         | 0/2105          | 0.94        | 4/2842 (0.1%)     |
| 46  | Cd    | 0.52         | 0/2438          | 0.86        | 4/3288 (0.1%)     |
| 47  | Cg    | 0.47         | 0/4025          | 0.95        | 11/5467 (0.2%)    |
| 48  | Ci    | 0.51         | 0/1388          | 1.00        | 5/1878 (0.3%)     |
| 49  | Cj    | 0.45         | 0/1842          | 0.89        | 4/2511 (0.2%)     |
| 50  | Ck    | 0.49         | 0/5696          | 0.90        | 6/7705 (0.1%)     |
| 51  | Cm    | 0.59         | 0/1616          | 1.02        | 4/2175 (0.2%)     |
| 52  | Cn    | 0.51         | 0/934           | 0.96        | 5/1248 (0.4%)     |
| 53  | Cp    | 0.46         | 0/1528          | 0.88        | 2/2072 (0.1%)     |
| 54  | Cq    | 0.52         | 0/2066          | 0.91        | 5/2815 (0.2%)     |
| 55  | Cr    | 0.45         | 0/2038          | 0.91        | 6/2759 (0.2%)     |
| 56  | Cv    | 0.51         | 0/8780          | 0.96        | 25/11901 (0.2%)   |
| 57  | CA    | 0.27         | 0/14679         | 0.45        | 0/22827           |
| All | All   | 0.47         | 1/181788 (0.0%) | 0.89        | 430/249026 (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                   | 2                   |
| 2   | DD    | 0                   | 3                   |
| 6   | DN    | 0                   | 1                   |
| 7   | DO    | 0                   | 2                   |
| 10  | DR    | 0                   | 2                   |
| 16  | DC    | 0                   | 2                   |
| 19  | DG    | 0                   | 2                   |
| 21  | DJ    | 0                   | 1                   |
| 23  | DT    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 26  | DX    | 0                   | 1                   |
| 31  | CH    | 0                   | 2                   |
| 33  | CJ    | 0                   | 2                   |
| 35  | CL    | 0                   | 3                   |
| 37  | CO    | 0                   | 2                   |
| 46  | Cd    | 0                   | 1                   |
| 47  | Cg    | 0                   | 1                   |
| 50  | Ck    | 0                   | 1                   |
| 56  | Cv    | 0                   | 2                   |
| All | All   | 0                   | 31                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | DA    | 529 | ILE  | C-O   | 5.61 | 1.30        | 1.24     |

All (430) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | DD    | 255 | VAL  | CA-C-N | 13.36  | 136.54      | 119.84   |
| 2   | DD    | 255 | VAL  | C-N-CA | 13.36  | 136.54      | 119.84   |
| 17  | DE    | 327 | ASN  | CA-C-N | -11.05 | 109.00      | 120.38   |
| 17  | DE    | 327 | ASN  | C-N-CA | -11.05 | 109.00      | 120.38   |
| 56  | Cv    | 945 | VAL  | CA-C-N | -9.94  | 110.19      | 120.03   |
| 56  | Cv    | 945 | VAL  | C-N-CA | -9.94  | 110.19      | 120.03   |
| 20  | DH    | 133 | CYS  | CA-C-N | -9.82  | 107.56      | 119.84   |
| 20  | DH    | 133 | CYS  | C-N-CA | -9.82  | 107.56      | 119.84   |
| 47  | Cg    | 16  | ARG  | CA-C-N | 9.40   | 130.06      | 120.38   |
| 47  | Cg    | 16  | ARG  | C-N-CA | 9.40   | 130.06      | 120.38   |
| 7   | DO    | 125 | LEU  | CA-C-N | -9.05  | 110.40      | 119.90   |
| 7   | DO    | 125 | LEU  | C-N-CA | -9.05  | 110.40      | 119.90   |
| 32  | CI    | 65  | MET  | CA-C-N | 9.00   | 128.60      | 119.24   |
| 32  | CI    | 65  | MET  | C-N-CA | 9.00   | 128.60      | 119.24   |
| 16  | DC    | 699 | VAL  | CA-C-N | 8.91   | 129.47      | 119.32   |
| 16  | DC    | 699 | VAL  | C-N-CA | 8.91   | 129.47      | 119.32   |
| 56  | Cv    | 440 | GLY  | CA-C-N | -8.77  | 110.75      | 119.87   |
| 56  | Cv    | 440 | GLY  | C-N-CA | -8.77  | 110.75      | 119.87   |
| 47  | Cg    | 49  | VAL  | CA-C-N | -8.77  | 108.88      | 119.84   |
| 47  | Cg    | 49  | VAL  | C-N-CA | -8.77  | 108.88      | 119.84   |
| 6   | DN    | 225 | GLY  | CA-C-N | 8.38   | 128.53      | 120.31   |
| 6   | DN    | 225 | GLY  | C-N-CA | 8.38   | 128.53      | 120.31   |
| 50  | Ck    | 687 | ARG  | N-CA-C | 8.35   | 123.69      | 113.17   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | DD    | 248  | ASP  | CA-C-N  | -8.34 | 111.01      | 119.93   |
| 2   | DD    | 248  | ASP  | C-N-CA  | -8.34 | 111.01      | 119.93   |
| 44  | Ca    | 32   | PRO  | N-CA-CB | 8.03  | 110.87      | 103.08   |
| 38  | CP    | 80   | THR  | CA-C-N  | 7.92  | 127.58      | 119.82   |
| 38  | CP    | 80   | THR  | C-N-CA  | 7.92  | 127.58      | 119.82   |
| 56  | Cv    | 59   | ILE  | N-CA-C  | 7.89  | 119.70      | 112.29   |
| 15  | DB    | 944  | HIS  | N-CA-C  | 7.87  | 121.37      | 111.69   |
| 56  | Cv    | 545  | THR  | CA-C-N  | 7.87  | 129.67      | 119.84   |
| 56  | Cv    | 545  | THR  | C-N-CA  | 7.87  | 129.67      | 119.84   |
| 15  | DB    | 672  | VAL  | N-CA-C  | 7.86  | 118.41      | 110.23   |
| 47  | Cg    | 451  | ASN  | CA-C-N  | 7.83  | 127.11      | 118.97   |
| 47  | Cg    | 451  | ASN  | C-N-CA  | 7.83  | 127.11      | 118.97   |
| 51  | Cm    | 43   | THR  | N-CA-C  | -7.76 | 102.14      | 111.69   |
| 1   | DA    | 1484 | PRO  | N-CA-CB | 7.75  | 110.67      | 103.46   |
| 55  | Cr    | 28   | PRO  | N-CA-CB | 7.74  | 110.58      | 103.08   |
| 50  | Ck    | 88   | ASP  | CA-C-N  | 7.70  | 127.60      | 120.21   |
| 50  | Ck    | 88   | ASP  | C-N-CA  | 7.70  | 127.60      | 120.21   |
| 47  | Cg    | 17   | PRO  | CA-C-N  | 7.69  | 129.45      | 119.84   |
| 47  | Cg    | 17   | PRO  | C-N-CA  | 7.69  | 129.45      | 119.84   |
| 4   | DL    | 229  | THR  | CA-C-N  | 7.65  | 127.19      | 118.85   |
| 4   | DL    | 229  | THR  | C-N-CA  | 7.65  | 127.19      | 118.85   |
| 40  | CR    | 317  | ILE  | N-CA-C  | 7.51  | 121.62      | 113.43   |
| 2   | DD    | 355  | SER  | CA-C-N  | -7.51 | 110.45      | 119.84   |
| 2   | DD    | 355  | SER  | C-N-CA  | -7.51 | 110.45      | 119.84   |
| 5   | DM    | 2    | GLU  | N-CA-C  | 7.49  | 120.16      | 111.02   |
| 21  | DJ    | 156  | LYS  | CA-C-N  | 7.49  | 125.05      | 119.66   |
| 21  | DJ    | 156  | LYS  | C-N-CA  | 7.49  | 125.05      | 119.66   |
| 33  | CJ    | 485  | GLU  | N-CA-C  | 7.49  | 119.13      | 110.97   |
| 38  | CP    | 21   | TRP  | N-CA-C  | 7.41  | 121.62      | 112.58   |
| 33  | CJ    | 712  | THR  | CA-C-N  | -7.36 | 110.64      | 119.84   |
| 33  | CJ    | 712  | THR  | C-N-CA  | -7.36 | 110.64      | 119.84   |
| 48  | Ci    | 151  | GLY  | N-CA-C  | -7.35 | 104.19      | 115.66   |
| 33  | CJ    | 461  | HIS  | N-CA-C  | 7.33  | 121.53      | 112.59   |
| 4   | DL    | 270  | THR  | CA-C-N  | -7.26 | 111.50      | 119.19   |
| 4   | DL    | 270  | THR  | C-N-CA  | -7.26 | 111.50      | 119.19   |
| 33  | CJ    | 783  | ILE  | CA-C-N  | 7.25  | 127.70      | 120.52   |
| 33  | CJ    | 783  | ILE  | C-N-CA  | 7.25  | 127.70      | 120.52   |
| 49  | Cj    | 38   | MET  | CA-C-N  | 7.24  | 126.74      | 118.85   |
| 49  | Cj    | 38   | MET  | C-N-CA  | 7.24  | 126.74      | 118.85   |
| 33  | CJ    | 32   | ALA  | CA-C-N  | 7.24  | 126.91      | 119.82   |
| 33  | CJ    | 32   | ALA  | C-N-CA  | 7.24  | 126.91      | 119.82   |
| 44  | Ca    | 35   | PRO  | N-CA-CB | 7.21  | 110.81      | 103.25   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 44  | Ca    | 33   | PRO  | N-CA-CB | 7.20  | 110.80      | 103.25   |
| 36  | CN    | 108  | VAL  | CA-C-N  | 7.19  | 127.03      | 119.05   |
| 36  | CN    | 108  | VAL  | C-N-CA  | 7.19  | 127.03      | 119.05   |
| 1   | DA    | 1314 | GLY  | N-CA-C  | 7.15  | 126.92      | 112.34   |
| 48  | Ci    | 93   | LEU  | CA-C-N  | 6.98  | 126.66      | 119.82   |
| 48  | Ci    | 93   | LEU  | C-N-CA  | 6.98  | 126.66      | 119.82   |
| 1   | DA    | 1004 | GLY  | N-CA-C  | -6.89 | 105.12      | 115.32   |
| 29  | CE    | 87   | ILE  | N-CA-C  | -6.87 | 103.51      | 111.00   |
| 41  | CS    | 130  | SER  | CA-C-N  | 6.84  | 126.82      | 119.78   |
| 41  | CS    | 130  | SER  | C-N-CA  | 6.84  | 126.82      | 119.78   |
| 16  | DC    | 601  | GLU  | N-CA-C  | 6.80  | 118.38      | 110.97   |
| 39  | CQ    | 64   | THR  | N-CA-C  | 6.79  | 121.72      | 113.17   |
| 37  | CO    | 87   | THR  | CA-C-N  | -6.79 | 112.67      | 119.93   |
| 37  | CO    | 87   | THR  | C-N-CA  | -6.79 | 112.67      | 119.93   |
| 37  | CO    | 396  | LYS  | N-CA-C  | 6.79  | 121.84      | 113.50   |
| 52  | Cn    | 157  | TYR  | CA-C-N  | -6.78 | 111.36      | 119.84   |
| 52  | Cn    | 157  | TYR  | C-N-CA  | -6.78 | 111.36      | 119.84   |
| 43  | CZ    | 296  | PRO  | N-CA-CB | 6.78  | 110.37      | 103.25   |
| 10  | DR    | 257  | GLY  | N-CA-C  | -6.77 | 104.65      | 115.08   |
| 44  | Ca    | 168  | TYR  | CA-C-N  | 6.75  | 126.35      | 119.19   |
| 44  | Ca    | 168  | TYR  | C-N-CA  | 6.75  | 126.35      | 119.19   |
| 38  | CP    | 65   | GLY  | N-CA-C  | 6.75  | 120.06      | 111.09   |
| 6   | DN    | 130  | ASN  | CA-C-N  | 6.74  | 126.70      | 120.03   |
| 6   | DN    | 130  | ASN  | C-N-CA  | 6.74  | 126.70      | 120.03   |
| 31  | CH    | 174  | SER  | N-CA-C  | 6.74  | 121.21      | 112.92   |
| 22  | DK    | 242  | HIS  | CA-C-N  | 6.70  | 126.21      | 119.24   |
| 22  | DK    | 242  | HIS  | C-N-CA  | 6.70  | 126.21      | 119.24   |
| 1   | DA    | 949  | ARG  | CA-C-N  | 6.68  | 126.37      | 119.82   |
| 1   | DA    | 949  | ARG  | C-N-CA  | 6.68  | 126.37      | 119.82   |
| 35  | CL    | 26   | SER  | CA-C-N  | 6.68  | 127.59      | 120.11   |
| 35  | CL    | 26   | SER  | C-N-CA  | 6.68  | 127.59      | 120.11   |
| 41  | CS    | 145  | LYS  | CA-C-N  | 6.68  | 125.92      | 118.97   |
| 41  | CS    | 145  | LYS  | C-N-CA  | 6.68  | 125.92      | 118.97   |
| 44  | Ca    | 524  | VAL  | CA-C-N  | 6.67  | 126.71      | 119.90   |
| 44  | Ca    | 524  | VAL  | C-N-CA  | 6.67  | 126.71      | 119.90   |
| 55  | Cr    | 31   | PRO  | N-CA-CB | 6.67  | 110.26      | 103.25   |
| 9   | DQ    | 257  | GLY  | N-CA-C  | -6.67 | 106.03      | 115.43   |
| 7   | DO    | 116  | ALA  | N-CA-C  | -6.62 | 105.21      | 113.28   |
| 16  | DC    | 921  | HIS  | CA-C-N  | 6.62  | 128.11      | 119.84   |
| 16  | DC    | 921  | HIS  | C-N-CA  | 6.62  | 128.11      | 119.84   |
| 17  | DE    | 591  | LEU  | CA-C-N  | -6.61 | 112.97      | 119.90   |
| 17  | DE    | 591  | LEU  | C-N-CA  | -6.61 | 112.97      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | DJ    | 16   | ASN  | CA-C-N  | 6.60  | 126.73      | 119.87   |
| 21  | DJ    | 16   | ASN  | C-N-CA  | 6.60  | 126.73      | 119.87   |
| 17  | DE    | 588  | PRO  | CA-C-N  | 6.58  | 126.27      | 119.82   |
| 17  | DE    | 588  | PRO  | C-N-CA  | 6.58  | 126.27      | 119.82   |
| 49  | Cj    | 200  | ASP  | CA-C-N  | 6.55  | 126.00      | 118.85   |
| 49  | Cj    | 200  | ASP  | C-N-CA  | 6.55  | 126.00      | 118.85   |
| 56  | Cv    | 1021 | SER  | N-CA-C  | -6.55 | 104.07      | 111.14   |
| 39  | CQ    | 68   | SER  | N-CA-C  | -6.48 | 105.12      | 113.16   |
| 19  | DG    | 252  | VAL  | CA-C-N  | 6.47  | 126.23      | 119.76   |
| 19  | DG    | 252  | VAL  | C-N-CA  | 6.47  | 126.23      | 119.76   |
| 33  | CJ    | 345  | VAL  | CA-C-N  | 6.47  | 125.97      | 119.24   |
| 33  | CJ    | 345  | VAL  | C-N-CA  | 6.47  | 125.97      | 119.24   |
| 50  | Ck    | 659  | GLY  | CA-C-N  | -6.45 | 114.13      | 120.52   |
| 50  | Ck    | 659  | GLY  | C-N-CA  | -6.45 | 114.13      | 120.52   |
| 15  | DB    | 987  | GLU  | CA-C-N  | 6.43  | 126.45      | 119.89   |
| 15  | DB    | 987  | GLU  | C-N-CA  | 6.43  | 126.45      | 119.89   |
| 1   | DA    | 1457 | HIS  | CA-C-N  | 6.43  | 126.05      | 119.56   |
| 1   | DA    | 1457 | HIS  | C-N-CA  | 6.43  | 126.05      | 119.56   |
| 37  | CO    | 313  | THR  | N-CA-C  | 6.42  | 119.96      | 111.75   |
| 18  | DF    | 569  | GLN  | CA-C-N  | 6.41  | 127.85      | 119.84   |
| 18  | DF    | 569  | GLN  | C-N-CA  | 6.41  | 127.85      | 119.84   |
| 55  | Cr    | 29   | PRO  | N-CA-CB | 6.37  | 109.94      | 103.25   |
| 1   | DA    | 883  | ASN  | CA-C-N  | 6.35  | 126.05      | 119.64   |
| 1   | DA    | 883  | ASN  | C-N-CA  | 6.35  | 126.05      | 119.64   |
| 1   | DA    | 311  | THR  | CA-C-N  | 6.33  | 127.75      | 119.84   |
| 1   | DA    | 311  | THR  | C-N-CA  | 6.33  | 127.75      | 119.84   |
| 33  | CJ    | 46   | ASP  | CA-C-N  | 6.33  | 125.55      | 118.97   |
| 33  | CJ    | 46   | ASP  | C-N-CA  | 6.33  | 125.55      | 118.97   |
| 18  | DF    | 192  | LEU  | CA-C-N  | 6.31  | 126.01      | 119.82   |
| 18  | DF    | 192  | LEU  | C-N-CA  | 6.31  | 126.01      | 119.82   |
| 15  | DB    | 608  | LEU  | CA-C-N  | 6.31  | 126.26      | 119.76   |
| 15  | DB    | 608  | LEU  | C-N-CA  | 6.31  | 126.26      | 119.76   |
| 52  | Cn    | 234  | GLY  | N-CA-C  | 6.29  | 120.25      | 112.64   |
| 33  | CJ    | 454  | THR  | CA-C-N  | -6.28 | 114.07      | 120.85   |
| 33  | CJ    | 454  | THR  | C-N-CA  | -6.28 | 114.07      | 120.85   |
| 17  | DE    | 739  | PRO  | CA-C-N  | 6.24  | 126.44      | 119.32   |
| 17  | DE    | 739  | PRO  | C-N-CA  | 6.24  | 126.44      | 119.32   |
| 17  | DE    | 190  | PHE  | CA-C-N  | 6.23  | 125.45      | 118.97   |
| 17  | DE    | 190  | PHE  | C-N-CA  | 6.23  | 125.45      | 118.97   |
| 17  | DE    | 613  | ILE  | N-CA-C  | 6.21  | 116.85      | 110.82   |
| 1   | DA    | 1526 | GLY  | CA-C-N  | 6.20  | 125.82      | 119.56   |
| 1   | DA    | 1526 | GLY  | C-N-CA  | 6.20  | 125.82      | 119.56   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | CR    | 80   | LEU  | N-CA-C  | 6.20  | 118.55      | 111.11   |
| 15  | DB    | 388  | VAL  | N-CA-C  | 6.15  | 118.07      | 112.29   |
| 4   | DL    | 251  | PHE  | N-CA-C  | 6.14  | 117.85      | 111.03   |
| 41  | CS    | 95   | THR  | N-CA-C  | -6.13 | 104.68      | 111.36   |
| 56  | Cv    | 1123 | GLN  | CA-C-N  | 6.12  | 126.29      | 119.32   |
| 56  | Cv    | 1123 | GLN  | C-N-CA  | 6.12  | 126.29      | 119.32   |
| 7   | DO    | 239  | LYS  | CA-C-N  | 6.12  | 125.80      | 119.56   |
| 7   | DO    | 239  | LYS  | C-N-CA  | 6.12  | 125.80      | 119.56   |
| 29  | CE    | 256  | LEU  | CB-CA-C | -6.11 | 108.92      | 117.23   |
| 1   | DA    | 224  | VAL  | N-CA-C  | 6.09  | 120.71      | 113.22   |
| 16  | DC    | 776  | ASN  | N-CA-C  | -6.08 | 105.15      | 113.30   |
| 27  | DY    | 141  | VAL  | CA-C-N  | 6.07  | 125.47      | 118.85   |
| 27  | DY    | 141  | VAL  | C-N-CA  | 6.07  | 125.47      | 118.85   |
| 45  | Cb    | 70   | THR  | CA-C-N  | -6.07 | 113.79      | 122.77   |
| 45  | Cb    | 70   | THR  | C-N-CA  | -6.07 | 113.79      | 122.77   |
| 51  | Cm    | 101  | MET  | N-CA-C  | -6.06 | 104.23      | 111.69   |
| 19  | DG    | 560  | GLU  | CA-C-N  | 6.05  | 127.41      | 119.84   |
| 19  | DG    | 560  | GLU  | C-N-CA  | 6.05  | 127.41      | 119.84   |
| 56  | Cv    | 213  | GLY  | N-CA-C  | -6.04 | 102.56      | 110.29   |
| 2   | DD    | 469  | GLY  | N-CA-C  | -6.03 | 102.17      | 111.64   |
| 38  | CP    | 182  | ARG  | CA-C-N  | 6.01  | 126.03      | 119.90   |
| 38  | CP    | 182  | ARG  | C-N-CA  | 6.01  | 126.03      | 119.90   |
| 1   | DA    | 890  | VAL  | CA-C-N  | 6.00  | 126.20      | 119.90   |
| 1   | DA    | 890  | VAL  | C-N-CA  | 6.00  | 126.20      | 119.90   |
| 43  | CZ    | 292  | ALA  | CA-C-N  | 5.98  | 126.17      | 120.31   |
| 43  | CZ    | 292  | ALA  | C-N-CA  | 5.98  | 126.17      | 120.31   |
| 33  | CJ    | 803  | ILE  | CA-C-N  | -5.96 | 114.65      | 123.11   |
| 33  | CJ    | 803  | ILE  | C-N-CA  | -5.96 | 114.65      | 123.11   |
| 18  | DF    | 427  | GLY  | CA-C-N  | 5.94  | 125.56      | 119.56   |
| 18  | DF    | 427  | GLY  | C-N-CA  | 5.94  | 125.56      | 119.56   |
| 37  | CO    | 411  | ARG  | N-CA-C  | -5.93 | 106.09      | 113.38   |
| 33  | CJ    | 373  | PHE  | N-CA-C  | 5.92  | 117.85      | 108.79   |
| 2   | DD    | 339  | ARG  | CB-CA-C | -5.90 | 108.10      | 115.89   |
| 44  | Ca    | 400  | TYR  | N-CA-C  | -5.89 | 105.94      | 113.01   |
| 44  | Ca    | 254  | ARG  | N-CA-C  | 5.89  | 118.45      | 111.33   |
| 16  | DC    | 164  | SER  | CA-C-N  | 5.88  | 127.19      | 119.84   |
| 16  | DC    | 164  | SER  | C-N-CA  | 5.88  | 127.19      | 119.84   |
| 17  | DE    | 481  | ASN  | N-CA-C  | -5.88 | 98.27       | 110.80   |
| 38  | CP    | 125  | PRO  | O-C-N   | 5.87  | 123.91      | 121.15   |
| 11  | DS    | 130  | VAL  | N-CA-C  | -5.86 | 105.97      | 111.48   |
| 31  | CH    | 17   | PRO  | CA-C-N  | 5.86  | 127.16      | 119.84   |
| 31  | CH    | 17   | PRO  | C-N-CA  | 5.86  | 127.16      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 35  | CL    | 71   | GLY  | N-CA-C | 5.86  | 122.97      | 112.77   |
| 2   | DD    | 255  | VAL  | N-CA-C | 5.86  | 121.53      | 108.88   |
| 56  | Cv    | 619  | THR  | CA-C-N | 5.86  | 123.94      | 119.66   |
| 56  | Cv    | 619  | THR  | C-N-CA | 5.86  | 123.94      | 119.66   |
| 12  | DU    | 124  | SER  | CA-C-N | 5.84  | 125.54      | 119.82   |
| 12  | DU    | 124  | SER  | C-N-CA | 5.84  | 125.54      | 119.82   |
| 30  | CF    | 72   | GLY  | N-CA-C | -5.84 | 102.52      | 112.51   |
| 33  | CJ    | 35   | SER  | N-CA-C | 5.84  | 118.32      | 107.99   |
| 20  | DH    | 452  | ARG  | CA-C-N | 5.83  | 125.84      | 119.89   |
| 20  | DH    | 452  | ARG  | C-N-CA | 5.83  | 125.84      | 119.89   |
| 56  | Cv    | 914  | ASN  | CA-C-N | -5.81 | 112.58      | 119.84   |
| 56  | Cv    | 914  | ASN  | C-N-CA | -5.81 | 112.58      | 119.84   |
| 4   | DL    | 276  | HIS  | N-CA-C | 5.80  | 119.97      | 113.01   |
| 2   | DD    | 679  | ASN  | CA-C-N | 5.80  | 125.93      | 119.32   |
| 2   | DD    | 679  | ASN  | C-N-CA | 5.80  | 125.93      | 119.32   |
| 15  | DB    | 1127 | MET  | CA-C-N | 5.79  | 125.33      | 119.19   |
| 15  | DB    | 1127 | MET  | C-N-CA | 5.79  | 125.33      | 119.19   |
| 6   | DN    | 276  | GLN  | N-CA-C | 5.79  | 116.73      | 108.74   |
| 6   | DN    | 235  | ASN  | CA-C-N | -5.75 | 113.10      | 119.19   |
| 6   | DN    | 235  | ASN  | C-N-CA | -5.75 | 113.10      | 119.19   |
| 53  | Cp    | 14   | GLY  | CA-C-N | 5.75  | 125.75      | 119.89   |
| 53  | Cp    | 14   | GLY  | C-N-CA | 5.75  | 125.75      | 119.89   |
| 31  | CH    | 215  | THR  | N-CA-C | -5.74 | 106.32      | 113.38   |
| 15  | DB    | 876  | LEU  | CA-C-N | 5.74  | 125.92      | 119.90   |
| 15  | DB    | 876  | LEU  | C-N-CA | 5.74  | 125.92      | 119.90   |
| 18  | DF    | 142  | ASN  | N-CA-C | 5.73  | 119.97      | 112.92   |
| 37  | CO    | 320  | ASP  | CA-C-N | 5.73  | 125.43      | 119.82   |
| 37  | CO    | 320  | ASP  | C-N-CA | 5.73  | 125.43      | 119.82   |
| 1   | DA    | 149  | GLY  | N-CA-C | 5.71  | 121.88      | 115.08   |
| 17  | DE    | 69   | GLY  | CA-C-N | -5.71 | 113.21      | 120.23   |
| 17  | DE    | 69   | GLY  | C-N-CA | -5.71 | 113.21      | 120.23   |
| 1   | DA    | 161  | GLU  | CA-C-N | 5.71  | 125.81      | 119.87   |
| 1   | DA    | 161  | GLU  | C-N-CA | 5.71  | 125.81      | 119.87   |
| 16  | DC    | 1123 | SER  | CA-C-N | 5.70  | 125.80      | 119.87   |
| 16  | DC    | 1123 | SER  | C-N-CA | 5.70  | 125.80      | 119.87   |
| 44  | Ca    | 438  | SER  | N-CA-C | 5.69  | 115.62      | 108.45   |
| 37  | CO    | 77   | TYR  | CA-C-N | 5.69  | 125.37      | 119.56   |
| 37  | CO    | 77   | TYR  | C-N-CA | 5.69  | 125.37      | 119.56   |
| 33  | CJ    | 703  | ALA  | N-CA-C | 5.69  | 119.03      | 111.75   |
| 55  | Cr    | 173  | SER  | CA-C-N | 5.69  | 125.30      | 119.56   |
| 55  | Cr    | 173  | SER  | C-N-CA | 5.69  | 125.30      | 119.56   |
| 35  | CL    | 72   | GLY  | N-CA-C | -5.68 | 104.43      | 111.70   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 33  | CJ    | 34   | GLN  | N-CA-C  | 5.67  | 118.29      | 110.35   |
| 20  | DH    | 81   | LYS  | CB-CA-C | -5.66 | 109.53      | 117.23   |
| 44  | Ca    | 224  | SER  | CA-C-N  | 5.63  | 125.83      | 120.31   |
| 44  | Ca    | 224  | SER  | C-N-CA  | 5.63  | 125.83      | 120.31   |
| 46  | Cd    | 194  | VAL  | N-CA-C  | 5.63  | 121.05      | 109.34   |
| 54  | Cq    | 146  | PRO  | CA-C-N  | 5.62  | 126.17      | 120.38   |
| 54  | Cq    | 146  | PRO  | C-N-CA  | 5.62  | 126.17      | 120.38   |
| 15  | DB    | 190  | HIS  | CA-C-N  | 5.62  | 125.73      | 119.32   |
| 15  | DB    | 190  | HIS  | C-N-CA  | 5.62  | 125.73      | 119.32   |
| 33  | CJ    | 549  | GLY  | N-CA-C  | -5.61 | 107.52      | 115.43   |
| 2   | DD    | 151  | SER  | N-CA-C  | -5.61 | 106.10      | 113.17   |
| 13  | DZ    | 53   | TRP  | CA-C-N  | 5.61  | 125.14      | 119.19   |
| 13  | DZ    | 53   | TRP  | C-N-CA  | 5.61  | 125.14      | 119.19   |
| 52  | Cn    | 219  | ASP  | CA-C-N  | 5.60  | 125.07      | 119.24   |
| 52  | Cn    | 219  | ASP  | C-N-CA  | 5.60  | 125.07      | 119.24   |
| 2   | DD    | 691  | PHE  | CA-C-N  | 5.60  | 125.58      | 120.03   |
| 2   | DD    | 691  | PHE  | C-N-CA  | 5.60  | 125.58      | 120.03   |
| 17  | DE    | 187  | GLN  | CA-C-N  | 5.60  | 125.97      | 119.47   |
| 17  | DE    | 187  | GLN  | C-N-CA  | 5.60  | 125.97      | 119.47   |
| 24  | DV    | 109  | ILE  | CA-C-N  | 5.60  | 125.61      | 119.90   |
| 24  | DV    | 109  | ILE  | C-N-CA  | 5.60  | 125.61      | 119.90   |
| 19  | DG    | 245  | ILE  | CA-C-N  | 5.60  | 125.13      | 119.19   |
| 19  | DG    | 245  | ILE  | C-N-CA  | 5.60  | 125.13      | 119.19   |
| 34  | CK    | 185  | MET  | CA-C-N  | -5.60 | 114.49      | 120.03   |
| 34  | CK    | 185  | MET  | C-N-CA  | -5.60 | 114.49      | 120.03   |
| 1   | DA    | 1088 | ALA  | N-CA-C  | -5.57 | 103.28      | 110.19   |
| 1   | DA    | 1590 | ARG  | N-CA-C  | -5.57 | 106.34      | 113.02   |
| 16  | DC    | 626  | ALA  | CA-C-N  | 5.56  | 125.66      | 119.32   |
| 16  | DC    | 626  | ALA  | C-N-CA  | 5.56  | 125.66      | 119.32   |
| 28  | CC    | 10   | VAL  | N-CA-C  | 5.55  | 118.33      | 112.83   |
| 1   | DA    | 1260 | VAL  | CA-C-N  | 5.54  | 126.77      | 119.84   |
| 1   | DA    | 1260 | VAL  | C-N-CA  | 5.54  | 126.77      | 119.84   |
| 15  | DB    | 908  | GLN  | CA-C-N  | 5.54  | 125.89      | 119.47   |
| 15  | DB    | 908  | GLN  | C-N-CA  | 5.54  | 125.89      | 119.47   |
| 44  | Ca    | 429  | GLY  | CA-C-N  | 5.53  | 125.89      | 119.47   |
| 44  | Ca    | 429  | GLY  | C-N-CA  | 5.53  | 125.89      | 119.47   |
| 51  | Cm    | 34   | THR  | N-CA-C  | 5.53  | 117.17      | 111.03   |
| 6   | DN    | 111  | ILE  | N-CA-C  | 5.51  | 115.92      | 107.77   |
| 45  | Cb    | 296  | PHE  | CA-C-N  | 5.50  | 125.59      | 119.87   |
| 45  | Cb    | 296  | PHE  | C-N-CA  | 5.50  | 125.59      | 119.87   |
| 29  | CE    | 41   | ARG  | N-CA-C  | 5.49  | 118.78      | 111.75   |
| 19  | DG    | 592  | THR  | N-CA-C  | -5.48 | 106.17      | 112.92   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 44  | Ca    | 563  | LEU  | N-CA-C  | 5.47  | 118.00      | 111.71   |
| 46  | Cd    | 208  | HIS  | CA-C-N  | 5.47  | 124.66      | 118.97   |
| 46  | Cd    | 208  | HIS  | C-N-CA  | 5.47  | 124.66      | 118.97   |
| 6   | DN    | 63   | LEU  | CA-C-N  | 5.45  | 125.10      | 119.05   |
| 6   | DN    | 63   | LEU  | C-N-CA  | 5.45  | 125.10      | 119.05   |
| 23  | DT    | 237  | GLY  | CA-C-N  | 5.45  | 124.64      | 118.97   |
| 23  | DT    | 237  | GLY  | C-N-CA  | 5.45  | 124.64      | 118.97   |
| 55  | Cr    | 170  | ALA  | CB-CA-C | -5.45 | 110.27      | 116.54   |
| 4   | DL    | 204  | MET  | N-CA-C  | -5.45 | 103.34      | 110.53   |
| 5   | DM    | 208  | HIS  | N-CA-C  | 5.43  | 120.01      | 113.17   |
| 17  | DE    | 479  | PRO  | CA-C-N  | -5.43 | 113.66      | 122.34   |
| 17  | DE    | 479  | PRO  | C-N-CA  | -5.43 | 113.66      | 122.34   |
| 2   | DD    | 752  | PHE  | CA-C-N  | 5.41  | 126.60      | 119.84   |
| 2   | DD    | 752  | PHE  | C-N-CA  | 5.41  | 126.60      | 119.84   |
| 16  | DC    | 54   | LEU  | CB-CA-C | -5.40 | 110.36      | 116.63   |
| 18  | DF    | 242  | VAL  | CB-CA-C | -5.40 | 106.92      | 114.00   |
| 25  | DW    | 51   | GLY  | CA-C-N  | 5.40  | 124.91      | 119.19   |
| 25  | DW    | 51   | GLY  | C-N-CA  | 5.40  | 124.91      | 119.19   |
| 1   | DA    | 774  | GLY  | N-CA-C  | 5.40  | 122.28      | 114.67   |
| 56  | Cv    | 235  | MET  | N-CA-C  | 5.40  | 117.86      | 111.33   |
| 39  | CQ    | 156  | TYR  | N-CA-C  | 5.38  | 119.95      | 113.17   |
| 21  | DJ    | 34   | LEU  | CA-C-N  | -5.37 | 116.23      | 121.65   |
| 21  | DJ    | 34   | LEU  | C-N-CA  | -5.37 | 116.23      | 121.65   |
| 28  | CC    | 11   | HIS  | N-CA-C  | 5.37  | 117.19      | 110.91   |
| 29  | CE    | 307  | ILE  | N-CA-C  | -5.36 | 105.27      | 110.42   |
| 19  | DG    | 13   | ILE  | CA-C-N  | 5.35  | 125.27      | 119.76   |
| 19  | DG    | 13   | ILE  | C-N-CA  | 5.35  | 125.27      | 119.76   |
| 27  | DY    | 161  | ARG  | N-CA-C  | 5.34  | 116.80      | 110.97   |
| 31  | CH    | 125  | LYS  | CA-C-N  | 5.34  | 125.76      | 119.99   |
| 31  | CH    | 125  | LYS  | C-N-CA  | 5.34  | 125.76      | 119.99   |
| 48  | Ci    | 62   | SER  | CA-C-N  | 5.32  | 125.03      | 119.82   |
| 48  | Ci    | 62   | SER  | C-N-CA  | 5.32  | 125.03      | 119.82   |
| 16  | DC    | 600  | ASP  | N-CA-C  | 5.30  | 118.91      | 112.23   |
| 16  | DC    | 774  | ASP  | CA-C-N  | -5.30 | 115.49      | 122.85   |
| 16  | DC    | 774  | ASP  | C-N-CA  | -5.30 | 115.49      | 122.85   |
| 56  | Cv    | 1084 | GLU  | CA-C-N  | 5.29  | 125.35      | 119.32   |
| 56  | Cv    | 1084 | GLU  | C-N-CA  | 5.29  | 125.35      | 119.32   |
| 33  | CJ    | 727  | THR  | N-CA-C  | 5.28  | 117.95      | 111.82   |
| 23  | DT    | 210  | GLY  | CA-C-N  | 5.28  | 125.59      | 119.47   |
| 23  | DT    | 210  | GLY  | C-N-CA  | 5.28  | 125.59      | 119.47   |
| 31  | CH    | 140  | VAL  | N-CA-C  | 5.27  | 113.51      | 109.19   |
| 5   | DM    | 284  | ARG  | CA-C-N  | -5.26 | 113.88      | 119.98   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | DM    | 284  | ARG  | C-N-CA | -5.26 | 113.88      | 119.98   |
| 56  | Cv    | 219  | VAL  | CA-C-N | 5.26  | 125.31      | 119.32   |
| 56  | Cv    | 219  | VAL  | C-N-CA | 5.26  | 125.31      | 119.32   |
| 29  | CE    | 255  | ASN  | N-CA-C | 5.25  | 118.96      | 111.92   |
| 47  | Cg    | 19   | VAL  | N-CA-C | 5.25  | 115.92      | 107.73   |
| 33  | CJ    | 405  | LEU  | CA-C-N | 5.25  | 125.33      | 119.87   |
| 33  | CJ    | 405  | LEU  | C-N-CA | 5.25  | 125.33      | 119.87   |
| 19  | DG    | 113  | GLU  | N-CA-C | 5.24  | 116.68      | 111.07   |
| 1   | DA    | 509  | LEU  | CA-C-N | 5.24  | 126.39      | 119.84   |
| 1   | DA    | 509  | LEU  | C-N-CA | 5.24  | 126.39      | 119.84   |
| 23  | DT    | 154  | GLN  | N-CA-C | -5.24 | 102.29      | 110.10   |
| 33  | CJ    | 158  | THR  | N-CA-C | 5.24  | 117.05      | 110.24   |
| 7   | DO    | 235  | LEU  | CA-C-N | -5.24 | 115.19      | 120.85   |
| 7   | DO    | 235  | LEU  | C-N-CA | -5.24 | 115.19      | 120.85   |
| 4   | DL    | 284  | PRO  | O-C-N  | 5.24  | 123.61      | 121.15   |
| 19  | DG    | 411  | TYR  | CA-C-N | 5.22  | 125.53      | 119.47   |
| 19  | DG    | 411  | TYR  | C-N-CA | 5.22  | 125.53      | 119.47   |
| 33  | CJ    | 800  | LEU  | CA-C-N | -5.22 | 113.65      | 119.19   |
| 33  | CJ    | 800  | LEU  | C-N-CA | -5.22 | 113.65      | 119.19   |
| 2   | DD    | 526  | GLY  | N-CA-C | -5.22 | 105.06      | 112.37   |
| 9   | DQ    | 196  | LEU  | N-CA-C | -5.21 | 101.20      | 109.96   |
| 28  | CC    | 7    | ILE  | N-CA-C | 5.21  | 115.15      | 107.75   |
| 24  | DV    | 100  | LYS  | N-CA-C | -5.21 | 106.92      | 113.28   |
| 1   | DA    | 1148 | GLY  | N-CA-C | 5.21  | 118.94      | 112.64   |
| 56  | Cv    | 995  | VAL  | N-CA-C | 5.21  | 120.17      | 109.34   |
| 8   | DP    | 85   | GLY  | N-CA-C | 5.20  | 122.96      | 112.34   |
| 39  | CQ    | 76   | TRP  | CA-C-N | -5.19 | 113.35      | 119.84   |
| 39  | CQ    | 76   | TRP  | C-N-CA | -5.19 | 113.35      | 119.84   |
| 18  | DF    | 156  | ALA  | N-CA-C | 5.19  | 119.70      | 113.17   |
| 37  | CO    | 427  | GLY  | CA-C-N | 5.19  | 125.23      | 119.32   |
| 37  | CO    | 427  | GLY  | C-N-CA | 5.19  | 125.23      | 119.32   |
| 33  | CJ    | 58   | GLY  | CA-C-N | 5.18  | 125.26      | 119.87   |
| 33  | CJ    | 58   | GLY  | C-N-CA | 5.18  | 125.26      | 119.87   |
| 21  | DJ    | 311  | SER  | CA-C-N | 5.18  | 124.98      | 119.28   |
| 21  | DJ    | 311  | SER  | C-N-CA | 5.18  | 124.98      | 119.28   |
| 44  | Ca    | 31   | GLU  | CA-C-N | 5.17  | 125.71      | 120.38   |
| 44  | Ca    | 31   | GLU  | C-N-CA | 5.17  | 125.71      | 120.38   |
| 2   | DD    | 370  | PRO  | CA-C-N | 5.17  | 124.48      | 118.85   |
| 2   | DD    | 370  | PRO  | C-N-CA | 5.17  | 124.48      | 118.85   |
| 21  | DJ    | 35   | PRO  | CA-C-O | -5.17 | 117.40      | 121.38   |
| 28  | CC    | 68   | PHE  | N-CA-C | 5.17  | 117.31      | 111.11   |
| 47  | Cg    | 192  | THR  | N-CA-C | 5.17  | 116.76      | 111.03   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | DC    | 245 | GLY  | N-CA-C  | 5.16  | 120.36      | 110.86   |
| 18  | DF    | 59  | GLY  | CA-C-N  | 5.16  | 125.46      | 119.47   |
| 18  | DF    | 59  | GLY  | C-N-CA  | 5.16  | 125.46      | 119.47   |
| 16  | DC    | 578 | VAL  | N-CA-C  | 5.16  | 112.97      | 107.76   |
| 23  | DT    | 154 | GLN  | CA-C-N  | -5.16 | 115.56      | 122.42   |
| 23  | DT    | 154 | GLN  | C-N-CA  | -5.16 | 115.56      | 122.42   |
| 3   | DI    | 314 | GLN  | N-CA-C  | 5.15  | 117.30      | 111.11   |
| 46  | Cd    | 195 | GLU  | N-CA-C  | 5.15  | 116.80      | 108.41   |
| 29  | CE    | 162 | TRP  | CA-C-N  | -5.14 | 116.67      | 122.48   |
| 29  | CE    | 162 | TRP  | C-N-CA  | -5.14 | 116.67      | 122.48   |
| 15  | DB    | 589 | ASP  | N-CA-C  | 5.14  | 117.48      | 110.24   |
| 6   | DN    | 204 | SER  | CA-C-N  | 5.13  | 124.85      | 119.82   |
| 6   | DN    | 204 | SER  | C-N-CA  | 5.13  | 124.85      | 119.82   |
| 10  | DR    | 92  | LEU  | CA-C-N  | 5.13  | 125.13      | 119.89   |
| 10  | DR    | 92  | LEU  | C-N-CA  | 5.13  | 125.13      | 119.89   |
| 50  | Ck    | 573 | THR  | N-CA-C  | -5.13 | 106.86      | 113.02   |
| 10  | DR    | 188 | LYS  | N-CA-C  | -5.13 | 105.24      | 112.12   |
| 56  | Cv    | 204 | ILE  | CB-CA-C | -5.12 | 108.83      | 113.70   |
| 17  | DE    | 304 | ASN  | N-CA-C  | 5.12  | 116.77      | 109.14   |
| 10  | DR    | 103 | ASP  | CA-C-N  | 5.12  | 124.43      | 118.85   |
| 10  | DR    | 103 | ASP  | C-N-CA  | 5.12  | 124.43      | 118.85   |
| 26  | DX    | 78  | GLU  | CA-C-N  | 5.11  | 124.72      | 119.56   |
| 26  | DX    | 78  | GLU  | C-N-CA  | 5.11  | 124.72      | 119.56   |
| 16  | DC    | 556 | GLN  | N-CA-C  | 5.11  | 120.51      | 113.77   |
| 44  | Ca    | 439 | GLU  | N-CA-C  | 5.11  | 117.24      | 111.11   |
| 24  | DV    | 78  | ASP  | CA-C-N  | 5.10  | 124.55      | 119.24   |
| 24  | DV    | 78  | ASP  | C-N-CA  | 5.10  | 124.55      | 119.24   |
| 54  | Cq    | 186 | GLY  | N-CA-C  | 5.10  | 116.91      | 110.38   |
| 27  | DY    | 72  | LYS  | CA-C-N  | 5.10  | 123.33      | 119.66   |
| 27  | DY    | 72  | LYS  | C-N-CA  | 5.10  | 123.33      | 119.66   |
| 2   | DD    | 683 | ASP  | N-CA-C  | 5.09  | 117.96      | 111.69   |
| 54  | Cq    | 140 | ARG  | CA-C-N  | 5.09  | 124.54      | 119.24   |
| 54  | Cq    | 140 | ARG  | C-N-CA  | 5.09  | 124.54      | 119.24   |
| 26  | DX    | 145 | ASN  | CA-C-N  | 5.09  | 125.02      | 119.78   |
| 26  | DX    | 145 | ASN  | C-N-CA  | 5.09  | 125.02      | 119.78   |
| 24  | DV    | 32  | PRO  | CA-C-N  | 5.09  | 124.99      | 119.85   |
| 24  | DV    | 32  | PRO  | C-N-CA  | 5.09  | 124.99      | 119.85   |
| 38  | CP    | 14  | LYS  | N-CA-C  | -5.08 | 101.48      | 109.25   |
| 51  | Cm    | 65  | GLY  | N-CA-C  | -5.08 | 107.99      | 115.30   |
| 2   | DD    | 810 | GLY  | CA-C-N  | 5.08  | 124.68      | 119.05   |
| 2   | DD    | 810 | GLY  | C-N-CA  | 5.08  | 124.68      | 119.05   |
| 6   | DN    | 58  | SER  | CA-C-N  | 5.07  | 126.17      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | DN    | 58   | SER  | C-N-CA  | 5.07  | 126.17      | 119.84   |
| 44  | Ca    | 599  | ILE  | N-CA-C  | 5.06  | 119.81      | 108.88   |
| 5   | DM    | 76   | ASN  | CA-C-N  | -5.05 | 114.45      | 119.56   |
| 5   | DM    | 76   | ASN  | C-N-CA  | -5.05 | 114.45      | 119.56   |
| 20  | DH    | 307  | ARG  | N-CA-C  | -5.04 | 102.17      | 109.59   |
| 18  | DF    | 348  | CYS  | N-CA-C  | 5.04  | 116.78      | 111.28   |
| 10  | DR    | 239  | PRO  | CA-C-N  | 5.04  | 125.04      | 119.90   |
| 10  | DR    | 239  | PRO  | C-N-CA  | 5.04  | 125.04      | 119.90   |
| 33  | CJ    | 668  | GLU  | CA-C-N  | 5.04  | 124.64      | 119.05   |
| 33  | CJ    | 668  | GLU  | C-N-CA  | 5.04  | 124.64      | 119.05   |
| 1   | DA    | 1544 | ASN  | N-CA-C  | 5.04  | 116.33      | 109.18   |
| 56  | Cv    | 60   | GLN  | N-CA-C  | 5.04  | 117.85      | 110.30   |
| 2   | DD    | 713  | GLY  | CA-C-N  | 5.03  | 124.64      | 119.56   |
| 2   | DD    | 713  | GLY  | C-N-CA  | 5.03  | 124.64      | 119.56   |
| 1   | DA    | 254  | PHE  | CA-C-N  | -5.03 | 115.69      | 123.14   |
| 1   | DA    | 254  | PHE  | C-N-CA  | -5.03 | 115.69      | 123.14   |
| 1   | DA    | 441  | SER  | CA-C-N  | 5.03  | 125.31      | 119.47   |
| 1   | DA    | 441  | SER  | C-N-CA  | 5.03  | 125.31      | 119.47   |
| 9   | DQ    | 199  | ASN  | CA-C-N  | 5.03  | 124.69      | 119.56   |
| 9   | DQ    | 199  | ASN  | C-N-CA  | 5.03  | 124.69      | 119.56   |
| 1   | DA    | 1607 | MET  | CA-C-N  | 5.03  | 125.30      | 119.47   |
| 1   | DA    | 1607 | MET  | C-N-CA  | 5.03  | 125.30      | 119.47   |
| 56  | Cv    | 302  | GLY  | N-CA-C  | -5.03 | 107.76      | 115.00   |
| 56  | Cv    | 210  | ASP  | N-CA-C  | 5.02  | 118.30      | 110.32   |
| 15  | DB    | 1079 | TRP  | N-CA-C  | 5.01  | 117.47      | 111.71   |
| 17  | DE    | 613  | ILE  | CB-CA-C | -5.01 | 105.48      | 112.04   |
| 26  | DX    | 163  | TYR  | N-CA-C  | 5.01  | 118.43      | 112.72   |
| 33  | CJ    | 294  | PRO  | N-CA-C  | -5.00 | 107.02      | 113.57   |
| 47  | Cg    | 365  | ASP  | N-CA-C  | 5.00  | 119.07      | 112.92   |

There are no chirality outliers.

All (31) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 31  | CH    | 17  | PRO  | Peptide |
| 31  | CH    | 92  | PRO  | Peptide |
| 33  | CJ    | 100 | ARG  | Peptide |
| 33  | CJ    | 798 | GLN  | Peptide |
| 35  | CL    | 70  | GLY  | Peptide |
| 35  | CL    | 71  | GLY  | Peptide |
| 35  | CL    | 79  | VAL  | Peptide |
| 37  | CO    | 70  | HIS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 37  | CO    | 86  | PRO  | Peptide |
| 46  | Cd    | 192 | ASN  | Peptide |
| 47  | Cg    | 50  | PRO  | Peptide |
| 50  | Ck    | 230 | LEU  | Peptide |
| 56  | Cv    | 545 | THR  | Peptide |
| 56  | Cv    | 943 | LEU  | Peptide |
| 1   | DA    | 166 | TYR  | Peptide |
| 1   | DA    | 273 | ASP  | Peptide |
| 16  | DC    | 497 | PRO  | Peptide |
| 16  | DC    | 775 | ALA  | Peptide |
| 2   | DD    | 247 | VAL  | Peptide |
| 2   | DD    | 255 | VAL  | Peptide |
| 2   | DD    | 351 | SER  | Peptide |
| 19  | DG    | 184 | ALA  | Peptide |
| 19  | DG    | 592 | THR  | Peptide |
| 21  | DJ    | 35  | PRO  | Peptide |
| 6   | DN    | 142 | ARG  | Peptide |
| 7   | DO    | 124 | CYS  | Peptide |
| 7   | DO    | 251 | ASN  | Peptide |
| 10  | DR    | 189 | GLU  | Peptide |
| 10  | DR    | 23  | VAL  | Peptide |
| 23  | DT    | 43  | ASP  | Peptide |
| 26  | DX    | 127 | MET  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | DA    | 12482 | 0        | 12152    | 306     | 0            |
| 2   | DD    | 6523  | 0        | 6307     | 195     | 0            |
| 3   | DI    | 3182  | 0        | 3153     | 69      | 0            |
| 4   | DL    | 2287  | 0        | 2275     | 61      | 0            |
| 5   | DM    | 2430  | 0        | 2427     | 68      | 0            |
| 6   | DN    | 2091  | 0        | 2076     | 77      | 0            |
| 7   | DO    | 1804  | 0        | 1752     | 58      | 0            |
| 8   | DP    | 1613  | 0        | 1581     | 52      | 0            |
| 9   | DQ    | 2061  | 0        | 2041     | 69      | 0            |
| 10  | DR    | 2025  | 0        | 2029     | 62      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | DS    | 1904  | 0        | 1855     | 65      | 0            |
| 12  | DU    | 1754  | 0        | 1687     | 61      | 0            |
| 13  | DZ    | 697   | 0        | 644      | 28      | 0            |
| 14  | Da    | 501   | 0        | 473      | 26      | 0            |
| 15  | DB    | 9148  | 0        | 8834     | 223     | 0            |
| 16  | DC    | 8748  | 0        | 8532     | 180     | 0            |
| 17  | DE    | 4831  | 0        | 4789     | 115     | 0            |
| 18  | DF    | 4747  | 0        | 4723     | 128     | 0            |
| 19  | DG    | 4575  | 0        | 4490     | 130     | 0            |
| 20  | DH    | 4578  | 0        | 4520     | 100     | 0            |
| 21  | DJ    | 2572  | 0        | 2495     | 75      | 0            |
| 22  | DK    | 2007  | 0        | 1998     | 41      | 0            |
| 23  | DT    | 2058  | 0        | 1928     | 86      | 0            |
| 24  | DV    | 1346  | 0        | 1335     | 38      | 0            |
| 25  | DW    | 1359  | 0        | 1342     | 41      | 0            |
| 26  | DX    | 1196  | 0        | 1189     | 30      | 0            |
| 27  | DY    | 1293  | 0        | 1287     | 33      | 0            |
| 28  | CC    | 646   | 0        | 679      | 29      | 0            |
| 29  | CE    | 3399  | 0        | 3376     | 139     | 0            |
| 30  | CF    | 1292  | 0        | 1261     | 44      | 0            |
| 31  | CH    | 2228  | 0        | 2204     | 59      | 0            |
| 32  | CI    | 3386  | 0        | 3374     | 103     | 0            |
| 33  | CJ    | 6516  | 0        | 6261     | 207     | 0            |
| 34  | CK    | 2418  | 0        | 2360     | 118     | 0            |
| 35  | CL    | 733   | 0        | 741      | 29      | 0            |
| 36  | CN    | 1322  | 0        | 1304     | 60      | 0            |
| 37  | CO    | 3003  | 0        | 2995     | 115     | 0            |
| 38  | CP    | 1489  | 0        | 1510     | 66      | 0            |
| 39  | CQ    | 1584  | 0        | 1601     | 55      | 0            |
| 40  | CR    | 2567  | 0        | 2508     | 101     | 0            |
| 41  | CS    | 1175  | 0        | 1191     | 43      | 0            |
| 42  | CU    | 1538  | 0        | 1539     | 74      | 0            |
| 43  | CZ    | 1212  | 0        | 1178     | 21      | 0            |
| 44  | Ca    | 5004  | 0        | 4776     | 219     | 0            |
| 45  | Cb    | 2056  | 0        | 2031     | 79      | 0            |
| 46  | Cd    | 2386  | 0        | 2220     | 79      | 0            |
| 47  | Cg    | 3904  | 0        | 3786     | 92      | 0            |
| 48  | Ci    | 1348  | 0        | 1306     | 65      | 0            |
| 49  | Cj    | 1792  | 0        | 1744     | 73      | 0            |
| 50  | Ck    | 5596  | 0        | 5613     | 182     | 0            |
| 51  | Cm    | 1577  | 0        | 1505     | 71      | 0            |
| 52  | Cn    | 912   | 0        | 969      | 49      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 53  | Cp    | 1483   | 0        | 1438     | 66      | 0            |
| 54  | Cq    | 2005   | 0        | 1916     | 47      | 0            |
| 55  | Cr    | 1999   | 0        | 2007     | 53      | 0            |
| 56  | Cv    | 8557   | 0        | 8252     | 262     | 0            |
| 57  | CA    | 13122  | 0        | 6563     | 279     | 0            |
| 58  | UO    | 30     | 0        | 33       | 3       | 0            |
| 59  | UP    | 42     | 0        | 46       | 1       | 0            |
| 60  | UQ    | 192    | 0        | 194      | 0       | 0            |
| 61  | UR    | 48     | 0        | 50       | 4       | 0            |
| 62  | US    | 324    | 0        | 326      | 5       | 0            |
| 63  | UT    | 264    | 0        | 268      | 4       | 0            |
| 64  | Cr    | 1      | 0        | 0        | 0       | 0            |
| 64  | DA    | 1      | 0        | 0        | 0       | 0            |
| 64  | DS    | 2      | 0        | 0        | 0       | 0            |
| 65  | DJ    | 29     | 0        | 11       | 2       | 0            |
| 66  | CA    | 35     | 0        | 0        | 0       | 0            |
| 66  | CQ    | 1      | 0        | 0        | 0       | 0            |
| 66  | Ca    | 1      | 0        | 0        | 0       | 0            |
| 66  | Cg    | 1      | 0        | 0        | 0       | 0            |
| 66  | Cv    | 1      | 0        | 0        | 0       | 0            |
| 67  | Cg    | 32     | 0        | 12       | 6       | 0            |
| 68  | CA    | 40     | 0        | 76       | 3       | 0            |
| 69  | CA    | 14     | 0        | 26       | 0       | 0            |
| 70  | Cg    | 3      | 0        | 0        | 1       | 0            |
| All | All   | 177122 | 0        | 167164   | 4189    | 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 12.

All (4189) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:Cd:137:ARG:HG2 | 46:Cd:137:ARG:HH11 | 1.23                     | 1.03              |
| 44:Ca:536:ARG:NH1 | 44:Ca:539:GLN:OE1  | 1.94                     | 0.99              |
| 30:CF:129:ASN:HB3 | 40:CR:125:ASN:HD22 | 1.31                     | 0.96              |
| 19:DG:628:LEU:O   | 47:Cg:124:LYS:NZ   | 2.00                     | 0.95              |
| 57:CA:564:U:H3    | 57:CA:570:A:H61    | 1.06                     | 0.95              |
| 33:CJ:698:HIS:HB3 | 36:CN:65:LYS:HZ1   | 1.32                     | 0.94              |
| 4:DL:273:THR:HG23 | 4:DL:276:HIS:HB2   | 1.49                     | 0.94              |
| 33:CJ:698:HIS:HB3 | 36:CN:65:LYS:NZ    | 1.82                     | 0.94              |
| 47:Cg:109:PHE:HA  | 67:Cg:501:GTP:HN21 | 1.32                     | 0.93              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:CK:315:LEU:O    | 56:Cv:175:ARG:NH1  | 2.02                     | 0.91              |
| 51:Cm:210:ARG:NH2  | 57:CA:358:U:OP2    | 2.03                     | 0.91              |
| 5:DM:27:GLN:HE22   | 56:Cv:1013:ARG:H   | 1.19                     | 0.90              |
| 1:DA:59:HIS:HD2    | 1:DA:86:TYR:H      | 1.20                     | 0.89              |
| 44:Ca:299:ARG:HH11 | 44:Ca:299:ARG:HG3  | 1.37                     | 0.89              |
| 40:CR:318:LYS:NZ   | 57:CA:590:A:OP1    | 2.05                     | 0.88              |
| 44:Ca:367:ASN:HA   | 56:Cv:954:ARG:HH22 | 1.36                     | 0.88              |
| 53:Cp:52:TYR:O     | 53:Cp:62:ARG:NH1   | 2.06                     | 0.88              |
| 56:Cv:702:ILE:HG21 | 56:Cv:761:MET:HB2  | 1.53                     | 0.88              |
| 10:DR:18:LYS:NZ    | 57:CA:165:A:OP1    | 2.07                     | 0.88              |
| 18:DF:38:GLY:H     | 18:DF:41:ASN:HD22  | 1.20                     | 0.88              |
| 19:DG:300:ASP:OD2  | 32:CI:59:ARG:NH1   | 2.08                     | 0.87              |
| 11:DS:54:ASN:HB3   | 11:DS:87:ARG:HG2   | 1.54                     | 0.86              |
| 31:CH:68:GLN:NE2   | 57:CA:4:A:N1       | 2.23                     | 0.86              |
| 1:DA:1590:ARG:HB3  | 1:DA:1593:ALA:HB3  | 1.57                     | 0.86              |
| 44:Ca:332:ARG:NH1  | 44:Ca:333:ASP:OD1  | 2.08                     | 0.85              |
| 32:CI:326:ASN:ND2  | 32:CI:330:ASN:O    | 2.09                     | 0.85              |
| 52:Cn:236:LYS:H    | 52:Cn:245:LYS:HZ3  | 1.20                     | 0.85              |
| 29:CE:71:ILE:HG23  | 29:CE:320:GLY:HA2  | 1.58                     | 0.85              |
| 29:CE:102:GLU:HG2  | 29:CE:105:GLN:HE22 | 1.42                     | 0.84              |
| 34:CK:180:ASP:HA   | 46:Cd:182:GLN:HE21 | 1.42                     | 0.84              |
| 34:CK:262:ARG:NH1  | 34:CK:269:MET:SD   | 2.50                     | 0.84              |
| 37:CO:151:LYS:NZ   | 37:CO:179:ASP:OD2  | 2.10                     | 0.84              |
| 56:Cv:590:THR:O    | 56:Cv:787:LYS:NZ   | 2.09                     | 0.84              |
| 29:CE:231:ARG:NH1  | 57:CA:16:U:O4      | 2.11                     | 0.84              |
| 19:DG:244:GLU:HG2  | 19:DG:251:ARG:HG3  | 1.58                     | 0.84              |
| 55:Cr:125:GLN:HE21 | 55:Cr:162:PRO:HD2  | 1.43                     | 0.83              |
| 18:DF:548:ARG:HD2  | 50:Ck:116:THR:HG22 | 1.58                     | 0.83              |
| 19:DG:574:ARG:HG2  | 32:CI:2:GLN:HE22   | 1.41                     | 0.83              |
| 24:DV:31:HIS:H     | 24:DV:83:GLN:HE22  | 1.23                     | 0.83              |
| 54:Cq:195:VAL:HG23 | 54:Cq:196:HIS:HD2  | 1.42                     | 0.82              |
| 2:DD:28:MET:HE1    | 31:CH:236:MET:HB3  | 1.60                     | 0.82              |
| 53:Cp:20:LYS:NZ    | 57:CA:201:A:OP2    | 2.12                     | 0.82              |
| 40:CR:112:GLY:H    | 40:CR:149:PRO:HB2  | 1.43                     | 0.82              |
| 19:DG:476:GLN:HE22 | 19:DG:560:GLU:H    | 1.24                     | 0.82              |
| 33:CJ:684:THR:OG1  | 36:CN:70:LYS:NZ    | 2.09                     | 0.82              |
| 37:CO:411:ARG:HH11 | 37:CO:424:LYS:HD2  | 1.45                     | 0.82              |
| 1:DA:79:LEU:HD21   | 38:CP:53:ARG:HH11  | 1.45                     | 0.81              |
| 6:DN:214:MET:O     | 44:Ca:308:LYS:NZ   | 2.11                     | 0.81              |
| 33:CJ:83:HIS:HD2   | 33:CJ:86:ASP:HB3   | 1.45                     | 0.81              |
| 54:Cq:177:THR:OG1  | 55:Cr:64:ARG:NH1   | 2.13                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Ck:188:LEU:HD11 | 50:Ck:224:LYS:HB3  | 1.63                     | 0.81              |
| 50:Ck:129:THR:HG22 | 50:Ck:131:ASN:H    | 1.47                     | 0.80              |
| 20:DH:520:GLY:HA2  | 23:DT:122:MET:HE3  | 1.63                     | 0.80              |
| 10:DR:249:GLU:HG3  | 10:DR:265:MET:HG2  | 1.64                     | 0.80              |
| 32:CI:89:ARG:HD2   | 34:CK:114:MET:HE2  | 1.63                     | 0.80              |
| 31:CH:176:ILE:HD13 | 31:CH:179:ARG:HH12 | 1.46                     | 0.80              |
| 10:DR:255:PRO:O    | 10:DR:268:HIS:ND1  | 2.13                     | 0.80              |
| 43:CZ:234:ILE:HG12 | 43:CZ:240:VAL:HG21 | 1.64                     | 0.80              |
| 2:DD:746:PRO:HD3   | 31:CH:77:VAL:HG12  | 1.63                     | 0.79              |
| 55:Cr:18:LEU:HD23  | 55:Cr:90:ILE:HG13  | 1.65                     | 0.79              |
| 2:DD:249:PRO:HD3   | 2:DD:329:VAL:HB    | 1.64                     | 0.79              |
| 52:Cn:243:ARG:HH12 | 57:CA:336:U:H6     | 1.28                     | 0.79              |
| 1:DA:1505:ASP:HB2  | 5:DM:163:THR:HG23  | 1.64                     | 0.79              |
| 5:DM:168:LYS:NZ    | 29:CE:342:GLY:O    | 2.16                     | 0.79              |
| 9:DQ:79:LEU:HB3    | 9:DQ:83:ASN:HD21   | 1.45                     | 0.79              |
| 1:DA:235:THR:HG23  | 1:DA:281:MET:HE2   | 1.65                     | 0.79              |
| 42:CU:115:LYS:NZ   | 51:Cm:142:GLU:OE1  | 2.12                     | 0.79              |
| 2:DD:129:ARG:HA    | 39:CQ:88:PRO:HB3   | 1.64                     | 0.79              |
| 11:DS:150:GLN:HE22 | 11:DS:176:ARG:HH21 | 1.32                     | 0.78              |
| 47:Cg:270:MET:HG2  | 47:Cg:338:GLY:HA3  | 1.64                     | 0.78              |
| 1:DA:1465:ASP:HA   | 1:DA:1605:ARG:HH12 | 1.47                     | 0.78              |
| 51:Cm:88:SER:HB2   | 57:CA:394:A:H5'    | 1.65                     | 0.78              |
| 6:DN:12:MET:HE3    | 6:DN:171:LEU:HD13  | 1.64                     | 0.78              |
| 16:DC:87:MET:HE3   | 16:DC:90:GLY:HA2   | 1.66                     | 0.78              |
| 32:CI:90:GLU:H     | 34:CK:114:MET:HE3  | 1.46                     | 0.78              |
| 42:CU:77:ARG:HH11  | 56:Cv:175:ARG:HH22 | 1.29                     | 0.78              |
| 3:DI:349:THR:HG23  | 3:DI:350:TYR:HD1   | 1.49                     | 0.77              |
| 29:CE:106:TRP:CZ2  | 44:Ca:257:ILE:HG22 | 2.18                     | 0.77              |
| 30:CF:50:ARG:HD3   | 42:CU:35:ILE:HD11  | 1.67                     | 0.77              |
| 18:DF:502:ARG:HD2  | 18:DF:579:GLU:HG3  | 1.66                     | 0.77              |
| 2:DD:149:SER:O     | 2:DD:153:THR:OG1   | 2.02                     | 0.77              |
| 11:DS:201:HIS:HD2  | 11:DS:203:ASP:H    | 1.33                     | 0.77              |
| 12:DU:206:PRO:O    | 37:CO:390:PHE:HB3  | 1.85                     | 0.77              |
| 24:DV:120:ARG:HH22 | 24:DV:131:GLN:HG2  | 1.50                     | 0.77              |
| 56:Cv:67:THR:HG22  | 56:Cv:69:GLN:H     | 1.50                     | 0.77              |
| 2:DD:626:ARG:NH1   | 49:Cj:156:THR:O    | 2.18                     | 0.76              |
| 19:DG:390:GLY:O    | 19:DG:497:ARG:NH2  | 2.18                     | 0.76              |
| 1:DA:1058:ARG:NH1  | 54:Cq:253:ARG:HH12 | 1.83                     | 0.76              |
| 16:DC:991:LYS:HG2  | 16:DC:1003:ARG:HG2 | 1.66                     | 0.76              |
| 1:DA:695:MET:HE2   | 1:DA:713:PHE:HB3   | 1.65                     | 0.76              |
| 48:Ci:101:LEU:HD13 | 50:Ck:697:MET:HE1  | 1.66                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Ck:775:ARG:HG3  | 50:Ck:775:ARG:HH11 | 1.50                     | 0.76              |
| 1:DA:225:GLY:HA3   | 1:DA:233:ARG:HH11  | 1.51                     | 0.76              |
| 10:DR:266:TRP:CG   | 49:Cj:210:PRO:HA   | 2.21                     | 0.76              |
| 29:CE:308:ARG:HA   | 29:CE:311:LYS:HZ1  | 1.49                     | 0.76              |
| 17:DE:144:PRO:HG2  | 17:DE:147:MET:HG3  | 1.68                     | 0.75              |
| 15:DB:559:GLU:OE2  | 15:DB:567:ARG:NH1  | 2.19                     | 0.75              |
| 41:CS:88:ASN:HD21  | 41:CS:105:VAL:H    | 1.32                     | 0.75              |
| 6:DN:288:PHE:O     | 29:CE:118:ARG:NH1  | 2.17                     | 0.75              |
| 12:DU:83:ARG:NH1   | 12:DU:159:ASP:OD1  | 2.20                     | 0.75              |
| 38:CP:73:LYS:NZ    | 53:Cp:29:LYS:O     | 2.19                     | 0.75              |
| 51:Cm:27:ASN:HD22  | 51:Cm:32:LYS:HG3   | 1.51                     | 0.75              |
| 33:CJ:460:HIS:O    | 33:CJ:465:SER:OG   | 2.02                     | 0.75              |
| 42:CU:142:PRO:HB2  | 42:CU:145:ALA:HB2  | 1.67                     | 0.75              |
| 18:DF:499:THR:HG22 | 20:DH:272:HIS:NE2  | 2.01                     | 0.75              |
| 56:Cv:286:THR:HG21 | 56:Cv:402:ALA:HB1  | 1.67                     | 0.75              |
| 15:DB:1053:ALA:HB2 | 20:DH:345:VAL:HG13 | 1.69                     | 0.75              |
| 56:Cv:255:PHE:HB3  | 56:Cv:292:LYS:HG3  | 1.69                     | 0.75              |
| 18:DF:15:HIS:HE1   | 21:DJ:278:GLY:HA2  | 1.50                     | 0.75              |
| 48:Ci:107:ILE:HD11 | 48:Ci:113:ALA:HB2  | 1.68                     | 0.74              |
| 50:Ck:775:ARG:HH11 | 50:Ck:775:ARG:CG   | 1.99                     | 0.74              |
| 20:DH:111:ASP:OD1  | 20:DH:170:ARG:NH2  | 2.20                     | 0.74              |
| 37:CO:127:THR:HG22 | 37:CO:131:LYS:NZ   | 2.01                     | 0.74              |
| 24:DV:60:LEU:HD13  | 24:DV:82:VAL:HG13  | 1.70                     | 0.74              |
| 37:CO:285:ASP:OD1  | 37:CO:285:ASP:N    | 2.14                     | 0.74              |
| 30:CF:136:ALA:HB3  | 34:CK:171:GLN:HB3  | 1.67                     | 0.74              |
| 49:Cj:132:LEU:HD21 | 49:Cj:135:ILE:HG13 | 1.69                     | 0.74              |
| 34:CK:214:LYS:HB3  | 34:CK:214:LYS:NZ   | 2.02                     | 0.74              |
| 2:DD:734:ARG:NH2   | 3:DI:164:GLU:OE2   | 2.21                     | 0.74              |
| 15:DB:490:ARG:HB2  | 15:DB:962:MET:HE1  | 1.69                     | 0.74              |
| 34:CK:111:ASN:HD22 | 34:CK:114:MET:HG3  | 1.51                     | 0.74              |
| 19:DG:12:ASN:O     | 33:CJ:415:ARG:NH2  | 2.21                     | 0.74              |
| 1:DA:1042:HIS:HD2  | 1:DA:1045:ILE:H    | 1.33                     | 0.74              |
| 1:DA:1662:ARG:HH22 | 29:CE:402:ARG:HH12 | 1.36                     | 0.73              |
| 42:CU:185:ARG:NH1  | 42:CU:189:ARG:O    | 2.21                     | 0.73              |
| 26:DX:50:ARG:NH2   | 41:CS:122:PHE:O    | 2.20                     | 0.73              |
| 44:Ca:359:ARG:HH21 | 56:Cv:257:LYS:HD3  | 1.53                     | 0.73              |
| 19:DG:334:MET:HE1  | 19:DG:384:VAL:O    | 1.87                     | 0.73              |
| 24:DV:123:PRO:O    | 24:DV:144:ARG:NH2  | 2.20                     | 0.73              |
| 56:Cv:95:ARG:HH11  | 56:Cv:95:ARG:HG3   | 1.51                     | 0.73              |
| 5:DM:265:ILE:HD13  | 29:CE:57:THR:HG21  | 1.68                     | 0.73              |
| 56:Cv:470:PHE:HD1  | 56:Cv:556:PHE:HE2  | 1.36                     | 0.73              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:CK:310:ILE:HG21 | 42:CU:38:PHE:HB3    | 1.70                     | 0.73              |
| 56:Cv:283:ASP:HB3  | 56:Cv:398:ARG:HD2   | 1.68                     | 0.73              |
| 9:DQ:32:GLY:HA3    | 10:DR:12:ARG:HE     | 1.52                     | 0.72              |
| 56:Cv:305:ASP:OD1  | 56:Cv:305:ASP:N     | 2.20                     | 0.72              |
| 57:CA:309:A:O2'    | 57:CA:350:U:O2'     | 2.06                     | 0.72              |
| 16:DC:119:THR:HG23 | 16:DC:132:SER:HB2   | 1.71                     | 0.72              |
| 55:Cr:242:LYS:HE2  | 55:Cr:246:GLU:OE2   | 1.89                     | 0.72              |
| 1:DA:1194:LEU:HB3  | 1:DA:1277:LEU:HD21  | 1.72                     | 0.72              |
| 16:DC:844:ALA:HB1  | 17:DE:68:PRO:HB3    | 1.70                     | 0.72              |
| 29:CE:311:LYS:NZ   | 44:Ca:368:ARG:O     | 2.22                     | 0.72              |
| 42:CU:77:ARG:NH1   | 56:Cv:175:ARG:HH22  | 1.87                     | 0.72              |
| 50:Ck:333:SER:OG   | 50:Ck:590:ARG:NH1   | 2.23                     | 0.72              |
| 51:Cm:83:LYS:NZ    | 57:CA:393:U:H5'     | 2.04                     | 0.72              |
| 41:CS:32:LYS:NZ    | 57:CA:493:U:O3'     | 2.22                     | 0.72              |
| 51:Cm:81:GLN:OE1   | 51:Cm:144:ASN:ND2   | 2.22                     | 0.72              |
| 17:DE:732:ASP:OD1  | 17:DE:735:ARG:NH2   | 2.21                     | 0.72              |
| 21:DJ:31:HIS:HD2   | 21:DJ:33:ASN:H      | 1.36                     | 0.71              |
| 1:DA:1416:VAL:HG11 | 1:DA:1442:VAL:HG13  | 1.71                     | 0.71              |
| 2:DD:736:TYR:HB3   | 31:CH:84:PRO:HG3    | 1.71                     | 0.71              |
| 26:DX:136:ARG:HH21 | 27:DY:11:THR:HG22   | 1.55                     | 0.71              |
| 38:CP:53:ARG:HH21  | 38:CP:59:ARG:HH12   | 1.38                     | 0.71              |
| 52:Cn:208:LYS:NZ   | 52:Cn:213:LYS:O     | 2.19                     | 0.71              |
| 53:Cp:93:ARG:HG3   | 53:Cp:102:ARG:NH1   | 2.05                     | 0.71              |
| 16:DC:1152:PRO:HG2 | 16:DC:1160:GLN:HE22 | 1.56                     | 0.71              |
| 27:DY:37:ARG:HH21  | 27:DY:106:GLN:HE22  | 1.37                     | 0.71              |
| 47:Cg:259:ILE:O    | 47:Cg:262:GLN:NE2   | 2.22                     | 0.71              |
| 2:DD:537:ARG:HA    | 10:DR:218:TRP:HZ3   | 1.55                     | 0.71              |
| 17:DE:431:SER:O    | 17:DE:532:TYR:HB2   | 1.91                     | 0.71              |
| 18:DF:131:ARG:NH2  | 57:CA:433:U:OP1     | 2.21                     | 0.71              |
| 4:DL:25:PRO:O      | 23:DT:202:LYS:NZ    | 2.22                     | 0.71              |
| 50:Ck:414:MET:O    | 50:Ck:541:ARG:NH2   | 2.24                     | 0.71              |
| 47:Cg:109:PHE:HA   | 67:Cg:501:GTP:N2    | 2.05                     | 0.71              |
| 9:DQ:68:ARG:NH2    | 12:DU:29:GLU:O      | 2.23                     | 0.71              |
| 37:CO:411:ARG:NH1  | 37:CO:424:LYS:HD2   | 2.03                     | 0.71              |
| 56:Cv:626:VAL:HB   | 56:Cv:628:LYS:NZ    | 2.06                     | 0.71              |
| 34:CK:53:ARG:HH21  | 40:CR:232:GLY:HA2   | 1.55                     | 0.71              |
| 2:DD:149:SER:HB2   | 2:DD:152:ALA:HB3    | 1.72                     | 0.71              |
| 19:DG:625:VAL:HG11 | 32:CI:35:GLY:HA3    | 1.73                     | 0.71              |
| 67:Cg:501:GTP:O2A  | 70:Cg:601:HOH:O     | 2.09                     | 0.71              |
| 15:DB:544:ARG:NH2  | 15:DB:572:ASP:OD1   | 2.24                     | 0.70              |
| 41:CS:158:LYS:NZ   | 43:CZ:327:LYS:O     | 2.24                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:615:ALA:HB1   | 1:DA:628:LEU:HD12  | 1.71                     | 0.70              |
| 18:DF:257:GLY:HA3  | 18:DF:265:SER:HB2  | 1.72                     | 0.70              |
| 26:DX:85:LYS:HA    | 26:DX:87:PHE:H     | 1.56                     | 0.70              |
| 7:DO:60:MET:HE1    | 7:DO:111:ARG:HB3   | 1.72                     | 0.70              |
| 19:DG:199:LEU:HD12 | 19:DG:206:LEU:HD12 | 1.74                     | 0.70              |
| 19:DG:293:ARG:HE   | 19:DG:299:PHE:HE1  | 1.36                     | 0.70              |
| 1:DA:79:LEU:HD21   | 38:CP:53:ARG:NH1   | 2.06                     | 0.70              |
| 31:CH:132:ASP:OD1  | 31:CH:132:ASP:N    | 2.24                     | 0.70              |
| 34:CK:205:TYR:HD2  | 34:CK:221:THR:HG23 | 1.56                     | 0.70              |
| 4:DL:189:THR:HB    | 40:CR:73:ASP:OD2   | 1.92                     | 0.70              |
| 37:CO:301:TRP:HZ2  | 39:CQ:182:VAL:HG21 | 1.56                     | 0.70              |
| 1:DA:59:HIS:CD2    | 1:DA:86:TYR:H      | 2.08                     | 0.70              |
| 33:CJ:792:HIS:HD2  | 33:CJ:795:LYS:H    | 1.40                     | 0.70              |
| 53:Cp:135:THR:HG21 | 53:Cp:139:SER:H    | 1.56                     | 0.70              |
| 55:Cr:22:LEU:HD22  | 55:Cr:90:ILE:HD13  | 1.73                     | 0.70              |
| 1:DA:916:ASP:HB2   | 6:DN:11:ARG:HA     | 1.72                     | 0.70              |
| 18:DF:57:ARG:HG2   | 18:DF:57:ARG:HH11  | 1.56                     | 0.70              |
| 52:Cn:171:MET:HE2  | 57:CA:555:A:H4'    | 1.72                     | 0.70              |
| 52:Cn:236:LYS:N    | 52:Cn:245:LYS:HZ3  | 1.89                     | 0.70              |
| 11:DS:108:ASN:ND2  | 11:DS:110:SER:OG   | 2.25                     | 0.70              |
| 15:DB:1023:ARG:NH2 | 33:CJ:263:ASP:OD1  | 2.25                     | 0.70              |
| 19:DG:394:PRO:O    | 19:DG:451:ARG:NH1  | 2.25                     | 0.70              |
| 21:DJ:22:MET:HG2   | 28:CC:67:ASN:HB2   | 1.73                     | 0.70              |
| 23:DT:183:LEU:HB2  | 23:DT:219:GLN:HE22 | 1.56                     | 0.70              |
| 49:Cj:124:GLY:O    | 49:Cj:207:LYS:NZ   | 2.19                     | 0.70              |
| 5:DM:52:VAL:HG22   | 5:DM:63:VAL:HG22   | 1.74                     | 0.70              |
| 18:DF:216:LYS:NZ   | 33:CJ:472:SER:O    | 2.25                     | 0.70              |
| 23:DT:44:ARG:H     | 23:DT:218:MET:HE1  | 1.55                     | 0.70              |
| 40:CR:105:ILE:HD12 | 42:CU:106:LYS:HD2  | 1.72                     | 0.70              |
| 55:Cr:275:TYR:HD1  | 55:Cr:280:ARG:NH1  | 1.90                     | 0.70              |
| 19:DG:196:ARG:NH1  | 19:DG:211:TYR:OH   | 2.24                     | 0.70              |
| 34:CK:215:ARG:NH2  | 57:CA:298:U:O2'    | 2.24                     | 0.70              |
| 13:DZ:27:MET:HE2   | 44:Ca:209:MET:HE3  | 1.73                     | 0.69              |
| 19:DG:485:MET:HE2  | 19:DG:543:VAL:HG22 | 1.73                     | 0.69              |
| 1:DA:1113:LEU:HB3  | 1:DA:1145:THR:HG21 | 1.74                     | 0.69              |
| 6:DN:237:ARG:NH2   | 44:Ca:350:GLU:OE2  | 2.25                     | 0.69              |
| 19:DG:467:THR:O    | 19:DG:478:LYS:NZ   | 2.25                     | 0.69              |
| 25:DW:168:MET:HE1  | 47:Cg:16:ARG:HH12  | 1.57                     | 0.69              |
| 29:CE:149:MET:HE2  | 29:CE:161:GLN:HB3  | 1.74                     | 0.69              |
| 34:CK:15:ARG:NH2   | 57:CA:527:A:OP2    | 2.25                     | 0.69              |
| 6:DN:222:LEU:HD11  | 44:Ca:301:ILE:HD11 | 1.74                     | 0.69              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:DB:576:GLU:O    | 15:DB:643:HIS:ND1   | 2.21                     | 0.69              |
| 6:DN:227:LYS:HE2   | 6:DN:287:ARG:HH22   | 1.57                     | 0.69              |
| 15:DB:1080:ARG:NH1 | 18:DF:177:ASP:OD1   | 2.25                     | 0.69              |
| 54:Cq:99:THR:HG23  | 54:Cq:101:LEU:H     | 1.57                     | 0.69              |
| 15:DB:118:VAL:HG21 | 15:DB:318:LEU:HD22  | 1.75                     | 0.69              |
| 28:CC:13:LYS:HD2   | 28:CC:15:ILE:HG12   | 1.73                     | 0.69              |
| 57:CA:350:U:O2'    | 57:CA:351:A:OP2     | 2.11                     | 0.69              |
| 8:DP:44:GLU:HG2    | 8:DP:59:THR:HG23    | 1.75                     | 0.69              |
| 17:DE:651:ASN:HD21 | 17:DE:654:VAL:HG23  | 1.57                     | 0.69              |
| 27:DY:36:GLU:OE2   | 27:DY:40:ARG:NH1    | 2.25                     | 0.69              |
| 37:CO:164:ARG:HH22 | 37:CO:201:PHE:HD1   | 1.41                     | 0.69              |
| 39:CQ:16:THR:HG21  | 53:Cp:18:SER:HA     | 1.74                     | 0.69              |
| 1:DA:1052:ALA:HB1  | 32:CI:202:LEU:HD21  | 1.73                     | 0.69              |
| 11:DS:225:GLU:HB3  | 11:DS:229:ARG:HH12  | 1.58                     | 0.69              |
| 31:CH:97:ARG:HG2   | 56:Cv:246:ARG:HD2   | 1.75                     | 0.69              |
| 50:Ck:179:GLU:HB3  | 50:Ck:183:ARG:HH21  | 1.57                     | 0.69              |
| 57:CA:564:U:H3     | 57:CA:570:A:N6      | 1.87                     | 0.69              |
| 38:CP:32:ARG:NH1   | 38:CP:52:LYS:HD3    | 2.08                     | 0.68              |
| 47:Cg:356:CYS:SG   | 47:Cg:357:THR:N     | 2.65                     | 0.68              |
| 50:Ck:568:LEU:HD12 | 50:Ck:569:GLY:H     | 1.58                     | 0.68              |
| 57:CA:263:A:HO2'   | 57:CA:264:A:H8      | 1.40                     | 0.68              |
| 8:DP:103:SER:O     | 49:Cj:139:ARG:NH2   | 2.25                     | 0.68              |
| 2:DD:350:LYS:O     | 2:DD:354:HIS:HB2    | 1.94                     | 0.68              |
| 4:DL:64:ILE:HG23   | 29:CE:126:ASP:HB3   | 1.74                     | 0.68              |
| 4:DL:181:ARG:NH2   | 56:Cv:494:THR:O     | 2.26                     | 0.68              |
| 15:DB:281:GLN:HB3  | 15:DB:285:MET:HE3   | 1.75                     | 0.68              |
| 33:CJ:226:ARG:HD2  | 33:CJ:815:ASN:HD21  | 1.57                     | 0.68              |
| 56:Cv:1108:GLN:HA  | 56:Cv:1108:GLN:HE21 | 1.58                     | 0.68              |
| 27:DY:77:VAL:HG22  | 27:DY:84:LYS:HZ1    | 1.56                     | 0.68              |
| 37:CO:206:MET:HE2  | 37:CO:210:ARG:HH21  | 1.59                     | 0.68              |
| 57:CA:518:G:H4'    | 57:CA:519:U:H5''    | 1.76                     | 0.68              |
| 5:DM:271:ARG:NH2   | 54:Cq:21:MET:SD     | 2.66                     | 0.68              |
| 16:DC:862:PRO:HG2  | 16:DC:865:CYS:HB2   | 1.75                     | 0.68              |
| 46:Cd:137:ARG:HG2  | 46:Cd:137:ARG:NH1   | 2.03                     | 0.68              |
| 3:DI:113:VAL:HG22  | 3:DI:114:PRO:HD2    | 1.75                     | 0.68              |
| 6:DN:118:LEU:HB3   | 6:DN:127:VAL:HG23   | 1.75                     | 0.68              |
| 16:DC:219:LEU:HD11 | 16:DC:249:LYS:HA    | 1.76                     | 0.68              |
| 57:CA:197:A:O2'    | 57:CA:199:U:OP2     | 2.11                     | 0.68              |
| 18:DF:343:GLU:HB3  | 18:DF:345:LEU:HG    | 1.76                     | 0.68              |
| 29:CE:60:TYR:HB3   | 29:CE:85:ASN:HD21   | 1.57                     | 0.68              |
| 32:CI:99:VAL:O     | 45:Cb:103:ARG:NH1   | 2.23                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:CK:203:ASN:HD22 | 34:CK:228:LYS:HZ1  | 1.41                     | 0.68              |
| 5:DM:51:VAL:HA     | 56:Cv:987:SER:HB3  | 1.76                     | 0.68              |
| 48:Ci:60:SER:HB2   | 48:Ci:69:THR:HG22  | 1.76                     | 0.68              |
| 53:Cp:53:VAL:HG11  | 53:Cp:59:PHE:HD1   | 1.59                     | 0.68              |
| 7:DO:114:GLY:O     | 7:DO:116:ALA:N     | 2.25                     | 0.68              |
| 17:DE:527:TYR:HB3  | 17:DE:543:ARG:HD2  | 1.74                     | 0.68              |
| 50:Ck:135:ASN:ND2  | 50:Ck:137:THR:O    | 2.27                     | 0.68              |
| 36:CN:108:VAL:HG21 | 36:CN:118:MET:HG3  | 1.76                     | 0.67              |
| 15:DB:1165:SER:H   | 25:DW:10:THR:HG21  | 1.57                     | 0.67              |
| 16:DC:1102:GLY:HA2 | 20:DH:59:MET:HE2   | 1.76                     | 0.67              |
| 17:DE:570:GLU:HA   | 17:DE:573:GLN:HB2  | 1.77                     | 0.67              |
| 18:DF:266:ARG:NH2  | 18:DF:293:VAL:O    | 2.26                     | 0.67              |
| 20:DH:269:ARG:NH1  | 33:CJ:288:GLN:OE1  | 2.27                     | 0.67              |
| 15:DB:1032:ASP:HB2 | 15:DB:1036:MET:HB2 | 1.73                     | 0.67              |
| 33:CJ:151:ASN:HD21 | 33:CJ:209:GLN:HB3  | 1.59                     | 0.67              |
| 55:Cr:103:VAL:HG23 | 55:Cr:184:VAL:HG13 | 1.75                     | 0.67              |
| 1:DA:212:ARG:HD2   | 11:DS:134:GLN:NE2  | 2.10                     | 0.67              |
| 1:DA:1312:TRP:CZ2  | 1:DA:1314:GLY:HA2  | 2.28                     | 0.67              |
| 16:DC:910:GLU:HG3  | 16:DC:937:LEU:HD11 | 1.77                     | 0.67              |
| 15:DB:1065:ASP:OD2 | 33:CJ:437:ARG:NH2  | 2.28                     | 0.67              |
| 16:DC:115:ASP:OD1  | 16:DC:116:TYR:N    | 2.26                     | 0.67              |
| 24:DV:61:ARG:NH2   | 57:CA:503:A:OP2    | 2.28                     | 0.67              |
| 34:CK:184:GLU:OE1  | 40:CR:181:ARG:NE   | 2.28                     | 0.67              |
| 56:Cv:26:LEU:N     | 57:CA:372:U:HO2'   | 1.92                     | 0.67              |
| 55:Cr:282:GLU:HG3  | 55:Cr:285:ARG:HH21 | 1.60                     | 0.67              |
| 36:CN:83:LYS:HB3   | 36:CN:83:LYS:HZ3   | 1.59                     | 0.67              |
| 45:Cb:216:LYS:NZ   | 45:Cb:279:ALA:O    | 2.28                     | 0.67              |
| 1:DA:874:ARG:NH2   | 1:DA:914:THR:O     | 2.28                     | 0.67              |
| 11:DS:182:TYR:OH   | 11:DS:189:ARG:NH2  | 2.28                     | 0.67              |
| 15:DB:110:ARG:HH21 | 15:DB:116:GLY:HA2  | 1.58                     | 0.67              |
| 51:Cm:53:THR:H     | 51:Cm:56:ASN:HB3   | 1.59                     | 0.67              |
| 55:Cr:67:PRO:HG2   | 55:Cr:70:GLU:HB2   | 1.76                     | 0.67              |
| 2:DD:605:ARG:NH1   | 2:DD:642:ASP:OD2   | 2.27                     | 0.66              |
| 11:DS:166:THR:HG21 | 11:DS:194:GLU:HG3  | 1.77                     | 0.66              |
| 13:DZ:48:ARG:H     | 44:Ca:586:ILE:HD11 | 1.59                     | 0.66              |
| 16:DC:330:ARG:HB2  | 16:DC:344:MET:HE1  | 1.77                     | 0.66              |
| 27:DY:33:ALA:HB2   | 27:DY:62:GLN:HG2   | 1.77                     | 0.66              |
| 36:CN:83:LYS:HB3   | 36:CN:83:LYS:NZ    | 2.09                     | 0.66              |
| 15:DB:876:LEU:HD21 | 15:DB:949:THR:HG21 | 1.76                     | 0.66              |
| 19:DG:70:TYR:HB3   | 19:DG:90:MET:HE2   | 1.77                     | 0.66              |
| 55:Cr:41:LEU:O     | 55:Cr:45:THR:OG1   | 2.12                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:DL:114:SER:O     | 4:DL:117:ASP:HB2   | 1.95                     | 0.66              |
| 37:CO:353:GLU:HB3  | 39:CQ:104:LEU:HD21 | 1.78                     | 0.66              |
| 21:DJ:316:TYR:CZ   | 23:DT:212:PHE:HB3  | 2.31                     | 0.66              |
| 26:DX:76:ARG:NH2   | 26:DX:169:ASP:OD1  | 2.25                     | 0.66              |
| 33:CJ:376:SER:HB2  | 57:CA:452:A:O2'    | 1.95                     | 0.66              |
| 3:DI:293:ILE:HG12  | 3:DI:298:VAL:HG13  | 1.77                     | 0.66              |
| 5:DM:10:ARG:HH12   | 29:CE:325:LEU:H    | 1.43                     | 0.66              |
| 6:DN:165:GLU:HG3   | 6:DN:171:LEU:H     | 1.59                     | 0.66              |
| 12:DU:122:ASN:O    | 37:CO:371:LYS:NZ   | 2.27                     | 0.66              |
| 19:DG:77:CYS:O     | 19:DG:108:ARG:NH1  | 2.28                     | 0.66              |
| 23:DT:82:HIS:HD2   | 23:DT:128:PRO:HB3  | 1.60                     | 0.66              |
| 34:CK:71:SER:O     | 34:CK:73:GLN:NE2   | 2.28                     | 0.66              |
| 45:Cb:303:GLU:HB2  | 55:Cr:105:ARG:NH1  | 2.10                     | 0.66              |
| 8:DP:15:ARG:HE     | 53:Cp:141:ARG:NH1  | 1.93                     | 0.66              |
| 14:Da:32:SER:HB3   | 31:CH:227:ARG:NH1  | 2.10                     | 0.66              |
| 18:DF:383:ASP:HB3  | 18:DF:468:MET:HE1  | 1.78                     | 0.66              |
| 22:DK:254:GLU:HG3  | 22:DK:261:SER:HB3  | 1.77                     | 0.66              |
| 42:CU:44:MET:HE1   | 42:CU:65:VAL:HG22  | 1.77                     | 0.66              |
| 1:DA:74:LYS:O      | 38:CP:59:ARG:NH2   | 2.28                     | 0.66              |
| 6:DN:293:PRO:HD2   | 29:CE:109:LYS:HD2  | 1.78                     | 0.66              |
| 15:DB:754:VAL:HG12 | 59:UP:7:UNK:HB1    | 1.78                     | 0.66              |
| 47:Cg:88:PHE:O     | 47:Cg:167:ARG:NH1  | 2.28                     | 0.66              |
| 50:Ck:119:GLU:OE1  | 50:Ck:132:TYR:OH   | 2.13                     | 0.66              |
| 51:Cm:153:ASP:OD1  | 51:Cm:153:ASP:N    | 2.27                     | 0.66              |
| 51:Cm:210:ARG:O    | 57:CA:357:A:N6     | 2.28                     | 0.66              |
| 57:CA:253:U:H2'    | 57:CA:254:A:C8     | 2.30                     | 0.66              |
| 58:UO:3:UNK:HG2    | 58:UO:5:UNK:HG3    | 1.78                     | 0.66              |
| 30:CF:41:ASN:ND2   | 46:Cd:163:GLU:O    | 2.25                     | 0.66              |
| 31:CH:16:VAL:HG13  | 31:CH:17:PRO:HD3   | 1.78                     | 0.66              |
| 34:CK:156:LYS:HB2  | 34:CK:156:LYS:NZ   | 2.10                     | 0.66              |
| 3:DI:27:THR:H      | 3:DI:30:GLN:HE21   | 1.42                     | 0.66              |
| 6:DN:10:PHE:HE1    | 6:DN:12:MET:HE2    | 1.61                     | 0.66              |
| 8:DP:143:ASN:HB2   | 49:Cj:141:GLY:HA3  | 1.78                     | 0.66              |
| 1:DA:286:VAL:HG11  | 1:DA:370:GLN:HB3   | 1.78                     | 0.66              |
| 1:DA:1090:GLY:O    | 1:DA:1384:ARG:NH2  | 2.26                     | 0.66              |
| 22:DK:306:GLU:OE2  | 23:DT:143:TYR:OH   | 2.14                     | 0.66              |
| 34:CK:304:VAL:HG12 | 42:CU:48:VAL:HG21  | 1.77                     | 0.66              |
| 8:DP:90:LEU:HD13   | 8:DP:127:ASP:HB3   | 1.77                     | 0.65              |
| 13:DZ:13:ALA:HB2   | 44:Ca:89:ARG:HA    | 1.77                     | 0.65              |
| 16:DC:1088:PHE:CE1 | 22:DK:241:VAL:HG21 | 2.31                     | 0.65              |
| 23:DT:87:ARG:HD3   | 23:DT:139:HIS:CE1  | 2.31                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:DH:558:GLU:O    | 20:DH:565:ASN:ND2  | 2.29                     | 0.65              |
| 40:CR:24:ASN:HD22  | 56:Cv:144:PHE:HA   | 1.61                     | 0.65              |
| 52:Cn:243:ARG:HG3  | 52:Cn:244:PRO:HD2  | 1.77                     | 0.65              |
| 7:DO:94:ILE:HG23   | 7:DO:99:LEU:HB2    | 1.76                     | 0.65              |
| 7:DO:236:PRO:HG2   | 7:DO:239:LYS:HG3   | 1.77                     | 0.65              |
| 27:DY:37:ARG:NH2   | 27:DY:106:GLN:HE22 | 1.93                     | 0.65              |
| 36:CN:12:HIS:NE2   | 57:CA:483:A:OP1    | 2.28                     | 0.65              |
| 37:CO:127:THR:HG22 | 37:CO:131:LYS:HZ1  | 1.60                     | 0.65              |
| 47:Cg:289:ASN:HD21 | 47:Cg:358:THR:H    | 1.44                     | 0.65              |
| 50:Ck:735:ILE:O    | 50:Ck:738:GLN:NE2  | 2.29                     | 0.65              |
| 1:DA:653:LYS:HB2   | 1:DA:726:GLU:HB2   | 1.77                     | 0.65              |
| 34:CK:188:TYR:HA   | 34:CK:192:MET:HE3  | 1.78                     | 0.65              |
| 34:CK:203:ASN:OD1  | 34:CK:204:THR:N    | 2.29                     | 0.65              |
| 47:Cg:193:ILE:HD11 | 47:Cg:267:LYS:HD2  | 1.78                     | 0.65              |
| 56:Cv:692:LYS:HD3  | 56:Cv:732:LEU:HD22 | 1.77                     | 0.65              |
| 20:DH:421:THR:O    | 33:CJ:16:ARG:NH2   | 2.30                     | 0.65              |
| 50:Ck:316:ASP:OD1  | 50:Ck:316:ASP:N    | 2.24                     | 0.65              |
| 2:DD:774:VAL:HG23  | 29:CE:294:HIS:CE1  | 2.30                     | 0.65              |
| 4:DL:276:HIS:HE1   | 57:CA:466:G:H5"    | 1.61                     | 0.65              |
| 15:DB:112:PHE:HA   | 15:DB:115:GLY:HA2  | 1.78                     | 0.65              |
| 35:CL:25:MET:HE3   | 35:CL:52:ARG:HH21  | 1.60                     | 0.65              |
| 44:Ca:189:GLU:HA   | 44:Ca:192:GLN:HB3  | 1.77                     | 0.65              |
| 44:Ca:507:MET:O    | 44:Ca:513:ASN:ND2  | 2.28                     | 0.65              |
| 55:Cr:19:LEU:HD21  | 55:Cr:41:LEU:HD11  | 1.77                     | 0.65              |
| 3:DI:349:THR:HG23  | 3:DI:350:TYR:CD1   | 2.31                     | 0.65              |
| 50:Ck:817:LEU:HD22 | 50:Ck:836:THR:HG22 | 1.78                     | 0.65              |
| 11:DS:49:VAL:HG11  | 11:DS:51:ARG:HH21  | 1.61                     | 0.65              |
| 16:DC:1088:PHE:HE1 | 22:DK:241:VAL:HG21 | 1.60                     | 0.65              |
| 32:CI:115:LEU:HD21 | 34:CK:82:MET:HE1   | 1.79                     | 0.65              |
| 51:Cm:171:ALA:HB1  | 56:Cv:54:ASN:HB3   | 1.78                     | 0.65              |
| 8:DP:33:THR:O      | 8:DP:36:GLN:NE2    | 2.21                     | 0.65              |
| 29:CE:22:ARG:HH21  | 29:CE:240:ASP:HB3  | 1.61                     | 0.65              |
| 1:DA:1662:ARG:HH22 | 29:CE:402:ARG:NH1  | 1.94                     | 0.64              |
| 19:DG:324:LEU:HD23 | 19:DG:361:SER:HB2  | 1.79                     | 0.64              |
| 24:DV:42:PHE:O     | 24:DV:43:ASN:ND2   | 2.22                     | 0.64              |
| 48:CI:69:THR:HG21  | 48:CI:73:MET:HE3   | 1.78                     | 0.64              |
| 56:Cv:813:ARG:HG2  | 56:Cv:813:ARG:NH1  | 2.12                     | 0.64              |
| 8:DP:10:ALA:N      | 57:CA:55:U:O4      | 2.30                     | 0.64              |
| 8:DP:111:THR:HG22  | 8:DP:113:ASP:H     | 1.62                     | 0.64              |
| 16:DC:88:LEU:HG    | 16:DC:93:ARG:HD2   | 1.79                     | 0.64              |
| 20:DH:518:LYS:O    | 20:DH:523:ARG:NH1  | 2.30                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:Ca:70:ASP:HA    | 44:Ca:79:MET:HB3   | 1.79                     | 0.64              |
| 47:Cg:155:LYS:HB3  | 47:Cg:356:CYS:SG   | 2.37                     | 0.64              |
| 52:Cn:145:LYS:NZ   | 57:CA:364:U:OP2    | 2.30                     | 0.64              |
| 10:DR:113:LEU:HD21 | 10:DR:140:PHE:HE1  | 1.63                     | 0.64              |
| 19:DG:65:ASN:HD21  | 32:CI:294:ILE:H    | 1.44                     | 0.64              |
| 42:CU:185:ARG:HD2  | 42:CU:187:ASN:O    | 1.98                     | 0.64              |
| 53:Cp:67:ARG:HA    | 53:Cp:124:LYS:HE2  | 1.79                     | 0.64              |
| 55:Cr:114:LEU:HD12 | 55:Cr:115:PRO:HD2  | 1.79                     | 0.64              |
| 56:Cv:292:LYS:NZ   | 56:Cv:511:HIS:O    | 2.29                     | 0.64              |
| 1:DA:1658:GLU:HB3  | 29:CE:394:ARG:HG3  | 1.80                     | 0.64              |
| 3:DI:268:LEU:HD13  | 3:DI:292:TYR:HD1   | 1.62                     | 0.64              |
| 15:DB:519:PHE:HD2  | 15:DB:522:MET:HE2  | 1.62                     | 0.64              |
| 19:DG:64:ARG:HH21  | 40:CR:249:GLN:HE22 | 1.46                     | 0.64              |
| 40:CR:320:VAL:HG12 | 46:Cd:280:SER:HB3  | 1.79                     | 0.64              |
| 20:DH:80:ARG:HG2   | 20:DH:85:LEU:HG    | 1.79                     | 0.64              |
| 22:DK:167:THR:HG22 | 22:DK:168:PRO:HD2  | 1.80                     | 0.64              |
| 33:CJ:109:ALA:HA   | 33:CJ:112:ARG:NH1  | 2.12                     | 0.64              |
| 56:Cv:304:THR:HG22 | 56:Cv:306:TYR:H    | 1.62                     | 0.64              |
| 15:DB:511:ARG:NH2  | 50:Ck:44:ALA:O     | 2.30                     | 0.64              |
| 31:CH:249:ARG:HD3  | 31:CH:266:ILE:HD13 | 1.79                     | 0.64              |
| 51:Cm:118:GLU:N    | 51:Cm:118:GLU:OE1  | 2.31                     | 0.64              |
| 56:Cv:626:VAL:HB   | 56:Cv:628:LYS:HZ2  | 1.62                     | 0.64              |
| 12:DU:142:ASP:HB2  | 12:DU:145:LYS:HG2  | 1.79                     | 0.64              |
| 15:DB:801:LEU:HB2  | 15:DB:805:GLU:HB2  | 1.79                     | 0.64              |
| 19:DG:83:MET:HE3   | 19:DG:105:LEU:HD23 | 1.80                     | 0.64              |
| 25:DW:44:ASN:O     | 25:DW:58:ARG:NH2   | 2.31                     | 0.64              |
| 33:CJ:119:ARG:HG2  | 33:CJ:119:ARG:HH11 | 1.63                     | 0.64              |
| 34:CK:28:VAL:O     | 34:CK:33:LYS:NZ    | 2.29                     | 0.64              |
| 5:DM:174:ASP:OD1   | 5:DM:177:ARG:NH2   | 2.31                     | 0.64              |
| 18:DF:136:ALA:O    | 18:DF:182:ARG:NH2  | 2.29                     | 0.64              |
| 15:DB:393:PRO:HB2  | 23:DT:113:GLN:HG3  | 1.79                     | 0.64              |
| 15:DB:749:THR:HG23 | 15:DB:750:GLU:HG3  | 1.80                     | 0.64              |
| 44:Ca:189:GLU:H    | 44:Ca:189:GLU:CD   | 2.05                     | 0.64              |
| 52:Cn:247:LYS:NZ   | 57:CA:599:A:OP1    | 2.27                     | 0.64              |
| 57:CA:73:U:H4'     | 57:CA:74:G:H5'     | 1.80                     | 0.64              |
| 1:DA:174:HIS:HA    | 38:CP:171:MET:HE2  | 1.80                     | 0.63              |
| 2:DD:575:THR:HG22  | 2:DD:577:LYS:HB2   | 1.80                     | 0.63              |
| 2:DD:700:ASP:HB2   | 2:DD:709:ARG:HD3   | 1.80                     | 0.63              |
| 19:DG:99:VAL:HG23  | 33:CJ:187:GLY:HA2  | 1.79                     | 0.63              |
| 25:DW:119:GLN:NE2  | 57:CA:400:U:O2     | 2.31                     | 0.63              |
| 33:CJ:716:ARG:NH2  | 48:CI:77:ARG:HD2   | 2.13                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:Cb:291:GLU:HB3  | 45:Cb:296:PHE:O    | 1.98                     | 0.63              |
| 49:Cj:213:ASP:N    | 49:Cj:213:ASP:OD1  | 2.30                     | 0.63              |
| 32:CI:203:ASP:N    | 32:CI:203:ASP:OD1  | 2.31                     | 0.63              |
| 41:CS:31:LEU:HD12  | 41:CS:39:GLY:HA2   | 1.78                     | 0.63              |
| 45:Cb:157:LYS:HE2  | 54:Cq:94:ARG:HG2   | 1.80                     | 0.63              |
| 45:Cb:222:SER:OG   | 45:Cb:273:VAL:O    | 2.12                     | 0.63              |
| 1:DA:568:SER:OG    | 6:DN:144:ARG:NH1   | 2.30                     | 0.63              |
| 1:DA:715:GLY:HA3   | 1:DA:721:ILE:HG12  | 1.81                     | 0.63              |
| 16:DC:1156:PRO:O   | 20:DH:41:LYS:NZ    | 2.32                     | 0.63              |
| 40:CR:37:PRO:HD3   | 45:Cb:110:MET:HG3  | 1.80                     | 0.63              |
| 47:Cg:273:LEU:O    | 47:Cg:351:LYS:NZ   | 2.32                     | 0.63              |
| 50:Ck:775:ARG:HG3  | 50:Ck:775:ARG:NH1  | 2.11                     | 0.63              |
| 54:Cq:92:LEU:O     | 54:Cq:96:THR:OG1   | 2.15                     | 0.63              |
| 5:DM:164:ILE:HD12  | 29:CE:333:ASN:HB3  | 1.81                     | 0.63              |
| 9:DQ:79:LEU:HB3    | 9:DQ:83:ASN:ND2    | 2.14                     | 0.63              |
| 9:DQ:134:ILE:HG21  | 9:DQ:248:LEU:HD22  | 1.80                     | 0.63              |
| 12:DU:46:THR:HG22  | 12:DU:48:PHE:H     | 1.63                     | 0.63              |
| 33:CJ:639:ARG:HH21 | 33:CJ:646:THR:HG22 | 1.64                     | 0.63              |
| 38:CP:87:HIS:CD2   | 44:Ca:476:PRO:HG3  | 2.33                     | 0.63              |
| 42:CU:16:HIS:HD2   | 42:CU:18:LYS:H     | 1.47                     | 0.63              |
| 45:Cb:101:LYS:NZ   | 45:Cb:101:LYS:HB3  | 2.13                     | 0.63              |
| 50:Ck:644:HIS:HD2  | 50:Ck:669:ASN:H    | 1.46                     | 0.63              |
| 56:Cv:367:ASP:OD1  | 56:Cv:367:ASP:N    | 2.31                     | 0.63              |
| 57:CA:83:U:H3'     | 57:CA:84:U:H5'     | 1.80                     | 0.63              |
| 1:DA:577:ASP:OD1   | 1:DA:578:LYS:N     | 2.30                     | 0.63              |
| 2:DD:264:LEU:HD12  | 2:DD:272:LYS:HE3   | 1.79                     | 0.63              |
| 4:DL:246:GLU:CD    | 51:Cm:61:ARG:HH12  | 2.06                     | 0.63              |
| 14:Da:27:LYS:NZ    | 57:CA:368:A:OP2    | 2.25                     | 0.63              |
| 30:CF:71:MET:HG3   | 30:CF:76:MET:HE3   | 1.80                     | 0.63              |
| 34:CK:77:MET:HG2   | 45:Cb:286:LEU:HD13 | 1.80                     | 0.63              |
| 41:CS:129:ASN:O    | 41:CS:131:PRO:HD3  | 1.99                     | 0.63              |
| 42:CU:62:MET:HB3   | 42:CU:171:VAL:HG11 | 1.80                     | 0.63              |
| 56:Cv:969:ASP:OD1  | 56:Cv:969:ASP:N    | 2.30                     | 0.63              |
| 18:DF:373:ASP:OD1  | 18:DF:373:ASP:N    | 2.31                     | 0.63              |
| 30:CF:35:LEU:HD21  | 37:CO:187:LYS:HD3  | 1.79                     | 0.63              |
| 33:CJ:793:HIS:CD2  | 33:CJ:794:GLU:HG2  | 2.33                     | 0.63              |
| 3:DI:290:PHE:HB2   | 3:DI:301:ILE:HB    | 1.80                     | 0.63              |
| 22:DK:3:PHE:O      | 22:DK:7:ASN:ND2    | 2.31                     | 0.63              |
| 44:Ca:46:ARG:NH2   | 56:Cv:1113:TYR:O   | 2.32                     | 0.63              |
| 53:Cp:93:ARG:HG3   | 53:Cp:102:ARG:HH12 | 1.63                     | 0.63              |
| 56:Cv:617:ASP:OD1  | 56:Cv:617:ASP:N    | 2.32                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:DA:446:ARG:NH1   | 1:DA:503:SER:OG     | 2.31                     | 0.63              |
| 1:DA:1060:LEU:HD13 | 1:DA:1163:MET:HE1   | 1.81                     | 0.63              |
| 9:DQ:41:GLN:NE2    | 12:DU:123:GLN:H     | 1.96                     | 0.63              |
| 21:DJ:322:SER:OG   | 23:DT:187:LYS:O     | 2.16                     | 0.63              |
| 22:DK:7:ASN:OD1    | 22:DK:135:ARG:NH1   | 2.32                     | 0.63              |
| 23:DT:106:ASP:OD1  | 23:DT:106:ASP:N     | 2.20                     | 0.63              |
| 30:CF:149:PHE:HA   | 56:Cv:627:LEU:HD11  | 1.81                     | 0.63              |
| 38:CP:28:ILE:HG13  | 38:CP:29:ILE:N      | 2.14                     | 0.63              |
| 46:Cd:141:ARG:NH2  | 56:Cv:198:HIS:O     | 2.32                     | 0.63              |
| 1:DA:150:ILE:HG12  | 1:DA:151:PRO:HD2    | 1.81                     | 0.62              |
| 1:DA:914:THR:HG21  | 1:DA:917:ARG:HH21   | 1.63                     | 0.62              |
| 16:DC:967:LEU:HD13 | 16:DC:1059:LEU:HD11 | 1.81                     | 0.62              |
| 20:DH:91:LEU:HD13  | 20:DH:119:LEU:HD21  | 1.80                     | 0.62              |
| 29:CE:81:LYS:NZ    | 56:Cv:512:MET:O     | 2.28                     | 0.62              |
| 42:CU:13:MET:HE3   | 57:CA:314:A:H5"     | 1.80                     | 0.62              |
| 1:DA:151:PRO:HG3   | 2:DD:280:LEU:HD21   | 1.80                     | 0.62              |
| 17:DE:248:THR:O    | 17:DE:252:ASP:HB2   | 1.98                     | 0.62              |
| 49:Cj:138:ASP:OD1  | 49:Cj:138:ASP:N     | 2.28                     | 0.62              |
| 5:DM:76:ASN:ND2    | 56:Cv:971:LEU:H     | 1.98                     | 0.62              |
| 7:DO:202:GLU:OE1   | 7:DO:256:ARG:NH1    | 2.31                     | 0.62              |
| 14:Da:53:ARG:HB2   | 14:Da:54:TRP:CE3    | 2.34                     | 0.62              |
| 41:CS:164:TYR:HB3  | 41:CS:170:LEU:HD13  | 1.81                     | 0.62              |
| 47:Cg:325:LEU:HD13 | 47:Cg:326:PRO:HD2   | 1.82                     | 0.62              |
| 56:Cv:930:ARG:HB3  | 56:Cv:930:ARG:HH11  | 1.64                     | 0.62              |
| 7:DO:177:MET:HG3   | 7:DO:184:MET:HE1    | 1.81                     | 0.62              |
| 20:DH:85:LEU:H     | 20:DH:85:LEU:HD12   | 1.65                     | 0.62              |
| 34:CK:324:VAL:HG11 | 42:CU:181:ILE:HG13  | 1.81                     | 0.62              |
| 48:Ci:39:ARG:NH2   | 50:Ck:773:ASP:OD1   | 2.31                     | 0.62              |
| 1:DA:1045:ILE:HD12 | 5:DM:291:ILE:HG23   | 1.81                     | 0.62              |
| 1:DA:1440:ILE:HD11 | 1:DA:1562:GLN:HG3   | 1.82                     | 0.62              |
| 6:DN:209:ARG:HD3   | 6:DN:211:TRP:CZ2    | 2.35                     | 0.62              |
| 8:DP:183:ASP:HB3   | 8:DP:186:HIS:CD2    | 2.34                     | 0.62              |
| 15:DB:917:LEU:HD13 | 15:DB:930:GLU:HB3   | 1.81                     | 0.62              |
| 43:CZ:254:ILE:HG21 | 43:CZ:318:LEU:HD21  | 1.81                     | 0.62              |
| 50:Ck:36:ARG:HH11  | 50:Ck:36:ARG:HG2    | 1.65                     | 0.62              |
| 56:Cv:408:THR:HG21 | 56:Cv:422:SER:HA    | 1.80                     | 0.62              |
| 1:DA:130:ALA:N     | 31:CH:260:ASN:HD21  | 1.98                     | 0.62              |
| 45:Cb:294:THR:HG23 | 55:Cr:283:LYS:HB3   | 1.82                     | 0.62              |
| 51:Cm:146:TRP:NE1  | 51:Cm:150:ASN:HD22  | 1.96                     | 0.62              |
| 54:Cq:146:PRO:HG3  | 54:Cq:167:MET:HE2   | 1.82                     | 0.62              |
| 56:Cv:925:ASP:HA   | 56:Cv:928:ARG:HH11  | 1.64                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:1068:GLY:HA2 | 50:Ck:660:PRO:HG3  | 1.81                     | 0.62              |
| 16:DC:200:VAL:HG13 | 16:DC:205:GLN:HB2  | 1.82                     | 0.62              |
| 18:DF:443:LEU:HD13 | 18:DF:452:VAL:HG11 | 1.80                     | 0.62              |
| 20:DH:175:ALA:HB1  | 20:DH:206:ILE:HD13 | 1.81                     | 0.62              |
| 33:CJ:544:THR:OG1  | 33:CJ:545:SER:N    | 2.32                     | 0.62              |
| 34:CK:320:MET:H    | 42:CU:81:GLU:HG2   | 1.65                     | 0.62              |
| 39:CQ:132:ALA:HB2  | 39:CQ:147:ILE:HD11 | 1.81                     | 0.62              |
| 51:Cm:202:THR:HG23 | 57:CA:338:U:H3     | 1.65                     | 0.62              |
| 1:DA:434:GLU:OE2   | 1:DA:437:LYS:NZ    | 2.30                     | 0.62              |
| 1:DA:1065:ALA:H    | 1:DA:1161:GLY:HA3  | 1.63                     | 0.62              |
| 4:DL:276:HIS:CE1   | 57:CA:466:G:H5''   | 2.35                     | 0.62              |
| 16:DC:949:PHE:O    | 16:DC:1055:ARG:NH2 | 2.33                     | 0.62              |
| 19:DG:111:ARG:NH2  | 32:CI:152:GLN:HG2  | 2.14                     | 0.62              |
| 19:DG:143:HIS:CE1  | 19:DG:202:LEU:HD13 | 2.35                     | 0.62              |
| 34:CK:53:ARG:NH1   | 34:CK:53:ARG:HB2   | 2.15                     | 0.62              |
| 34:CK:201:ARG:HE   | 42:CU:180:GLN:HE21 | 1.45                     | 0.62              |
| 46:Cd:187:GLU:HG3  | 46:Cd:191:GLY:HA2  | 1.81                     | 0.62              |
| 55:Cr:152:VAL:HG12 | 55:Cr:181:PRO:HA   | 1.81                     | 0.62              |
| 9:DQ:135:GLN:HA    | 9:DQ:138:MET:HE2   | 1.82                     | 0.62              |
| 13:DZ:11:LYS:O     | 44:Ca:89:ARG:NH1   | 2.33                     | 0.62              |
| 23:DT:30:PHE:HD1   | 23:DT:203:ARG:HH22 | 1.46                     | 0.62              |
| 30:CF:93:LEU:HB3   | 40:CR:168:ILE:HD13 | 1.81                     | 0.62              |
| 34:CK:158:ARG:NH2  | 56:Cv:617:ASP:OD2  | 2.32                     | 0.62              |
| 38:CP:88:LEU:HD21  | 53:Cp:33:ILE:HD13  | 1.81                     | 0.62              |
| 49:Cj:46:TYR:HA    | 49:Cj:165:PHE:HE2  | 1.65                     | 0.62              |
| 51:Cm:210:ARG:HG2  | 57:CA:288:U:H5''   | 1.81                     | 0.62              |
| 57:CA:38:U:H4'     | 57:CA:39:U:OP2     | 1.99                     | 0.62              |
| 1:DA:216:LEU:HB3   | 1:DA:238:VAL:HG22  | 1.80                     | 0.61              |
| 1:DA:1507:VAL:HB   | 5:DM:175:GLU:HG3   | 1.81                     | 0.61              |
| 25:DW:122:ARG:HD2  | 25:DW:126:ARG:HH21 | 1.64                     | 0.61              |
| 30:CF:2:VAL:HG13   | 30:CF:37:ARG:HD2   | 1.82                     | 0.61              |
| 40:CR:314:THR:HA   | 40:CR:318:LYS:HB2  | 1.80                     | 0.61              |
| 43:CZ:243:THR:HG21 | 43:CZ:245:LYS:HE3  | 1.80                     | 0.61              |
| 51:Cm:134:ARG:HD2  | 57:CA:396:A:H2     | 1.65                     | 0.61              |
| 56:Cv:458:PRO:HG3  | 56:Cv:828:ALA:HA   | 1.80                     | 0.61              |
| 7:DO:69:GLU:HA     | 7:DO:72:GLU:HB3    | 1.83                     | 0.61              |
| 13:DZ:62:ASP:OD1   | 13:DZ:62:ASP:N     | 2.29                     | 0.61              |
| 42:CU:74:GLN:HE21  | 42:CU:74:GLN:C     | 2.08                     | 0.61              |
| 43:CZ:236:ARG:O    | 43:CZ:237:ARG:HB3  | 1.99                     | 0.61              |
| 53:Cp:69:ARG:HG2   | 53:Cp:104:ALA:HB2  | 1.82                     | 0.61              |
| 1:DA:825:GLU:OE2   | 6:DN:189:ARG:NH2   | 2.32                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:DN:292:TYR:HH    | 29:CE:117:TRP:CD1  | 2.19                     | 0.61              |
| 17:DE:463:LEU:HD23 | 17:DE:486:ILE:HG23 | 1.82                     | 0.61              |
| 22:DK:220:PRO:HG2  | 22:DK:223:ALA:HB2  | 1.83                     | 0.61              |
| 47:Cg:82:ASN:OD1   | 47:Cg:107:ARG:NH1  | 2.34                     | 0.61              |
| 6:DN:212:THR:OG1   | 44:Ca:193:ARG:NH1  | 2.32                     | 0.61              |
| 47:Cg:383:ASP:OD1  | 47:Cg:383:ASP:N    | 2.32                     | 0.61              |
| 54:Cq:195:VAL:HG23 | 54:Cq:196:HIS:CD2  | 2.31                     | 0.61              |
| 11:DS:36:SER:OG    | 57:CA:199:U:OP1    | 2.19                     | 0.61              |
| 15:DB:725:LEU:HD22 | 15:DB:809:MET:HE1  | 1.81                     | 0.61              |
| 20:DH:233:MET:HE1  | 20:DH:244:THR:HG21 | 1.82                     | 0.61              |
| 21:DJ:132:ARG:NH2  | 65:DJ:401:UTP:O2B  | 2.33                     | 0.61              |
| 34:CK:79:TRP:HE1   | 45:Cb:289:LYS:NZ   | 1.98                     | 0.61              |
| 38:CP:108:CYS:O    | 46:Cd:58:ARG:NH2   | 2.33                     | 0.61              |
| 54:Cq:83:LEU:HD21  | 55:Cr:196:VAL:HG21 | 1.83                     | 0.61              |
| 1:DA:751:GLU:HG3   | 5:DM:197:LEU:HD22  | 1.83                     | 0.61              |
| 15:DB:557:ALA:O    | 18:DF:512:ASN:ND2  | 2.32                     | 0.61              |
| 17:DE:72:ARG:HB3   | 17:DE:194:HIS:HB2  | 1.81                     | 0.61              |
| 39:CQ:198:LEU:O    | 39:CQ:199:ASN:ND2  | 2.34                     | 0.61              |
| 1:DA:236:ARG:NH1   | 44:Ca:541:ARG:O    | 2.33                     | 0.61              |
| 1:DA:617:PRO:HG2   | 1:DA:746:GLN:NE2   | 2.16                     | 0.61              |
| 2:DD:64:HIS:HD2    | 44:Ca:447:ILE:HG21 | 1.64                     | 0.61              |
| 7:DO:131:ASP:HB3   | 7:DO:133:LYS:HG2   | 1.81                     | 0.61              |
| 20:DH:120:HIS:H    | 20:DH:123:HIS:HD2  | 1.47                     | 0.61              |
| 37:CO:73:ILE:HD13  | 52:Cn:226:LEU:HD23 | 1.82                     | 0.61              |
| 56:Cv:930:ARG:HB3  | 56:Cv:930:ARG:NH1  | 2.15                     | 0.61              |
| 56:Cv:938:ASP:OD1  | 56:Cv:938:ASP:N    | 2.28                     | 0.61              |
| 57:CA:35:U:H3'     | 57:CA:36:U:H5''    | 1.82                     | 0.61              |
| 1:DA:90:MET:O      | 2:DD:123:ARG:NH1   | 2.33                     | 0.61              |
| 1:DA:1278:THR:HG22 | 1:DA:1280:GLU:H    | 1.65                     | 0.61              |
| 2:DD:608:ASP:OD1   | 10:DR:221:ARG:NH2  | 2.34                     | 0.61              |
| 33:CJ:617:ARG:NH2  | 48:Ci:21:SER:OG    | 2.34                     | 0.61              |
| 43:CZ:305:HIS:HD2  | 43:CZ:307:LYS:HB2  | 1.65                     | 0.61              |
| 1:DA:562:LYS:HA    | 1:DA:567:ALA:HB3   | 1.82                     | 0.61              |
| 1:DA:650:LEU:HB3   | 1:DA:728:VAL:HG12  | 1.83                     | 0.61              |
| 21:DJ:242:LEU:HB3  | 21:DJ:294:MET:HE2  | 1.83                     | 0.61              |
| 30:CF:12:PRO:HG3   | 30:CF:62:ALA:HA    | 1.83                     | 0.61              |
| 33:CJ:431:PHE:HB2  | 50:Ck:678:GLU:HB2  | 1.82                     | 0.61              |
| 39:CQ:94:LYS:HD3   | 39:CQ:111:THR:HG21 | 1.83                     | 0.61              |
| 45:Cb:19:PRO:HD2   | 51:Cm:156:THR:HG21 | 1.82                     | 0.61              |
| 52:Cn:141:ARG:HD2  | 57:CA:280:A:N1     | 2.15                     | 0.61              |
| 15:DB:983:LEU:HD11 | 19:DG:123:LEU:HD13 | 1.83                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DT:82:HIS:CD2   | 23:DT:128:PRO:HB3  | 2.36                     | 0.61              |
| 23:DT:144:SER:OG   | 23:DT:161:ASN:ND2  | 2.34                     | 0.61              |
| 25:DW:103:PRO:HB3  | 27:DY:97:ARG:NH1   | 2.16                     | 0.61              |
| 29:CE:15:TRP:CD1   | 29:CE:18:LYS:HZ1   | 2.18                     | 0.61              |
| 7:DO:139:GLU:HB3   | 7:DO:176:THR:HG23  | 1.83                     | 0.60              |
| 27:DY:128:GLN:C    | 27:DY:128:GLN:HE21 | 2.09                     | 0.60              |
| 41:CS:158:LYS:HZ3  | 43:CZ:328:SER:HA   | 1.66                     | 0.60              |
| 29:CE:173:LYS:HB3  | 45:Cb:45:PHE:CE2   | 2.36                     | 0.60              |
| 38:CP:93:THR:HG22  | 44:Ca:447:ILE:HG12 | 1.84                     | 0.60              |
| 39:CQ:197:LYS:NZ   | 39:CQ:199:ASN:O    | 2.34                     | 0.60              |
| 44:Ca:570:THR:O    | 57:CA:30:U:O2'     | 2.18                     | 0.60              |
| 46:Cd:139:SER:O    | 46:Cd:143:GLN:HG2  | 2.01                     | 0.60              |
| 47:Cg:85:LEU:HD22  | 47:Cg:107:ARG:HG2  | 1.82                     | 0.60              |
| 1:DA:518:GLU:OE2   | 1:DA:837:ARG:NH2   | 2.35                     | 0.60              |
| 8:DP:36:GLN:HG2    | 12:DU:204:LEU:HG   | 1.82                     | 0.60              |
| 11:DS:33:LEU:HG    | 11:DS:35:TYR:HB2   | 1.81                     | 0.60              |
| 34:CK:200:ARG:NE   | 34:CK:205:TYR:OH   | 2.34                     | 0.60              |
| 54:Cq:175:TRP:HZ3  | 54:Cq:235:LEU:HD23 | 1.66                     | 0.60              |
| 4:DL:283:ILE:HG23  | 28:CC:75:ILE:HD11  | 1.82                     | 0.60              |
| 15:DB:83:GLU:OE2   | 15:DB:154:ARG:NH2  | 2.34                     | 0.60              |
| 15:DB:625:ASN:OD1  | 15:DB:625:ASN:N    | 2.32                     | 0.60              |
| 29:CE:312:GLY:O    | 29:CE:314:MET:N    | 2.31                     | 0.60              |
| 34:CK:280:ARG:HA   | 34:CK:308:GLU:O    | 2.01                     | 0.60              |
| 5:DM:217:ALA:O     | 5:DM:221:LYS:NZ    | 2.35                     | 0.60              |
| 34:CK:174:VAL:HG13 | 56:Cv:648:VAL:HB   | 1.82                     | 0.60              |
| 53:Cp:123:THR:HG21 | 57:CA:45:G:H22     | 1.65                     | 0.60              |
| 2:DD:500:LEU:H     | 2:DD:500:LEU:HD12  | 1.65                     | 0.60              |
| 6:DN:118:LEU:HD22  | 6:DN:129:LEU:HD11  | 1.82                     | 0.60              |
| 27:DY:139:ASP:OD2  | 27:DY:145:ARG:NH1  | 2.34                     | 0.60              |
| 33:CJ:374:TRP:CZ3  | 36:CN:106:GLU:HB3  | 2.37                     | 0.60              |
| 37:CO:82:ASN:ND2   | 52:Cn:142:TRP:H    | 2.00                     | 0.60              |
| 44:Ca:264:ARG:HH11 | 44:Ca:264:ARG:HG3  | 1.67                     | 0.60              |
| 47:Cg:249:TRP:O    | 47:Cg:261:ARG:NH1  | 2.35                     | 0.60              |
| 54:Cq:26:MET:HG2   | 54:Cq:30:ILE:HD11  | 1.84                     | 0.60              |
| 1:DA:251:SER:OG    | 1:DA:253:ASP:OD1   | 2.12                     | 0.60              |
| 22:DK:4:ARG:NH2    | 23:DT:131:SER:O    | 2.34                     | 0.60              |
| 50:Ck:834:MET:HA   | 50:Ck:838:LEU:HB3  | 1.84                     | 0.60              |
| 56:Cv:333:ILE:HG12 | 56:Cv:336:ARG:HH21 | 1.67                     | 0.60              |
| 5:DM:1:MET:HE3     | 5:DM:2:GLU:N       | 2.17                     | 0.60              |
| 15:DB:925:ASP:OD1  | 15:DB:925:ASP:N    | 2.32                     | 0.60              |
| 26:DX:57:ARG:NH2   | 41:CS:64:MET:HG3   | 2.17                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:CL:84:ARG:NH2   | 57:CA:265:U:O2     | 2.35                     | 0.60              |
| 39:CQ:103:MET:HB2  | 39:CQ:106:THR:HB   | 1.84                     | 0.60              |
| 1:DA:551:LYS:HA    | 1:DA:554:GLU:HG2   | 1.84                     | 0.60              |
| 1:DA:1486:ALA:O    | 1:DA:1488:GLN:NE2  | 2.34                     | 0.60              |
| 6:DN:57:ARG:HG3    | 6:DN:66:GLY:HA3    | 1.84                     | 0.60              |
| 19:DG:186:ARG:HH12 | 19:DG:189:LYS:HD3  | 1.66                     | 0.60              |
| 27:DY:148:ARG:NH1  | 57:CA:517:U:OP2    | 2.35                     | 0.60              |
| 33:CJ:541:LEU:HD22 | 33:CJ:552:ILE:HG13 | 1.82                     | 0.60              |
| 44:Ca:225:PRO:HG2  | 44:Ca:228:LYS:HB2  | 1.84                     | 0.60              |
| 50:Ck:682:ASN:HD22 | 50:Ck:682:ASN:H    | 1.50                     | 0.60              |
| 50:Ck:775:ARG:HH11 | 50:Ck:775:ARG:CB   | 2.14                     | 0.60              |
| 52:Cn:214:ARG:H    | 52:Cn:214:ARG:HD3  | 1.66                     | 0.60              |
| 56:Cv:441:PRO:HD3  | 56:Cv:447:PRO:HD3  | 1.82                     | 0.60              |
| 56:Cv:470:PHE:CD1  | 56:Cv:556:PHE:HE2  | 2.19                     | 0.60              |
| 16:DC:952:GLU:H    | 16:DC:952:GLU:CD   | 2.10                     | 0.60              |
| 19:DG:96:LYS:HB3   | 33:CJ:188:ARG:HD2  | 1.83                     | 0.60              |
| 34:CK:203:ASN:HD22 | 34:CK:228:LYS:NZ   | 1.99                     | 0.60              |
| 35:CL:15:ARG:HE    | 35:CL:42:PHE:HE2   | 1.50                     | 0.60              |
| 50:Ck:287:GLU:O    | 50:Ck:293:ARG:NH2  | 2.35                     | 0.60              |
| 1:DA:938:ILE:HD12  | 5:DM:122:LYS:HB2   | 1.83                     | 0.59              |
| 2:DD:248:ASP:OD1   | 12:DU:31:SER:HB2   | 2.02                     | 0.59              |
| 8:DP:115:LEU:HD21  | 8:DP:135:LEU:HD13  | 1.84                     | 0.59              |
| 33:CJ:463:MET:HE1  | 48:Ci:85:PRO:HB2   | 1.83                     | 0.59              |
| 2:DD:799:ASP:OD1   | 2:DD:799:ASP:N     | 2.31                     | 0.59              |
| 33:CJ:239:ARG:O    | 33:CJ:239:ARG:NH1  | 2.30                     | 0.59              |
| 40:CR:153:GLU:HA   | 56:Cv:183:LEU:HD23 | 1.84                     | 0.59              |
| 44:Ca:67:ARG:NH1   | 44:Ca:79:MET:O     | 2.35                     | 0.59              |
| 47:Cg:109:PHE:CA   | 67:Cg:501:GTP:HN21 | 2.12                     | 0.59              |
| 9:DQ:49:ARG:HH12   | 37:CO:361:ALA:HA   | 1.66                     | 0.59              |
| 11:DS:52:ASP:OD1   | 11:DS:55:ARG:NH1   | 2.35                     | 0.59              |
| 15:DB:635:MET:HG3  | 50:Ck:373:ARG:HD3  | 1.83                     | 0.59              |
| 19:DG:476:GLN:NE2  | 19:DG:560:GLU:H    | 1.99                     | 0.59              |
| 33:CJ:17:MET:HE2   | 33:CJ:18:PRO:HD2   | 1.84                     | 0.59              |
| 35:CL:69:GLU:HG2   | 35:CL:70:GLY:N     | 2.17                     | 0.59              |
| 57:CA:360:C:H2'    | 57:CA:361:A:H5'    | 1.84                     | 0.59              |
| 2:DD:802:LYS:HA    | 2:DD:807:ARG:HE    | 1.67                     | 0.59              |
| 7:DO:194:TYR:HB3   | 7:DO:253:PRO:HB2   | 1.84                     | 0.59              |
| 8:DP:30:LYS:HG3    | 53:Cp:144:PRO:HG2  | 1.85                     | 0.59              |
| 15:DB:455:ARG:NH1  | 15:DB:461:GLN:O    | 2.36                     | 0.59              |
| 15:DB:898:GLN:HE21 | 50:Ck:270:TYR:HB2  | 1.67                     | 0.59              |
| 22:DK:5:TYR:HD2    | 23:DT:78:GLU:HG2   | 1.67                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:130:ARG:NH2  | 50:Ck:308:ARG:O    | 2.35                     | 0.59              |
| 33:CJ:405:LEU:HD23 | 33:CJ:406:PRO:HD2  | 1.83                     | 0.59              |
| 34:CK:282:MET:HG2  | 34:CK:310:ILE:O    | 2.02                     | 0.59              |
| 36:CN:160:VAL:HG13 | 36:CN:165:ARG:HH21 | 1.65                     | 0.59              |
| 40:CR:25:GLU:H     | 56:Cv:143:THR:HG21 | 1.68                     | 0.59              |
| 44:Ca:76:GLN:HA    | 44:Ca:79:MET:HE2   | 1.84                     | 0.59              |
| 57:CA:460:U:O2     | 57:CA:461:A:N6     | 2.35                     | 0.59              |
| 1:DA:714:LEU:HB3   | 1:DA:721:ILE:HD13  | 1.84                     | 0.59              |
| 2:DD:735:GLY:HA3   | 3:DI:96:CYS:SG     | 2.42                     | 0.59              |
| 6:DN:223:GLN:HB2   | 44:Ca:256:GLU:OE2  | 2.03                     | 0.59              |
| 9:DQ:92:MET:HE1    | 9:DQ:210:VAL:HG11  | 1.84                     | 0.59              |
| 37:CO:72:ALA:HA    | 37:CO:87:THR:HG21  | 1.84                     | 0.59              |
| 37:CO:76:TRP:HB2   | 37:CO:83:PRO:HB3   | 1.85                     | 0.59              |
| 6:DN:270:HIS:O     | 6:DN:273:SER:OG    | 2.21                     | 0.59              |
| 10:DR:101:VAL:HG21 | 10:DR:123:VAL:HG12 | 1.84                     | 0.59              |
| 29:CE:42:ARG:HB2   | 29:CE:102:GLU:OE2  | 2.02                     | 0.59              |
| 31:CH:148:LEU:N    | 31:CH:225:ASP:OD1  | 2.27                     | 0.59              |
| 42:CU:157:ALA:HA   | 42:CU:160:ARG:HH11 | 1.66                     | 0.59              |
| 44:Ca:597:LYS:HB2  | 44:Ca:597:LYS:NZ   | 2.17                     | 0.59              |
| 4:DL:171:ARG:NH1   | 45:Cb:80:THR:OG1   | 2.36                     | 0.59              |
| 6:DN:251:PHE:CD2   | 6:DN:273:SER:HB3   | 2.38                     | 0.59              |
| 12:DU:73:ARG:NH1   | 12:DU:73:ARG:O     | 2.35                     | 0.59              |
| 15:DB:333:ALA:HB1  | 17:DE:33:ILE:HD13  | 1.83                     | 0.59              |
| 18:DF:154:ASN:ND2  | 18:DF:157:THR:OG1  | 2.35                     | 0.59              |
| 19:DG:473:CYS:HB3  | 19:DG:477:GLN:HE22 | 1.67                     | 0.59              |
| 27:DY:33:ALA:CB    | 27:DY:62:GLN:HG2   | 2.33                     | 0.59              |
| 29:CE:83:MET:HE1   | 29:CE:307:ILE:HD11 | 1.85                     | 0.59              |
| 29:CE:308:ARG:HA   | 29:CE:311:LYS:NZ   | 2.16                     | 0.59              |
| 55:Cr:168:MET:HE1  | 55:Cr:177:LEU:HD12 | 1.85                     | 0.59              |
| 12:DU:94:TRP:CH2   | 12:DU:196:MET:HE1  | 2.38                     | 0.59              |
| 17:DE:503:ASP:N    | 17:DE:503:ASP:OD1  | 2.34                     | 0.59              |
| 23:DT:52:ARG:NH1   | 23:DT:213:ASP:OD1  | 2.35                     | 0.59              |
| 44:Ca:367:ASN:HA   | 56:Cv:954:ARG:NH2  | 2.15                     | 0.59              |
| 45:Cb:56:ARG:NH1   | 45:Cb:57:MET:HE1   | 2.18                     | 0.59              |
| 45:Cb:90:GLU:OE1   | 45:Cb:90:GLU:N     | 2.29                     | 0.59              |
| 47:Cg:301:HIS:HD2  | 47:Cg:303:ASP:H    | 1.49                     | 0.59              |
| 1:DA:230:PHE:O     | 11:DS:62:ARG:NH2   | 2.36                     | 0.59              |
| 2:DD:83:THR:O      | 2:DD:87:MET:N      | 2.34                     | 0.59              |
| 16:DC:119:THR:HG21 | 16:DC:136:TRP:NE1  | 2.18                     | 0.59              |
| 17:DE:566:ARG:NH2  | 20:DH:528:GLU:OE2  | 2.35                     | 0.59              |
| 24:DV:114:VAL:HG22 | 24:DV:115:PRO:HD2  | 1.84                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 44:Ca:299:ARG:HG3  | 44:Ca:299:ARG:NH1   | 2.08                     | 0.59              |
| 45:Cb:165:ALA:HB1  | 54:Cq:117:ALA:HB1   | 1.85                     | 0.59              |
| 50:Ck:153:VAL:HG21 | 50:Ck:247:LEU:HB3   | 1.84                     | 0.59              |
| 1:DA:212:ARG:HD2   | 11:DS:134:GLN:HE22  | 1.68                     | 0.59              |
| 1:DA:213:LEU:HD21  | 1:DA:274:LEU:HD11   | 1.84                     | 0.59              |
| 12:DU:227:SER:HA   | 49:Cj:161:VAL:HG13  | 1.84                     | 0.59              |
| 15:DB:1102:TYR:O   | 15:DB:1106:VAL:HG23 | 2.03                     | 0.59              |
| 18:DF:170:ARG:HG2  | 48:Ci:104:ARG:NH2   | 2.18                     | 0.59              |
| 23:DT:65:VAL:HG23  | 23:DT:160:TYR:HB3   | 1.85                     | 0.59              |
| 40:CR:184:LYS:HB2  | 40:CR:184:LYS:NZ    | 2.18                     | 0.59              |
| 45:Cb:169:LYS:HD2  | 45:Cb:176:THR:HG23  | 1.84                     | 0.59              |
| 53:Cp:162:LEU:HD12 | 53:Cp:163:PRO:HD2   | 1.84                     | 0.59              |
| 1:DA:70:ARG:NH2    | 57:CA:73:U:OP2      | 2.33                     | 0.58              |
| 1:DA:212:ARG:HA    | 11:DS:134:GLN:HE22  | 1.66                     | 0.58              |
| 14:Da:36:SER:OG    | 14:Da:38:ASP:OD1    | 2.21                     | 0.58              |
| 16:DC:211:LYS:NZ   | 16:DC:439:ALA:HA    | 2.17                     | 0.58              |
| 17:DE:319:ASN:OD1  | 17:DE:319:ASN:N     | 2.36                     | 0.58              |
| 44:Ca:423:GLN:HE21 | 44:Ca:479:THR:HA    | 1.67                     | 0.58              |
| 53:Cp:55:ASN:HB2   | 53:Cp:57:GLU:OE2    | 2.03                     | 0.58              |
| 49:Cj:73:ARG:NH1   | 53:Cp:169:ASN:HB3   | 2.18                     | 0.58              |
| 50:Ck:149:LEU:HG   | 50:Ck:254:ILE:HD11  | 1.85                     | 0.58              |
| 56:Cv:305:ASP:O    | 56:Cv:412:GLY:HA3   | 2.02                     | 0.58              |
| 57:CA:309:A:O2'    | 57:CA:351:A:OP2     | 2.20                     | 0.58              |
| 3:DI:356:ILE:HG21  | 3:DI:378:LEU:HD21   | 1.84                     | 0.58              |
| 6:DN:57:ARG:NH2    | 6:DN:70:GLU:OE2     | 2.37                     | 0.58              |
| 10:DR:112:ARG:HD2  | 49:Cj:158:THR:HG23  | 1.86                     | 0.58              |
| 13:DZ:17:LEU:HD21  | 56:Cv:1120:TRP:HB3  | 1.85                     | 0.58              |
| 18:DF:101:ALA:O    | 36:CN:78:GLN:NE2    | 2.37                     | 0.58              |
| 18:DF:288:MET:HE3  | 20:DH:363:PRO:HG3   | 1.85                     | 0.58              |
| 20:DH:518:LYS:HG3  | 20:DH:523:ARG:HH12  | 1.68                     | 0.58              |
| 21:DJ:261:PHE:O    | 21:DJ:305:ARG:NH2   | 2.36                     | 0.58              |
| 44:Ca:569:ARG:NH1  | 57:CA:143:U:H5''    | 2.17                     | 0.58              |
| 56:Cv:491:LEU:HB3  | 56:Cv:529:PHE:HB3   | 1.85                     | 0.58              |
| 57:CA:233:C:H4'    | 57:CA:234:C:H5''    | 1.85                     | 0.58              |
| 1:DA:985:LYS:HE3   | 1:DA:1205:THR:HG21  | 1.83                     | 0.58              |
| 2:DD:620:ALA:O     | 2:DD:623:TRP:HB2    | 2.03                     | 0.58              |
| 15:DB:447:PHE:CD1  | 20:DH:154:LYS:HG2   | 2.39                     | 0.58              |
| 29:CE:14:SER:O     | 29:CE:14:SER:OG     | 2.16                     | 0.58              |
| 49:Cj:209:TYR:CZ   | 49:Cj:212:TYR:HB2   | 2.38                     | 0.58              |
| 11:DS:57:LEU:HD11  | 11:DS:83:LEU:HD23   | 1.86                     | 0.58              |
| 17:DE:406:ASP:HB2  | 17:DE:410:ARG:HD3   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:DG:215:LEU:HD22 | 19:DG:224:LEU:HD12 | 1.85                     | 0.58              |
| 23:DT:85:ASP:OD2   | 23:DT:87:ARG:NH1   | 2.37                     | 0.58              |
| 42:CU:10:GLY:HA3   | 57:CA:344:C:OP1    | 2.03                     | 0.58              |
| 45:Cb:9:TYR:CD1    | 57:CA:612:U:H5''   | 2.39                     | 0.58              |
| 46:Cd:178:ASN:HB2  | 46:Cd:182:GLN:H    | 1.68                     | 0.58              |
| 50:Ck:834:MET:HG2  | 50:Ck:838:LEU:HD12 | 1.86                     | 0.58              |
| 56:Cv:78:ILE:HD11  | 56:Cv:80:TYR:CZ    | 2.38                     | 0.58              |
| 56:Cv:690:GLU:HB2  | 56:Cv:798:TYR:CE1  | 2.38                     | 0.58              |
| 4:DL:279:ARG:HD3   | 33:CJ:50:ASP:OD2   | 2.04                     | 0.58              |
| 6:DN:292:TYR:HH    | 29:CE:117:TRP:CG   | 2.20                     | 0.58              |
| 10:DR:117:ILE:HG22 | 10:DR:118:VAL:H    | 1.68                     | 0.58              |
| 17:DE:184:PHE:O    | 17:DE:536:ARG:NH1  | 2.37                     | 0.58              |
| 20:DH:446:PRO:HD3  | 21:DJ:40:ARG:NH1   | 2.19                     | 0.58              |
| 28:CC:65:ILE:HG12  | 28:CC:73:ILE:HG12  | 1.84                     | 0.58              |
| 33:CJ:385:LEU:HD11 | 41:CS:45:ARG:HD3   | 1.84                     | 0.58              |
| 36:CN:93:ASP:OD1   | 36:CN:114:SER:N    | 2.34                     | 0.58              |
| 39:CQ:140:VAL:HG21 | 39:CQ:172:ARG:HG3  | 1.86                     | 0.58              |
| 47:Cg:435:SER:O    | 47:Cg:440:LYS:HE3  | 2.03                     | 0.58              |
| 1:DA:300:THR:HG22  | 11:DS:61:ASN:HB2   | 1.85                     | 0.58              |
| 20:DH:508:LEU:HD22 | 20:DH:514:PRO:HB3  | 1.85                     | 0.58              |
| 26:DX:68:TYR:HB2   | 26:DX:164:THR:HG23 | 1.84                     | 0.58              |
| 32:CI:191:LEU:HD11 | 54:Cq:257:MET:HE3  | 1.86                     | 0.58              |
| 37:CO:317:ASP:OD1  | 37:CO:318:VAL:N    | 2.36                     | 0.58              |
| 37:CO:327:CYS:HB3  | 37:CO:330:THR:HB   | 1.86                     | 0.58              |
| 40:CR:134:ARG:HH21 | 40:CR:185:PHE:HB3  | 1.69                     | 0.58              |
| 44:Ca:61:LEU:HB2   | 44:Ca:76:GLN:NE2   | 2.19                     | 0.58              |
| 51:Cm:83:LYS:HZ2   | 57:CA:393:U:H5'    | 1.66                     | 0.58              |
| 2:DD:340:ARG:HG3   | 2:DD:341:PRO:HD2   | 1.86                     | 0.58              |
| 16:DC:79:VAL:HG21  | 16:DC:712:LEU:HD23 | 1.85                     | 0.58              |
| 23:DT:164:GLY:O    | 23:DT:168:GLU:HB2  | 2.03                     | 0.58              |
| 40:CR:167:ARG:NH1  | 57:CA:317:U:O4     | 2.37                     | 0.58              |
| 49:Cj:73:ARG:HH11  | 53:Cp:169:ASN:HB3  | 1.69                     | 0.58              |
| 54:Cq:76:GLN:OE1   | 54:Cq:228:LEU:HB2  | 2.03                     | 0.58              |
| 56:Cv:813:ARG:HG2  | 56:Cv:813:ARG:HH11 | 1.69                     | 0.58              |
| 1:DA:776:GLY:O     | 1:DA:925:SER:HA    | 2.04                     | 0.58              |
| 1:DA:945:ILE:HB    | 5:DM:128:ILE:HD11  | 1.85                     | 0.58              |
| 1:DA:1662:ARG:NH2  | 29:CE:402:ARG:HH12 | 2.02                     | 0.58              |
| 3:DI:405:LEU:HD13  | 31:CH:116:HIS:CD2  | 2.38                     | 0.58              |
| 7:DO:114:GLY:C     | 7:DO:116:ALA:H     | 2.08                     | 0.58              |
| 34:CK:202:ARG:NH1  | 57:CA:306:A:OP2    | 2.33                     | 0.58              |
| 36:CN:15:GLN:OE1   | 57:CA:416:U:N3     | 2.37                     | 0.58              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 38:CP:18:PRO:HG2    | 57:CA:176:A:C2     | 2.38                     | 0.58              |
| 40:CR:261:ILE:HG13  | 40:CR:262:SER:H    | 1.69                     | 0.58              |
| 49:Cj:50:VAL:HG22   | 57:CA:51:U:H2'     | 1.86                     | 0.58              |
| 56:Cv:292:LYS:O     | 56:Cv:405:PRO:HG2  | 2.03                     | 0.58              |
| 56:Cv:687:GLU:O     | 56:Cv:788:ARG:NH2  | 2.37                     | 0.58              |
| 1:DA:1566:ARG:O     | 1:DA:1570:ASN:ND2  | 2.37                     | 0.58              |
| 2:DD:431:LEU:HD11   | 2:DD:469:GLY:HA3   | 1.85                     | 0.58              |
| 5:DM:23:MET:HE3     | 5:DM:28:PHE:HB2    | 1.86                     | 0.58              |
| 16:DC:993:VAL:HG13  | 16:DC:1001:SER:HB3 | 1.86                     | 0.58              |
| 18:DF:516:ARG:HD2   | 18:DF:542:HIS:ND1  | 2.19                     | 0.58              |
| 57:CA:536:U:H2'     | 57:CA:537:A:H8     | 1.68                     | 0.58              |
| 6:DN:26:ARG:HD2     | 44:Ca:406:MET:O    | 2.03                     | 0.57              |
| 15:DB:358:ASN:HB3   | 20:DH:542:LEU:HD21 | 1.85                     | 0.57              |
| 15:DB:1024:PRO:HG2  | 15:DB:1044:PRO:HB3 | 1.86                     | 0.57              |
| 20:DH:307:ARG:HB3   | 33:CJ:286:LEU:HD11 | 1.87                     | 0.57              |
| 23:DT:214:ARG:O     | 23:DT:218:MET:HG3  | 2.04                     | 0.57              |
| 31:CH:154:ASP:OD1   | 31:CH:173:PRO:HG3  | 2.04                     | 0.57              |
| 31:CH:176:ILE:HD13  | 31:CH:179:ARG:NH1  | 2.18                     | 0.57              |
| 33:CJ:243:VAL:HG21  | 33:CJ:408:GLN:HB2  | 1.84                     | 0.57              |
| 34:CK:289:GLN:HE22  | 42:CU:59:ARG:HG2   | 1.68                     | 0.57              |
| 50:Ck:188:LEU:HD21  | 50:Ck:224:LYS:HD3  | 1.85                     | 0.57              |
| 52:Cn:179:ARG:HD2   | 52:Cn:183:ARG:NH1  | 2.19                     | 0.57              |
| 6:DN:62:ARG:NH2     | 44:Ca:390:GLN:OE1  | 2.37                     | 0.57              |
| 16:DC:1055:ARG:HH11 | 16:DC:1055:ARG:HA  | 1.68                     | 0.57              |
| 18:DF:27:ARG:HB2    | 57:CA:435:G:C6     | 2.39                     | 0.57              |
| 33:CJ:436:ARG:NH2   | 50:Ck:671:PRO:HB2  | 2.19                     | 0.57              |
| 37:CO:93:ARG:HH21   | 57:CA:358:U:H3     | 1.50                     | 0.57              |
| 47:Cg:102:PRO:HG2   | 47:Cg:105:HIS:HB2  | 1.86                     | 0.57              |
| 49:Cj:47:VAL:HG22   | 49:Cj:48:PRO:HD2   | 1.85                     | 0.57              |
| 15:DB:635:MET:HE1   | 50:Ck:374:ARG:HE   | 1.70                     | 0.57              |
| 16:DC:155:VAL:HG13  | 16:DC:168:PHE:HE1  | 1.69                     | 0.57              |
| 18:DF:55:ARG:HB2    | 18:DF:59:GLY:HA3   | 1.86                     | 0.57              |
| 41:CS:158:LYS:NZ    | 43:CZ:328:SER:HA   | 2.18                     | 0.57              |
| 46:Cd:137:ARG:HH11  | 46:Cd:137:ARG:CG   | 2.06                     | 0.57              |
| 47:Cg:205:ARG:HD3   | 47:Cg:258:SER:HB3  | 1.86                     | 0.57              |
| 56:Cv:937:MET:SD    | 56:Cv:937:MET:N    | 2.78                     | 0.57              |
| 56:Cv:1003:HIS:HB3  | 56:Cv:1006:GLU:O   | 2.03                     | 0.57              |
| 4:DL:159:GLN:N      | 4:DL:240:GLU:OE2   | 2.26                     | 0.57              |
| 5:DM:265:ILE:HG21   | 29:CE:57:THR:HG23  | 1.87                     | 0.57              |
| 7:DO:186:MET:HE1    | 46:Cd:132:PHE:HD2  | 1.68                     | 0.57              |
| 16:DC:1134:HIS:NE2  | 16:DC:1136:GLU:HB2 | 2.20                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:DE:166:ARG:O    | 17:DE:170:ILE:HG12 | 2.05                     | 0.57              |
| 19:DG:130:LEU:O    | 33:CJ:188:ARG:NH2  | 2.37                     | 0.57              |
| 34:CK:26:ARG:HB2   | 57:CA:460:U:C5     | 2.39                     | 0.57              |
| 37:CO:400:ARG:NH1  | 57:CA:157:G:O3'    | 2.37                     | 0.57              |
| 47:Cg:292:SER:HG   | 47:Cg:388:TYR:HE2  | 1.52                     | 0.57              |
| 3:DI:161:MET:O     | 3:DI:165:ARG:HG3   | 2.04                     | 0.57              |
| 4:DL:287:TRP:CD2   | 33:CJ:75:TYR:HA    | 2.39                     | 0.57              |
| 8:DP:139:ARG:NH1   | 8:DP:176:PRO:O     | 2.38                     | 0.57              |
| 20:DH:19:THR:HG22  | 20:DH:21:LEU:H     | 1.69                     | 0.57              |
| 33:CJ:83:HIS:CD2   | 33:CJ:86:ASP:HB3   | 2.35                     | 0.57              |
| 33:CJ:460:HIS:CE1  | 36:CN:57:LYS:HG3   | 2.40                     | 0.57              |
| 34:CK:322:ARG:HH11 | 34:CK:326:LYS:HE2  | 1.68                     | 0.57              |
| 37:CO:332:ARG:NH1  | 37:CO:337:VAL:HG12 | 2.19                     | 0.57              |
| 40:CR:23:TRP:CD2   | 56:Cv:494:THR:HG21 | 2.39                     | 0.57              |
| 51:Cm:211:LEU:HD23 | 51:Cm:212:PRO:HD2  | 1.87                     | 0.57              |
| 1:DA:971:GLU:HG2   | 1:DA:972:PRO:HD3   | 1.87                     | 0.57              |
| 2:DD:390:VAL:HG13  | 2:DD:457:LEU:HD22  | 1.86                     | 0.57              |
| 4:DL:164:ARG:O     | 4:DL:168:SER:OG    | 2.17                     | 0.57              |
| 14:Da:32:SER:HB3   | 31:CH:227:ARG:HH12 | 1.70                     | 0.57              |
| 15:DB:194:GLN:HE22 | 17:DE:470:LYS:HB3  | 1.68                     | 0.57              |
| 15:DB:488:ASN:OD1  | 15:DB:493:ARG:NH1  | 2.37                     | 0.57              |
| 15:DB:1132:ARG:HD3 | 33:CJ:709:GLU:OE2  | 2.05                     | 0.57              |
| 31:CH:106:THR:HG21 | 56:Cv:232:GLN:O    | 2.05                     | 0.57              |
| 32:CI:333:ILE:HG23 | 32:CI:370:ALA:HB3  | 1.87                     | 0.57              |
| 34:CK:203:ASN:ND2  | 34:CK:228:LYS:HZ1  | 2.02                     | 0.57              |
| 43:CZ:212:HIS:HB3  | 43:CZ:226:ARG:NH1  | 2.20                     | 0.57              |
| 44:Ca:409:GLU:H    | 44:Ca:409:GLU:CD   | 2.12                     | 0.57              |
| 1:DA:949:ARG:HD2   | 5:DM:18:HIS:HA     | 1.87                     | 0.57              |
| 8:DP:130:TYR:OH    | 49:Cj:71:ILE:O     | 2.18                     | 0.57              |
| 18:DF:259:SER:O    | 57:CA:423:A:H1'    | 2.05                     | 0.57              |
| 33:CJ:261:ALA:O    | 33:CJ:265:CYS:HB2  | 2.04                     | 0.57              |
| 44:Ca:335:ARG:NH2  | 44:Ca:391:ASP:OD1  | 2.38                     | 0.57              |
| 50:Ck:264:ASN:HD22 | 50:Ck:267:TYR:H    | 1.52                     | 0.57              |
| 50:Ck:411:CYS:HA   | 50:Ck:414:MET:HE2  | 1.86                     | 0.57              |
| 1:DA:1399:ASN:HD21 | 1:DA:1502:PHE:H    | 1.53                     | 0.57              |
| 2:DD:527:THR:HG21  | 10:DR:224:ALA:H    | 1.70                     | 0.57              |
| 15:DB:981:HIS:HD2  | 15:DB:983:LEU:HB2  | 1.69                     | 0.57              |
| 16:DC:155:VAL:HG13 | 16:DC:168:PHE:CE1  | 2.39                     | 0.57              |
| 17:DE:293:TYR:O    | 17:DE:297:VAL:HG23 | 2.04                     | 0.57              |
| 18:DF:56:TYR:CZ    | 57:CA:485:U:H5'    | 2.39                     | 0.57              |
| 34:CK:321:PRO:HD3  | 42:CU:16:HIS:CE1   | 2.39                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:Cd:47:ARG:HH21  | 49:Cj:24:SER:HA    | 1.69                     | 0.57              |
| 56:Cv:79:ASP:O     | 56:Cv:83:TRP:HB2   | 2.05                     | 0.57              |
| 9:DQ:77:LEU:HG     | 9:DQ:117:LEU:HD11  | 1.85                     | 0.57              |
| 13:DZ:44:PHE:CZ    | 29:CE:24:GLY:HA3   | 2.39                     | 0.57              |
| 15:DB:394:ASP:OD2  | 20:DH:492:ARG:NH1  | 2.38                     | 0.57              |
| 20:DH:35:TYR:OH    | 21:DJ:46:ARG:NH2   | 2.38                     | 0.57              |
| 32:CI:313:ASP:C    | 32:CI:315:GLU:H    | 2.12                     | 0.57              |
| 44:Ca:381:ASP:OD2  | 44:Ca:383:TYR:N    | 2.35                     | 0.57              |
| 53:Cp:10:ASP:HB2   | 57:CA:28:U:OP1     | 2.04                     | 0.57              |
| 55:Cr:143:ARG:HD3  | 55:Cr:187:VAL:HG21 | 1.86                     | 0.57              |
| 57:CA:110:U:H5'    | 57:CA:111:A:OP2    | 2.04                     | 0.57              |
| 1:DA:904:TRP:CE2   | 44:Ca:399:ASN:HA   | 2.40                     | 0.57              |
| 15:DB:472:GLY:HA3  | 50:Ck:93:THR:O     | 2.05                     | 0.57              |
| 16:DC:372:ASP:OD1  | 16:DC:373:GLY:N    | 2.37                     | 0.57              |
| 18:DF:467:LEU:HB3  | 18:DF:475:TYR:HB2  | 1.87                     | 0.57              |
| 50:Ck:201:THR:HG23 | 50:Ck:600:LEU:HD11 | 1.86                     | 0.57              |
| 51:Cm:96:CYS:HB3   | 51:Cm:125:CYS:SG   | 2.44                     | 0.57              |
| 52:Cn:206:GLU:OE1  | 52:Cn:206:GLU:N    | 2.35                     | 0.57              |
| 1:DA:324:GLN:HG2   | 1:DA:330:TRP:NE1   | 2.20                     | 0.56              |
| 1:DA:349:PRO:HG2   | 1:DA:350:TYR:CD2   | 2.40                     | 0.56              |
| 2:DD:742:ASP:N     | 2:DD:742:ASP:OD1   | 2.38                     | 0.56              |
| 4:DL:241:GLU:OE1   | 4:DL:242:ARG:N     | 2.38                     | 0.56              |
| 13:DZ:20:ARG:HD2   | 44:Ca:172:PHE:CE2  | 2.40                     | 0.56              |
| 21:DJ:31:HIS:CD2   | 21:DJ:33:ASN:H     | 2.22                     | 0.56              |
| 34:CK:78:ASP:HB2   | 45:Cb:178:ARG:NH1  | 2.19                     | 0.56              |
| 43:CZ:359:MET:HA   | 43:CZ:359:MET:HE2  | 1.85                     | 0.56              |
| 47:Cg:110:LEU:H    | 67:Cg:501:GTP:HN1  | 1.52                     | 0.56              |
| 47:Cg:289:ASN:ND2  | 47:Cg:358:THR:H    | 2.02                     | 0.56              |
| 51:Cm:85:ILE:HG12  | 51:Cm:140:CYS:HB2  | 1.86                     | 0.56              |
| 57:CA:443:U:O2'    | 57:CA:483:A:OP2    | 2.22                     | 0.56              |
| 1:DA:237:HIS:HE1   | 1:DA:310:ASP:HB2   | 1.70                     | 0.56              |
| 2:DD:247:VAL:HG21  | 12:DU:35:PRO:HD3   | 1.87                     | 0.56              |
| 4:DL:266:GLY:HA3   | 34:CK:22:PRO:HD3   | 1.86                     | 0.56              |
| 21:DJ:187:ASP:N    | 21:DJ:187:ASP:OD1  | 2.36                     | 0.56              |
| 34:CK:102:ASP:OD2  | 45:Cb:104:LEU:HB2  | 2.06                     | 0.56              |
| 37:CO:78:PRO:HG2   | 52:Cn:185:TYR:HB3  | 1.86                     | 0.56              |
| 44:Ca:474:ARG:NH1  | 44:Ca:478:GLY:O    | 2.38                     | 0.56              |
| 1:DA:192:ASP:OD1   | 1:DA:192:ASP:N     | 2.38                     | 0.56              |
| 1:DA:364:LEU:HD23  | 1:DA:380:PHE:CE1   | 2.39                     | 0.56              |
| 1:DA:999:SER:HB3   | 32:CI:260:LEU:HD21 | 1.86                     | 0.56              |
| 2:DD:778:PRO:HB3   | 29:CE:32:TRP:CD2   | 2.40                     | 0.56              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:DQ:142:PHE:HE2   | 9:DQ:246:VAL:HG11   | 1.70                     | 0.56              |
| 15:DB:749:THR:HG21 | 50:Ck:157:SER:HB3   | 1.87                     | 0.56              |
| 17:DE:333:ASP:HA   | 17:DE:336:ILE:HD12  | 1.85                     | 0.56              |
| 20:DH:475:ASP:HB2  | 23:DT:197:VAL:HG11  | 1.87                     | 0.56              |
| 29:CE:32:TRP:CD1   | 29:CE:33:MET:HG3    | 2.39                     | 0.56              |
| 29:CE:144:ILE:HD11 | 29:CE:190:LYS:HD2   | 1.85                     | 0.56              |
| 32:CI:110:ARG:HG2  | 32:CI:110:ARG:HH11  | 1.70                     | 0.56              |
| 32:CI:195:ILE:HG12 | 54:Cq:254:TYR:CE1   | 2.41                     | 0.56              |
| 37:CO:211:TYR:CD2  | 37:CO:226:VAL:HG21  | 2.40                     | 0.56              |
| 38:CP:53:ARG:HE    | 38:CP:59:ARG:NH1    | 2.03                     | 0.56              |
| 38:CP:102:TRP:HB3  | 38:CP:108:CYS:SG    | 2.44                     | 0.56              |
| 40:CR:219:ARG:HG3  | 40:CR:219:ARG:HH11  | 1.70                     | 0.56              |
| 44:Ca:444:PHE:HB2  | 44:Ca:472:VAL:HG12  | 1.86                     | 0.56              |
| 44:Ca:466:GLU:OE1  | 44:Ca:466:GLU:N     | 2.29                     | 0.56              |
| 44:Ca:577:PRO:HG2  | 44:Ca:579:VAL:HG12  | 1.87                     | 0.56              |
| 54:Cq:131:ASN:HB3  | 54:Cq:187:TRP:CE2   | 2.41                     | 0.56              |
| 56:Cv:162:SER:H    | 56:Cv:166:HIS:CD2   | 2.23                     | 0.56              |
| 56:Cv:1030:ARG:HG2 | 56:Cv:1034:ARG:HH12 | 1.70                     | 0.56              |
| 1:DA:333:VAL:HG13  | 13:DZ:62:ASP:HB2    | 1.88                     | 0.56              |
| 8:DP:13:ARG:NH1    | 57:CA:55:U:OP1      | 2.33                     | 0.56              |
| 18:DF:15:HIS:CE1   | 21:DJ:278:GLY:HA2   | 2.37                     | 0.56              |
| 19:DG:399:ARG:HB2  | 19:DG:409:LYS:O     | 2.06                     | 0.56              |
| 31:CH:150:THR:C    | 31:CH:152:ILE:H     | 2.12                     | 0.56              |
| 33:CJ:792:HIS:CD2  | 33:CJ:795:LYS:H     | 2.21                     | 0.56              |
| 56:Cv:292:LYS:HE2  | 56:Cv:512:MET:HE3   | 1.86                     | 0.56              |
| 9:DQ:73:HIS:CE1    | 9:DQ:250:ARG:HB2    | 2.41                     | 0.56              |
| 33:CJ:119:ARG:HG2  | 33:CJ:119:ARG:NH1   | 2.20                     | 0.56              |
| 34:CK:203:ASN:ND2  | 34:CK:228:LYS:NZ    | 2.53                     | 0.56              |
| 44:Ca:62:TRP:CD1   | 44:Ca:79:MET:HE1    | 2.41                     | 0.56              |
| 46:Cd:129:ARG:HD3  | 56:Cv:209:VAL:O     | 2.06                     | 0.56              |
| 2:DD:298:MET:HG2   | 2:DD:314:PHE:CZ     | 2.41                     | 0.56              |
| 10:DR:252:ALA:HA   | 10:DR:262:ARG:HG3   | 1.88                     | 0.56              |
| 11:DS:51:ARG:O     | 11:DS:52:ASP:HB2    | 2.04                     | 0.56              |
| 15:DB:908:GLN:H    | 15:DB:908:GLN:CD    | 2.13                     | 0.56              |
| 16:DC:77:ASP:H     | 16:DC:81:HIS:CD2    | 2.22                     | 0.56              |
| 16:DC:747:GLU:HG2  | 16:DC:748:TRP:H     | 1.70                     | 0.56              |
| 19:DG:333:LEU:O    | 19:DG:336:MET:HB2   | 2.05                     | 0.56              |
| 21:DJ:285:ARG:NH1  | 65:DJ:401:UTP:O2B   | 2.38                     | 0.56              |
| 34:CK:104:MET:HA   | 45:Cb:103:ARG:HD3   | 1.87                     | 0.56              |
| 36:CN:104:THR:HG21 | 41:CS:48:ARG:HH12   | 1.70                     | 0.56              |
| 44:Ca:65:ARG:NH2   | 44:Ca:80:ASP:OD1    | 2.36                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:Ca:323:LYS:HG3  | 44:Ca:330:TRP:CD2  | 2.41                     | 0.56              |
| 51:Cm:77:PRO:HB3   | 51:Cm:155:HIS:CE1  | 2.40                     | 0.56              |
| 6:DN:160:CYS:HB3   | 6:DN:162:LEU:H     | 1.70                     | 0.56              |
| 15:DB:536:ARG:HA   | 15:DB:585:MET:HE1  | 1.88                     | 0.56              |
| 29:CE:156:PRO:HG2  | 40:CR:307:ARG:HE   | 1.71                     | 0.56              |
| 33:CJ:639:ARG:NH2  | 33:CJ:646:THR:HG22 | 2.21                     | 0.56              |
| 35:CL:58:PHE:HB2   | 44:Ca:15:LYS:HA    | 1.87                     | 0.56              |
| 40:CR:317:ILE:HG21 | 57:CA:588:U:C5     | 2.39                     | 0.56              |
| 50:Ck:167:PHE:CE2  | 50:Ck:235:GLY:HA2  | 2.40                     | 0.56              |
| 57:CA:360:C:C2'    | 57:CA:361:A:H5'    | 2.34                     | 0.56              |
| 2:DD:537:ARG:HA    | 10:DR:218:TRP:CZ3  | 2.38                     | 0.56              |
| 3:DI:74:ASP:OD1    | 3:DI:75:GLN:N      | 2.38                     | 0.56              |
| 9:DQ:103:CYS:HA    | 9:DQ:106:MET:HE3   | 1.88                     | 0.56              |
| 16:DC:202:ASN:HB2  | 16:DC:205:GLN:HG3  | 1.87                     | 0.56              |
| 16:DC:871:GLN:HG2  | 17:DE:43:HIS:HA    | 1.87                     | 0.56              |
| 16:DC:954:LEU:HD23 | 16:DC:1055:ARG:HD2 | 1.85                     | 0.56              |
| 20:DH:440:VAL:HG22 | 28:CC:77:THR:HG23  | 1.87                     | 0.56              |
| 33:CJ:451:ASP:OD2  | 50:Ck:783:TYR:HE1  | 1.88                     | 0.56              |
| 33:CJ:716:ARG:HD2  | 48:Ci:46:GLU:OE2   | 2.06                     | 0.56              |
| 45:Cb:221:VAL:HG21 | 55:Cr:303:LEU:HD11 | 1.88                     | 0.56              |
| 50:Ck:42:HIS:O     | 50:Ck:93:THR:HB    | 2.06                     | 0.56              |
| 1:DA:420:ASN:ND2   | 1:DA:491:VAL:O     | 2.39                     | 0.56              |
| 3:DI:161:MET:HA    | 3:DI:161:MET:HE2   | 1.88                     | 0.56              |
| 6:DN:141:MET:HB2   | 6:DN:149:ASP:HB3   | 1.87                     | 0.56              |
| 6:DN:235:ASN:OD1   | 6:DN:238:ASN:ND2   | 2.39                     | 0.56              |
| 6:DN:291:PRO:HB3   | 29:CE:106:TRP:CG   | 2.41                     | 0.56              |
| 18:DF:181:ARG:HH21 | 57:CA:423:A:H5'    | 1.71                     | 0.56              |
| 27:DY:39:VAL:HG21  | 47:Cg:461:GLN:HG2  | 1.86                     | 0.56              |
| 42:CU:108:PHE:HZ   | 51:Cm:85:ILE:HG23  | 1.71                     | 0.56              |
| 55:Cr:10:ARG:HH12  | 55:Cr:13:ARG:CB    | 2.19                     | 0.56              |
| 56:Cv:95:ARG:HG3   | 56:Cv:95:ARG:NH1   | 2.21                     | 0.56              |
| 4:DL:120:PHE:HE1   | 4:DL:213:SER:HA    | 1.70                     | 0.56              |
| 9:DQ:105:PRO:HG2   | 9:DQ:221:LEU:HD21  | 1.86                     | 0.56              |
| 10:DR:22:LEU:HB3   | 37:CO:389:LYS:HZ2  | 1.71                     | 0.56              |
| 15:DB:276:VAL:O    | 15:DB:486:HIS:HE1  | 1.88                     | 0.56              |
| 19:DG:248:LEU:HD11 | 19:DG:313:SER:HB2  | 1.88                     | 0.56              |
| 25:DW:85:GLU:HA    | 25:DW:88:ARG:HD2   | 1.86                     | 0.56              |
| 37:CO:124:ILE:HD13 | 37:CO:128:ARG:NH1  | 2.21                     | 0.56              |
| 54:Cq:55:PHE:H     | 54:Cq:93:ASN:HD21  | 1.54                     | 0.56              |
| 57:CA:82:U:H2'     | 57:CA:83:U:O4'     | 2.05                     | 0.56              |
| 8:DP:20:MET:HE1    | 8:DP:29:TRP:HB2    | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:DQ:227:GLN:HG3   | 9:DQ:230:TRP:CZ2   | 2.41                     | 0.55              |
| 14:Da:40:ARG:HH12  | 57:CA:330:U:H5     | 1.54                     | 0.55              |
| 15:DB:544:ARG:NH1  | 15:DB:849:ASP:OD2  | 2.37                     | 0.55              |
| 23:DT:194:GLY:O    | 23:DT:207:THR:OG1  | 2.16                     | 0.55              |
| 26:DX:50:ARG:NH1   | 41:CS:145:LYS:O    | 2.37                     | 0.55              |
| 33:CJ:382:PHE:CD1  | 41:CS:48:ARG:HB2   | 2.41                     | 0.55              |
| 37:CO:251:VAL:HG22 | 57:CA:285:A:C5     | 2.40                     | 0.55              |
| 48:Ci:28:ALA:HB3   | 50:Ck:785:PRO:HA   | 1.87                     | 0.55              |
| 2:DD:323:LEU:HD22  | 2:DD:448:ARG:HH21  | 1.71                     | 0.55              |
| 2:DD:487:LYS:HA    | 2:DD:490:LEU:HD23  | 1.88                     | 0.55              |
| 13:DZ:88:PHE:HD2   | 44:Ca:201:ARG:HE   | 1.54                     | 0.55              |
| 16:DC:855:ARG:NH2  | 16:DC:866:GLU:OE2  | 2.39                     | 0.55              |
| 18:DF:310:LEU:HD11 | 18:DF:345:LEU:HD21 | 1.87                     | 0.55              |
| 34:CK:53:ARG:NH2   | 40:CR:232:GLY:HA2  | 2.22                     | 0.55              |
| 50:Ck:611:ASN:H    | 50:Ck:611:ASN:HD22 | 1.54                     | 0.55              |
| 3:DI:130:VAL:HG22  | 3:DI:145:LEU:HD23  | 1.87                     | 0.55              |
| 5:DM:74:ARG:HB3    | 56:Cv:971:LEU:HD11 | 1.87                     | 0.55              |
| 8:DP:188:ARG:HB3   | 8:DP:193:GLU:HB2   | 1.87                     | 0.55              |
| 15:DB:893:ILE:HG12 | 50:Ck:312:VAL:HB   | 1.88                     | 0.55              |
| 19:DG:160:ARG:NH1  | 19:DG:163:GLN:OE1  | 2.39                     | 0.55              |
| 20:DH:69:VAL:HG22  | 20:DH:96:ARG:HH11  | 1.70                     | 0.55              |
| 23:DT:176:ASP:OD1  | 23:DT:176:ASP:N    | 2.35                     | 0.55              |
| 33:CJ:661:ARG:O    | 33:CJ:663:PRO:HD3  | 2.07                     | 0.55              |
| 33:CJ:674:GLN:HG2  | 33:CJ:678:ASP:OD2  | 2.06                     | 0.55              |
| 33:CJ:698:HIS:HB3  | 36:CN:65:LYS:HZ3   | 1.69                     | 0.55              |
| 44:Ca:272:PHE:CE1  | 44:Ca:309:ALA:HB1  | 2.41                     | 0.55              |
| 5:DM:289:GLU:OE1   | 5:DM:289:GLU:N     | 2.39                     | 0.55              |
| 26:DX:129:PRO:HG2  | 47:Cg:296:HIS:HB2  | 1.86                     | 0.55              |
| 29:CE:308:ARG:O    | 29:CE:311:LYS:NZ   | 2.38                     | 0.55              |
| 48:Ci:69:THR:HG23  | 48:Ci:71:TYR:H     | 1.72                     | 0.55              |
| 50:Ck:36:ARG:HG2   | 50:Ck:36:ARG:NH1   | 2.20                     | 0.55              |
| 51:Cm:95:MET:HE2   | 51:Cm:129:VAL:HG13 | 1.87                     | 0.55              |
| 56:Cv:95:ARG:O     | 56:Cv:98:ARG:NH1   | 2.35                     | 0.55              |
| 56:Cv:681:HIS:HE2  | 56:Cv:695:SER:HG   | 1.47                     | 0.55              |
| 1:DA:80:PRO:HD3    | 57:CA:154:G:N2     | 2.21                     | 0.55              |
| 7:DO:138:LEU:HD23  | 7:DO:176:THR:HG21  | 1.87                     | 0.55              |
| 14:Da:11:ALA:HB2   | 57:CA:149:U:H5"    | 1.89                     | 0.55              |
| 21:DJ:12:TYR:HD1   | 48:Ci:132:THR:HG22 | 1.70                     | 0.55              |
| 29:CE:88:ASP:OD2   | 29:CE:91:ASN:HB2   | 2.06                     | 0.55              |
| 44:Ca:62:TRP:HB3   | 44:Ca:79:MET:HE1   | 1.89                     | 0.55              |
| 48:Ci:96:ASN:HD21  | 50:Ck:697:MET:HG3  | 1.72                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:631:ALA:HB1   | 2:DD:635:LEU:HD23  | 1.88                     | 0.55              |
| 9:DQ:202:ASP:OD1   | 9:DQ:203:SER:N     | 2.39                     | 0.55              |
| 15:DB:153:HIS:HE1  | 15:DB:173:ARG:CZ   | 2.20                     | 0.55              |
| 20:DH:37:SER:O     | 21:DJ:49:ALA:HB1   | 2.06                     | 0.55              |
| 34:CK:113:ARG:NH2  | 40:CR:192:GLU:OE1  | 2.39                     | 0.55              |
| 45:Cb:175:ILE:HG23 | 45:Cb:179:GLU:HB2  | 1.87                     | 0.55              |
| 1:DA:1185:ARG:HA   | 1:DA:1185:ARG:HH11 | 1.71                     | 0.55              |
| 14:Da:35:ALA:HB2   | 14:Da:42:ARG:HD2   | 1.88                     | 0.55              |
| 18:DF:383:ASP:O    | 18:DF:387:VAL:HG23 | 2.06                     | 0.55              |
| 37:CO:245:ASN:OD1  | 37:CO:245:ASN:N    | 2.39                     | 0.55              |
| 40:CR:122:MET:HE1  | 56:Cv:192:LEU:HA   | 1.89                     | 0.55              |
| 51:Cm:89:GLY:O     | 51:Cm:92:GLN:HB3   | 2.07                     | 0.55              |
| 53:Cp:88:ASP:O     | 53:Cp:92:LEU:HB2   | 2.07                     | 0.55              |
| 53:Cp:151:ARG:H    | 53:Cp:154:GLN:HE21 | 1.53                     | 0.55              |
| 57:CA:310:A:N3     | 57:CA:310:A:H2'    | 2.21                     | 0.55              |
| 2:DD:704:ASP:OD1   | 2:DD:704:ASP:N     | 2.35                     | 0.55              |
| 5:DM:76:ASN:HD21   | 56:Cv:971:LEU:H    | 1.53                     | 0.55              |
| 6:DN:128:VAL:HB    | 44:Ca:405:ARG:HB3  | 1.88                     | 0.55              |
| 11:DS:57:LEU:HD23  | 11:DS:67:ILE:HD13  | 1.87                     | 0.55              |
| 16:DC:1104:MET:HE1 | 20:DH:146:GLN:HE21 | 1.71                     | 0.55              |
| 29:CE:62:ARG:HH22  | 56:Cv:491:LEU:HD11 | 1.71                     | 0.55              |
| 34:CK:212:GLU:OE1  | 34:CK:212:GLU:N    | 2.40                     | 0.55              |
| 44:Ca:66:PRO:HD3   | 44:Ca:530:ALA:HB2  | 1.89                     | 0.55              |
| 45:Cb:52:TYR:O     | 45:Cb:56:ARG:HB2   | 2.07                     | 0.55              |
| 1:DA:1224:PHE:HD1  | 1:DA:1275:MET:HE1  | 1.71                     | 0.55              |
| 16:DC:635:MET:HE3  | 16:DC:656:ILE:HG12 | 1.89                     | 0.55              |
| 16:DC:819:LEU:HD13 | 16:DC:885:LEU:HD11 | 1.89                     | 0.55              |
| 32:CI:315:GLU:OE2  | 36:CN:144:LYS:HD2  | 2.07                     | 0.55              |
| 33:CJ:463:MET:HG2  | 48:Ci:89:MET:HG3   | 1.87                     | 0.55              |
| 33:CJ:551:ARG:HB3  | 33:CJ:553:ARG:HH21 | 1.72                     | 0.55              |
| 40:CR:198:THR:HB   | 40:CR:200:SER:H    | 1.72                     | 0.55              |
| 49:Cj:51:VAL:HG12  | 49:Cj:52:LEU:HD23  | 1.88                     | 0.55              |
| 50:Ck:337:VAL:HG22 | 50:Ck:338:PRO:HD2  | 1.89                     | 0.55              |
| 56:Cv:293:LEU:HD11 | 56:Cv:407:MET:HB2  | 1.88                     | 0.55              |
| 57:CA:253:U:H2'    | 57:CA:254:A:H8     | 1.69                     | 0.55              |
| 2:DD:702:TYR:HB3   | 31:CH:233:SER:HB2  | 1.88                     | 0.55              |
| 3:DI:296:ASN:HA    | 3:DI:334:ILE:HD11  | 1.87                     | 0.55              |
| 5:DM:293:ARG:HE    | 54:Cq:59:ARG:HB2   | 1.72                     | 0.55              |
| 9:DQ:255:PRO:HG3   | 9:DQ:260:HIS:HB2   | 1.88                     | 0.55              |
| 15:DB:978:ASN:OD1  | 15:DB:978:ASN:N    | 2.35                     | 0.55              |
| 16:DC:506:SER:HB3  | 16:DC:509:LYS:HG3  | 1.89                     | 0.55              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:DT:44:ARG:HB2    | 23:DT:218:MET:HE2  | 1.88                     | 0.55              |
| 33:CJ:386:GLU:O     | 33:CJ:389:THR:OG1  | 2.25                     | 0.55              |
| 40:CR:89:VAL:HG21   | 54:Cq:112:LYS:HG3  | 1.88                     | 0.55              |
| 47:Cg:413:LEU:HD23  | 47:Cg:441:LEU:HD12 | 1.88                     | 0.55              |
| 55:Cr:46:GLY:HA3    | 55:Cr:176:LEU:HD11 | 1.89                     | 0.55              |
| 2:DD:700:ASP:HB3    | 2:DD:704:ASP:OD1   | 2.07                     | 0.54              |
| 3:DI:243:LEU:HD11   | 3:DI:375:ILE:HD11  | 1.88                     | 0.54              |
| 15:DB:423:THR:HG22  | 15:DB:426:HIS:CE1  | 2.42                     | 0.54              |
| 21:DJ:229:ASP:O     | 21:DJ:233:VAL:HG23 | 2.07                     | 0.54              |
| 27:DY:95:TYR:OH     | 40:CR:269:SER:O    | 2.15                     | 0.54              |
| 32:CI:307:VAL:HG22  | 32:CI:322:LEU:HD22 | 1.89                     | 0.54              |
| 33:CJ:619:HIS:N     | 33:CJ:622:ASP:OD2  | 2.37                     | 0.54              |
| 41:CS:103:ARG:HD2   | 57:CA:488:A:C4     | 2.41                     | 0.54              |
| 12:DU:174:ARG:HG2   | 12:DU:175:PRO:HD2  | 1.89                     | 0.54              |
| 15:DB:1051:GLN:HE21 | 21:DJ:41:PRO:HA    | 1.73                     | 0.54              |
| 18:DF:166:ARG:NH1   | 57:CA:421:G:OP1    | 2.34                     | 0.54              |
| 18:DF:521:THR:HG22  | 18:DF:523:LEU:H    | 1.70                     | 0.54              |
| 33:CJ:452:PRO:HB2   | 33:CJ:454:THR:O    | 2.07                     | 0.54              |
| 33:CJ:783:ILE:HD13  | 48:CI:53:TRP:HZ3   | 1.72                     | 0.54              |
| 63:UT:36:UNK:HB2    | 63:UT:39:UNK:HG3   | 1.89                     | 0.54              |
| 3:DI:367:SER:H      | 3:DI:370:GLN:HE21  | 1.53                     | 0.54              |
| 10:DR:118:VAL:HG22  | 10:DR:144:LEU:HG   | 1.88                     | 0.54              |
| 20:DH:391:GLU:O     | 20:DH:394:ARG:HG2  | 2.07                     | 0.54              |
| 46:Cd:12:ILE:HG23   | 53:Cp:120:ARG:HE   | 1.71                     | 0.54              |
| 47:Cg:174:LEU:HB2   | 47:Cg:283:ILE:HG23 | 1.90                     | 0.54              |
| 1:DA:418:LEU:HB2    | 1:DA:481:TYR:CZ    | 2.43                     | 0.54              |
| 1:DA:1180:SER:HB3   | 54:Cq:148:PRO:HG3  | 1.89                     | 0.54              |
| 3:DI:234:SER:O      | 3:DI:237:ARG:HG3   | 2.08                     | 0.54              |
| 4:DL:296:PRO:HB2    | 33:CJ:61:VAL:HG21  | 1.89                     | 0.54              |
| 6:DN:69:VAL:O       | 6:DN:113:ALA:HA    | 2.07                     | 0.54              |
| 8:DP:70:TRP:CD2     | 12:DU:182:GLU:HG2  | 2.42                     | 0.54              |
| 18:DF:92:MET:HE2    | 41:CS:104:GLN:NE2  | 2.22                     | 0.54              |
| 18:DF:112:ARG:HH22  | 18:DF:118:THR:HG23 | 1.72                     | 0.54              |
| 19:DG:64:ARG:HH22   | 19:DG:98:ASP:CG    | 2.16                     | 0.54              |
| 19:DG:624:ARG:NH1   | 24:DV:181:LYS:O    | 2.41                     | 0.54              |
| 48:CI:114:MET:HE2   | 50:Ck:690:TRP:CH2  | 2.43                     | 0.54              |
| 56:Cv:147:HIS:HD2   | 56:Cv:149:ASP:H    | 1.56                     | 0.54              |
| 56:Cv:946:PRO:O     | 56:Cv:947:THR:HB   | 2.06                     | 0.54              |
| 5:DM:3:VAL:HG21     | 29:CE:318:PRO:HD2  | 1.90                     | 0.54              |
| 5:DM:245:ASN:HD22   | 29:CE:108:HIS:HE1  | 1.55                     | 0.54              |
| 14:Da:53:ARG:NH1    | 57:CA:333:U:OP2    | 2.40                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:DE:311:VAL:HA   | 17:DE:324:LEU:HD21 | 1.88                     | 0.54              |
| 19:DG:524:PHE:HZ   | 19:DG:582:VAL:HG11 | 1.73                     | 0.54              |
| 29:CE:171:SER:C    | 29:CE:173:LYS:H    | 2.15                     | 0.54              |
| 32:CI:420:ARG:O    | 34:CK:27:ARG:HB3   | 2.07                     | 0.54              |
| 44:Ca:10:ARG:HB3   | 44:Ca:10:ARG:NH1   | 2.22                     | 0.54              |
| 55:Cr:10:ARG:HH12  | 55:Cr:13:ARG:HB2   | 1.73                     | 0.54              |
| 55:Cr:10:ARG:HH22  | 55:Cr:13:ARG:HB2   | 1.73                     | 0.54              |
| 56:Cv:813:ARG:HH11 | 56:Cv:813:ARG:CG   | 2.21                     | 0.54              |
| 57:CA:350:U:H5'    | 57:CA:351:A:H5''   | 1.89                     | 0.54              |
| 2:DD:527:THR:HB    | 10:DR:223:GLN:HG3  | 1.90                     | 0.54              |
| 2:DD:797:PHE:HB2   | 2:DD:803:GLN:HE21  | 1.72                     | 0.54              |
| 3:DI:280:SER:OG    | 3:DI:281:GLY:N     | 2.41                     | 0.54              |
| 17:DE:221:ILE:HB   | 17:DE:405:ILE:HD11 | 1.87                     | 0.54              |
| 18:DF:57:ARG:HG2   | 18:DF:57:ARG:NH1   | 2.21                     | 0.54              |
| 21:DJ:213:GLU:HG3  | 21:DJ:245:VAL:HA   | 1.90                     | 0.54              |
| 33:CJ:507:ASN:CG   | 33:CJ:519:ILE:HG12 | 2.33                     | 0.54              |
| 37:CO:128:ARG:NH2  | 37:CO:209:GLU:OE1  | 2.35                     | 0.54              |
| 40:CR:12:ALA:HA    | 56:Cv:689:CYS:SG   | 2.47                     | 0.54              |
| 42:CU:27:LYS:HG2   | 57:CA:297:G:H1     | 1.72                     | 0.54              |
| 44:Ca:443:MET:HG2  | 44:Ca:473:ILE:HG12 | 1.89                     | 0.54              |
| 45:Cb:56:ARG:HH11  | 45:Cb:57:MET:CE    | 2.21                     | 0.54              |
| 56:Cv:84:GLY:HA2   | 56:Cv:87:GLN:HG3   | 1.89                     | 0.54              |
| 57:CA:47:U:H2'     | 57:CA:48:U:C6      | 2.42                     | 0.54              |
| 57:CA:526:A:H2'    | 57:CA:527:A:H5''   | 1.89                     | 0.54              |
| 1:DA:1107:ARG:HH11 | 1:DA:1169:PRO:HB2  | 1.73                     | 0.54              |
| 9:DQ:250:ARG:HD3   | 9:DQ:252:LYS:HE3   | 1.89                     | 0.54              |
| 17:DE:210:MET:HG3  | 17:DE:426:PHE:HZ   | 1.71                     | 0.54              |
| 23:DT:138:SER:OG   | 23:DT:176:ASP:OD2  | 2.16                     | 0.54              |
| 37:CO:427:GLY:HA3  | 39:CQ:156:TYR:CE2  | 2.43                     | 0.54              |
| 44:Ca:205:LEU:HA   | 44:Ca:208:VAL:HG22 | 1.89                     | 0.54              |
| 46:Cd:13:ARG:CZ    | 46:Cd:26:ARG:HH21  | 2.20                     | 0.54              |
| 56:Cv:200:ASP:HB2  | 56:Cv:612:THR:HG23 | 1.89                     | 0.54              |
| 10:DR:108:GLN:HE22 | 49:Cj:147:TYR:HB2  | 1.73                     | 0.54              |
| 15:DB:1133:PRO:HA  | 15:DB:1137:MET:HB2 | 1.90                     | 0.54              |
| 49:Cj:90:ARG:NE    | 49:Cj:94:ILE:HD11  | 2.23                     | 0.54              |
| 57:CA:134:U:H2'    | 57:CA:135:U:H5''   | 1.89                     | 0.54              |
| 57:CA:536:U:H2'    | 57:CA:537:A:C8     | 2.43                     | 0.54              |
| 13:DZ:39:ASN:ND2   | 57:CA:225:A:OP1    | 2.38                     | 0.54              |
| 17:DE:152:ALA:HA   | 17:DE:157:ARG:HD3  | 1.90                     | 0.54              |
| 18:DF:326:ASP:OD2  | 18:DF:462:ARG:NH2  | 2.41                     | 0.54              |
| 19:DG:206:LEU:N    | 19:DG:234:GLU:OE2  | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:CF:131:SER:O    | 30:CF:134:THR:OG1  | 2.26                     | 0.54              |
| 32:CI:175:ARG:NH1  | 32:CI:179:CYS:SG   | 2.81                     | 0.54              |
| 36:CN:165:ARG:O    | 50:Ck:740:ARG:NH1  | 2.41                     | 0.54              |
| 46:Cd:287:GLU:HA   | 46:Cd:290:VAL:HB   | 1.88                     | 0.54              |
| 56:Cv:843:LYS:HG3  | 56:Cv:933:LEU:HG   | 1.90                     | 0.54              |
| 57:CA:83:U:H5'     | 57:CA:84:U:OP2     | 2.07                     | 0.54              |
| 57:CA:521:G:H2'    | 57:CA:522:A:O4'    | 2.07                     | 0.54              |
| 61:UR:6:UNK:HG2    | 61:UR:8:UNK:HG2    | 1.90                     | 0.54              |
| 1:DA:1058:ARG:HH11 | 54:Cq:253:ARG:HH12 | 1.54                     | 0.54              |
| 2:DD:140:SER:HB2   | 57:CA:86:G:H22     | 1.72                     | 0.54              |
| 15:DB:635:MET:HG3  | 50:Ck:373:ARG:NH1  | 2.23                     | 0.54              |
| 21:DJ:305:ARG:HB3  | 21:DJ:305:ARG:HH11 | 1.71                     | 0.54              |
| 32:CI:132:GLY:HA3  | 40:CR:225:LEU:HD13 | 1.90                     | 0.54              |
| 50:Ck:711:ILE:HG21 | 50:Ck:730:GLU:HG3  | 1.88                     | 0.54              |
| 53:Cp:178:GLU:O    | 53:Cp:182:GLN:HB2  | 2.07                     | 0.54              |
| 56:Cv:559:GLN:OE1  | 56:Cv:565:ILE:HG12 | 2.08                     | 0.54              |
| 2:DD:177:TYR:CE2   | 2:DD:200:MET:HG3   | 2.43                     | 0.53              |
| 7:DO:276:GLY:C     | 56:Cv:685:ARG:HH12 | 2.16                     | 0.53              |
| 15:DB:543:GLN:HE22 | 15:DB:580:PHE:HA   | 1.73                     | 0.53              |
| 15:DB:975:LYS:HG2  | 19:DG:92:GLN:HE22  | 1.74                     | 0.53              |
| 16:DC:353:LEU:O    | 16:DC:357:GLN:HB2  | 2.08                     | 0.53              |
| 18:DF:122:LEU:HD23 | 36:CN:37:ARG:HH21  | 1.72                     | 0.53              |
| 29:CE:253:ARG:NH1  | 29:CE:256:LEU:O    | 2.41                     | 0.53              |
| 33:CJ:556:GLU:CD   | 33:CJ:556:GLU:H    | 2.16                     | 0.53              |
| 34:CK:244:HIS:CD2  | 34:CK:294:ALA:HB2  | 2.42                     | 0.53              |
| 34:CK:258:LEU:HD13 | 34:CK:275:VAL:HG21 | 1.90                     | 0.53              |
| 42:CU:77:ARG:HH11  | 56:Cv:175:ARG:NH2  | 2.04                     | 0.53              |
| 44:Ca:589:ARG:NH1  | 57:CA:259:U:OP2    | 2.40                     | 0.53              |
| 46:Cd:10:ARG:HE    | 57:CA:47:U:H4'     | 1.72                     | 0.53              |
| 47:Cg:202:ASP:OD1  | 47:Cg:205:ARG:NH2  | 2.41                     | 0.53              |
| 5:DM:266:ALA:HB2   | 29:CE:61:PHE:CE2   | 2.44                     | 0.53              |
| 6:DN:227:LYS:HE2   | 6:DN:287:ARG:NH2   | 2.23                     | 0.53              |
| 8:DP:88:THR:HG22   | 8:DP:90:LEU:H      | 1.72                     | 0.53              |
| 15:DB:944:HIS:O    | 33:CJ:342:ASN:HB3  | 2.09                     | 0.53              |
| 15:DB:1080:ARG:HD2 | 18:DF:176:VAL:HG12 | 1.90                     | 0.53              |
| 19:DG:38:ARG:HB3   | 33:CJ:88:ARG:NH1   | 2.23                     | 0.53              |
| 19:DG:118:ASP:OD1  | 50:Ck:406:ARG:NH2  | 2.42                     | 0.53              |
| 19:DG:335:GLU:HG3  | 19:DG:387:ARG:HD3  | 1.88                     | 0.53              |
| 24:DV:30:ASP:OD1   | 48:Ci:59:ARG:NH2   | 2.41                     | 0.53              |
| 29:CE:240:ASP:HA   | 29:CE:243:CYS:HB2  | 1.90                     | 0.53              |
| 47:Cg:144:GLY:HA3  | 47:Cg:353:PHE:O    | 2.09                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Cm:88:SER:CB    | 57:CA:394:A:H5'    | 2.38                     | 0.53              |
| 1:DA:193:GLU:N     | 1:DA:193:GLU:OE1   | 2.41                     | 0.53              |
| 5:DM:26:ARG:HH22   | 44:Ca:266:GLU:HG3  | 1.74                     | 0.53              |
| 6:DN:267:GLU:CD    | 6:DN:267:GLU:H     | 2.16                     | 0.53              |
| 15:DB:190:HIS:HD2  | 15:DB:192:ILE:H    | 1.56                     | 0.53              |
| 16:DC:752:VAL:HG22 | 16:DC:774:ASP:HB2  | 1.90                     | 0.53              |
| 19:DG:445:LEU:HD22 | 19:DG:531:ASP:HB3  | 1.88                     | 0.53              |
| 23:DT:114:LEU:HD23 | 23:DT:119:PHE:HA   | 1.89                     | 0.53              |
| 29:CE:40:ARG:CZ    | 29:CE:94:ARG:HD2   | 2.38                     | 0.53              |
| 37:CO:138:LEU:HD23 | 37:CO:138:LEU:H    | 1.72                     | 0.53              |
| 43:CZ:351:ARG:NH1  | 57:CA:235:A:H5''   | 2.23                     | 0.53              |
| 49:Cj:10:ARG:NH2   | 57:CA:77:A:OP2     | 2.39                     | 0.53              |
| 56:Cv:200:ASP:N    | 56:Cv:200:ASP:OD1  | 2.38                     | 0.53              |
| 2:DD:181:MET:HE1   | 2:DD:215:TYR:HD1   | 1.74                     | 0.53              |
| 13:DZ:48:ARG:H     | 44:Ca:586:ILE:CD1  | 2.21                     | 0.53              |
| 15:DB:562:GLN:NE2  | 18:DF:571:LEU:HA   | 2.24                     | 0.53              |
| 16:DC:1012:ALA:HB2 | 22:DK:111:LEU:HD13 | 1.90                     | 0.53              |
| 17:DE:186:ARG:NH2  | 17:DE:190:PHE:O    | 2.41                     | 0.53              |
| 19:DG:394:PRO:HA   | 19:DG:488:TYR:OH   | 2.08                     | 0.53              |
| 23:DT:24:ILE:HB    | 23:DT:206:LEU:HD21 | 1.90                     | 0.53              |
| 25:DW:102:MET:HE1  | 40:CR:271:MET:HE1  | 1.88                     | 0.53              |
| 32:CI:136:GLN:HB2  | 32:CI:140:GLU:OE2  | 2.09                     | 0.53              |
| 37:CO:140:ALA:O    | 37:CO:144:ARG:HB2  | 2.08                     | 0.53              |
| 37:CO:411:ARG:HH21 | 57:CA:68:A:H5'     | 1.74                     | 0.53              |
| 56:Cv:911:PRO:HG2  | 56:Cv:913:TRP:CZ2  | 2.43                     | 0.53              |
| 57:CA:610:U:H2'    | 57:CA:611:U:C6     | 2.44                     | 0.53              |
| 2:DD:342:ARG:HB3   | 9:DQ:29:ILE:O      | 2.09                     | 0.53              |
| 18:DF:43:THR:HG22  | 18:DF:44:ALA:H     | 1.74                     | 0.53              |
| 34:CK:125:LYS:HA   | 34:CK:128:SER:HB3  | 1.90                     | 0.53              |
| 35:CL:80:LYS:NZ    | 57:CA:378:A:OP1    | 2.40                     | 0.53              |
| 44:Ca:507:MET:HE3  | 44:Ca:557:PHE:HB3  | 1.89                     | 0.53              |
| 45:Cb:202:LEU:O    | 45:Cb:205:LYS:HG3  | 2.09                     | 0.53              |
| 49:Cj:28:LYS:NZ    | 49:Cj:28:LYS:HB3   | 2.23                     | 0.53              |
| 55:Cr:243:LYS:O    | 55:Cr:247:ILE:HG23 | 2.08                     | 0.53              |
| 56:Cv:797:ALA:HA   | 56:Cv:800:VAL:HG12 | 1.91                     | 0.53              |
| 1:DA:696:LEU:HD23  | 1:DA:714:LEU:HD22  | 1.89                     | 0.53              |
| 1:DA:1592:GLY:O    | 1:DA:1596:VAL:N    | 2.34                     | 0.53              |
| 2:DD:364:ARG:HD3   | 10:DR:188:LYS:HD2  | 1.91                     | 0.53              |
| 4:DL:230:PRO:HG2   | 4:DL:231:TRP:CD1   | 2.43                     | 0.53              |
| 10:DR:51:LEU:HD11  | 10:DR:63:ILE:HD11  | 1.91                     | 0.53              |
| 14:Da:14:TYR:OH    | 57:CA:150:A:OP2    | 2.23                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:233:ASP:N    | 15:DB:233:ASP:OD1  | 2.38                     | 0.53              |
| 18:DF:170:ARG:HG2  | 48:Ci:104:ARG:HH22 | 1.73                     | 0.53              |
| 21:DJ:87:PRO:HB3   | 21:DJ:92:LEU:HD12  | 1.91                     | 0.53              |
| 30:CF:16:ARG:HB2   | 30:CF:16:ARG:NH1   | 2.24                     | 0.53              |
| 33:CJ:52:PHE:CD1   | 33:CJ:53:PRO:HD2   | 2.43                     | 0.53              |
| 39:CQ:48:ARG:NH2   | 57:CA:375:A:O2'    | 2.42                     | 0.53              |
| 47:Cg:414:ARG:HH11 | 47:Cg:418:ASN:ND2  | 2.06                     | 0.53              |
| 2:DD:773:MET:SD    | 44:Ca:335:ARG:HD3  | 2.49                     | 0.53              |
| 6:DN:293:PRO:HD2   | 29:CE:109:LYS:CD   | 2.38                     | 0.53              |
| 8:DP:87:GLU:O      | 8:DP:92:LYS:NZ     | 2.42                     | 0.53              |
| 11:DS:128:SER:H    | 11:DS:168:LYS:HE2  | 1.74                     | 0.53              |
| 15:DB:527:GLU:N    | 15:DB:530:GLU:HG3  | 2.23                     | 0.53              |
| 16:DC:1134:HIS:HD2 | 16:DC:1136:GLU:H   | 1.57                     | 0.53              |
| 17:DE:183:LEU:O    | 17:DE:186:ARG:NH1  | 2.38                     | 0.53              |
| 17:DE:406:ASP:OD1  | 17:DE:406:ASP:N    | 2.37                     | 0.53              |
| 19:DG:186:ARG:HD2  | 34:CK:54:LEU:HB3   | 1.90                     | 0.53              |
| 19:DG:447:ALA:O    | 19:DG:451:ARG:HD2  | 2.08                     | 0.53              |
| 22:DK:283:ARG:HD3  | 23:DT:124:GLY:HA3  | 1.91                     | 0.53              |
| 23:DT:70:MET:HE3   | 23:DT:162:TYR:CD2  | 2.44                     | 0.53              |
| 44:Ca:243:THR:HG22 | 44:Ca:245:GLU:H    | 1.73                     | 0.53              |
| 50:Ck:132:TYR:CZ   | 50:Ck:140:ARG:HG3  | 2.44                     | 0.53              |
| 56:Cv:836:GLU:OE1  | 56:Cv:836:GLU:N    | 2.42                     | 0.53              |
| 1:DA:651:ARG:HG3   | 1:DA:726:GLU:HB3   | 1.90                     | 0.53              |
| 1:DA:910:HIS:CD2   | 44:Ca:318:ASP:HB2  | 2.44                     | 0.53              |
| 1:DA:1016:MET:HG2  | 29:CE:110:LEU:HD11 | 1.90                     | 0.53              |
| 2:DD:442:PHE:HD2   | 2:DD:486:ARG:CZ    | 2.22                     | 0.53              |
| 2:DD:504:ASN:N     | 2:DD:504:ASN:OD1   | 2.39                     | 0.53              |
| 9:DQ:39:ASP:HB2    | 10:DR:27:LYS:HE3   | 1.91                     | 0.53              |
| 9:DQ:40:VAL:HG22   | 12:DU:100:VAL:HB   | 1.91                     | 0.53              |
| 11:DS:128:SER:O    | 11:DS:130:VAL:N    | 2.40                     | 0.53              |
| 13:DZ:34:LYS:HG3   | 13:DZ:35:LYS:H     | 1.74                     | 0.53              |
| 15:DB:720:LYS:HD2  | 15:DB:722:ARG:HD2  | 1.91                     | 0.53              |
| 18:DF:29:ARG:H     | 21:DJ:314:GLN:HE22 | 1.56                     | 0.53              |
| 22:DK:24:ARG:NH1   | 22:DK:236:ILE:HG12 | 2.23                     | 0.53              |
| 33:CJ:440:ILE:HG13 | 50:Ck:660:PRO:HG2  | 1.90                     | 0.53              |
| 39:CQ:48:ARG:HH11  | 39:CQ:48:ARG:HG3   | 1.73                     | 0.53              |
| 44:Ca:430:PRO:HA   | 44:Ca:433:GLN:HB2  | 1.89                     | 0.53              |
| 51:Cm:56:ASN:HD21  | 51:Cm:62:ALA:CB    | 2.21                     | 0.53              |
| 55:Cr:39:ALA:O     | 55:Cr:43:VAL:HG23  | 2.07                     | 0.53              |
| 15:DB:110:ARG:NH2  | 15:DB:309:SER:O    | 2.41                     | 0.53              |
| 15:DB:339:ARG:HH21 | 20:DH:549:SER:HB3  | 1.74                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:831:ASN:HB3  | 15:DB:834:ILE:HD12 | 1.91                     | 0.53              |
| 16:DC:87:MET:HE2   | 16:DC:957:LYS:HA   | 1.91                     | 0.53              |
| 16:DC:393:THR:HG21 | 16:DC:457:LYS:HE3  | 1.89                     | 0.53              |
| 20:DH:474:ASP:OD1  | 20:DH:474:ASP:N    | 2.30                     | 0.53              |
| 33:CJ:716:ARG:HH21 | 48:CI:77:ARG:HD2   | 1.73                     | 0.53              |
| 33:CJ:762:GLN:OE1  | 33:CJ:763:ILE:N    | 2.38                     | 0.53              |
| 36:CN:158:ARG:NH1  | 36:CN:159:ASN:OD1  | 2.41                     | 0.53              |
| 37:CO:214:HIS:CD2  | 37:CO:216:PHE:H    | 2.27                     | 0.53              |
| 56:Cv:390:ARG:HH12 | 56:Cv:943:LEU:HA   | 1.73                     | 0.53              |
| 56:Cv:467:LEU:O    | 56:Cv:471:VAL:HG22 | 2.09                     | 0.53              |
| 56:Cv:808:SER:HB3  | 56:Cv:913:TRP:CE3  | 2.44                     | 0.53              |
| 1:DA:907:GLN:HE22  | 44:Ca:399:ASN:HD22 | 1.57                     | 0.53              |
| 6:DN:124:SER:O     | 44:Ca:383:TYR:OH   | 2.19                     | 0.53              |
| 11:DS:43:MET:HE1   | 57:CA:204:U:H5'    | 1.91                     | 0.53              |
| 16:DC:753:LEU:HD23 | 16:DC:930:ALA:HB1  | 1.91                     | 0.53              |
| 20:DH:19:THR:HG23  | 28:CC:68:PHE:O     | 2.09                     | 0.53              |
| 24:DV:107:ILE:HG12 | 33:CJ:754:VAL:HG22 | 1.90                     | 0.53              |
| 43:CZ:358:LYS:HD2  | 62:US:4:UNK:HG2    | 1.91                     | 0.53              |
| 47:Cg:107:ARG:HD2  | 47:Cg:107:ARG:N    | 2.25                     | 0.53              |
| 1:DA:467:PRO:O     | 56:Cv:1071:ARG:HD2 | 2.09                     | 0.52              |
| 13:DZ:71:ASP:OD1   | 44:Ca:195:ARG:NH2  | 2.42                     | 0.52              |
| 15:DB:1070:SER:HB3 | 15:DB:1074:SER:HB2 | 1.89                     | 0.52              |
| 16:DC:211:LYS:HZ1  | 16:DC:439:ALA:HA   | 1.74                     | 0.52              |
| 16:DC:863:LEU:HD21 | 17:DE:206:LEU:HG   | 1.91                     | 0.52              |
| 17:DE:611:LEU:HB3  | 17:DE:612:HIS:HD2  | 1.73                     | 0.52              |
| 21:DJ:22:MET:HE3   | 33:CJ:74:TRP:CH2   | 2.45                     | 0.52              |
| 31:CH:99:ASP:OD2   | 31:CH:113:LYS:HA   | 2.09                     | 0.52              |
| 37:CO:313:THR:OG1  | 39:CQ:166:GLU:OE1  | 2.26                     | 0.52              |
| 37:CO:349:LEU:HD13 | 37:CO:353:GLU:HB2  | 1.91                     | 0.52              |
| 40:CR:220:ARG:HH22 | 51:Cm:128:ARG:NH1  | 2.07                     | 0.52              |
| 44:Ca:522:GLU:HG2  | 44:Ca:588:LYS:HE3  | 1.91                     | 0.52              |
| 1:DA:1042:HIS:CD2  | 1:DA:1045:ILE:HG23 | 2.44                     | 0.52              |
| 2:DD:265:LEU:HD22  | 39:CQ:84:ILE:HD13  | 1.91                     | 0.52              |
| 10:DR:79:LEU:O     | 12:DU:139:LYS:NZ   | 2.41                     | 0.52              |
| 13:DZ:54:PRO:HG2   | 13:DZ:55:ILE:HG22  | 1.92                     | 0.52              |
| 16:DC:371:ILE:HD12 | 16:DC:374:LEU:HD12 | 1.91                     | 0.52              |
| 19:DG:305:VAL:HG21 | 19:DG:310:LEU:HD13 | 1.91                     | 0.52              |
| 28:CC:66:ASN:HB3   | 28:CC:72:ILE:HG23  | 1.90                     | 0.52              |
| 34:CK:307:PHE:HE1  | 42:CU:61:ILE:HD12  | 1.74                     | 0.52              |
| 44:Ca:89:ARG:HD2   | 44:Ca:177:GLN:NE2  | 2.25                     | 0.52              |
| 47:Cg:233:THR:HG23 | 47:Cg:237:GLU:HB3  | 1.90                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:Ci:42:GLN:HE21  | 48:Ci:42:GLN:HA    | 1.74                     | 0.52              |
| 56:Cv:33:GLU:CD    | 56:Cv:33:GLU:H     | 2.17                     | 0.52              |
| 1:DA:47:LEU:HD11   | 2:DD:38:ARG:HB3    | 1.91                     | 0.52              |
| 1:DA:853:LYS:HE3   | 56:Cv:1005:TRP:CE2 | 2.44                     | 0.52              |
| 3:DI:61:ASN:HA     | 3:DI:64:GLU:HG3    | 1.90                     | 0.52              |
| 7:DO:122:LEU:O     | 7:DO:163:ARG:NH1   | 2.41                     | 0.52              |
| 16:DC:546:LEU:HD22 | 16:DC:695:VAL:HG11 | 1.89                     | 0.52              |
| 16:DC:582:ARG:O    | 16:DC:622:TYR:HA   | 2.09                     | 0.52              |
| 17:DE:150:ARG:HG2  | 17:DE:151:PRO:HD2  | 1.91                     | 0.52              |
| 19:DG:314:LEU:O    | 19:DG:318:ILE:HG23 | 2.09                     | 0.52              |
| 39:CQ:56:ARG:HG3   | 57:CA:99:G:OP1     | 2.10                     | 0.52              |
| 44:Ca:124:ILE:HD11 | 56:Cv:1033:GLU:HA  | 1.90                     | 0.52              |
| 44:Ca:575:ARG:NH1  | 44:Ca:575:ARG:O    | 2.40                     | 0.52              |
| 47:Cg:112:ARG:HD2  | 47:Cg:408:GLU:OE2  | 2.09                     | 0.52              |
| 1:DA:463:VAL:HG11  | 1:DA:840:TYR:HB3   | 1.91                     | 0.52              |
| 2:DD:352:VAL:HG12  | 2:DD:359:LEU:HD22  | 1.90                     | 0.52              |
| 8:DP:133:GLN:HE22  | 49:Cj:66:LEU:HB2   | 1.74                     | 0.52              |
| 12:DU:83:ARG:NH2   | 12:DU:157:GLN:HG3  | 2.24                     | 0.52              |
| 27:DY:30:LYS:HE2   | 57:CA:531:G:C8     | 2.44                     | 0.52              |
| 27:DY:77:VAL:HG22  | 27:DY:84:LYS:NZ    | 2.25                     | 0.52              |
| 42:CU:16:HIS:CD2   | 42:CU:18:LYS:H     | 2.27                     | 0.52              |
| 50:Ck:204:LEU:O    | 50:Ck:250:ARG:NH2  | 2.43                     | 0.52              |
| 50:Ck:362:TYR:CD2  | 50:Ck:365:ILE:HB   | 2.45                     | 0.52              |
| 56:Cv:454:LEU:HA   | 56:Cv:457:ARG:HD2  | 1.92                     | 0.52              |
| 57:CA:370:A:O2'    | 57:CA:371:U:H5'    | 2.09                     | 0.52              |
| 1:DA:170:GLN:HB2   | 1:DA:173:ALA:HB2   | 1.91                     | 0.52              |
| 1:DA:1638:LEU:O    | 1:DA:1642:LEU:HB2  | 2.08                     | 0.52              |
| 1:DA:1650:MET:HE1  | 29:CE:425:PRO:HD2  | 1.91                     | 0.52              |
| 10:DR:68:HIS:HA    | 10:DR:87:LEU:HD11  | 1.92                     | 0.52              |
| 19:DG:547:MET:HE1  | 19:DG:561:PRO:HB3  | 1.91                     | 0.52              |
| 21:DJ:21:PRO:HD2   | 36:CN:126:ASN:O    | 2.09                     | 0.52              |
| 33:CJ:490:ASP:HA   | 33:CJ:493:ALA:HB3  | 1.91                     | 0.52              |
| 38:CP:31:MET:HB2   | 38:CP:114:PRO:HG3  | 1.91                     | 0.52              |
| 38:CP:79:ASP:OD2   | 53:Cp:28:ARG:HG3   | 2.09                     | 0.52              |
| 50:Ck:119:GLU:OE1  | 50:Ck:140:ARG:NH1  | 2.42                     | 0.52              |
| 62:US:46:UNK:HG3   | 62:US:49:UNK:HB2   | 1.92                     | 0.52              |
| 2:DD:588:ARG:HH12  | 2:DD:626:ARG:NH2   | 2.07                     | 0.52              |
| 7:DO:194:TYR:CZ    | 7:DO:251:ASN:HB3   | 2.44                     | 0.52              |
| 8:DP:20:MET:O      | 8:DP:23:LEU:HB2    | 2.10                     | 0.52              |
| 15:DB:232:ARG:HG2  | 16:DC:953:MET:HE3  | 1.92                     | 0.52              |
| 16:DC:1095:LEU:HG  | 22:DK:14:LYS:HG2   | 1.92                     | 0.52              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:DG:176:VAL:HG22  | 19:DG:188:LEU:HD11 | 1.92                     | 0.52              |
| 29:CE:286:ALA:HB2   | 44:Ca:355:PHE:CE1  | 2.45                     | 0.52              |
| 33:CJ:753:ASN:ND2   | 48:Ci:16:GLY:O     | 2.43                     | 0.52              |
| 34:CK:284:PHE:O     | 42:CU:71:ARG:NH2   | 2.29                     | 0.52              |
| 51:Cm:53:THR:OG1    | 51:Cm:56:ASN:HB2   | 2.10                     | 0.52              |
| 56:Cv:366:ALA:O     | 56:Cv:369:ARG:HB3  | 2.10                     | 0.52              |
| 56:Cv:573:GLU:OE2   | 56:Cv:798:TYR:HA   | 2.09                     | 0.52              |
| 1:DA:791:THR:HA     | 1:DA:794:ARG:NH2   | 2.25                     | 0.52              |
| 2:DD:248:ASP:CG     | 2:DD:249:PRO:HD2   | 2.34                     | 0.52              |
| 3:DI:291:LEU:HD13   | 3:DI:300:LEU:HD23  | 1.92                     | 0.52              |
| 4:DL:235:PRO:HG2    | 4:DL:236:LEU:HD12  | 1.92                     | 0.52              |
| 6:DN:288:PHE:HD1    | 6:DN:288:PHE:H     | 1.57                     | 0.52              |
| 12:DU:64:TYR:CE1    | 37:CO:330:THR:HG23 | 2.45                     | 0.52              |
| 16:DC:1041:LEU:HD13 | 22:DK:48:VAL:HG21  | 1.91                     | 0.52              |
| 17:DE:451:THR:HB    | 17:DE:501:HIS:HD2  | 1.75                     | 0.52              |
| 33:CJ:426:GLN:HA    | 50:Ck:683:LEU:HD21 | 1.90                     | 0.52              |
| 36:CN:18:PRO:O      | 57:CA:442:A:O2'    | 2.24                     | 0.52              |
| 37:CO:131:LYS:HA    | 37:CO:134:GLU:HG2  | 1.91                     | 0.52              |
| 40:CR:60:PHE:CE2    | 40:CR:62:GLN:HB3   | 2.44                     | 0.52              |
| 44:Ca:191:MET:HA    | 44:Ca:194:LEU:HB2  | 1.91                     | 0.52              |
| 54:Cq:253:ARG:O     | 54:Cq:257:MET:HG3  | 2.10                     | 0.52              |
| 57:CA:30:U:H2'      | 57:CA:31:U:C6      | 2.45                     | 0.52              |
| 1:DA:897:SER:OG     | 1:DA:898:VAL:N     | 2.42                     | 0.52              |
| 1:DA:907:GLN:NE2    | 44:Ca:399:ASN:HD22 | 2.06                     | 0.52              |
| 4:DL:292:ARG:HH21   | 33:CJ:389:THR:H    | 1.58                     | 0.52              |
| 9:DQ:148:LEU:HD23   | 9:DQ:176:ARG:NH2   | 2.24                     | 0.52              |
| 18:DF:262:PHE:HE1   | 21:DJ:59:VAL:HG12  | 1.75                     | 0.52              |
| 19:DG:149:SER:O     | 19:DG:149:SER:OG   | 2.27                     | 0.52              |
| 31:CH:218:VAL:HG22  | 31:CH:282:HIS:CE1  | 2.45                     | 0.52              |
| 33:CJ:583:LYS:NZ    | 33:CJ:597:LEU:HD11 | 2.24                     | 0.52              |
| 42:CU:85:SER:HB3    | 57:CA:609:A:H5''   | 1.92                     | 0.52              |
| 50:Ck:203:PHE:HB3   | 50:Ck:210:PHE:HB2  | 1.91                     | 0.52              |
| 50:Ck:277:VAL:HG21  | 50:Ck:348:LEU:HD13 | 1.92                     | 0.52              |
| 51:Cm:106:CYS:SG    | 51:Cm:107:MET:N    | 2.83                     | 0.52              |
| 55:Cr:125:GLN:HE22  | 55:Cr:161:ARG:HG3  | 1.75                     | 0.52              |
| 56:Cv:636:ALA:HB3   | 56:Cv:650:HIS:CE1  | 2.44                     | 0.52              |
| 2:DD:794:ARG:CZ     | 2:DD:808:THR:HG23  | 2.40                     | 0.52              |
| 16:DC:589:VAL:HG21  | 16:DC:604:VAL:O    | 2.10                     | 0.52              |
| 16:DC:629:VAL:HG12  | 16:DC:633:LYS:HE3  | 1.92                     | 0.52              |
| 18:DF:237:LEU:HB3   | 18:DF:253:ILE:HD13 | 1.91                     | 0.52              |
| 19:DG:391:ALA:HA    | 19:DG:497:ARG:HH22 | 1.75                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:DG:395:TRP:NE1  | 19:DG:528:TYR:OH   | 2.38                     | 0.52              |
| 25:DW:86:PHE:CE1   | 47:Cg:103:PRO:HG3  | 2.44                     | 0.52              |
| 37:CO:112:LYS:HB2  | 37:CO:112:LYS:NZ   | 2.25                     | 0.52              |
| 38:CP:177:GLU:OE1  | 38:CP:177:GLU:N    | 2.42                     | 0.52              |
| 47:Cg:112:ARG:HH21 | 47:Cg:154:GLY:HA3  | 1.74                     | 0.52              |
| 1:DA:1455:THR:HG23 | 1:DA:1580:ASN:HD22 | 1.73                     | 0.52              |
| 2:DD:209:THR:HG21  | 2:DD:290:ARG:HB2   | 1.91                     | 0.52              |
| 2:DD:612:MET:O     | 2:DD:616:LEU:HB2   | 2.10                     | 0.52              |
| 17:DE:601:ILE:HD13 | 17:DE:635:ILE:HG23 | 1.91                     | 0.52              |
| 23:DT:93:MET:HE1   | 23:DT:102:TRP:CE2  | 2.45                     | 0.52              |
| 37:CO:87:THR:OG1   | 37:CO:88:PRO:HD2   | 2.09                     | 0.52              |
| 43:CZ:343:ARG:NH1  | 57:CA:577:A:O2'    | 2.43                     | 0.52              |
| 44:Ca:423:GLN:NE2  | 44:Ca:479:THR:HA   | 2.24                     | 0.52              |
| 56:Cv:594:LEU:HD23 | 56:Cv:600:GLY:HA2  | 1.92                     | 0.52              |
| 1:DA:967:GLU:OE2   | 44:Ca:255:TYR:OH   | 2.27                     | 0.51              |
| 3:DI:107:ILE:HG12  | 3:DI:145:LEU:HD12  | 1.91                     | 0.51              |
| 3:DI:148:ALA:O     | 3:DI:152:LEU:HB2   | 2.09                     | 0.51              |
| 6:DN:141:MET:N     | 6:DN:141:MET:SD    | 2.82                     | 0.51              |
| 15:DB:1018:ARG:HB3 | 19:DG:31:TYR:CE1   | 2.45                     | 0.51              |
| 16:DC:963:SER:N    | 16:DC:1062:GLN:HG2 | 2.25                     | 0.51              |
| 18:DF:580:ASP:HB3  | 18:DF:583:ARG:HB2  | 1.91                     | 0.51              |
| 25:DW:130:ARG:HB3  | 40:CR:286:LEU:HB2  | 1.92                     | 0.51              |
| 33:CJ:365:GLU:HB3  | 33:CJ:813:GLU:HG3  | 1.92                     | 0.51              |
| 37:CO:248:ILE:HD11 | 57:CA:287:A:N3     | 2.24                     | 0.51              |
| 37:CO:334:ARG:HD2  | 39:CQ:164:ILE:HG12 | 1.92                     | 0.51              |
| 39:CQ:193:ARG:HH12 | 52:Cn:194:PRO:HD3  | 1.75                     | 0.51              |
| 42:CU:79:TYR:HD2   | 42:CU:80:GLN:HG2   | 1.76                     | 0.51              |
| 46:Cd:63:ARG:HD2   | 46:Cd:67:GLU:OE2   | 2.10                     | 0.51              |
| 46:Cd:170:GLY:O    | 46:Cd:171:LYS:HG2  | 2.09                     | 0.51              |
| 46:Cd:287:GLU:OE1  | 46:Cd:287:GLU:N    | 2.40                     | 0.51              |
| 54:Cq:57:GLN:NE2   | 54:Cq:81:TYR:O     | 2.41                     | 0.51              |
| 57:CA:153:A:C4     | 57:CA:154:G:C8     | 2.98                     | 0.51              |
| 57:CA:182:U:H5''   | 57:CA:183:U:OP1    | 2.10                     | 0.51              |
| 4:DL:118:ASP:OD2   | 4:DL:159:GLN:NE2   | 2.43                     | 0.51              |
| 9:DQ:181:VAL:O     | 9:DQ:184:ILE:HG13  | 2.10                     | 0.51              |
| 11:DS:260:ALA:HB1  | 38:CP:165:LEU:HD13 | 1.91                     | 0.51              |
| 15:DB:1095:GLU:OE1 | 15:DB:1095:GLU:N   | 2.43                     | 0.51              |
| 19:DG:176:VAL:HG23 | 19:DG:192:MET:HE3  | 1.91                     | 0.51              |
| 21:DJ:247:ASN:HD22 | 21:DJ:250:VAL:HG23 | 1.76                     | 0.51              |
| 29:CE:308:ARG:HD3  | 44:Ca:368:ARG:NH1  | 2.24                     | 0.51              |
| 32:CI:392:ARG:HD3  | 32:CI:415:LEU:HD22 | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:Ca:88:ARG:NH2   | 56:Cv:1110:GLU:OE1 | 2.41                     | 0.51              |
| 44:Ca:399:ASN:OD1  | 44:Ca:399:ASN:N    | 2.38                     | 0.51              |
| 56:Cv:311:LEU:H    | 56:Cv:311:LEU:HD12 | 1.75                     | 0.51              |
| 58:UO:3:UNK:O      | 58:UO:5:UNK:N      | 2.43                     | 0.51              |
| 1:DA:59:HIS:HD2    | 1:DA:86:TYR:N      | 2.00                     | 0.51              |
| 1:DA:324:GLN:HG2   | 1:DA:330:TRP:HE1   | 1.74                     | 0.51              |
| 2:DD:588:ARG:HH12  | 2:DD:626:ARG:HH22  | 1.57                     | 0.51              |
| 3:DI:294:ASN:ND2   | 3:DI:365:ARG:HH21  | 2.08                     | 0.51              |
| 15:DB:80:LEU:HD23  | 17:DE:539:ARG:HH22 | 1.76                     | 0.51              |
| 15:DB:231:ASP:OD1  | 15:DB:232:ARG:N    | 2.43                     | 0.51              |
| 15:DB:361:ARG:NH2  | 20:DH:539:ASP:OD1  | 2.43                     | 0.51              |
| 15:DB:891:GLN:HG3  | 50:Ck:310:ASP:HA   | 1.91                     | 0.51              |
| 18:DF:271:LEU:HD13 | 18:DF:294:MET:HB2  | 1.92                     | 0.51              |
| 18:DF:519:TRP:CZ3  | 18:DF:531:ARG:HD2  | 2.45                     | 0.51              |
| 19:DG:560:GLU:HB3  | 19:DG:622:ARG:NH2  | 2.25                     | 0.51              |
| 34:CK:79:TRP:HE1   | 45:Cb:289:LYS:HZ2  | 1.56                     | 0.51              |
| 34:CK:202:ARG:NH1  | 57:CA:305:A:OP2    | 2.43                     | 0.51              |
| 41:CS:122:PHE:CD2  | 41:CS:123:PRO:HA   | 2.45                     | 0.51              |
| 44:Ca:78:PHE:HE1   | 44:Ca:176:ILE:HG13 | 1.75                     | 0.51              |
| 44:Ca:575:ARG:NH1  | 44:Ca:575:ARG:HG2  | 2.25                     | 0.51              |
| 49:Cj:94:ILE:HG23  | 49:Cj:98:LYS:HG2   | 1.92                     | 0.51              |
| 52:Cn:144:ALA:HA   | 57:CA:280:A:N6     | 2.25                     | 0.51              |
| 52:Cn:144:ALA:HA   | 57:CA:280:A:H61    | 1.75                     | 0.51              |
| 57:CA:63:G:N1      | 57:CA:156:U:O2'    | 2.43                     | 0.51              |
| 6:DN:113:ALA:HB3   | 6:DN:133:PHE:CE2   | 2.46                     | 0.51              |
| 12:DU:34:TYR:CD1   | 12:DU:35:PRO:HD2   | 2.46                     | 0.51              |
| 15:DB:887:SER:HB3  | 50:Ck:283:GLU:OE2  | 2.10                     | 0.51              |
| 18:DF:129:ILE:O    | 18:DF:163:ARG:NH1  | 2.43                     | 0.51              |
| 19:DG:87:TYR:HA    | 19:DG:90:MET:HG2   | 1.92                     | 0.51              |
| 20:DH:557:VAL:HG12 | 20:DH:558:GLU:H    | 1.74                     | 0.51              |
| 21:DJ:304:ILE:HD12 | 23:DT:42:PHE:CD2   | 2.44                     | 0.51              |
| 23:DT:92:LYS:HD2   | 23:DT:174:TYR:CD1  | 2.45                     | 0.51              |
| 29:CE:220:ASP:HB2  | 56:Cv:44:ARG:HH12  | 1.75                     | 0.51              |
| 32:CI:191:LEU:O    | 32:CI:195:ILE:HG13 | 2.11                     | 0.51              |
| 32:CI:294:ILE:HD11 | 32:CI:408:ILE:HD11 | 1.93                     | 0.51              |
| 33:CJ:419:ILE:HA   | 33:CJ:422:TRP:NE1  | 2.24                     | 0.51              |
| 34:CK:278:VAL:HG13 | 34:CK:306:TYR:HB2  | 1.93                     | 0.51              |
| 36:CN:51:LEU:O     | 36:CN:68:GLN:NE2   | 2.44                     | 0.51              |
| 42:CU:69:ARG:HA    | 42:CU:72:HIS:CD2   | 2.46                     | 0.51              |
| 44:Ca:359:ARG:NH2  | 56:Cv:257:LYS:HD3  | 2.25                     | 0.51              |
| 45:Cb:305:PRO:HG2  | 55:Cr:38:ALA:HB3   | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Ck:331:ARG:NH2  | 50:Ck:595:ASP:OD1  | 2.34                     | 0.51              |
| 50:Ck:617:VAL:HG21 | 50:Ck:638:ARG:HD2  | 1.91                     | 0.51              |
| 1:DA:182:ARG:HH22  | 44:Ca:414:THR:HG22 | 1.74                     | 0.51              |
| 1:DA:1064:ASP:HB2  | 1:DA:1067:GLY:H    | 1.75                     | 0.51              |
| 1:DA:1153:SER:HB3  | 1:DA:1165:ALA:HB1  | 1.92                     | 0.51              |
| 2:DD:763:TYR:CD1   | 44:Ca:387:GLN:HG2  | 2.45                     | 0.51              |
| 8:DP:27:ASP:OD1    | 8:DP:27:ASP:N      | 2.40                     | 0.51              |
| 11:DS:122:CYS:O    | 11:DS:125:LYS:HB2  | 2.11                     | 0.51              |
| 16:DC:119:THR:HG21 | 16:DC:136:TRP:HE1  | 1.75                     | 0.51              |
| 16:DC:929:TRP:O    | 16:DC:933:ARG:HB2  | 2.10                     | 0.51              |
| 24:DV:32:PRO:HG3   | 24:DV:52:ARG:HH12  | 1.75                     | 0.51              |
| 34:CK:20:MET:HE2   | 34:CK:20:MET:HA    | 1.93                     | 0.51              |
| 34:CK:113:ARG:HG2  | 34:CK:113:ARG:HH11 | 1.75                     | 0.51              |
| 38:CP:34:HIS:O     | 38:CP:41:GLN:NE2   | 2.43                     | 0.51              |
| 44:Ca:153:LYS:HZ2  | 44:Ca:157:LYS:HE3  | 1.73                     | 0.51              |
| 44:Ca:570:THR:HG21 | 53:Cp:16:HIS:CE1   | 2.45                     | 0.51              |
| 51:Cm:33:PRO:HB3   | 51:Cm:45:LEU:HD11  | 1.92                     | 0.51              |
| 54:Cq:216:LEU:HB3  | 54:Cq:251:ALA:HB1  | 1.93                     | 0.51              |
| 56:Cv:235:MET:HE3  | 56:Cv:251:ASN:HD22 | 1.75                     | 0.51              |
| 1:DA:1278:THR:HA   | 54:Cq:152:GLU:OE2  | 2.11                     | 0.51              |
| 1:DA:1558:ASN:HA   | 1:DA:1596:VAL:HG21 | 1.92                     | 0.51              |
| 2:DD:414:ARG:NH1   | 2:DD:568:GLU:OE1   | 2.44                     | 0.51              |
| 9:DQ:215:PRO:HA    | 9:DQ:218:ARG:NH1   | 2.26                     | 0.51              |
| 11:DS:49:VAL:HB    | 44:Ca:600:PRO:HG3  | 1.92                     | 0.51              |
| 12:DU:206:PRO:HB2  | 12:DU:208:TYR:CE1  | 2.46                     | 0.51              |
| 14:Da:20:ARG:NH2   | 57:CA:371:U:OP1    | 2.39                     | 0.51              |
| 15:DB:801:LEU:HD11 | 15:DB:807:ILE:HD11 | 1.92                     | 0.51              |
| 19:DG:444:THR:HG22 | 19:DG:445:LEU:H    | 1.74                     | 0.51              |
| 30:CF:141:GLN:HE22 | 56:Cv:653:ALA:HA   | 1.76                     | 0.51              |
| 39:CQ:55:THR:OG1   | 39:CQ:56:ARG:N     | 2.43                     | 0.51              |
| 46:Cd:100:LYS:O    | 46:Cd:104:GLU:HG2  | 2.11                     | 0.51              |
| 46:Cd:195:GLU:HB3  | 46:Cd:216:HIS:HB2  | 1.93                     | 0.51              |
| 50:Ck:158:PRO:HA   | 50:Ck:161:GLU:OE2  | 2.10                     | 0.51              |
| 50:Ck:568:LEU:HD12 | 50:Ck:569:GLY:N    | 2.24                     | 0.51              |
| 56:Cv:172:THR:HG21 | 56:Cv:178:GLU:HB3  | 1.92                     | 0.51              |
| 1:DA:1259:VAL:HG22 | 15:DB:628:LEU:HD13 | 1.91                     | 0.51              |
| 3:DI:327:ARG:NH1   | 7:DO:226:ILE:O     | 2.44                     | 0.51              |
| 7:DO:105:ARG:HE    | 7:DO:147:ARG:HD2   | 1.75                     | 0.51              |
| 15:DB:72:TRP:CD1   | 15:DB:72:TRP:H     | 2.28                     | 0.51              |
| 15:DB:527:GLU:H    | 15:DB:530:GLU:HG3  | 1.76                     | 0.51              |
| 19:DG:366:ASP:HA   | 19:DG:370:ARG:HH12 | 1.75                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:CI:49:LYS:O     | 32:CI:52:SER:OG    | 2.25                     | 0.51              |
| 48:CI:69:THR:HG21  | 48:CI:73:MET:HG2   | 1.92                     | 0.51              |
| 56:Cv:296:LEU:HD21 | 56:Cv:421:LEU:HD21 | 1.92                     | 0.51              |
| 9:DQ:232:ASP:OD1   | 9:DQ:232:ASP:N     | 2.44                     | 0.51              |
| 12:DU:90:VAL:O     | 12:DU:210:ALA:HA   | 2.11                     | 0.51              |
| 15:DB:983:LEU:HD22 | 19:DG:84:LEU:HD21  | 1.93                     | 0.51              |
| 16:DC:905:ALA:HB1  | 16:DC:941:MET:HE3  | 1.93                     | 0.51              |
| 17:DE:344:ARG:O    | 17:DE:348:ILE:HG13 | 2.10                     | 0.51              |
| 29:CE:80:ILE:HD11  | 56:Cv:517:VAL:HG12 | 1.93                     | 0.51              |
| 33:CJ:345:VAL:HG22 | 33:CJ:346:PRO:HD2  | 1.93                     | 0.51              |
| 33:CJ:556:GLU:HA   | 33:CJ:559:ALA:HB3  | 1.91                     | 0.51              |
| 33:CJ:733:TYR:OH   | 47:Cg:300:PRO:O    | 2.27                     | 0.51              |
| 37:CO:222:ALA:O    | 37:CO:226:VAL:HG23 | 2.10                     | 0.51              |
| 44:Ca:45:THR:HG22  | 44:Ca:47:ASP:H     | 1.76                     | 0.51              |
| 56:Cv:632:GLU:HG2  | 56:Cv:635:ARG:NH2  | 2.26                     | 0.51              |
| 56:Cv:914:ASN:CG   | 56:Cv:915:PRO:HD3  | 2.35                     | 0.51              |
| 56:Cv:1042:ARG:NH2 | 56:Cv:1046:ASN:HB2 | 2.25                     | 0.51              |
| 1:DA:90:MET:HE1    | 2:DD:122:GLN:HE22  | 1.75                     | 0.51              |
| 1:DA:414:HIS:HD2   | 1:DA:416:HIS:H     | 1.59                     | 0.51              |
| 1:DA:518:GLU:CD    | 1:DA:837:ARG:HH22  | 2.19                     | 0.51              |
| 2:DD:181:MET:HE1   | 2:DD:215:TYR:HA    | 1.92                     | 0.51              |
| 3:DI:307:ASN:HB2   | 3:DI:310:LEU:HB2   | 1.93                     | 0.51              |
| 9:DQ:51:ASN:HD22   | 37:CO:339:ARG:HD2  | 1.76                     | 0.51              |
| 23:DT:55:ALA:HA    | 23:DT:58:HIS:CD2   | 2.45                     | 0.51              |
| 23:DT:143:TYR:HE1  | 23:DT:177:MET:HE3  | 1.75                     | 0.51              |
| 29:CE:40:ARG:NE    | 29:CE:94:ARG:HD2   | 2.25                     | 0.51              |
| 29:CE:417:ASN:HD22 | 29:CE:419:ARG:H    | 1.58                     | 0.51              |
| 39:CQ:92:SER:HA    | 39:CQ:149:GLN:HB2  | 1.92                     | 0.51              |
| 39:CQ:144:LEU:HB3  | 39:CQ:166:GLU:HB3  | 1.92                     | 0.51              |
| 40:CR:91:ASP:OD2   | 40:CR:94:MET:HB2   | 2.10                     | 0.51              |
| 43:CZ:276:HIS:HB3  | 43:CZ:305:HIS:NE2  | 2.26                     | 0.51              |
| 50:Ck:130:MET:HG3  | 50:Ck:275:TRP:NE1  | 2.26                     | 0.51              |
| 54:Cq:107:GLU:O    | 54:Cq:110:ILE:N    | 2.44                     | 0.51              |
| 2:DD:156:GLN:NE2   | 46:Cd:70:ARG:HH11  | 2.09                     | 0.51              |
| 5:DM:176:VAL:HG21  | 5:DM:226:PRO:HD3   | 1.93                     | 0.51              |
| 8:DP:132:LEU:HD21  | 8:DP:154:PHE:CE1   | 2.47                     | 0.51              |
| 14:Da:10:ILE:N     | 57:CA:270:U:OP1    | 2.43                     | 0.51              |
| 16:DC:1023:ASN:N   | 16:DC:1023:ASN:OD1 | 2.44                     | 0.51              |
| 17:DE:101:GLU:O    | 17:DE:105:ASN:ND2  | 2.44                     | 0.51              |
| 23:DT:33:HIS:O     | 23:DT:36:GLU:HG2   | 2.10                     | 0.51              |
| 30:CF:41:ASN:HB2   | 46:Cd:163:GLU:HB3  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:CK:153:ASP:N    | 34:CK:153:ASP:OD1  | 2.37                     | 0.51              |
| 45:Cb:288:GLU:HA   | 45:Cb:291:GLU:OE1  | 2.10                     | 0.51              |
| 49:Cj:80:LEU:HD12  | 49:Cj:84:ARG:HH12  | 1.76                     | 0.51              |
| 49:Cj:209:TYR:CE2  | 49:Cj:212:TYR:HB2  | 2.46                     | 0.51              |
| 50:Ck:325:LEU:HD13 | 50:Ck:632:MET:HE2  | 1.93                     | 0.51              |
| 50:Ck:832:THR:HG22 | 50:Ck:834:MET:H    | 1.76                     | 0.51              |
| 56:Cv:871:ILE:HD13 | 56:Cv:890:PRO:HG2  | 1.92                     | 0.51              |
| 56:Cv:945:VAL:HG13 | 56:Cv:946:PRO:HD3  | 1.92                     | 0.51              |
| 2:DD:11:ARG:NH2    | 52:Cn:157:TYR:O    | 2.44                     | 0.50              |
| 12:DU:46:THR:HG23  | 37:CO:332:ARG:HA   | 1.93                     | 0.50              |
| 17:DE:174:VAL:HG11 | 17:DE:550:ALA:HB2  | 1.92                     | 0.50              |
| 17:DE:602:LYS:HE3  | 17:DE:611:LEU:HD11 | 1.92                     | 0.50              |
| 41:CS:122:PHE:CG   | 41:CS:123:PRO:HA   | 2.46                     | 0.50              |
| 44:Ca:579:VAL:O    | 57:CA:260:U:O2'    | 2.25                     | 0.50              |
| 56:Cv:559:GLN:NE2  | 61:UR:3:UNK:HG1    | 2.26                     | 0.50              |
| 1:DA:53:ARG:HH12   | 2:DD:63:GLN:HE22   | 1.58                     | 0.50              |
| 1:DA:74:LYS:NZ     | 57:CA:71:U:OP1     | 2.45                     | 0.50              |
| 1:DA:1048:ASN:HD21 | 1:DA:1051:ASN:HA   | 1.76                     | 0.50              |
| 1:DA:1191:ILE:O    | 1:DA:1195:VAL:HG23 | 2.11                     | 0.50              |
| 8:DP:101:PHE:CD2   | 8:DP:110:PRO:HG3   | 2.46                     | 0.50              |
| 15:DB:131:GLU:HG3  | 15:DB:228:THR:HG23 | 1.93                     | 0.50              |
| 15:DB:383:ARG:NH1  | 23:DT:113:GLN:O    | 2.44                     | 0.50              |
| 16:DC:493:TYR:O    | 16:DC:496:LYS:HB2  | 2.11                     | 0.50              |
| 21:DJ:55:ASN:ND2   | 57:CA:433:U:O4     | 2.43                     | 0.50              |
| 23:DT:139:HIS:HB2  | 23:DT:176:ASP:OD1  | 2.11                     | 0.50              |
| 33:CJ:315:ASP:OD1  | 33:CJ:315:ASP:N    | 2.44                     | 0.50              |
| 33:CJ:585:SER:C    | 33:CJ:594:GLU:HB2  | 2.36                     | 0.50              |
| 37:CO:82:ASN:HD21  | 52:Cn:142:TRP:H    | 1.58                     | 0.50              |
| 40:CR:8:ILE:HG22   | 40:CR:9:TYR:HD1    | 1.76                     | 0.50              |
| 40:CR:119:GLU:H    | 40:CR:119:GLU:CD   | 2.18                     | 0.50              |
| 47:Cg:279:LEU:HD23 | 47:Cg:280:PRO:HD2  | 1.92                     | 0.50              |
| 51:Cm:168:HIS:CD2  | 51:Cm:168:HIS:H    | 2.29                     | 0.50              |
| 56:Cv:247:THR:HG23 | 56:Cv:263:GLU:HG3  | 1.93                     | 0.50              |
| 2:DD:347:GLU:HG3   | 10:DR:30:TRP:NE1   | 2.26                     | 0.50              |
| 5:DM:65:THR:HG22   | 5:DM:69:PHE:HB3    | 1.94                     | 0.50              |
| 15:DB:335:LYS:O    | 15:DB:339:ARG:HB2  | 2.11                     | 0.50              |
| 15:DB:748:HIS:CD2  | 15:DB:751:THR:H    | 2.29                     | 0.50              |
| 21:DJ:304:ILE:HD12 | 23:DT:42:PHE:HD2   | 1.76                     | 0.50              |
| 22:DK:225:THR:HG22 | 22:DK:226:LEU:HD13 | 1.94                     | 0.50              |
| 32:CI:40:TRP:CE2   | 33:CJ:163:MET:HE2  | 2.46                     | 0.50              |
| 32:CI:137:SER:HB3  | 32:CI:182:ARG:HH21 | 1.77                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:394:PHE:HE1  | 36:CN:127:LEU:HD11 | 1.76                     | 0.50              |
| 37:CO:71:PRO:HB2   | 52:Cn:191:ALA:HB3  | 1.93                     | 0.50              |
| 44:Ca:46:ARG:HH11  | 44:Ca:46:ARG:HG3   | 1.76                     | 0.50              |
| 46:Cd:36:ARG:NH1   | 46:Cd:39:MET:SD    | 2.84                     | 0.50              |
| 48:Ci:96:ASN:ND2   | 50:Ck:697:MET:HG3  | 2.26                     | 0.50              |
| 49:Cj:73:ARG:HB2   | 53:Cp:169:ASN:HA   | 1.93                     | 0.50              |
| 51:Cm:48:PHE:O     | 51:Cm:52:THR:OG1   | 2.29                     | 0.50              |
| 7:DO:254:ASP:OD1   | 7:DO:254:ASP:N     | 2.44                     | 0.50              |
| 14:Da:64:PRO:HG2   | 37:CO:279:ARG:HG2  | 1.92                     | 0.50              |
| 16:DC:116:TYR:CE2  | 17:DE:572:VAL:HG11 | 2.47                     | 0.50              |
| 26:DX:43:HIS:CE1   | 41:CS:123:PRO:HB2  | 2.46                     | 0.50              |
| 56:Cv:292:LYS:HG2  | 56:Cv:512:MET:HE3  | 1.93                     | 0.50              |
| 56:Cv:902:ILE:HG22 | 56:Cv:903:ASP:OD1  | 2.11                     | 0.50              |
| 1:DA:521:GLU:O     | 1:DA:525:LEU:HG    | 2.12                     | 0.50              |
| 2:DD:88:TYR:HD1    | 2:DD:92:MET:HE2    | 1.77                     | 0.50              |
| 2:DD:131:PRO:HG3   | 37:CO:331:GLY:HA3  | 1.92                     | 0.50              |
| 2:DD:357:TRP:O     | 2:DD:626:ARG:NH2   | 2.44                     | 0.50              |
| 7:DO:136:ASP:HA    | 7:DO:139:GLU:HG3   | 1.93                     | 0.50              |
| 17:DE:570:GLU:OE1  | 20:DH:527:VAL:N    | 2.42                     | 0.50              |
| 18:DF:499:THR:HG21 | 18:DF:578:LYS:HD2  | 1.93                     | 0.50              |
| 20:DH:120:HIS:H    | 20:DH:123:HIS:CD2  | 2.29                     | 0.50              |
| 22:DK:36:ARG:NH1   | 22:DK:106:SER:HB3  | 2.27                     | 0.50              |
| 26:DX:48:LYS:O     | 26:DX:52:GLU:HG2   | 2.12                     | 0.50              |
| 27:DY:32:TRP:O     | 27:DY:37:ARG:NH1   | 2.44                     | 0.50              |
| 31:CH:147:ASN:ND2  | 31:CH:224:TYR:HB3  | 2.27                     | 0.50              |
| 34:CK:71:SER:HB3   | 45:Cb:280:ASN:HD22 | 1.77                     | 0.50              |
| 44:Ca:130:TYR:HB3  | 44:Ca:131:MET:HE2  | 1.94                     | 0.50              |
| 46:Cd:198:GLU:OE1  | 46:Cd:198:GLU:N    | 2.43                     | 0.50              |
| 53:Cp:82:ASN:O     | 53:Cp:86:THR:OG1   | 2.11                     | 0.50              |
| 56:Cv:498:MET:HE3  | 56:Cv:502:ILE:HG13 | 1.93                     | 0.50              |
| 3:DI:313:ARG:HH11  | 3:DI:407:LEU:C     | 2.19                     | 0.50              |
| 10:DR:244:LEU:HD22 | 10:DR:269:TRP:CE2  | 2.47                     | 0.50              |
| 16:DC:1075:GLU:OE1 | 17:DE:582:GLU:N    | 2.34                     | 0.50              |
| 23:DT:119:PHE:CD1  | 23:DT:127:LYS:HB2  | 2.46                     | 0.50              |
| 29:CE:376:LEU:HD11 | 29:CE:416:VAL:HG12 | 1.93                     | 0.50              |
| 29:CE:417:ASN:ND2  | 29:CE:419:ARG:H    | 2.09                     | 0.50              |
| 30:CF:141:GLN:HB3  | 56:Cv:633:MET:HE3  | 1.92                     | 0.50              |
| 35:CL:84:ARG:HG2   | 44:Ca:11:TYR:CD2   | 2.46                     | 0.50              |
| 37:CO:182:ASN:HB2  | 46:Cd:146:ASN:OD1  | 2.12                     | 0.50              |
| 44:Ca:295:PHE:CD2  | 44:Ca:299:ARG:NH1  | 2.80                     | 0.50              |
| 44:Ca:589:ARG:HD2  | 57:CA:259:U:H5"    | 1.92                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:Cj:118:ARG:NH2  | 49:Cj:168:VAL:HB   | 2.26                     | 0.50              |
| 56:Cv:1010:SER:OG  | 56:Cv:1011:SER:N   | 2.44                     | 0.50              |
| 1:DA:222:GLU:CD    | 1:DA:222:GLU:H     | 2.20                     | 0.50              |
| 1:DA:961:LYS:NZ    | 1:DA:983:GLU:OE1   | 2.40                     | 0.50              |
| 2:DD:650:THR:HG23  | 49:Cj:211:TYR:CD2  | 2.47                     | 0.50              |
| 9:DQ:63:PRO:HG2    | 9:DQ:66:SER:HB3    | 1.94                     | 0.50              |
| 11:DS:211:CYS:HB2  | 11:DS:214:CYS:HB2  | 1.94                     | 0.50              |
| 18:DF:27:ARG:NH1   | 57:CA:435:G:O2'    | 2.45                     | 0.50              |
| 20:DH:268:LEU:HB3  | 20:DH:276:ILE:HD11 | 1.92                     | 0.50              |
| 33:CJ:372:GLU:HG3  | 33:CJ:391:HIS:CD2  | 2.46                     | 0.50              |
| 34:CK:53:ARG:HH12  | 47:Cg:488:ARG:NH2  | 2.10                     | 0.50              |
| 47:Cg:224:LEU:HD11 | 47:Cg:241:GLN:C    | 2.35                     | 0.50              |
| 50:Ck:170:VAL:HG13 | 50:Ck:174:LYS:HD2  | 1.92                     | 0.50              |
| 53:Cp:151:ARG:O    | 53:Cp:154:GLN:HG2  | 2.11                     | 0.50              |
| 54:Cq:64:VAL:HG11  | 54:Cq:77:PHE:CD2   | 2.47                     | 0.50              |
| 56:Cv:612:THR:HG22 | 56:Cv:613:LEU:HD22 | 1.94                     | 0.50              |
| 7:DO:106:GLU:H     | 7:DO:106:GLU:CD    | 2.20                     | 0.50              |
| 33:CJ:54:MET:HE1   | 33:CJ:59:PRO:HA    | 1.93                     | 0.50              |
| 38:CP:143:GLU:OE1  | 38:CP:143:GLU:N    | 2.27                     | 0.50              |
| 44:Ca:10:ARG:HB3   | 44:Ca:10:ARG:CZ    | 2.42                     | 0.50              |
| 50:Ck:96:ASN:OD1   | 50:Ck:97:GLN:NE2   | 2.44                     | 0.50              |
| 50:Ck:611:ASN:H    | 50:Ck:611:ASN:ND2  | 2.09                     | 0.50              |
| 57:CA:293:A:H2'    | 57:CA:294:A:C8     | 2.47                     | 0.50              |
| 1:DA:258:TYR:CE2   | 1:DA:259:LEU:HD13  | 2.46                     | 0.50              |
| 7:DO:105:ARG:HE    | 7:DO:147:ARG:CD    | 2.25                     | 0.50              |
| 12:DU:205:ALA:HB1  | 12:DU:206:PRO:HD2  | 1.94                     | 0.50              |
| 13:DZ:73:HIS:HA    | 13:DZ:76:TYR:CE2   | 2.47                     | 0.50              |
| 15:DB:185:GLU:OE2  | 15:DB:207:LYS:HE3  | 2.12                     | 0.50              |
| 15:DB:635:MET:HG3  | 50:Ck:373:ARG:HH11 | 1.77                     | 0.50              |
| 17:DE:145:PRO:HB2  | 20:DH:535:VAL:HG13 | 1.94                     | 0.50              |
| 34:CK:26:ARG:NH1   | 57:CA:465:U:OP1    | 2.44                     | 0.50              |
| 35:CL:17:VAL:HB    | 35:CL:40:ALA:HB1   | 1.93                     | 0.50              |
| 40:CR:320:VAL:HG21 | 42:CU:178:MET:HB3  | 1.94                     | 0.50              |
| 45:Cb:168:ALA:HB2  | 55:Cr:144:ARG:HD3  | 1.93                     | 0.50              |
| 50:Ck:167:PHE:HE2  | 50:Ck:235:GLY:HA2  | 1.76                     | 0.50              |
| 53:Cp:54:PRO:HD2   | 53:Cp:58:THR:HG21  | 1.93                     | 0.50              |
| 56:Cv:35:ARG:HD3   | 56:Cv:37:LEU:HD21  | 1.92                     | 0.50              |
| 56:Cv:813:ARG:HG2  | 56:Cv:926:ILE:HD13 | 1.93                     | 0.50              |
| 1:DA:617:PRO:HG2   | 1:DA:746:GLN:HE22  | 1.77                     | 0.49              |
| 1:DA:717:ASP:O     | 1:DA:721:ILE:HG13  | 2.12                     | 0.49              |
| 2:DD:347:GLU:HG3   | 10:DR:30:TRP:HE1   | 1.77                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:DI:51:VAL:HG13   | 3:DI:182:PHE:HE1    | 1.76                     | 0.49              |
| 7:DO:131:ASP:OD1   | 7:DO:132:ALA:N      | 2.42                     | 0.49              |
| 7:DO:246:MET:HE2   | 56:Cv:208:LYS:HD3   | 1.94                     | 0.49              |
| 9:DQ:77:LEU:HB2    | 9:DQ:115:ILE:HB     | 1.94                     | 0.49              |
| 12:DU:83:ARG:CZ    | 12:DU:157:GLN:HG3   | 2.42                     | 0.49              |
| 16:DC:1082:ARG:NH2 | 23:DT:75:ARG:HD3    | 2.27                     | 0.49              |
| 17:DE:572:VAL:HA   | 17:DE:575:CYS:HB3   | 1.94                     | 0.49              |
| 19:DG:529:ASP:OD1  | 19:DG:529:ASP:N     | 2.44                     | 0.49              |
| 21:DJ:259:PHE:CD1  | 21:DJ:301:HIS:HE1   | 2.30                     | 0.49              |
| 24:DV:31:HIS:H     | 24:DV:83:GLN:NE2    | 2.00                     | 0.49              |
| 25:DW:22:THR:HG21  | 41:CS:149:ASP:O     | 2.12                     | 0.49              |
| 27:DY:49:GLY:HA3   | 47:Cg:103:PRO:HG2   | 1.94                     | 0.49              |
| 33:CJ:555:TRP:HE1  | 33:CJ:581:GLN:HA    | 1.77                     | 0.49              |
| 33:CJ:618:VAL:HG22 | 33:CJ:654:VAL:HG22  | 1.94                     | 0.49              |
| 34:CK:205:TYR:CD2  | 34:CK:221:THR:HG23  | 2.43                     | 0.49              |
| 34:CK:207:VAL:HG13 | 34:CK:219:THR:HA    | 1.92                     | 0.49              |
| 40:CR:265:ARG:HG2  | 40:CR:266:ASN:N     | 2.26                     | 0.49              |
| 48:Ci:34:ARG:NH1   | 48:Ci:43:GLU:OE1    | 2.38                     | 0.49              |
| 49:Cj:227:ASP:O    | 53:Cp:47:ARG:NH2    | 2.44                     | 0.49              |
| 50:Ck:593:ILE:HG23 | 50:Ck:597:LEU:HD12  | 1.93                     | 0.49              |
| 51:Cm:83:LYS:HZ1   | 57:CA:393:U:H5'     | 1.76                     | 0.49              |
| 51:Cm:191:LYS:NZ   | 57:CA:337:U:OP2     | 2.45                     | 0.49              |
| 56:Cv:62:LEU:O     | 56:Cv:99:VAL:HG22   | 2.11                     | 0.49              |
| 56:Cv:1005:TRP:CD1 | 56:Cv:1006:GLU:H    | 2.30                     | 0.49              |
| 5:DM:227:LEU:HD21  | 5:DM:229:ILE:HD11   | 1.94                     | 0.49              |
| 6:DN:280:GLN:HB2   | 29:CE:117:TRP:NE1   | 2.27                     | 0.49              |
| 9:DQ:58:ARG:O      | 12:DU:39:ARG:NH1    | 2.46                     | 0.49              |
| 15:DB:815:ASP:OD2  | 18:DF:555:ARG:HA    | 2.12                     | 0.49              |
| 16:DC:109:PRO:HB3  | 16:DC:1062:GLN:HE21 | 1.76                     | 0.49              |
| 20:DH:171:TRP:HA   | 20:DH:174:LEU:HD22  | 1.93                     | 0.49              |
| 24:DV:137:ARG:O    | 24:DV:138:ASN:HB2   | 2.12                     | 0.49              |
| 33:CJ:293:ASP:HB2  | 33:CJ:296:LEU:H     | 1.77                     | 0.49              |
| 35:CL:25:MET:HG2   | 35:CL:76:LEU:HD11   | 1.94                     | 0.49              |
| 40:CR:137:THR:HG23 | 40:CR:139:THR:H     | 1.77                     | 0.49              |
| 44:Ca:225:PRO:HD2  | 44:Ca:228:LYS:HD2   | 1.94                     | 0.49              |
| 47:Cg:238:ARG:HH21 | 47:Cg:241:GLN:HE22  | 1.59                     | 0.49              |
| 1:DA:939:GLU:HA    | 1:DA:942:LEU:HB2    | 1.92                     | 0.49              |
| 1:DA:1094:VAL:O    | 1:DA:1098:LEU:HB2   | 2.12                     | 0.49              |
| 2:DD:665:GLU:HG3   | 44:Ca:426:ILE:O     | 2.12                     | 0.49              |
| 2:DD:696:ALA:HB2   | 44:Ca:456:LEU:HD11  | 1.95                     | 0.49              |
| 3:DI:284:CYS:SG    | 7:DO:238:ASN:ND2    | 2.85                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:DN:48:LEU:HD22   | 6:DN:52:TRP:CZ3    | 2.47                     | 0.49              |
| 16:DC:612:TRP:CZ2  | 16:DC:618:ARG:HB2  | 2.47                     | 0.49              |
| 18:DF:262:PHE:O    | 21:DJ:90:ARG:NH2   | 2.43                     | 0.49              |
| 19:DG:483:THR:HA   | 19:DG:565:CYS:HB2  | 1.94                     | 0.49              |
| 22:DK:2:SER:HA     | 23:DT:133:ASP:OD2  | 2.12                     | 0.49              |
| 24:DV:71:GLN:HG2   | 24:DV:72:GLY:N     | 2.26                     | 0.49              |
| 28:CC:25:HIS:CD2   | 28:CC:27:PHE:HB2   | 2.47                     | 0.49              |
| 33:CJ:32:ALA:HB1   | 33:CJ:33:PRO:HD2   | 1.93                     | 0.49              |
| 33:CJ:758:TRP:CG   | 33:CJ:759:PRO:HA   | 2.47                     | 0.49              |
| 52:Cn:152:PHE:O    | 52:Cn:152:PHE:CG   | 2.64                     | 0.49              |
| 56:Cv:305:ASP:OD2  | 56:Cv:413:LYS:HE3  | 2.12                     | 0.49              |
| 1:DA:502:LYS:NZ    | 1:DA:502:LYS:HB3   | 2.27                     | 0.49              |
| 5:DM:21:ARG:HB3    | 5:DM:236:MET:HE2   | 1.94                     | 0.49              |
| 8:DP:61:PRO:HG2    | 8:DP:64:MET:SD     | 2.52                     | 0.49              |
| 9:DQ:35:VAL:HG12   | 9:DQ:36:GLU:HG3    | 1.93                     | 0.49              |
| 11:DS:31:MET:HG3   | 57:CA:207:A:H5'    | 1.95                     | 0.49              |
| 16:DC:158:TYR:HB2  | 16:DC:168:PHE:CZ   | 2.48                     | 0.49              |
| 18:DF:112:ARG:O    | 36:CN:37:ARG:HA    | 2.13                     | 0.49              |
| 25:DW:64:TYR:HB2   | 47:Cg:376:ASP:O    | 2.12                     | 0.49              |
| 35:CL:57:CYS:HA    | 44:Ca:14:ASN:HB3   | 1.95                     | 0.49              |
| 37:CO:379:ARG:HH11 | 37:CO:379:ARG:HG3  | 1.77                     | 0.49              |
| 51:Cm:56:ASN:HD21  | 51:Cm:62:ALA:HB2   | 1.78                     | 0.49              |
| 56:Cv:577:PHE:HD2  | 56:Cv:792:TYR:CE2  | 2.30                     | 0.49              |
| 57:CA:233:C:H4'    | 57:CA:234:C:C5'    | 2.42                     | 0.49              |
| 1:DA:760:ILE:HD13  | 1:DA:765:LEU:HA    | 1.95                     | 0.49              |
| 2:DD:115:GLU:O     | 31:CH:53:ARG:NH2   | 2.46                     | 0.49              |
| 9:DQ:218:ARG:HD2   | 9:DQ:223:ASP:OD1   | 2.12                     | 0.49              |
| 16:DC:381:LEU:O    | 16:DC:385:THR:OG1  | 2.21                     | 0.49              |
| 19:DG:143:HIS:HD2  | 45:Cb:198:HIS:CE1  | 2.30                     | 0.49              |
| 19:DG:335:GLU:HB2  | 19:DG:387:ARG:HH11 | 1.78                     | 0.49              |
| 32:CI:240:ASN:N    | 32:CI:240:ASN:OD1  | 2.45                     | 0.49              |
| 33:CJ:428:SER:HA   | 50:Ck:682:ASN:HD21 | 1.77                     | 0.49              |
| 33:CJ:798:GLN:HA   | 33:CJ:805:HIS:HB2  | 1.94                     | 0.49              |
| 35:CL:28:ARG:NH1   | 57:CA:575:U:OP1    | 2.44                     | 0.49              |
| 38:CP:184:VAL:C    | 38:CP:188:LEU:HB3  | 2.37                     | 0.49              |
| 44:Ca:51:MET:HE3   | 56:Cv:1127:HIS:HE1 | 1.77                     | 0.49              |
| 50:Ck:282:VAL:O    | 50:Ck:286:GLU:HG3  | 2.12                     | 0.49              |
| 56:Cv:318:PHE:HE1  | 56:Cv:887:ARG:HB2  | 1.78                     | 0.49              |
| 56:Cv:1084:GLU:H   | 56:Cv:1084:GLU:CD  | 2.20                     | 0.49              |
| 56:Cv:1114:ASP:OD1 | 56:Cv:1117:TYR:N   | 2.32                     | 0.49              |
| 1:DA:647:ARG:HG2   | 1:DA:731:ALA:HB3   | 1.95                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:DA:854:LYS:HE2    | 44:Ca:264:ARG:HG2   | 1.93                     | 0.49              |
| 2:DD:70:SER:O       | 11:DS:28:TYR:OH     | 2.27                     | 0.49              |
| 7:DO:59:ALA:HA      | 7:DO:62:LEU:HD23    | 1.95                     | 0.49              |
| 13:DZ:27:MET:HE1    | 44:Ca:209:MET:HB3   | 1.94                     | 0.49              |
| 16:DC:771:PRO:HG3   | 16:DC:896:SER:HB2   | 1.95                     | 0.49              |
| 28:CC:54:ILE:HD12   | 33:CJ:29:PRO:HG3    | 1.95                     | 0.49              |
| 29:CE:222:VAL:HG21  | 29:CE:267:HIS:HB3   | 1.95                     | 0.49              |
| 33:CJ:792:HIS:CD2   | 33:CJ:795:LYS:HB2   | 2.48                     | 0.49              |
| 38:CP:96:ILE:HD11   | 44:Ca:470:ARG:NH2   | 2.27                     | 0.49              |
| 44:Ca:121:ALA:HB2   | 56:Cv:1054:VAL:HG13 | 1.94                     | 0.49              |
| 45:Cb:175:ILE:H     | 54:Cq:116:ASP:HA    | 1.77                     | 0.49              |
| 55:Cr:86:LEU:HG     | 55:Cr:90:ILE:HD12   | 1.94                     | 0.49              |
| 56:Cv:311:LEU:HD22  | 56:Cv:389:LEU:HD23  | 1.93                     | 0.49              |
| 1:DA:1060:LEU:O     | 54:Cq:140:ARG:NE    | 2.37                     | 0.49              |
| 2:DD:52:LYS:NZ      | 57:CA:138:U:O4      | 2.46                     | 0.49              |
| 7:DO:274:LYS:HG2    | 56:Cv:693:ILE:HD13  | 1.94                     | 0.49              |
| 9:DQ:35:VAL:HG21    | 10:DR:13:PHE:HB3    | 1.93                     | 0.49              |
| 18:DF:452:VAL:HG12  | 18:DF:453:MET:HE2   | 1.95                     | 0.49              |
| 20:DH:253:SER:HA    | 20:DH:258:MET:HE1   | 1.93                     | 0.49              |
| 21:DJ:22:MET:SD     | 28:CC:67:ASN:HB2    | 2.52                     | 0.49              |
| 24:DV:99:TRP:CE2    | 33:CJ:771:PRO:HG2   | 2.48                     | 0.49              |
| 33:CJ:253:TRP:O     | 33:CJ:256:HIS:HB2   | 2.12                     | 0.49              |
| 52:Cn:226:LEU:O     | 52:Cn:230:VAL:HG23  | 2.12                     | 0.49              |
| 55:Cr:9:LEU:HG      | 55:Cr:100:TYR:CG    | 2.47                     | 0.49              |
| 56:Cv:175:ARG:HB3   | 56:Cv:176:PRO:HD2   | 1.95                     | 0.49              |
| 57:CA:593:A:H2'     | 57:CA:594:U:C6      | 2.48                     | 0.49              |
| 1:DA:424:LEU:HD21   | 1:DA:438:ALA:HA     | 1.95                     | 0.49              |
| 1:DA:492:ASN:HD22   | 1:DA:495:GLU:HB2    | 1.78                     | 0.49              |
| 1:DA:779:LEU:O      | 1:DA:812:PRO:HD3    | 2.13                     | 0.49              |
| 1:DA:886:ALA:HA     | 6:DN:207:VAL:HG21   | 1.95                     | 0.49              |
| 7:DO:114:GLY:H      | 56:Cv:780:PRO:HG3   | 1.78                     | 0.49              |
| 9:DQ:185:ARG:HH21   | 9:DQ:204:TYR:HB2    | 1.77                     | 0.49              |
| 11:DS:128:SER:C     | 11:DS:130:VAL:H     | 2.21                     | 0.49              |
| 15:DB:453:GLU:HB3   | 17:DE:712:MET:HE1   | 1.94                     | 0.49              |
| 15:DB:1121:VAL:HG21 | 41:CS:84:LEU:HD11   | 1.94                     | 0.49              |
| 16:DC:295:VAL:HG21  | 16:DC:367:MET:HE3   | 1.95                     | 0.49              |
| 16:DC:708:TYR:CE1   | 22:DK:166:ALA:HA    | 2.48                     | 0.49              |
| 17:DE:317:GLU:HG2   | 17:DE:318:PRO:HD2   | 1.93                     | 0.49              |
| 18:DF:8:SER:O       | 48:Ci:160:SER:HB3   | 2.12                     | 0.49              |
| 24:DV:103:ASP:OD1   | 24:DV:103:ASP:N     | 2.46                     | 0.49              |
| 30:CF:9:VAL:HG12    | 30:CF:90:LEU:HB2    | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:CF:15:ARG:HH11  | 30:CF:15:ARG:HG3   | 1.78                     | 0.49              |
| 34:CK:53:ARG:HB2   | 34:CK:53:ARG:CZ    | 2.42                     | 0.49              |
| 34:CK:281:VAL:H    | 34:CK:309:ASP:HA   | 1.78                     | 0.49              |
| 34:CK:316:ASN:OD1  | 34:CK:317:GLY:N    | 2.46                     | 0.49              |
| 37:CO:112:LYS:HB2  | 37:CO:112:LYS:HZ3  | 1.78                     | 0.49              |
| 37:CO:261:HIS:O    | 37:CO:265:ARG:HG3  | 2.12                     | 0.49              |
| 40:CR:103:PHE:CD2  | 40:CR:196:PRO:HB3  | 2.48                     | 0.49              |
| 40:CR:271:MET:HE3  | 40:CR:272:GLU:H    | 1.77                     | 0.49              |
| 43:CZ:278:THR:HG22 | 43:CZ:279:SER:OG   | 2.13                     | 0.49              |
| 44:Ca:272:PHE:O    | 44:Ca:276:SER:OG   | 2.22                     | 0.49              |
| 47:Cg:139:THR:HG22 | 47:Cg:145:PHE:CZ   | 2.47                     | 0.49              |
| 50:Ck:218:ILE:HD12 | 50:Ck:243:LYS:HG3  | 1.95                     | 0.49              |
| 51:Cm:146:TRP:CD1  | 51:Cm:150:ASN:HD22 | 2.30                     | 0.49              |
| 53:Cp:135:THR:HG22 | 53:Cp:138:TYR:H    | 1.78                     | 0.49              |
| 55:Cr:10:ARG:O     | 55:Cr:10:ARG:HD3   | 2.12                     | 0.49              |
| 56:Cv:581:HIS:ND1  | 61:UR:8:UNK:O      | 2.46                     | 0.49              |
| 57:CA:52:C:H5''    | 57:CA:53:A:C8      | 2.48                     | 0.49              |
| 2:DD:693:ASP:OD1   | 2:DD:694:ARG:N     | 2.46                     | 0.49              |
| 6:DN:45:ARG:HB3    | 6:DN:132:TYR:CE2   | 2.48                     | 0.49              |
| 10:DR:27:LYS:HB2   | 12:DU:97:ARG:NE    | 2.28                     | 0.49              |
| 12:DU:207:ARG:HA   | 57:CA:160:U:C5     | 2.47                     | 0.49              |
| 15:DB:285:MET:HE2  | 50:Ck:36:ARG:HH21  | 1.78                     | 0.49              |
| 15:DB:511:ARG:HH11 | 15:DB:511:ARG:HG3  | 1.78                     | 0.49              |
| 19:DG:102:MET:HE1  | 19:DG:134:PRO:HA   | 1.95                     | 0.49              |
| 19:DG:155:GLU:HG2  | 50:Ck:414:MET:HG3  | 1.95                     | 0.49              |
| 19:DG:624:ARG:NH2  | 32:CI:33:SER:HB2   | 2.27                     | 0.49              |
| 29:CE:66:ASP:OD2   | 29:CE:69:GLU:HB2   | 2.13                     | 0.49              |
| 32:CI:100:PRO:O    | 45:Cb:103:ARG:NH1  | 2.44                     | 0.49              |
| 36:CN:37:ARG:NH1   | 36:CN:38:ASP:OD2   | 2.43                     | 0.49              |
| 44:Ca:233:ARG:NH1  | 44:Ca:233:ARG:HB3  | 2.28                     | 0.49              |
| 44:Ca:461:LEU:HD22 | 44:Ca:488:MET:HE2  | 1.95                     | 0.49              |
| 45:Cb:12:PRO:HG2   | 45:Cb:15:MET:CG    | 2.43                     | 0.49              |
| 57:CA:414:A:O2'    | 57:CA:484:A:OP1    | 2.29                     | 0.49              |
| 4:DL:84:GLU:OE1    | 4:DL:209:ARG:NH1   | 2.46                     | 0.49              |
| 20:DH:246:GLU:HG2  | 20:DH:280:SER:HB3  | 1.94                     | 0.49              |
| 31:CH:142:ARG:HH22 | 56:Cv:74:ASN:ND2   | 2.10                     | 0.49              |
| 32:CI:325:GLU:OE2  | 33:CJ:178:SER:HB2  | 2.13                     | 0.49              |
| 33:CJ:246:LYS:HB2  | 33:CJ:432:HIS:HB2  | 1.95                     | 0.49              |
| 50:Ck:343:GLU:HG3  | 50:Ck:589:GLN:HE22 | 1.76                     | 0.49              |
| 2:DD:154:ILE:HG22  | 2:DD:156:GLN:H     | 1.77                     | 0.48              |
| 2:DD:238:GLU:OE1   | 2:DD:238:GLU:N     | 2.41                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:DI:51:VAL:HG13   | 3:DI:182:PHE:CE1   | 2.47                     | 0.48              |
| 15:DB:885:PHE:HE2  | 15:DB:929:MET:HE2  | 1.78                     | 0.48              |
| 18:DF:389:PRO:HB2  | 18:DF:393:ARG:NH2  | 2.28                     | 0.48              |
| 21:DJ:22:MET:CG    | 28:CC:67:ASN:HB2   | 2.40                     | 0.48              |
| 23:DT:9:GLN:O      | 57:CA:438:U:N3     | 2.36                     | 0.48              |
| 35:CL:43:TYR:HE1   | 62:US:35:UNK:HA    | 1.78                     | 0.48              |
| 38:CP:32:ARG:HH12  | 38:CP:52:LYS:HD3   | 1.76                     | 0.48              |
| 41:CS:59:LYS:HE3   | 57:CA:411:A:OP1    | 2.13                     | 0.48              |
| 41:CS:70:TYR:CE1   | 57:CA:505:U:H2'    | 2.48                     | 0.48              |
| 42:CU:189:ARG:HH11 | 42:CU:189:ARG:HG3  | 1.77                     | 0.48              |
| 44:Ca:509:TRP:HA   | 44:Ca:514:THR:OG1  | 2.13                     | 0.48              |
| 44:Ca:548:GLU:OE1  | 44:Ca:548:GLU:N    | 2.45                     | 0.48              |
| 46:Cd:102:ARG:HG3  | 46:Cd:103:ILE:N    | 2.26                     | 0.48              |
| 47:Cg:84:GLU:N     | 47:Cg:84:GLU:CD    | 2.71                     | 0.48              |
| 50:Ck:113:ASN:O    | 50:Ck:140:ARG:NH2  | 2.46                     | 0.48              |
| 50:Ck:395:MET:HE1  | 50:Ck:567:LYS:HD2  | 1.95                     | 0.48              |
| 57:CA:309:A:H2'    | 57:CA:309:A:N3     | 2.28                     | 0.48              |
| 1:DA:481:TYR:CD1   | 1:DA:496:VAL:HG21  | 2.48                     | 0.48              |
| 5:DM:104:LYS:O     | 5:DM:107:GLU:HG2   | 2.13                     | 0.48              |
| 6:DN:217:MET:HG3   | 44:Ca:263:VAL:HG13 | 1.94                     | 0.48              |
| 9:DQ:142:PHE:HB3   | 9:DQ:267:LEU:HD21  | 1.95                     | 0.48              |
| 9:DQ:185:ARG:HD3   | 9:DQ:196:LEU:HD13  | 1.95                     | 0.48              |
| 14:Da:53:ARG:HB2   | 14:Da:54:TRP:CZ3   | 2.48                     | 0.48              |
| 15:DB:303:PRO:O    | 17:DE:489:ARG:NH2  | 2.45                     | 0.48              |
| 16:DC:104:PRO:HG2  | 16:DC:112:TYR:CE1  | 2.48                     | 0.48              |
| 17:DE:301:TYR:O    | 17:DE:437:LYS:NZ   | 2.46                     | 0.48              |
| 27:DY:14:THR:HG21  | 57:CA:501:A:OP2    | 2.13                     | 0.48              |
| 39:CQ:49:ASN:ND2   | 57:CA:566:U:OP1    | 2.43                     | 0.48              |
| 54:Cq:25:PHE:O     | 54:Cq:27:PRO:HD3   | 2.12                     | 0.48              |
| 1:DA:1417:PHE:C    | 1:DA:1419:GLY:H    | 2.22                     | 0.48              |
| 2:DD:20:PHE:CD2    | 29:CE:225:LEU:HB2  | 2.48                     | 0.48              |
| 9:DQ:167:ARG:HH11  | 37:CO:344:SER:HB2  | 1.76                     | 0.48              |
| 11:DS:201:HIS:HB2  | 53:Cp:41:ILE:O     | 2.13                     | 0.48              |
| 13:DZ:20:ARG:HD2   | 44:Ca:172:PHE:CD2  | 2.48                     | 0.48              |
| 16:DC:203:MET:HB3  | 16:DC:504:TYR:HD1  | 1.79                     | 0.48              |
| 16:DC:327:GLU:O    | 16:DC:330:ARG:HB3  | 2.13                     | 0.48              |
| 16:DC:801:HIS:HB3  | 16:DC:804:TYR:HD2  | 1.78                     | 0.48              |
| 31:CH:138:LYS:NZ   | 31:CH:138:LYS:HB2  | 2.28                     | 0.48              |
| 32:CI:32:LYS:O     | 32:CI:37:ARG:NH2   | 2.46                     | 0.48              |
| 33:CJ:37:ASN:ND2   | 51:Cm:49:GLY:O     | 2.46                     | 0.48              |
| 33:CJ:257:VAL:HG13 | 33:CJ:399:ARG:HB2  | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:322:PHE:CE1  | 50:Ck:642:VAL:HG22 | 2.48                     | 0.48              |
| 34:CK:200:ARG:NH2  | 42:CU:20:MET:O     | 2.46                     | 0.48              |
| 37:CO:75:LEU:HD11  | 52:Cn:230:VAL:HG22 | 1.93                     | 0.48              |
| 44:Ca:451:VAL:HA   | 44:Ca:460:GLU:OE2  | 2.12                     | 0.48              |
| 46:Cd:13:ARG:NH2   | 46:Cd:26:ARG:HE    | 2.11                     | 0.48              |
| 46:Cd:13:ARG:NH1   | 53:Cp:126:GLU:OE2  | 2.35                     | 0.48              |
| 50:Ck:156:LEU:HD11 | 50:Ck:244:ARG:HB3  | 1.94                     | 0.48              |
| 53:Cp:53:VAL:HG11  | 53:Cp:59:PHE:CD1   | 2.43                     | 0.48              |
| 53:Cp:80:ASP:OD2   | 53:Cp:82:ASN:N     | 2.46                     | 0.48              |
| 57:CA:282:A:C6     | 57:CA:283:U:O4     | 2.66                     | 0.48              |
| 1:DA:213:LEU:HD23  | 1:DA:271:LEU:HD13  | 1.96                     | 0.48              |
| 1:DA:824:GLU:OE1   | 1:DA:824:GLU:N     | 2.46                     | 0.48              |
| 1:DA:1382:SER:HA   | 1:DA:1389:VAL:HG21 | 1.95                     | 0.48              |
| 6:DN:17:MET:HE1    | 6:DN:162:LEU:HD11  | 1.94                     | 0.48              |
| 9:DQ:142:PHE:CE2   | 9:DQ:246:VAL:HG21  | 2.48                     | 0.48              |
| 11:DS:111:VAL:HG12 | 11:DS:117:ALA:HB2  | 1.94                     | 0.48              |
| 12:DU:141:LEU:HB3  | 12:DU:150:TYR:HE2  | 1.77                     | 0.48              |
| 14:Da:36:SER:O     | 14:Da:40:ARG:HG2   | 2.13                     | 0.48              |
| 16:DC:45:LEU:HG    | 23:DT:75:ARG:NH2   | 2.28                     | 0.48              |
| 17:DE:147:MET:HE1  | 17:DE:567:HIS:CE1  | 2.49                     | 0.48              |
| 18:DF:505:LYS:HG2  | 18:DF:517:VAL:HB   | 1.95                     | 0.48              |
| 21:DJ:101:ILE:HG23 | 21:DJ:139:LEU:HD11 | 1.95                     | 0.48              |
| 25:DW:79:LEU:HD13  | 47:Cg:89:PHE:O     | 2.13                     | 0.48              |
| 32:CI:313:ASP:HA   | 32:CI:421:ARG:O    | 2.13                     | 0.48              |
| 33:CJ:489:TRP:HA   | 33:CJ:513:ILE:HD11 | 1.94                     | 0.48              |
| 34:CK:320:MET:N    | 42:CU:81:GLU:HG2   | 2.28                     | 0.48              |
| 35:CL:19:PHE:HB2   | 35:CL:66:PHE:CE1   | 2.48                     | 0.48              |
| 49:Cj:141:GLY:C    | 49:Cj:143:LYS:H    | 2.20                     | 0.48              |
| 2:DD:438:ILE:HD11  | 2:DD:461:ILE:HG12  | 1.94                     | 0.48              |
| 11:DS:34:SER:HA    | 11:DS:39:ARG:HB3   | 1.96                     | 0.48              |
| 17:DE:204:VAL:HG13 | 17:DE:208:LYS:HE2  | 1.94                     | 0.48              |
| 24:DV:127:THR:HG23 | 50:Ck:742:GLY:HA2  | 1.94                     | 0.48              |
| 30:CF:75:GLU:CD    | 30:CF:75:GLU:H     | 2.20                     | 0.48              |
| 40:CR:119:GLU:OE1  | 40:CR:119:GLU:N    | 2.30                     | 0.48              |
| 47:Cg:427:TRP:CE2  | 47:Cg:434:SER:HB3  | 2.48                     | 0.48              |
| 51:Cm:164:HIS:HB3  | 57:CA:611:U:H5"    | 1.96                     | 0.48              |
| 1:DA:253:ASP:OD1   | 1:DA:253:ASP:N     | 2.42                     | 0.48              |
| 2:DD:66:TRP:CE2    | 38:CP:66:LYS:HD3   | 2.49                     | 0.48              |
| 3:DI:236:LEU:HG    | 3:DI:240:MET:HE2   | 1.96                     | 0.48              |
| 5:DM:169:ALA:HB2   | 29:CE:343:TYR:CE2  | 2.48                     | 0.48              |
| 7:DO:105:ARG:HH21  | 7:DO:147:ARG:HG2   | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:DU:90:VAL:HG12  | 12:DU:211:ARG:N    | 2.27                     | 0.48              |
| 20:DH:140:ILE:HD12 | 20:DH:156:LEU:HG   | 1.94                     | 0.48              |
| 20:DH:405:ARG:NE   | 21:DJ:48:PHE:HB3   | 2.29                     | 0.48              |
| 21:DJ:86:LEU:HD13  | 21:DJ:123:LYS:HB3  | 1.95                     | 0.48              |
| 30:CF:22:LEU:HD11  | 30:CF:65:ILE:HD13  | 1.95                     | 0.48              |
| 32:CI:89:ARG:HE    | 40:CR:193:ASN:HD21 | 1.60                     | 0.48              |
| 33:CJ:724:THR:HG21 | 47:Cg:302:PRO:HG3  | 1.94                     | 0.48              |
| 39:CQ:182:VAL:HG12 | 39:CQ:183:PRO:HD2  | 1.96                     | 0.48              |
| 46:Cd:63:ARG:HG3   | 46:Cd:64:GLN:N     | 2.28                     | 0.48              |
| 49:Cj:107:ALA:HB2  | 49:Cj:173:MET:HE1  | 1.96                     | 0.48              |
| 50:Ck:253:TYR:OH   | 50:Ck:257:ARG:NH1  | 2.46                     | 0.48              |
| 55:Cr:65:LYS:NZ    | 55:Cr:65:LYS:HB2   | 2.29                     | 0.48              |
| 56:Cv:428:CYS:O    | 56:Cv:489:THR:OG1  | 2.27                     | 0.48              |
| 57:CA:263:A:O2'    | 57:CA:264:A:H8     | 1.95                     | 0.48              |
| 1:DA:103:ARG:HD2   | 31:CH:231:GLU:HG3  | 1.94                     | 0.48              |
| 1:DA:1077:ARG:NH2  | 1:DA:1085:GLU:OE1  | 2.46                     | 0.48              |
| 2:DD:93:PRO:HA     | 39:CQ:12:TRP:CE2   | 2.49                     | 0.48              |
| 11:DS:93:ARG:HB3   | 11:DS:106:ARG:HD2  | 1.96                     | 0.48              |
| 18:DF:23:ARG:NH1   | 23:DT:236:GLU:O    | 2.45                     | 0.48              |
| 18:DF:372:ASN:OD1  | 18:DF:372:ASN:N    | 2.44                     | 0.48              |
| 20:DH:342:ILE:O    | 20:DH:345:VAL:HG22 | 2.14                     | 0.48              |
| 24:DV:177:MET:HB3  | 24:DV:183:LEU:HD22 | 1.95                     | 0.48              |
| 33:CJ:713:PRO:HB3  | 57:CA:507:A:C2     | 2.49                     | 0.48              |
| 39:CQ:69:GLN:OE1   | 57:CA:96:U:H5'     | 2.13                     | 0.48              |
| 44:Ca:76:GLN:HG3   | 56:Cv:1120:TRP:HZ2 | 1.79                     | 0.48              |
| 1:DA:602:LEU:HB3   | 1:DA:803:LEU:HB2   | 1.95                     | 0.48              |
| 1:DA:1565:ARG:HH21 | 1:DA:1592:GLY:HA3  | 1.79                     | 0.48              |
| 2:DD:458:LEU:HD23  | 2:DD:504:ASN:ND2   | 2.29                     | 0.48              |
| 11:DS:238:ARG:HG3  | 11:DS:239:SER:H    | 1.79                     | 0.48              |
| 15:DB:98:ASP:O     | 15:DB:103:TYR:N    | 2.46                     | 0.48              |
| 15:DB:688:VAL:HG13 | 17:DE:657:VAL:HG13 | 1.96                     | 0.48              |
| 17:DE:467:MET:HE1  | 17:DE:486:ILE:HD13 | 1.94                     | 0.48              |
| 17:DE:597:PHE:O    | 17:DE:601:ILE:HG22 | 2.14                     | 0.48              |
| 17:DE:649:TYR:CD2  | 17:DE:721:ASP:HB2  | 2.49                     | 0.48              |
| 18:DF:56:TYR:CE1   | 57:CA:485:U:H5'    | 2.49                     | 0.48              |
| 18:DF:57:ARG:HH11  | 18:DF:57:ARG:CG    | 2.23                     | 0.48              |
| 26:DX:57:ARG:HH22  | 41:CS:64:MET:HG3   | 1.77                     | 0.48              |
| 29:CE:304:LEU:O    | 44:Ca:368:ARG:HD3  | 2.13                     | 0.48              |
| 44:Ca:102:TRP:CZ3  | 44:Ca:159:LEU:HD22 | 2.48                     | 0.48              |
| 46:Cd:283:GLU:HB2  | 46:Cd:287:GLU:OE2  | 2.13                     | 0.48              |
| 51:Cm:162:ARG:HG3  | 51:Cm:165:ASP:OD2  | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:95:THR:O      | 2:DD:269:LYS:NZ    | 2.47                     | 0.48              |
| 1:DA:779:LEU:HD11  | 1:DA:922:ASN:HB2   | 1.96                     | 0.48              |
| 8:DP:101:PHE:O     | 49:Cj:139:ARG:HD2  | 2.14                     | 0.48              |
| 12:DU:90:VAL:HG12  | 12:DU:211:ARG:H    | 1.79                     | 0.48              |
| 27:DY:61:ILE:HD11  | 27:DY:98:ILE:HD12  | 1.95                     | 0.48              |
| 29:CE:116:GLN:HA   | 29:CE:122:TRP:CG   | 2.49                     | 0.48              |
| 33:CJ:406:PRO:O    | 50:Ck:655:ARG:NH1  | 2.46                     | 0.48              |
| 37:CO:253:ALA:O    | 37:CO:257:ARG:HG3  | 2.12                     | 0.48              |
| 45:Cb:56:ARG:HH11  | 45:Cb:57:MET:HE1   | 1.76                     | 0.48              |
| 47:Cg:23:THR:O     | 47:Cg:26:CYS:HB2   | 2.13                     | 0.48              |
| 47:Cg:414:ARG:HH11 | 47:Cg:418:ASN:HD21 | 1.61                     | 0.48              |
| 50:Ck:35:ASP:OD2   | 50:Ck:35:ASP:N     | 2.47                     | 0.48              |
| 56:Cv:47:GLN:OE1   | 56:Cv:47:GLN:N     | 2.41                     | 0.48              |
| 56:Cv:112:ILE:HD11 | 56:Cv:150:LEU:HB3  | 1.96                     | 0.48              |
| 1:DA:853:LYS:HZ1   | 56:Cv:1005:TRP:CG  | 2.32                     | 0.48              |
| 2:DD:13:GLY:O      | 52:Cn:155:ARG:NH2  | 2.47                     | 0.48              |
| 4:DL:119:MET:HE3   | 4:DL:153:ALA:HB2   | 1.95                     | 0.48              |
| 4:DL:163:PHE:O     | 4:DL:167:GLU:HG2   | 2.12                     | 0.48              |
| 5:DM:186:TRP:O     | 5:DM:192:GLY:HA3   | 2.14                     | 0.48              |
| 16:DC:874:THR:OG1  | 16:DC:878:ASP:HB2  | 2.13                     | 0.48              |
| 17:DE:729:ARG:NH2  | 50:Ck:78:PRO:HA    | 2.29                     | 0.48              |
| 19:DG:186:ARG:C    | 19:DG:186:ARG:HD3  | 2.39                     | 0.48              |
| 21:DJ:192:THR:HG22 | 21:DJ:226:VAL:HG21 | 1.95                     | 0.48              |
| 23:DT:87:ARG:HD2   | 23:DT:93:MET:HB3   | 1.95                     | 0.48              |
| 30:CF:119:ASP:O    | 30:CF:123:ARG:HD3  | 2.14                     | 0.48              |
| 31:CH:60:LEU:HD23  | 31:CH:60:LEU:HA    | 1.76                     | 0.48              |
| 33:CJ:583:LYS:HZ3  | 33:CJ:597:LEU:HD11 | 1.78                     | 0.48              |
| 37:CO:207:TYR:HB3  | 37:CO:226:VAL:HG11 | 1.96                     | 0.48              |
| 38:CP:49:HIS:HD2   | 38:CP:59:ARG:HG2   | 1.77                     | 0.48              |
| 55:Cr:125:GLN:HE22 | 55:Cr:161:ARG:HA   | 1.78                     | 0.48              |
| 1:DA:47:LEU:HD23   | 1:DA:52:MET:HB3    | 1.95                     | 0.47              |
| 1:DA:82:ILE:HG21   | 2:DD:48:MET:HE3    | 1.96                     | 0.47              |
| 1:DA:287:HIS:HD2   | 1:DA:290:TYR:CD1   | 2.32                     | 0.47              |
| 2:DD:94:LYS:HE3    | 2:DD:99:THR:O      | 2.13                     | 0.47              |
| 10:DR:142:GLY:HA2  | 10:DR:173:ASN:ND2  | 2.29                     | 0.47              |
| 15:DB:433:ARG:HA   | 15:DB:442:LEU:HD21 | 1.96                     | 0.47              |
| 16:DC:77:ASP:H     | 16:DC:81:HIS:HD2   | 1.62                     | 0.47              |
| 24:DV:32:PRO:HG3   | 24:DV:52:ARG:NH1   | 2.29                     | 0.47              |
| 24:DV:110:PRO:HB3  | 48:Ci:27:CYS:HB3   | 1.96                     | 0.47              |
| 25:DW:121:HIS:HD2  | 25:DW:123:ALA:H    | 1.62                     | 0.47              |
| 29:CE:156:PRO:HG2  | 40:CR:307:ARG:NE   | 2.28                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:CI:439:ARG:NH1  | 57:CA:496:U:O4     | 2.47                     | 0.47              |
| 34:CK:215:ARG:NH1  | 34:CK:218:ASN:HA   | 2.29                     | 0.47              |
| 37:CO:359:HIS:CE1  | 37:CO:366:ARG:HH12 | 2.32                     | 0.47              |
| 44:Ca:51:MET:HE3   | 56:Cv:1127:HIS:CE1 | 2.49                     | 0.47              |
| 44:Ca:457:LYS:HD2  | 44:Ca:492:TYR:CG   | 2.49                     | 0.47              |
| 47:Cg:329:PRO:HG2  | 47:Cg:332:ARG:HG2  | 1.94                     | 0.47              |
| 48:CI:19:HIS:CG    | 48:CI:20:PRO:HD2   | 2.49                     | 0.47              |
| 49:Cj:102:GLN:HE21 | 49:Cj:142:ASN:ND2  | 2.13                     | 0.47              |
| 54:Cq:104:HIS:HB3  | 54:Cq:108:THR:OG1  | 2.13                     | 0.47              |
| 56:Cv:207:PHE:C    | 56:Cv:208:LYS:HG2  | 2.39                     | 0.47              |
| 1:DA:512:GLU:OE1   | 1:DA:512:GLU:N     | 2.42                     | 0.47              |
| 1:DA:1203:CYS:HB3  | 15:DB:994:THR:HG23 | 1.96                     | 0.47              |
| 3:DI:307:ASN:OD1   | 46:Cd:107:GLN:HG2  | 2.14                     | 0.47              |
| 6:DN:17:MET:HB3    | 6:DN:17:MET:HE3    | 1.71                     | 0.47              |
| 15:DB:745:ASP:OD1  | 15:DB:754:VAL:HG13 | 2.15                     | 0.47              |
| 15:DB:800:GLN:HA   | 15:DB:805:GLU:O    | 2.14                     | 0.47              |
| 16:DC:475:LEU:HB2  | 16:DC:476:PHE:CD2  | 2.49                     | 0.47              |
| 17:DE:725:PRO:HG2  | 22:DK:146:TYR:CZ   | 2.49                     | 0.47              |
| 23:DT:14:THR:HG21  | 57:CA:438:U:O2     | 2.13                     | 0.47              |
| 26:DX:164:THR:HG22 | 26:DX:167:HIS:HB2  | 1.96                     | 0.47              |
| 28:CC:38:PHE:HB2   | 28:CC:77:THR:O     | 2.13                     | 0.47              |
| 33:CJ:99:PHE:H     | 33:CJ:105:ASN:ND2  | 2.13                     | 0.47              |
| 44:Ca:98:PRO:HB2   | 44:Ca:174:ASP:OD2  | 2.13                     | 0.47              |
| 47:Cg:93:LEU:HD12  | 47:Cg:98:PHE:HD1   | 1.78                     | 0.47              |
| 51:Cm:72:SER:HB3   | 51:Cm:155:HIS:CD2  | 2.50                     | 0.47              |
| 52:Cn:203:MET:HA   | 52:Cn:203:MET:HE2  | 1.96                     | 0.47              |
| 52:Cn:236:LYS:H    | 52:Cn:245:LYS:NZ   | 2.01                     | 0.47              |
| 53:Cp:138:TYR:CE2  | 57:CA:45:G:H5"     | 2.48                     | 0.47              |
| 56:Cv:236:GLN:HA   | 56:Cv:260:MET:HE1  | 1.95                     | 0.47              |
| 1:DA:469:ALA:N     | 56:Cv:1071:ARG:NH1 | 2.62                     | 0.47              |
| 1:DA:1510:GLU:OE1  | 1:DA:1510:GLU:N    | 2.43                     | 0.47              |
| 11:DS:142:GLN:O    | 11:DS:145:PRO:HD3  | 2.15                     | 0.47              |
| 17:DE:254:VAL:HG11 | 17:DE:413:GLU:HG2  | 1.95                     | 0.47              |
| 18:DF:268:GLY:HA3  | 18:DF:312:TRP:CG   | 2.49                     | 0.47              |
| 20:DH:131:LEU:HA   | 20:DH:131:LEU:HD23 | 1.66                     | 0.47              |
| 23:DT:29:TRP:CH2   | 48:CI:130:PRO:HG3  | 2.49                     | 0.47              |
| 29:CE:22:ARG:NH2   | 29:CE:240:ASP:HB3  | 2.27                     | 0.47              |
| 29:CE:415:ILE:HG12 | 29:CE:427:HIS:CG   | 2.49                     | 0.47              |
| 30:CF:47:PRO:HD2   | 30:CF:60:THR:O     | 2.12                     | 0.47              |
| 31:CH:196:ASP:HA   | 31:CH:203:PHE:HB2  | 1.95                     | 0.47              |
| 33:CJ:365:GLU:HG3  | 33:CJ:366:PRO:HD2  | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:CO:183:ASP:OD1  | 37:CO:183:ASP:N    | 2.46                     | 0.47              |
| 38:CP:55:ASN:OD1   | 38:CP:58:ILE:HG13  | 2.14                     | 0.47              |
| 42:CU:65:VAL:HG12  | 42:CU:71:ARG:N     | 2.29                     | 0.47              |
| 44:Ca:264:ARG:HG3  | 44:Ca:264:ARG:NH1  | 2.29                     | 0.47              |
| 49:Cj:72:ASP:HB2   | 49:Cj:75:SER:HB3   | 1.96                     | 0.47              |
| 56:Cv:842:PHE:HB2  | 56:Cv:943:LEU:HD22 | 1.97                     | 0.47              |
| 1:DA:80:PRO:HB3    | 57:CA:153:A:N1     | 2.30                     | 0.47              |
| 11:DS:238:ARG:O    | 11:DS:241:GLU:HG3  | 2.14                     | 0.47              |
| 16:DC:310:ARG:HG3  | 16:DC:315:LEU:HD11 | 1.97                     | 0.47              |
| 17:DE:594:LEU:O    | 17:DE:598:VAL:HG23 | 2.15                     | 0.47              |
| 18:DF:92:MET:HE2   | 41:CS:104:GLN:HE22 | 1.80                     | 0.47              |
| 32:CI:108:SER:OG   | 32:CI:110:ARG:HD3  | 2.13                     | 0.47              |
| 32:CI:183:PRO:HD2  | 40:CR:87:GLU:HG3   | 1.95                     | 0.47              |
| 33:CJ:266:MET:HE3  | 33:CJ:266:MET:HB2  | 1.68                     | 0.47              |
| 36:CN:137:TRP:CE3  | 36:CN:137:TRP:HA   | 2.48                     | 0.47              |
| 40:CR:136:LEU:HD13 | 40:CR:140:GLY:O    | 2.13                     | 0.47              |
| 43:CZ:311:GLU:H    | 43:CZ:311:GLU:CD   | 2.20                     | 0.47              |
| 44:Ca:293:LEU:HD13 | 44:Ca:297:LEU:HD13 | 1.96                     | 0.47              |
| 44:Ca:397:GLY:HA3  | 44:Ca:502:PHE:CZ   | 2.49                     | 0.47              |
| 50:Ck:724:PHE:CD2  | 50:Ck:725:VAL:HG23 | 2.50                     | 0.47              |
| 53:Cp:71:THR:HG23  | 53:Cp:105:ILE:HG12 | 1.95                     | 0.47              |
| 55:Cr:261:TRP:CE3  | 55:Cr:264:ILE:HD12 | 2.49                     | 0.47              |
| 56:Cv:615:PRO:HG2  | 56:Cv:616:TRP:CE3  | 2.49                     | 0.47              |
| 57:CA:153:A:H2'    | 57:CA:154:G:O4'    | 2.15                     | 0.47              |
| 1:DA:1656:ASN:ND2  | 1:DA:1659:ARG:HD2  | 2.29                     | 0.47              |
| 3:DI:288:ILE:HD13  | 3:DI:300:LEU:HD22  | 1.96                     | 0.47              |
| 5:DM:145:ILE:HG13  | 5:DM:146:GLY:N     | 2.29                     | 0.47              |
| 8:DP:45:MET:HE3    | 8:DP:57:PRO:HB3    | 1.95                     | 0.47              |
| 11:DS:32:PHE:O     | 57:CA:206:A:O2'    | 2.32                     | 0.47              |
| 11:DS:79:LEU:HD21  | 11:DS:93:ARG:O     | 2.14                     | 0.47              |
| 17:DE:335:GLU:H    | 17:DE:335:GLU:HG3  | 1.50                     | 0.47              |
| 20:DH:4:GLN:HE22   | 20:DH:411:LEU:H    | 1.60                     | 0.47              |
| 22:DK:280:PHE:CD2  | 23:DT:96:TRP:CD1   | 3.03                     | 0.47              |
| 23:DT:31:ASN:C     | 23:DT:205:VAL:HG22 | 2.38                     | 0.47              |
| 23:DT:114:LEU:O    | 23:DT:127:LYS:NZ   | 2.46                     | 0.47              |
| 32:CI:87:TYR:HE2   | 42:CU:161:GLN:HG2  | 1.78                     | 0.47              |
| 32:CI:313:ASP:O    | 32:CI:315:GLU:N    | 2.48                     | 0.47              |
| 33:CJ:109:ALA:HA   | 33:CJ:112:ARG:HH12 | 1.79                     | 0.47              |
| 33:CJ:370:MET:HA   | 33:CJ:393:GLU:HG2  | 1.96                     | 0.47              |
| 34:CK:18:ALA:HB2   | 57:CA:527:A:N6     | 2.30                     | 0.47              |
| 40:CR:199:TYR:CZ   | 42:CU:106:LYS:NZ   | 2.81                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:CS:107:THR:HG22 | 41:CS:109:GLN:H    | 1.79                     | 0.47              |
| 42:CU:104:LEU:O    | 42:CU:107:SER:OG   | 2.22                     | 0.47              |
| 50:Ck:166:MET:O    | 50:Ck:170:VAL:N    | 2.46                     | 0.47              |
| 56:Cv:27:LYS:NZ    | 56:Cv:29:LEU:HB2   | 2.28                     | 0.47              |
| 56:Cv:405:PRO:HB3  | 56:Cv:427:TYR:HE2  | 1.78                     | 0.47              |
| 1:DA:935:MET:HG3   | 5:DM:118:LEU:HD12  | 1.97                     | 0.47              |
| 1:DA:1066:LEU:HD22 | 1:DA:1143:LEU:HD21 | 1.96                     | 0.47              |
| 2:DD:271:LYS:HA    | 2:DD:271:LYS:HD2   | 1.76                     | 0.47              |
| 2:DD:293:GLU:O     | 2:DD:297:ARG:HG2   | 2.15                     | 0.47              |
| 2:DD:296:LEU:HG    | 2:DD:300:GLN:HE21  | 1.79                     | 0.47              |
| 5:DM:56:TRP:CD1    | 5:DM:56:TRP:C      | 2.93                     | 0.47              |
| 11:DS:72:VAL:HG13  | 11:DS:83:LEU:HD13  | 1.96                     | 0.47              |
| 12:DU:170:ARG:O    | 12:DU:174:ARG:NH1  | 2.48                     | 0.47              |
| 12:DU:184:THR:O    | 12:DU:188:VAL:HG23 | 2.14                     | 0.47              |
| 15:DB:641:ARG:HD2  | 50:Ck:555:PHE:CD2  | 2.49                     | 0.47              |
| 15:DB:830:LEU:HD13 | 15:DB:830:LEU:HA   | 1.66                     | 0.47              |
| 18:DF:258:ASP:O    | 18:DF:259:SER:OG   | 2.30                     | 0.47              |
| 20:DH:247:LEU:HA   | 20:DH:247:LEU:HD23 | 1.69                     | 0.47              |
| 24:DV:40:HIS:HB3   | 27:DY:16:SER:HA    | 1.96                     | 0.47              |
| 32:CI:437:LYS:NZ   | 57:CA:454:G:OP1    | 2.37                     | 0.47              |
| 33:CJ:668:GLU:HB3  | 33:CJ:671:LEU:HD22 | 1.95                     | 0.47              |
| 34:CK:111:ASN:ND2  | 34:CK:114:MET:HG3  | 2.25                     | 0.47              |
| 44:Ca:189:GLU:CD   | 44:Ca:189:GLU:N    | 2.72                     | 0.47              |
| 46:Cd:63:ARG:HH12  | 46:Cd:64:GLN:HG2   | 1.80                     | 0.47              |
| 48:CI:36:ALA:O     | 48:CI:40:ILE:HG13  | 2.14                     | 0.47              |
| 50:Ck:337:VAL:HG13 | 50:Ck:338:PRO:O    | 2.14                     | 0.47              |
| 50:Ck:415:ASN:HA   | 50:Ck:541:ARG:HH12 | 1.80                     | 0.47              |
| 2:DD:275:ASP:OD1   | 2:DD:275:ASP:N     | 2.33                     | 0.47              |
| 2:DD:417:THR:HG22  | 2:DD:419:ALA:H     | 1.80                     | 0.47              |
| 4:DL:157:MET:HE3   | 4:DL:161:THR:HG22  | 1.96                     | 0.47              |
| 9:DQ:74:PHE:HE1    | 9:DQ:76:SER:HB3    | 1.80                     | 0.47              |
| 10:DR:14:ARG:HD2   | 57:CA:87:U:OP2     | 2.13                     | 0.47              |
| 12:DU:83:ARG:HG2   | 12:DU:98:MET:HE3   | 1.97                     | 0.47              |
| 14:Da:10:ILE:HG23  | 14:Da:22:ARG:NH1   | 2.29                     | 0.47              |
| 15:DB:1015:ASP:OD2 | 19:DG:38:ARG:NH2   | 2.43                     | 0.47              |
| 16:DC:192:SER:O    | 16:DC:197:LYS:N    | 2.48                     | 0.47              |
| 16:DC:949:PHE:CG   | 16:DC:950:PRO:HD2  | 2.50                     | 0.47              |
| 17:DE:246:ILE:HG13 | 17:DE:423:PHE:CG   | 2.50                     | 0.47              |
| 18:DF:102:LEU:HD13 | 18:DF:143:ILE:HG22 | 1.97                     | 0.47              |
| 18:DF:187:ASN:HD22 | 18:DF:191:THR:HB   | 1.80                     | 0.47              |
| 18:DF:286:ARG:HD3  | 18:DF:286:ARG:HA   | 1.68                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:DF:358:MET:HE3  | 18:DF:368:ILE:HD12 | 1.95                     | 0.47              |
| 19:DG:160:ARG:NH2  | 50:Ck:406:ARG:HE   | 2.13                     | 0.47              |
| 21:DJ:12:TYR:HB2   | 36:CN:18:PRO:HG3   | 1.95                     | 0.47              |
| 24:DV:48:HIS:HD2   | 57:CA:499:U:O2'    | 1.98                     | 0.47              |
| 24:DV:81:THR:HA    | 33:CJ:790:MET:HE1  | 1.97                     | 0.47              |
| 26:DX:88:ASP:OD1   | 26:DX:89:ARG:N     | 2.47                     | 0.47              |
| 29:CE:91:ASN:O     | 29:CE:94:ARG:HG3   | 2.15                     | 0.47              |
| 29:CE:204:VAL:HG11 | 29:CE:247:PHE:CZ   | 2.49                     | 0.47              |
| 29:CE:396:LEU:HD23 | 29:CE:418:PRO:HA   | 1.96                     | 0.47              |
| 31:CH:16:VAL:O     | 31:CH:18:PRO:HD3   | 2.14                     | 0.47              |
| 32:CI:295:ASP:OD1  | 32:CI:295:ASP:N    | 2.46                     | 0.47              |
| 32:CI:426:GLN:HG2  | 36:CN:137:TRP:CZ2  | 2.50                     | 0.47              |
| 33:CJ:619:HIS:CD2  | 33:CJ:630:ARG:HH12 | 2.31                     | 0.47              |
| 33:CJ:685:ILE:HG23 | 36:CN:63:HIS:HE1   | 1.78                     | 0.47              |
| 34:CK:53:ARG:NH1   | 47:Cg:488:ARG:NH2  | 2.63                     | 0.47              |
| 34:CK:307:PHE:CE1  | 42:CU:61:ILE:HD12  | 2.49                     | 0.47              |
| 37:CO:122:VAL:HG22 | 37:CO:123:ASN:H    | 1.80                     | 0.47              |
| 39:CQ:172:ARG:HG2  | 39:CQ:172:ARG:HH11 | 1.80                     | 0.47              |
| 40:CR:23:TRP:CE2   | 56:Cv:494:THR:HG21 | 2.49                     | 0.47              |
| 40:CR:220:ARG:HH22 | 51:Cm:128:ARG:CZ   | 2.28                     | 0.47              |
| 40:CR:318:LYS:HA   | 40:CR:318:LYS:HD2  | 1.72                     | 0.47              |
| 41:CS:63:SER:HA    | 41:CS:75:MET:SD    | 2.55                     | 0.47              |
| 43:CZ:258:ARG:HH21 | 43:CZ:314:TRP:HB3  | 1.80                     | 0.47              |
| 44:Ca:575:ARG:HG2  | 44:Ca:575:ARG:HH11 | 1.78                     | 0.47              |
| 45:Cb:98:LEU:HD13  | 45:Cb:125:MET:HE2  | 1.96                     | 0.47              |
| 45:Cb:203:LEU:HA   | 45:Cb:206:GLU:OE2  | 2.14                     | 0.47              |
| 46:Cd:218:PRO:HD2  | 56:Cv:641:ARG:HH21 | 1.79                     | 0.47              |
| 47:Cg:469:TYR:O    | 47:Cg:472:THR:HB   | 2.15                     | 0.47              |
| 49:Cj:60:LEU:HD13  | 49:Cj:65:LEU:HD11  | 1.96                     | 0.47              |
| 50:Ck:757:ALA:O    | 50:Ck:760:VAL:HG22 | 2.14                     | 0.47              |
| 55:Cr:125:GLN:NE2  | 55:Cr:162:PRO:HD2  | 2.22                     | 0.47              |
| 57:CA:232:G:N1     | 57:CA:248:A:OP1    | 2.45                     | 0.47              |
| 57:CA:524:A:H2'    | 57:CA:525:A:H8     | 1.79                     | 0.47              |
| 3:DI:268:LEU:HD13  | 3:DI:292:TYR:CD1   | 2.47                     | 0.47              |
| 4:DL:194:ILE:HD12  | 40:CR:77:ILE:HD13  | 1.96                     | 0.47              |
| 10:DR:14:ARG:NH1   | 57:CA:87:U:OP2     | 2.45                     | 0.47              |
| 10:DR:249:GLU:O    | 10:DR:262:ARG:NH1  | 2.47                     | 0.47              |
| 15:DB:493:ARG:NH2  | 19:DG:29:ASP:OD1   | 2.48                     | 0.47              |
| 21:DJ:272:THR:HG22 | 21:DJ:276:LEU:HD22 | 1.96                     | 0.47              |
| 36:CN:46:ARG:HH12  | 48:CI:82:GLN:HE21  | 1.62                     | 0.47              |
| 37:CO:221:PRO:HG3  | 37:CO:269:VAL:HG21 | 1.97                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 37:CO:429:ASN:ND2   | 57:CA:92:A:OP1     | 2.48                     | 0.47              |
| 38:CP:157:ASP:OD1   | 38:CP:157:ASP:N    | 2.47                     | 0.47              |
| 40:CR:94:MET:HE2    | 40:CR:94:MET:HB3   | 1.73                     | 0.47              |
| 45:Cb:11:MET:HE2    | 57:CA:385:A:H1'    | 1.97                     | 0.47              |
| 49:Cj:26:GLY:O      | 57:CA:177:A:O2'    | 2.24                     | 0.47              |
| 50:Ck:268:LEU:HD23  | 50:Ck:348:LEU:HG   | 1.95                     | 0.47              |
| 50:Ck:561:SER:O     | 50:Ck:565:LEU:HB2  | 2.15                     | 0.47              |
| 52:Cn:243:ARG:HH22  | 57:CA:336:U:H5     | 1.62                     | 0.47              |
| 57:CA:88:A:H3'      | 57:CA:88:A:OP2     | 2.13                     | 0.47              |
| 1:DA:630:ASP:OD2    | 1:DA:694:ARG:NH1   | 2.48                     | 0.47              |
| 1:DA:945:ILE:HG22   | 5:DM:129:ARG:HB3   | 1.97                     | 0.47              |
| 2:DD:102:TRP:CZ3    | 2:DD:104:ARG:HD3   | 2.50                     | 0.47              |
| 2:DD:217:ASP:OD1    | 2:DD:297:ARG:HD2   | 2.15                     | 0.47              |
| 2:DD:297:ARG:O      | 2:DD:301:VAL:HG23  | 2.15                     | 0.47              |
| 6:DN:224:ARG:HB3    | 6:DN:287:ARG:HD2   | 1.96                     | 0.47              |
| 9:DQ:52:PHE:CE1     | 9:DQ:235:HIS:HE1   | 2.32                     | 0.47              |
| 15:DB:719:MET:HE2   | 15:DB:719:MET:HB3  | 1.76                     | 0.47              |
| 16:DC:475:LEU:HD21  | 23:DT:95:ARG:HG2   | 1.96                     | 0.47              |
| 17:DE:245:TYR:O     | 17:DE:248:THR:HB   | 2.15                     | 0.47              |
| 18:DF:78:ASN:HB2    | 26:DX:43:HIS:CD2   | 2.50                     | 0.47              |
| 20:DH:399:PHE:HD2   | 48:Di:119:LEU:HD22 | 1.79                     | 0.47              |
| 27:DY:76:ARG:HD3    | 27:DY:84:LYS:HE2   | 1.97                     | 0.47              |
| 28:CC:38:PHE:HB2    | 28:CC:77:THR:C     | 2.40                     | 0.47              |
| 29:CE:152:VAL:HG22  | 51:Cm:42:PRO:HG2   | 1.95                     | 0.47              |
| 33:CJ:67:GLU:H      | 33:CJ:67:GLU:CD    | 2.23                     | 0.47              |
| 33:CJ:552:ILE:HG22  | 33:CJ:557:GLU:CD   | 2.40                     | 0.47              |
| 33:CJ:797:LEU:HD12  | 33:CJ:797:LEU:HA   | 1.67                     | 0.47              |
| 34:CK:288:ARG:NH1   | 42:CU:62:MET:HG2   | 2.30                     | 0.47              |
| 44:Ca:511:ILE:HA    | 44:Ca:519:GLN:HE22 | 1.80                     | 0.47              |
| 50:Ck:723:GLN:O     | 50:Ck:778:GLN:NE2  | 2.47                     | 0.47              |
| 52:Cn:163:ARG:NH1   | 57:CA:591:A:O2'    | 2.48                     | 0.47              |
| 53:Cp:70:PRO:HB2    | 53:Cp:73:ASP:OD2   | 2.14                     | 0.47              |
| 53:Cp:128:LEU:HD23  | 53:Cp:128:LEU:HA   | 1.74                     | 0.47              |
| 55:Cr:172:ARG:HH21  | 55:Cr:176:LEU:HD23 | 1.79                     | 0.47              |
| 1:DA:414:HIS:CD2    | 1:DA:416:HIS:H     | 2.33                     | 0.47              |
| 1:DA:1386:ASP:HB3   | 29:CE:339:LEU:HD21 | 1.96                     | 0.47              |
| 3:DI:83:GLN:HE21    | 3:DI:175:GLN:HG2   | 1.79                     | 0.47              |
| 9:DQ:217:GLN:HB3    | 9:DQ:221:LEU:HD12  | 1.96                     | 0.47              |
| 11:DS:114:LYS:NZ    | 57:CA:206:A:OP1    | 2.25                     | 0.47              |
| 15:DB:609:PRO:HB2   | 15:DB:614:VAL:HG23 | 1.96                     | 0.47              |
| 16:DC:1082:ARG:HH22 | 23:DT:75:ARG:HD3   | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:DF:115:HIS:CD2  | 36:CN:37:ARG:HG3   | 2.50                     | 0.47              |
| 18:DF:341:VAL:HG22 | 18:DF:346:LEU:HD11 | 1.97                     | 0.47              |
| 20:DH:80:ARG:NH1   | 20:DH:86:PRO:HD2   | 2.29                     | 0.47              |
| 32:CI:183:PRO:HG2  | 40:CR:85:THR:HG22  | 1.97                     | 0.47              |
| 34:CK:88:GLU:OE1   | 34:CK:88:GLU:N     | 2.34                     | 0.47              |
| 40:CR:245:ALA:HA   | 40:CR:248:LYS:HD2  | 1.96                     | 0.47              |
| 41:CS:87:GLU:O     | 41:CS:104:GLN:HG3  | 2.15                     | 0.47              |
| 45:Cb:19:PRO:HD2   | 51:Cm:156:THR:CG2  | 2.45                     | 0.47              |
| 45:Cb:169:LYS:NZ   | 45:Cb:176:THR:OG1  | 2.39                     | 0.47              |
| 49:Cj:73:ARG:O     | 53:Cp:172:PRO:HD3  | 2.15                     | 0.47              |
| 49:Cj:226:LYS:HG3  | 49:Cj:231:LEU:HB2  | 1.97                     | 0.47              |
| 1:DA:1440:ILE:HD11 | 1:DA:1562:GLN:CG   | 2.45                     | 0.46              |
| 2:DD:20:PHE:HZ     | 29:CE:256:LEU:H    | 1.63                     | 0.46              |
| 3:DI:50:LEU:HD12   | 3:DI:50:LEU:HA     | 1.75                     | 0.46              |
| 3:DI:276:GLU:HG2   | 3:DI:277:SER:N     | 2.29                     | 0.46              |
| 4:DL:44:LYS:HB2    | 4:DL:44:LYS:HE3    | 1.71                     | 0.46              |
| 5:DM:36:TYR:OH     | 29:CE:309:ARG:NH2  | 2.37                     | 0.46              |
| 5:DM:129:ARG:HD2   | 5:DM:163:THR:HG21  | 1.98                     | 0.46              |
| 5:DM:227:LEU:HB2   | 56:Cv:1008:ARG:HD3 | 1.97                     | 0.46              |
| 10:DR:22:LEU:CB    | 37:CO:389:LYS:HZ2  | 2.28                     | 0.46              |
| 15:DB:678:PRO:HG2  | 15:DB:708:THR:HG23 | 1.98                     | 0.46              |
| 17:DE:725:PRO:HG2  | 22:DK:146:TYR:CE2  | 2.50                     | 0.46              |
| 18:DF:349:ASP:OD1  | 18:DF:349:ASP:N    | 2.48                     | 0.46              |
| 20:DH:325:MET:SD   | 20:DH:374:GLU:HG3  | 2.55                     | 0.46              |
| 26:DX:45:LYS:HB2   | 26:DX:45:LYS:HE3   | 1.57                     | 0.46              |
| 26:DX:50:ARG:NH2   | 41:CS:121:SER:HB3  | 2.30                     | 0.46              |
| 33:CJ:206:PHE:CD2  | 33:CJ:207:PRO:HA   | 2.50                     | 0.46              |
| 33:CJ:728:GLN:HE21 | 48:Ci:13:HIS:HB2   | 1.80                     | 0.46              |
| 40:CR:28:GLY:CA    | 45:Cb:91:ARG:HH12  | 2.29                     | 0.46              |
| 40:CR:105:ILE:O    | 40:CR:105:ILE:HG13 | 2.15                     | 0.46              |
| 45:Cb:67:GLN:NE2   | 45:Cb:73:PRO:HA    | 2.30                     | 0.46              |
| 46:Cd:106:ARG:HG3  | 46:Cd:107:GLN:N    | 2.30                     | 0.46              |
| 54:Cq:168:ASP:HA   | 54:Cq:171:ARG:HG2  | 1.96                     | 0.46              |
| 56:Cv:233:LYS:HG3  | 56:Cv:500:TYR:CG   | 2.51                     | 0.46              |
| 56:Cv:847:ARG:NE   | 56:Cv:938:ASP:OD2  | 2.42                     | 0.46              |
| 1:DA:1377:VAL:HG13 | 1:DA:1620:TYR:CD2  | 2.50                     | 0.46              |
| 1:DA:1432:CYS:O    | 1:DA:1613:TYR:OH   | 2.14                     | 0.46              |
| 10:DR:39:GLN:O     | 10:DR:42:MET:HB3   | 2.16                     | 0.46              |
| 16:DC:86:THR:HG23  | 16:DC:959:VAL:HG21 | 1.97                     | 0.46              |
| 17:DE:736:TRP:HE1  | 50:Ck:74:SER:H     | 1.63                     | 0.46              |
| 18:DF:258:ASP:C    | 18:DF:260:LYS:H    | 2.24                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:DH:82:GLN:H     | 20:DH:82:GLN:HG3   | 1.38                     | 0.46              |
| 21:DJ:46:ARG:HD3   | 21:DJ:46:ARG:HA    | 1.76                     | 0.46              |
| 29:CE:40:ARG:NE    | 29:CE:94:ARG:HH11  | 2.12                     | 0.46              |
| 29:CE:312:GLY:C    | 29:CE:314:MET:H    | 2.19                     | 0.46              |
| 30:CF:42:GLU:CD    | 46:Cd:179:PHE:HD1  | 2.23                     | 0.46              |
| 33:CJ:118:MET:HE3  | 33:CJ:139:PHE:CE2  | 2.50                     | 0.46              |
| 33:CJ:232:ASN:ND2  | 33:CJ:241:SER:OG   | 2.48                     | 0.46              |
| 33:CJ:541:LEU:HG   | 33:CJ:595:THR:O    | 2.15                     | 0.46              |
| 36:CN:127:LEU:HD13 | 36:CN:129:VAL:HG13 | 1.97                     | 0.46              |
| 38:CP:16:ARG:NH1   | 57:CA:44:U:C4      | 2.83                     | 0.46              |
| 40:CR:134:ARG:NH2  | 40:CR:185:PHE:HB3  | 2.30                     | 0.46              |
| 40:CR:319:LYS:HD3  | 42:CU:185:ARG:HH21 | 1.80                     | 0.46              |
| 44:Ca:285:GLU:OE1  | 44:Ca:285:GLU:N    | 2.48                     | 0.46              |
| 46:Cd:260:THR:CG2  | 51:Cm:104:ARG:HB3  | 2.45                     | 0.46              |
| 50:Ck:134:HIS:HE1  | 50:Ck:326:THR:OG1  | 1.98                     | 0.46              |
| 50:Ck:682:ASN:H    | 50:Ck:682:ASN:ND2  | 2.13                     | 0.46              |
| 50:Ck:688:TYR:O    | 50:Ck:691:GLN:HB3  | 2.15                     | 0.46              |
| 51:Cm:93:LEU:HD22  | 51:Cm:136:MET:HE1  | 1.97                     | 0.46              |
| 56:Cv:409:LEU:HD11 | 56:Cv:498:MET:HB3  | 1.98                     | 0.46              |
| 56:Cv:718:THR:N    | 56:Cv:757:ASP:HB2  | 2.29                     | 0.46              |
| 56:Cv:1005:TRP:CD1 | 56:Cv:1006:GLU:HG2 | 2.49                     | 0.46              |
| 2:DD:16:ARG:HD3    | 29:CE:223:ARG:NH1  | 2.31                     | 0.46              |
| 2:DD:465:PHE:CD2   | 2:DD:479:ARG:HD3   | 2.50                     | 0.46              |
| 3:DI:52:GLU:OE1    | 3:DI:165:ARG:NE    | 2.49                     | 0.46              |
| 12:DU:86:ILE:HG13  | 12:DU:97:ARG:O     | 2.15                     | 0.46              |
| 13:DZ:90:VAL:HG22  | 44:Ca:149:ARG:HH12 | 1.81                     | 0.46              |
| 19:DG:551:MET:SD   | 19:DG:561:PRO:HD3  | 2.56                     | 0.46              |
| 21:DJ:145:HIS:NE2  | 21:DJ:150:ALA:HB2  | 2.30                     | 0.46              |
| 25:DW:17:SER:O     | 25:DW:21:THR:OG1   | 2.33                     | 0.46              |
| 27:DY:111:ARG:HG2  | 27:DY:126:LYS:O    | 2.15                     | 0.46              |
| 29:CE:162:TRP:CD1  | 29:CE:184:PRO:HA   | 2.51                     | 0.46              |
| 32:CI:270:PHE:O    | 32:CI:274:LEU:HB2  | 2.15                     | 0.46              |
| 39:CQ:148:LYS:O    | 39:CQ:159:TYR:HA   | 2.15                     | 0.46              |
| 40:CR:54:GLY:HA2   | 45:Cb:21:PHE:HB3   | 1.97                     | 0.46              |
| 40:CR:62:GLN:OE1   | 40:CR:62:GLN:N     | 2.35                     | 0.46              |
| 45:Cb:301:THR:O    | 45:Cb:301:THR:OG1  | 2.33                     | 0.46              |
| 1:DA:903:LYS:NZ    | 44:Ca:551:TYR:OH   | 2.49                     | 0.46              |
| 1:DA:1039:SER:HB2  | 29:CE:54:GLU:OE1   | 2.15                     | 0.46              |
| 1:DA:1654:ARG:O    | 29:CE:393:ARG:NH1  | 2.49                     | 0.46              |
| 2:DD:27:MET:HE1    | 31:CH:239:ARG:HD2  | 1.96                     | 0.46              |
| 2:DD:527:THR:CB    | 10:DR:223:GLN:HG3  | 2.45                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:DN:292:TYR:HE2    | 44:Ca:252:ARG:HG2  | 1.81                     | 0.46              |
| 8:DP:82:ARG:HD3     | 49:Cj:72:ASP:OD2   | 2.16                     | 0.46              |
| 8:DP:132:LEU:HA     | 8:DP:132:LEU:HD23  | 1.82                     | 0.46              |
| 12:DU:189:LYS:NZ    | 12:DU:190:ARG:HB2  | 2.30                     | 0.46              |
| 27:DY:53:LEU:HD23   | 27:DY:53:LEU:HA    | 1.76                     | 0.46              |
| 29:CE:392:ARG:NH1   | 29:CE:392:ARG:HA   | 2.31                     | 0.46              |
| 31:CH:225:ASP:HB3   | 31:CH:227:ARG:H    | 1.80                     | 0.46              |
| 33:CJ:785:VAL:O     | 33:CJ:787:GLN:HG3  | 2.16                     | 0.46              |
| 37:CO:398:ASP:OD1   | 37:CO:398:ASP:N    | 2.48                     | 0.46              |
| 40:CR:109:ASP:HB3   | 40:CR:112:GLY:HA2  | 1.98                     | 0.46              |
| 44:Ca:106:ASN:HB3   | 44:Ca:155:ARG:HD3  | 1.96                     | 0.46              |
| 55:Cr:143:ARG:HE    | 55:Cr:143:ARG:HB3  | 1.51                     | 0.46              |
| 1:DA:584:PHE:HB3    | 1:DA:759:GLY:HA3   | 1.96                     | 0.46              |
| 1:DA:1384:ARG:HH12  | 1:DA:1628:ARG:HE   | 1.62                     | 0.46              |
| 2:DD:10:HIS:N       | 57:CA:23:A:HO2'    | 2.13                     | 0.46              |
| 9:DQ:58:ARG:NH2     | 12:DU:39:ARG:HB2   | 2.30                     | 0.46              |
| 10:DR:51:LEU:HD22   | 10:DR:84:LEU:HD21  | 1.98                     | 0.46              |
| 14:Da:33:LEU:HA     | 31:CH:144:ARG:NH1  | 2.31                     | 0.46              |
| 16:DC:33:TRP:CZ3    | 21:DJ:256:LYS:HA   | 2.51                     | 0.46              |
| 24:DV:127:THR:HG22  | 24:DV:128:ASP:OD1  | 2.15                     | 0.46              |
| 30:CF:37:ARG:NH1    | 30:CF:121:PHE:O    | 2.47                     | 0.46              |
| 34:CK:251:LEU:HD13  | 34:CK:298:ARG:HG3  | 1.96                     | 0.46              |
| 42:CU:24:LYS:HE3    | 57:CA:300:G:N2     | 2.31                     | 0.46              |
| 42:CU:67:HIS:HE1    | 57:CA:621:U:H5     | 1.64                     | 0.46              |
| 42:CU:182:HIS:HE1   | 42:CU:193:ASN:HA   | 1.80                     | 0.46              |
| 43:CZ:265:GLN:HG2   | 43:CZ:308:TYR:CE1  | 2.50                     | 0.46              |
| 44:Ca:102:TRP:CE2   | 44:Ca:159:LEU:HD13 | 2.50                     | 0.46              |
| 46:Cd:173:GLU:HB2   | 46:Cd:174:PRO:HD2  | 1.97                     | 0.46              |
| 47:Cg:294:GLU:HA    | 47:Cg:329:PRO:HA   | 1.97                     | 0.46              |
| 50:Ck:392:PHE:CD1   | 50:Ck:408:VAL:HG11 | 2.50                     | 0.46              |
| 53:Cp:125:GLU:OE2   | 53:Cp:125:GLU:HA   | 2.13                     | 0.46              |
| 55:Cr:42:ILE:HD11   | 55:Cr:95:SER:HA    | 1.98                     | 0.46              |
| 57:CA:565:A:H4'     | 57:CA:566:U:OP1    | 2.16                     | 0.46              |
| 3:DI:326:ARG:HH12   | 7:DO:201:GLU:CD    | 2.24                     | 0.46              |
| 6:DN:61:LEU:HD23    | 31:CH:56:LEU:HD12  | 1.96                     | 0.46              |
| 15:DB:1117:THR:HG23 | 41:CS:83:PHE:CD1   | 2.51                     | 0.46              |
| 17:DE:147:MET:HE1   | 17:DE:567:HIS:CG   | 2.51                     | 0.46              |
| 17:DE:182:ASP:OD1   | 17:DE:543:ARG:NH2  | 2.47                     | 0.46              |
| 17:DE:547:THR:O     | 17:DE:551:VAL:HG23 | 2.15                     | 0.46              |
| 18:DF:6:VAL:HG11    | 36:CN:10:MET:HE2   | 1.97                     | 0.46              |
| 20:DH:438:GLY:HA3   | 28:CC:40:ILE:HD11  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:CO:264:ARG:HH12 | 37:CO:303:TYR:HB3  | 1.80                     | 0.46              |
| 44:Ca:362:PHE:CD2  | 56:Cv:284:LYS:HE2  | 2.50                     | 0.46              |
| 44:Ca:601:GLU:OE2  | 44:Ca:601:GLU:HA   | 2.15                     | 0.46              |
| 45:Cb:168:ALA:O    | 45:Cb:171:THR:HG22 | 2.16                     | 0.46              |
| 47:Cg:154:GLY:HA2  | 67:Cg:501:GTP:N7   | 2.31                     | 0.46              |
| 48:Ci:162:ALA:O    | 48:Ci:165:PRO:HD3  | 2.16                     | 0.46              |
| 51:Cm:87:LEU:HD21  | 51:Cm:136:MET:HE2  | 1.97                     | 0.46              |
| 52:Cn:201:VAL:HG22 | 52:Cn:226:LEU:HD13 | 1.97                     | 0.46              |
| 1:DA:525:LEU:O     | 1:DA:529:ILE:HG13  | 2.15                     | 0.46              |
| 1:DA:1020:MET:HE3  | 1:DA:1020:MET:HB3  | 1.64                     | 0.46              |
| 7:DO:60:MET:HE1    | 7:DO:112:GLY:H     | 1.81                     | 0.46              |
| 7:DO:245:VAL:HA    | 46:Cd:129:ARG:HH22 | 1.81                     | 0.46              |
| 8:DP:11:SER:O      | 53:Cp:141:ARG:HD3  | 2.15                     | 0.46              |
| 10:DR:60:VAL:HG23  | 10:DR:61:PRO:HD2   | 1.97                     | 0.46              |
| 11:DS:227:VAL:HG21 | 38:CP:139:LEU:HD12 | 1.98                     | 0.46              |
| 15:DB:659:TYR:O    | 15:DB:663:VAL:HG22 | 2.15                     | 0.46              |
| 15:DB:746:LEU:HD12 | 15:DB:757:VAL:HG21 | 1.97                     | 0.46              |
| 15:DB:765:GLU:O    | 15:DB:769:VAL:HG23 | 2.16                     | 0.46              |
| 16:DC:984:THR:HA   | 16:DC:1008:GLY:HA3 | 1.97                     | 0.46              |
| 17:DE:301:TYR:HB2  | 17:DE:437:LYS:NZ   | 2.30                     | 0.46              |
| 17:DE:668:LEU:HD23 | 17:DE:668:LEU:HA   | 1.75                     | 0.46              |
| 19:DG:524:PHE:CZ   | 19:DG:582:VAL:HG11 | 2.50                     | 0.46              |
| 31:CH:91:LEU:HD12  | 56:Cv:315:ILE:HG12 | 1.96                     | 0.46              |
| 32:CI:61:ARG:HD3   | 47:Cg:431:TRP:CZ3  | 2.51                     | 0.46              |
| 33:CJ:540:PRO:HA   | 33:CJ:596:GLU:HG2  | 1.97                     | 0.46              |
| 34:CK:214:LYS:HB3  | 34:CK:214:LYS:HZ3  | 1.75                     | 0.46              |
| 34:CK:314:PRO:HB3  | 42:CU:15:TYR:CZ    | 2.51                     | 0.46              |
| 37:CO:251:VAL:HG22 | 57:CA:285:A:C6     | 2.50                     | 0.46              |
| 40:CR:60:PHE:HZ    | 40:CR:66:LEU:HD11  | 1.80                     | 0.46              |
| 41:CS:79:SER:HB2   | 57:CA:507:A:N1     | 2.30                     | 0.46              |
| 47:Cg:264:VAL:HG21 | 50:Ck:821:TYR:CE2  | 2.50                     | 0.46              |
| 56:Cv:78:ILE:HD11  | 56:Cv:80:TYR:CE2   | 2.51                     | 0.46              |
| 1:DA:410:ASP:OD1   | 1:DA:494:ARG:NH1   | 2.46                     | 0.46              |
| 2:DD:280:LEU:HD23  | 2:DD:280:LEU:HA    | 1.62                     | 0.46              |
| 3:DI:306:ASP:OD1   | 3:DI:306:ASP:N     | 2.37                     | 0.46              |
| 4:DL:128:MET:HE2   | 4:DL:231:TRP:CH2   | 2.51                     | 0.46              |
| 6:DN:26:ARG:HD3    | 6:DN:115:PRO:HG2   | 1.98                     | 0.46              |
| 9:DQ:171:GLU:HG2   | 37:CO:319:MET:HE2  | 1.96                     | 0.46              |
| 11:DS:225:GLU:HB3  | 11:DS:229:ARG:NH1  | 2.29                     | 0.46              |
| 14:Da:50:LYS:NZ    | 57:CA:362:A:H5'    | 2.30                     | 0.46              |
| 17:DE:697:THR:HG23 | 22:DK:59:TRP:HH2   | 1.79                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DX:42:PHE:CE1   | 41:CS:152:ASP:HB3  | 2.50                     | 0.46              |
| 26:DX:43:HIS:CE1   | 41:CS:124:SER:HB2  | 2.51                     | 0.46              |
| 29:CE:30:TYR:CE2   | 29:CE:206:LEU:HB2  | 2.51                     | 0.46              |
| 30:CF:144:MET:HE3  | 30:CF:144:MET:HB2  | 1.81                     | 0.46              |
| 36:CN:66:MET:HE2   | 36:CN:66:MET:HB2   | 1.66                     | 0.46              |
| 37:CO:259:LEU:HD13 | 37:CO:286:ILE:HD13 | 1.98                     | 0.46              |
| 40:CR:173:ARG:HG3  | 40:CR:173:ARG:HH11 | 1.81                     | 0.46              |
| 44:Ca:450:ASN:ND2  | 44:Ca:467:LYS:HD3  | 2.31                     | 0.46              |
| 45:Cb:292:ASP:N    | 45:Cb:292:ASP:OD1  | 2.47                     | 0.46              |
| 48:Ci:141:LYS:NZ   | 57:CA:440:U:H3'    | 2.31                     | 0.46              |
| 50:Ck:184:LYS:HD3  | 50:Ck:228:LEU:HD11 | 1.97                     | 0.46              |
| 50:Ck:330:ILE:HG21 | 50:Ck:591:PRO:HG2  | 1.96                     | 0.46              |
| 1:DA:150:ILE:HG23  | 1:DA:151:PRO:O     | 2.16                     | 0.46              |
| 1:DA:224:VAL:HG11  | 1:DA:287:HIS:HB3   | 1.97                     | 0.46              |
| 3:DI:310:LEU:HD12  | 3:DI:310:LEU:HA    | 1.74                     | 0.46              |
| 6:DN:47:VAL:HG22   | 6:DN:132:TYR:HB2   | 1.98                     | 0.46              |
| 6:DN:50:LEU:HD12   | 6:DN:133:PHE:HB3   | 1.98                     | 0.46              |
| 9:DQ:74:PHE:CE1    | 9:DQ:76:SER:HB3    | 2.51                     | 0.46              |
| 15:DB:450:MET:HE2  | 15:DB:450:MET:HA   | 1.98                     | 0.46              |
| 24:DV:56:ARG:NH2   | 33:CJ:775:ASP:OD1  | 2.48                     | 0.46              |
| 33:CJ:414:LYS:HE2  | 33:CJ:414:LYS:HB3  | 1.79                     | 0.46              |
| 37:CO:208:MET:HG2  | 37:CO:223:VAL:HG13 | 1.98                     | 0.46              |
| 37:CO:293:VAL:HG22 | 39:CQ:189:TYR:CE1  | 2.50                     | 0.46              |
| 38:CP:69:PRO:HA    | 38:CP:90:MET:HE1   | 1.98                     | 0.46              |
| 44:Ca:11:TYR:CE2   | 44:Ca:13:PHE:HB2   | 2.51                     | 0.46              |
| 44:Ca:138:LYS:NZ   | 44:Ca:141:THR:H    | 2.14                     | 0.46              |
| 48:Ci:24:PRO:O     | 48:Ci:25:VAL:HG23  | 2.16                     | 0.46              |
| 56:Cv:214:HIS:CD2  | 56:Cv:216:ASN:H    | 2.33                     | 0.46              |
| 56:Cv:448:TYR:HD1  | 56:Cv:841:GLU:HB3  | 1.80                     | 0.46              |
| 56:Cv:742:LEU:HD23 | 56:Cv:742:LEU:HA   | 1.74                     | 0.46              |
| 1:DA:369:VAL:HA    | 1:DA:408:LEU:HD22  | 1.99                     | 0.46              |
| 1:DA:1483:GLN:O    | 1:DA:1488:GLN:NE2  | 2.49                     | 0.46              |
| 2:DD:119:TYR:CD1   | 46:Cd:76:TYR:HD1   | 2.34                     | 0.46              |
| 2:DD:782:ILE:HG21  | 44:Ca:303:VAL:HG11 | 1.98                     | 0.46              |
| 5:DM:242:LEU:HD23  | 5:DM:242:LEU:HA    | 1.79                     | 0.46              |
| 7:DO:60:MET:HE2    | 7:DO:60:MET:HA     | 1.97                     | 0.46              |
| 10:DR:68:HIS:NE2   | 10:DR:93:PRO:HG3   | 2.31                     | 0.46              |
| 10:DR:269:TRP:H    | 49:Cj:126:TYR:HB2  | 1.81                     | 0.46              |
| 11:DS:17:SER:OG    | 11:DS:18:ARG:N     | 2.49                     | 0.46              |
| 11:DS:211:CYS:HB2  | 11:DS:214:CYS:H    | 1.81                     | 0.46              |
| 12:DU:198:MET:HE3  | 12:DU:199:GLN:HE21 | 1.81                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:778:LYS:HA   | 15:DB:783:VAL:HA   | 1.98                     | 0.46              |
| 16:DC:43:ALA:O     | 16:DC:46:ARG:HG3   | 2.16                     | 0.46              |
| 17:DE:198:CYS:HB3  | 17:DE:202:HIS:HB2  | 1.98                     | 0.46              |
| 24:DV:24:VAL:HA    | 32:CI:380:PRO:O    | 2.15                     | 0.46              |
| 24:DV:129:ILE:HD13 | 33:CJ:138:PRO:HD3  | 1.98                     | 0.46              |
| 25:DW:137:PRO:HA   | 25:DW:140:TRP:CD2  | 2.51                     | 0.46              |
| 27:DY:89:ALA:O     | 27:DY:93:THR:HG23  | 2.16                     | 0.46              |
| 29:CE:127:LEU:HD13 | 29:CE:194:ILE:HG21 | 1.98                     | 0.46              |
| 32:CI:82:HIS:HB2   | 51:Cm:128:ARG:HH21 | 1.79                     | 0.46              |
| 32:CI:100:PRO:HB3  | 40:CR:95:GLN:OE1   | 2.15                     | 0.46              |
| 32:CI:104:ASN:HD22 | 32:CI:105:THR:N    | 2.14                     | 0.46              |
| 32:CI:178:GLU:HG2  | 32:CI:183:PRO:HA   | 1.98                     | 0.46              |
| 32:CI:400:VAL:HG21 | 32:CI:416:LEU:HD11 | 1.98                     | 0.46              |
| 37:CO:247:ILE:HG22 | 37:CO:248:ILE:HG12 | 1.97                     | 0.46              |
| 49:Cj:10:ARG:N     | 49:Cj:10:ARG:HE    | 2.13                     | 0.46              |
| 50:Ck:364:LEU:HB3  | 50:Ck:372:LYS:HE3  | 1.97                     | 0.46              |
| 51:Cm:23:ASP:OD1   | 51:Cm:24:SER:N     | 2.48                     | 0.46              |
| 55:Cr:183:ALA:HB1  | 55:Cr:259:MET:HE1  | 1.98                     | 0.46              |
| 57:CA:43:A:H62     | 57:CA:173:A:H62    | 1.64                     | 0.46              |
| 1:DA:501:GLU:HG2   | 1:DA:889:VAL:HB    | 1.98                     | 0.45              |
| 1:DA:1645:GLU:HG2  | 29:CE:425:PRO:HB2  | 1.97                     | 0.45              |
| 5:DM:41:GLU:OE2    | 44:Ca:286:ARG:NH2  | 2.43                     | 0.45              |
| 5:DM:77:PRO:HD3    | 56:Cv:969:ASP:HA   | 1.98                     | 0.45              |
| 15:DB:315:GLN:HE21 | 15:DB:319:ARG:HH21 | 1.64                     | 0.45              |
| 15:DB:684:GLN:NE2  | 17:DE:660:GLN:HB3  | 2.30                     | 0.45              |
| 18:DF:371:ASN:HB2  | 18:DF:374:VAL:HG23 | 1.98                     | 0.45              |
| 21:DJ:55:ASN:O     | 57:CA:430:U:O2'    | 2.24                     | 0.45              |
| 29:CE:400:LEU:HD22 | 29:CE:405:LYS:HB2  | 1.96                     | 0.45              |
| 32:CI:9:THR:HG22   | 32:CI:10:ALA:H     | 1.80                     | 0.45              |
| 37:CO:126:GLU:H    | 37:CO:126:GLU:CD   | 2.24                     | 0.45              |
| 39:CQ:72:ARG:O     | 39:CQ:118:PRO:HD2  | 2.16                     | 0.45              |
| 40:CR:309:GLY:HA3  | 57:CA:388:U:O2     | 2.15                     | 0.45              |
| 44:Ca:138:LYS:HZ1  | 44:Ca:141:THR:HA   | 1.81                     | 0.45              |
| 45:Cb:91:ARG:O     | 45:Cb:95:ARG:HG2   | 2.16                     | 0.45              |
| 56:Cv:255:PHE:CD2  | 56:Cv:292:LYS:HE3  | 2.51                     | 0.45              |
| 56:Cv:681:HIS:NE2  | 56:Cv:695:SER:OG   | 2.33                     | 0.45              |
| 57:CA:194:A:O2'    | 57:CA:195:A:H2'    | 2.16                     | 0.45              |
| 6:DN:223:GLN:HB2   | 44:Ca:256:GLU:CD   | 2.42                     | 0.45              |
| 8:DP:32:TYR:OH     | 53:Cp:151:ARG:NH2  | 2.49                     | 0.45              |
| 8:DP:84:ASP:C      | 8:DP:86:PRO:HD3    | 2.41                     | 0.45              |
| 10:DR:60:VAL:HG22  | 10:DR:63:ILE:HG12  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:DG:577:LEU:HD23 | 19:DG:577:LEU:HA   | 1.79                     | 0.45              |
| 21:DJ:291:ASN:ND2  | 21:DJ:294:MET:H    | 2.14                     | 0.45              |
| 23:DT:93:MET:HE1   | 23:DT:102:TRP:NE1  | 2.31                     | 0.45              |
| 26:DX:123:ASN:HD22 | 47:Cg:318:ILE:HA   | 1.82                     | 0.45              |
| 33:CJ:541:LEU:HD13 | 33:CJ:551:ARG:HE   | 1.81                     | 0.45              |
| 44:Ca:55:ASP:OD1   | 44:Ca:55:ASP:N     | 2.49                     | 0.45              |
| 44:Ca:171:THR:HG22 | 44:Ca:173:GLY:H    | 1.82                     | 0.45              |
| 45:Cb:101:LYS:HB3  | 45:Cb:101:LYS:HZ3  | 1.82                     | 0.45              |
| 46:Cd:55:GLU:O     | 46:Cd:58:ARG:HB2   | 2.16                     | 0.45              |
| 47:Cg:139:THR:HG22 | 47:Cg:145:PHE:CE2  | 2.51                     | 0.45              |
| 51:Cm:50:ARG:HH11  | 51:Cm:50:ARG:HG3   | 1.80                     | 0.45              |
| 51:Cm:175:LEU:HD23 | 51:Cm:186:TYR:HE2  | 1.81                     | 0.45              |
| 56:Cv:626:VAL:HB   | 56:Cv:628:LYS:HZ1  | 1.80                     | 0.45              |
| 1:DA:776:GLY:O     | 1:DA:777:SER:HB2   | 2.16                     | 0.45              |
| 9:DQ:43:ARG:HH21   | 37:CO:371:LYS:NZ   | 2.14                     | 0.45              |
| 15:DB:587:VAL:HG11 | 15:DB:593:ARG:HE   | 1.80                     | 0.45              |
| 15:DB:993:ASP:O    | 15:DB:996:ALA:N    | 2.49                     | 0.45              |
| 16:DC:36:ASP:OD1   | 16:DC:36:ASP:N     | 2.49                     | 0.45              |
| 16:DC:293:ALA:O    | 16:DC:297:LYS:HG3  | 2.17                     | 0.45              |
| 16:DC:312:TRP:CE2  | 16:DC:320:ARG:HD3  | 2.51                     | 0.45              |
| 19:DG:395:TRP:HA   | 19:DG:451:ARG:HH12 | 1.82                     | 0.45              |
| 39:CQ:56:ARG:HH11  | 39:CQ:56:ARG:CG    | 2.30                     | 0.45              |
| 40:CR:29:LEU:HD13  | 45:Cb:127:LYS:HB2  | 1.99                     | 0.45              |
| 41:CS:32:LYS:HB2   | 41:CS:32:LYS:HE3   | 1.68                     | 0.45              |
| 42:CU:46:GLU:HG2   | 42:CU:57:VAL:HG13  | 1.99                     | 0.45              |
| 44:Ca:60:ASP:OD1   | 44:Ca:60:ASP:N     | 2.43                     | 0.45              |
| 49:Cj:11:ALA:HA    | 57:CA:81:U:P       | 2.56                     | 0.45              |
| 50:Ck:756:GLN:O    | 50:Ck:760:VAL:HG13 | 2.15                     | 0.45              |
| 51:Cm:101:MET:O    | 51:Cm:105:LEU:HG   | 2.16                     | 0.45              |
| 51:Cm:177:ARG:HD2  | 51:Cm:177:ARG:HA   | 1.49                     | 0.45              |
| 53:Cp:66:HIS:HB3   | 53:Cp:69:ARG:H     | 1.82                     | 0.45              |
| 56:Cv:336:ARG:HE   | 56:Cv:336:ARG:HB3  | 1.59                     | 0.45              |
| 1:DA:584:PHE:CZ    | 1:DA:766:PHE:HD2   | 2.34                     | 0.45              |
| 2:DD:94:LYS:HG3    | 39:CQ:12:TRP:CD1   | 2.50                     | 0.45              |
| 2:DD:247:VAL:HG23  | 12:DU:33:THR:O     | 2.16                     | 0.45              |
| 4:DL:270:THR:HG23  | 4:DL:271:PRO:HD3   | 1.97                     | 0.45              |
| 6:DN:27:ASP:OD1    | 6:DN:27:ASP:N      | 2.28                     | 0.45              |
| 9:DQ:187:ARG:HA    | 9:DQ:191:VAL:HG23  | 1.97                     | 0.45              |
| 11:DS:201:HIS:CD2  | 11:DS:203:ASP:H    | 2.23                     | 0.45              |
| 15:DB:189:VAL:HG22 | 17:DE:471:ARG:HA   | 1.97                     | 0.45              |
| 16:DC:410:ARG:HE   | 16:DC:453:LEU:HD23 | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:DC:713:TYR:CD1  | 16:DC:922:PRO:HB3  | 2.50                     | 0.45              |
| 19:DG:22:GLN:HG2   | 50:Ck:102:PRO:HD3  | 1.99                     | 0.45              |
| 19:DG:560:GLU:HB3  | 19:DG:622:ARG:HH21 | 1.81                     | 0.45              |
| 20:DH:76:LEU:HD12  | 20:DH:76:LEU:HA    | 1.78                     | 0.45              |
| 23:DT:29:TRP:O     | 23:DT:37:TYR:OH    | 2.29                     | 0.45              |
| 29:CE:398:ASP:OD1  | 29:CE:398:ASP:N    | 2.45                     | 0.45              |
| 34:CK:156:LYS:HB2  | 34:CK:156:LYS:HZ3  | 1.79                     | 0.45              |
| 34:CK:318:PRO:HD3  | 51:Cm:195:PHE:CD2  | 2.52                     | 0.45              |
| 34:CK:322:ARG:NH1  | 34:CK:326:LYS:HE2  | 2.30                     | 0.45              |
| 38:CP:135:MET:HE2  | 38:CP:135:MET:HB3  | 1.74                     | 0.45              |
| 39:CQ:180:LYS:HB3  | 39:CQ:180:LYS:HE2  | 1.74                     | 0.45              |
| 44:Ca:570:THR:HG21 | 53:Cp:16:HIS:CG    | 2.51                     | 0.45              |
| 56:Cv:229:GLU:HB2  | 56:Cv:300:GLN:HE21 | 1.81                     | 0.45              |
| 56:Cv:260:MET:HB3  | 56:Cv:299:ALA:HB2  | 1.97                     | 0.45              |
| 56:Cv:622:GLU:OE2  | 56:Cv:662:GLN:HG3  | 2.16                     | 0.45              |
| 1:DA:206:CYS:HB3   | 1:DA:266:VAL:HG21  | 1.98                     | 0.45              |
| 1:DA:252:LEU:HD13  | 44:Ca:497:TRP:CZ3  | 2.51                     | 0.45              |
| 1:DA:529:ILE:O     | 1:DA:532:ARG:N     | 2.49                     | 0.45              |
| 1:DA:1255:VAL:HG13 | 1:DA:1258:ASN:HD22 | 1.82                     | 0.45              |
| 3:DI:56:PHE:HZ     | 3:DI:93:TRP:CD1    | 2.34                     | 0.45              |
| 4:DL:267:HIS:CE1   | 68:CA:737:SPD:H42  | 2.52                     | 0.45              |
| 5:DM:77:PRO:HD3    | 56:Cv:968:LEU:O    | 2.16                     | 0.45              |
| 6:DN:258:ASP:OD2   | 6:DN:277:LYS:HG3   | 2.16                     | 0.45              |
| 16:DC:620:VAL:HG13 | 16:DC:766:VAL:HG23 | 1.98                     | 0.45              |
| 18:DF:119:HIS:CG   | 18:DF:120:ASP:N    | 2.84                     | 0.45              |
| 19:DG:192:MET:HG3  | 19:DG:214:TYR:CE2  | 2.52                     | 0.45              |
| 19:DG:411:TYR:OH   | 19:DG:451:ARG:HA   | 2.16                     | 0.45              |
| 22:DK:18:LEU:HD12  | 22:DK:18:LEU:HA    | 1.80                     | 0.45              |
| 29:CE:348:TYR:HE1  | 44:Ca:132:ARG:HH21 | 1.65                     | 0.45              |
| 32:CI:139:ASP:OD1  | 32:CI:139:ASP:N    | 2.45                     | 0.45              |
| 33:CJ:494:GLN:HE21 | 33:CJ:659:GLU:HA   | 1.82                     | 0.45              |
| 33:CJ:542:LYS:HA   | 33:CJ:542:LYS:HZ2  | 1.81                     | 0.45              |
| 34:CK:281:VAL:O    | 34:CK:309:ASP:HB2  | 2.16                     | 0.45              |
| 35:CL:18:LEU:HD23  | 35:CL:65:LEU:HB3   | 1.98                     | 0.45              |
| 35:CL:19:PHE:HB2   | 35:CL:66:PHE:HE1   | 1.81                     | 0.45              |
| 44:Ca:568:ARG:NH2  | 57:CA:144:A:OP2    | 2.44                     | 0.45              |
| 47:Cg:61:PRO:HG2   | 47:Cg:79:CYS:SG    | 2.56                     | 0.45              |
| 50:Ck:819:GLU:HG2  | 50:Ck:822:ARG:NH2  | 2.31                     | 0.45              |
| 56:Cv:604:LEU:HD23 | 56:Cv:766:THR:HG22 | 1.99                     | 0.45              |
| 57:CA:362:A:H2'    | 57:CA:363:A:O4'    | 2.17                     | 0.45              |
| 1:DA:43:TYR:HB3    | 2:DD:95:ARG:HA     | 1.99                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:DI:166:LEU:HD12   | 3:DI:166:LEU:HA    | 1.77                     | 0.45              |
| 4:DL:270:THR:HA     | 4:DL:273:THR:HB    | 1.98                     | 0.45              |
| 8:DP:180:TRP:CD1    | 8:DP:180:TRP:H     | 2.33                     | 0.45              |
| 12:DU:153:THR:HG23  | 12:DU:155:GLN:H    | 1.82                     | 0.45              |
| 17:DE:80:LEU:HD12   | 17:DE:80:LEU:HA    | 1.85                     | 0.45              |
| 20:DH:405:ARG:CZ    | 21:DJ:48:PHE:HB3   | 2.47                     | 0.45              |
| 21:DJ:271:THR:HG23  | 57:CA:434:A:OP1    | 2.16                     | 0.45              |
| 25:DW:75:MET:HA     | 47:Cg:98:PHE:CE2   | 2.52                     | 0.45              |
| 26:DX:64:SER:HA     | 26:DX:162:VAL:HG22 | 1.97                     | 0.45              |
| 29:CE:188:GLU:OE2   | 51:Cm:29:TYR:OH    | 2.34                     | 0.45              |
| 29:CE:223:ARG:N     | 29:CE:223:ARG:HD2  | 2.31                     | 0.45              |
| 30:CF:99:GLU:OE2    | 37:CO:170:ARG:NH2  | 2.49                     | 0.45              |
| 32:CI:97:GLU:OE2    | 34:CK:108:ARG:NH1  | 2.50                     | 0.45              |
| 33:CJ:792:HIS:HB3   | 33:CJ:795:LYS:HB2  | 1.98                     | 0.45              |
| 37:CO:127:THR:HG22  | 37:CO:131:LYS:HZ3  | 1.82                     | 0.45              |
| 40:CR:28:GLY:C      | 45:Cb:91:ARG:HH12  | 2.24                     | 0.45              |
| 44:Ca:290:MET:HB3   | 44:Ca:291:TYR:CD1  | 2.52                     | 0.45              |
| 50:Ck:391:ALA:O     | 50:Ck:395:MET:HG3  | 2.17                     | 0.45              |
| 51:Cm:71:PRO:HB3    | 51:Cm:148:ILE:HG12 | 1.98                     | 0.45              |
| 55:Cr:266:GLN:O     | 55:Cr:270:LYS:HG3  | 2.17                     | 0.45              |
| 1:DA:1191:ILE:HD12  | 1:DA:1309:ILE:HG23 | 1.98                     | 0.45              |
| 2:DD:359:LEU:HD23   | 2:DD:359:LEU:HA    | 1.79                     | 0.45              |
| 2:DD:685:VAL:HG22   | 38:CP:100:LYS:HD2  | 1.99                     | 0.45              |
| 2:DD:689:LEU:HA     | 2:DD:690:PRO:HD3   | 1.84                     | 0.45              |
| 4:DL:118:ASP:OD1    | 4:DL:119:MET:N     | 2.50                     | 0.45              |
| 5:DM:40:TYR:CE2     | 44:Ca:286:ARG:HD2  | 2.51                     | 0.45              |
| 7:DO:249:ASP:OD1    | 7:DO:249:ASP:N     | 2.48                     | 0.45              |
| 8:DP:194:GLN:HG3    | 8:DP:195:THR:H     | 1.82                     | 0.45              |
| 10:DR:266:TRP:CD2   | 49:Cj:210:PRO:HA   | 2.51                     | 0.45              |
| 12:DU:43:PRO:HB2    | 12:DU:64:TYR:OH    | 2.17                     | 0.45              |
| 12:DU:103:ILE:H     | 12:DU:103:ILE:HG13 | 1.47                     | 0.45              |
| 12:DU:114:VAL:O     | 12:DU:118:VAL:HG23 | 2.17                     | 0.45              |
| 15:DB:97:ARG:HA     | 15:DB:104:SER:O    | 2.17                     | 0.45              |
| 15:DB:150:PHE:O     | 15:DB:154:ARG:HG2  | 2.17                     | 0.45              |
| 15:DB:224:LEU:HD13  | 17:DE:636:TYR:CD2  | 2.51                     | 0.45              |
| 15:DB:1058:ILE:HG22 | 15:DB:1060:GLU:H   | 1.82                     | 0.45              |
| 16:DC:92:PHE:C      | 16:DC:94:ASN:H     | 2.23                     | 0.45              |
| 16:DC:881:MET:O     | 16:DC:885:LEU:HB2  | 2.16                     | 0.45              |
| 18:DF:66:GLY:HA2    | 41:CS:96:GLY:O     | 2.16                     | 0.45              |
| 19:DG:387:ARG:HH21  | 19:DG:480:GLU:CD   | 2.25                     | 0.45              |
| 20:DH:88:HIS:CE1    | 20:DH:89:VAL:HG23  | 2.52                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 20:DH:354:LEU:HD12 | 20:DH:354:LEU:HA    | 1.83                     | 0.45              |
| 21:DJ:48:PHE:HD1   | 21:DJ:49:ALA:N      | 2.15                     | 0.45              |
| 22:DK:303:TYR:HB2  | 22:DK:306:GLU:HG3   | 1.99                     | 0.45              |
| 27:DY:76:ARG:NH1   | 57:CA:534:A:O2'     | 2.42                     | 0.45              |
| 29:CE:83:MET:CE    | 29:CE:83:MET:H      | 2.29                     | 0.45              |
| 39:CQ:56:ARG:NH1   | 57:CA:99:G:OP1      | 2.47                     | 0.45              |
| 47:Cg:91:GLU:HA    | 47:Cg:210:TYR:CD2   | 2.52                     | 0.45              |
| 49:Cj:66:LEU:HD23  | 49:Cj:66:LEU:HA     | 1.84                     | 0.45              |
| 50:Ck:275:TRP:O    | 50:Ck:278:PHE:HB3   | 2.16                     | 0.45              |
| 50:Ck:414:MET:HE1  | 50:Ck:544:ARG:HD2   | 1.99                     | 0.45              |
| 54:Cq:250:LEU:O    | 54:Cq:253:ARG:HG3   | 2.17                     | 0.45              |
| 56:Cv:442:ASN:HA   | 56:Cv:807:GLN:HB3   | 1.99                     | 0.45              |
| 1:DA:285:TYR:OH    | 1:DA:292:PRO:O      | 2.16                     | 0.45              |
| 1:DA:1060:LEU:HD22 | 1:DA:1163:MET:HE1   | 1.98                     | 0.45              |
| 2:DD:343:TRP:CZ3   | 2:DD:345:PRO:HD3    | 2.52                     | 0.45              |
| 4:DL:109:VAL:HG11  | 32:CI:234:PHE:HE2   | 1.81                     | 0.45              |
| 4:DL:150:GLU:HG3   | 4:DL:204:MET:SD     | 2.57                     | 0.45              |
| 4:DL:174:ALA:HB2   | 56:Cv:501:HIS:CG    | 2.51                     | 0.45              |
| 15:DB:483:VAL:HG13 | 19:DG:31:TYR:HD2    | 1.82                     | 0.45              |
| 15:DB:700:TYR:O    | 15:DB:704:VAL:HG23  | 2.17                     | 0.45              |
| 15:DB:861:GLU:HG3  | 15:DB:941:ARG:HA    | 1.98                     | 0.45              |
| 15:DB:969:THR:HG22 | 15:DB:970:ASP:OD2   | 2.16                     | 0.45              |
| 16:DC:117:MET:HE3  | 17:DE:566:ARG:NH2   | 2.31                     | 0.45              |
| 16:DC:874:THR:HG22 | 16:DC:875:THR:H     | 1.81                     | 0.45              |
| 16:DC:1057:GLY:O   | 16:DC:1060:SER:OG   | 2.33                     | 0.45              |
| 16:DC:1152:PRO:CG  | 16:DC:1160:GLN:HE22 | 2.26                     | 0.45              |
| 23:DT:73:LEU:HD23  | 23:DT:73:LEU:HA     | 1.82                     | 0.45              |
| 25:DW:143:MET:HE2  | 27:DY:101:GLN:HE21  | 1.82                     | 0.45              |
| 26:DX:29:TRP:HB2   | 57:CA:472:G:O4'     | 2.17                     | 0.45              |
| 32:CI:56:GLU:HA    | 32:CI:59:ARG:NH1    | 2.31                     | 0.45              |
| 35:CL:76:LEU:HD12  | 35:CL:77:PRO:HD2    | 1.98                     | 0.45              |
| 42:CU:61:ILE:O     | 42:CU:65:VAL:HG23   | 2.16                     | 0.45              |
| 48:CI:33:LEU:HD11  | 50:Ck:785:PRO:HB3   | 1.98                     | 0.45              |
| 49:Cj:53:ASN:O     | 49:Cj:55:ARG:N      | 2.49                     | 0.45              |
| 56:Cv:718:THR:OG1  | 56:Cv:719:THR:N     | 2.50                     | 0.45              |
| 57:CA:152:U:H2'    | 57:CA:153:A:O4'     | 2.17                     | 0.45              |
| 1:DA:222:GLU:O     | 1:DA:233:ARG:HD3    | 2.17                     | 0.45              |
| 2:DD:544:ALA:O     | 2:DD:548:GLN:HG2    | 2.16                     | 0.45              |
| 7:DO:201:GLU:N     | 7:DO:230:ILE:HD11   | 2.32                     | 0.45              |
| 10:DR:30:TRP:CE3   | 12:DU:98:MET:HB2    | 2.52                     | 0.45              |
| 10:DR:114:SER:HB3  | 10:DR:120:VAL:HG23  | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:DU:83:ARG:HD3   | 12:DU:159:ASP:OD1  | 2.17                     | 0.45              |
| 15:DB:554:GLU:O    | 15:DB:567:ARG:HD2  | 2.17                     | 0.45              |
| 15:DB:562:GLN:HE22 | 18:DF:571:LEU:HA   | 1.81                     | 0.45              |
| 16:DC:164:SER:HA   | 16:DC:165:PRO:HD3  | 1.73                     | 0.45              |
| 16:DC:855:ARG:HH12 | 17:DE:202:HIS:CE1  | 2.35                     | 0.45              |
| 19:DG:117:VAL:HG13 | 19:DG:145:VAL:CG1  | 2.47                     | 0.45              |
| 20:DH:480:ASP:OD1  | 33:CJ:16:ARG:NH1   | 2.50                     | 0.45              |
| 20:DH:504:ARG:HH12 | 22:DK:287:ILE:HG12 | 1.82                     | 0.45              |
| 30:CF:138:ILE:HD13 | 56:Cv:634:PHE:CE1  | 2.52                     | 0.45              |
| 33:CJ:103:PRO:HD2  | 33:CJ:112:ARG:NH2  | 2.32                     | 0.45              |
| 33:CJ:555:TRP:HB3  | 33:CJ:566:VAL:HG13 | 1.99                     | 0.45              |
| 34:CK:26:ARG:HB2   | 57:CA:460:U:H5     | 1.80                     | 0.45              |
| 35:CL:9:LEU:HG     | 35:CL:81:TYR:HE1   | 1.82                     | 0.45              |
| 37:CO:123:ASN:OD1  | 37:CO:191:LYS:NZ   | 2.47                     | 0.45              |
| 40:CR:234:ALA:HA   | 40:CR:237:ARG:HB3  | 1.99                     | 0.45              |
| 40:CR:308:MET:HE3  | 57:CA:388:U:H5'    | 1.99                     | 0.45              |
| 44:Ca:95:TRP:CD1   | 44:Ca:95:TRP:H     | 2.35                     | 0.45              |
| 47:Cg:184:HIS:HA   | 47:Cg:296:HIS:CE1  | 2.52                     | 0.45              |
| 47:Cg:462:GLU:HA   | 47:Cg:465:TRP:NE1  | 2.32                     | 0.45              |
| 48:Ci:145:ASN:HD21 | 48:Ci:152:ASN:HD21 | 1.65                     | 0.45              |
| 50:Ck:700:VAL:O    | 50:Ck:703:ARG:HG3  | 2.17                     | 0.45              |
| 56:Cv:39:MET:HB3   | 56:Cv:44:ARG:HD2   | 1.99                     | 0.45              |
| 57:CA:261:U:OP2    | 68:CA:738:SPD:H42  | 2.17                     | 0.45              |
| 1:DA:112:GLN:HE22  | 39:CQ:83:LEU:HD21  | 1.80                     | 0.45              |
| 1:DA:441:SER:HA    | 1:DA:442:PRO:HD2   | 1.75                     | 0.45              |
| 2:DD:351:SER:O     | 2:DD:353:HIS:N     | 2.50                     | 0.45              |
| 3:DI:256:ARG:NH1   | 3:DI:271:TYR:O     | 2.50                     | 0.45              |
| 6:DN:77:LEU:HB3    | 6:DN:78:PRO:HD3    | 1.98                     | 0.45              |
| 11:DS:207:TRP:CZ2  | 38:CP:134:ILE:HG23 | 2.52                     | 0.45              |
| 15:DB:1099:LEU:HB2 | 18:DF:108:LEU:HD11 | 1.98                     | 0.45              |
| 15:DB:1101:GLN:HB2 | 33:CJ:680:LEU:HD22 | 1.99                     | 0.45              |
| 16:DC:114:GLU:OE1  | 16:DC:118:GLY:HA2  | 2.17                     | 0.45              |
| 16:DC:673:VAL:HG12 | 16:DC:674:THR:O    | 2.17                     | 0.45              |
| 19:DG:146:LEU:HD23 | 19:DG:202:LEU:HD11 | 1.99                     | 0.45              |
| 21:DJ:180:LEU:HD23 | 21:DJ:180:LEU:HA   | 1.80                     | 0.45              |
| 28:CC:17:GLN:O     | 28:CC:19:TYR:N     | 2.50                     | 0.45              |
| 30:CF:11:LYS:HD2   | 30:CF:53:ASP:OD2   | 2.16                     | 0.45              |
| 30:CF:143:GLU:OE2  | 34:CK:158:ARG:HD3  | 2.17                     | 0.45              |
| 32:CI:313:ASP:C    | 32:CI:315:GLU:N    | 2.74                     | 0.45              |
| 33:CJ:175:ARG:HG2  | 33:CJ:175:ARG:HH11 | 1.82                     | 0.45              |
| 34:CK:269:MET:HG3  | 34:CK:273:GLU:OE1  | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:CO:77:TYR:CZ    | 52:Cn:249:GLN:HG3  | 2.51                     | 0.45              |
| 37:CO:426:HIS:HE1  | 57:CA:105:G:OP1    | 2.00                     | 0.45              |
| 38:CP:184:VAL:O    | 38:CP:188:LEU:HB3  | 2.17                     | 0.45              |
| 46:Cd:194:VAL:HG12 | 46:Cd:195:GLU:HG3  | 1.97                     | 0.45              |
| 54:Cq:60:LEU:HD13  | 54:Cq:64:VAL:HG21  | 1.98                     | 0.45              |
| 55:Cr:126:PHE:CE2  | 55:Cr:132:LEU:HD13 | 2.52                     | 0.45              |
| 55:Cr:176:LEU:HD12 | 55:Cr:176:LEU:HA   | 1.80                     | 0.45              |
| 1:DA:1228:LEU:HD12 | 1:DA:1228:LEU:HA   | 1.84                     | 0.44              |
| 1:DA:1455:THR:HG23 | 1:DA:1580:ASN:ND2  | 2.32                     | 0.44              |
| 5:DM:162:ARG:HG3   | 29:CE:332:ASP:O    | 2.18                     | 0.44              |
| 13:DZ:50:MET:HE3   | 44:Ca:514:THR:HG21 | 1.98                     | 0.44              |
| 16:DC:441:VAL:HG11 | 16:DC:496:LYS:HD3  | 2.00                     | 0.44              |
| 16:DC:1112:ASP:HB3 | 20:DH:52:LYS:HD2   | 1.99                     | 0.44              |
| 17:DE:729:ARG:HH22 | 50:Ck:92:ARG:HH12  | 1.65                     | 0.44              |
| 19:DG:59:LEU:O     | 32:CI:293:ARG:HD3  | 2.17                     | 0.44              |
| 19:DG:381:ASP:O    | 19:DG:384:VAL:HG13 | 2.17                     | 0.44              |
| 19:DG:392:ARG:HB3  | 19:DG:488:TYR:HE1  | 1.82                     | 0.44              |
| 20:DH:327:HIS:CD2  | 20:DH:346:GLU:HG2  | 2.52                     | 0.44              |
| 20:DH:393:GLY:HA3  | 50:Ck:691:GLN:HG2  | 1.99                     | 0.44              |
| 20:DH:501:PRO:HD2  | 22:DK:303:TYR:CE2  | 2.52                     | 0.44              |
| 21:DJ:136:ALA:HB3  | 21:DJ:168:TYR:CZ   | 2.52                     | 0.44              |
| 33:CJ:542:LYS:HA   | 33:CJ:542:LYS:NZ   | 2.33                     | 0.44              |
| 40:CR:137:THR:OG1  | 40:CR:138:ARG:N    | 2.50                     | 0.44              |
| 44:Ca:102:TRP:CH2  | 44:Ca:159:LEU:HD22 | 2.52                     | 0.44              |
| 44:Ca:228:LYS:O    | 44:Ca:232:GLN:HG2  | 2.16                     | 0.44              |
| 44:Ca:566:MET:HE2  | 44:Ca:566:MET:HB3  | 1.80                     | 0.44              |
| 46:Cd:169:ALA:HA   | 46:Cd:186:LEU:HB3  | 2.00                     | 0.44              |
| 51:Cm:181:GLN:OE1  | 51:Cm:212:PRO:HG2  | 2.16                     | 0.44              |
| 56:Cv:91:ARG:H     | 56:Cv:91:ARG:HG3   | 1.52                     | 0.44              |
| 1:DA:781:ARG:H     | 1:DA:781:ARG:HG2   | 1.60                     | 0.44              |
| 2:DD:182:LYS:O     | 2:DD:186:SER:OG    | 2.25                     | 0.44              |
| 3:DI:344:LEU:HB2   | 56:Cv:879:ILE:HD12 | 2.00                     | 0.44              |
| 5:DM:169:ALA:HB2   | 29:CE:343:TYR:CZ   | 2.52                     | 0.44              |
| 6:DN:74:HIS:O      | 6:DN:109:ASN:ND2   | 2.50                     | 0.44              |
| 6:DN:148:LEU:HD11  | 31:CH:19:LEU:HD21  | 1.98                     | 0.44              |
| 9:DQ:63:PRO:HB3    | 12:DU:34:TYR:HD2   | 1.82                     | 0.44              |
| 15:DB:384:GLN:HG3  | 15:DB:396:ARG:HG2  | 1.99                     | 0.44              |
| 15:DB:572:ASP:OD2  | 15:DB:648:ARG:HG2  | 2.17                     | 0.44              |
| 15:DB:769:VAL:HG22 | 15:DB:774:ASN:O    | 2.18                     | 0.44              |
| 15:DB:958:ASN:HD22 | 15:DB:959:PRO:CD   | 2.30                     | 0.44              |
| 18:DF:38:GLY:H     | 18:DF:41:ASN:ND2   | 2.00                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:DX:29:TRP:N     | 57:CA:472:G:OP1     | 2.50                     | 0.44              |
| 27:DY:144:HIS:HD2  | 27:DY:145:ARG:N     | 2.15                     | 0.44              |
| 28:CC:22:LYS:HB2   | 28:CC:22:LYS:HE3    | 1.71                     | 0.44              |
| 29:CE:21:MET:HG2   | 29:CE:23:GLY:H      | 1.82                     | 0.44              |
| 29:CE:413:ILE:HG22 | 29:CE:415:ILE:H     | 1.82                     | 0.44              |
| 31:CH:150:THR:O    | 31:CH:152:ILE:N     | 2.49                     | 0.44              |
| 31:CH:201:ARG:HG2  | 31:CH:201:ARG:HH11  | 1.81                     | 0.44              |
| 33:CJ:23:LYS:H     | 33:CJ:23:LYS:HG2    | 1.42                     | 0.44              |
| 33:CJ:230:PHE:CD2  | 50:Ck:710:ARG:HD2   | 2.52                     | 0.44              |
| 33:CJ:374:TRP:CE3  | 36:CN:106:GLU:HB3   | 2.52                     | 0.44              |
| 34:CK:70:ILE:HD12  | 45:Cb:189:LYS:HD3   | 1.99                     | 0.44              |
| 37:CO:399:ILE:HD12 | 37:CO:400:ARG:N     | 2.32                     | 0.44              |
| 38:CP:16:ARG:C     | 38:CP:18:PRO:HD3    | 2.42                     | 0.44              |
| 43:CZ:305:HIS:CD2  | 43:CZ:307:LYS:HB2   | 2.48                     | 0.44              |
| 44:Ca:104:LEU:HD21 | 56:Cv:1091:ARG:HH12 | 1.82                     | 0.44              |
| 49:Cj:22:LEU:HD23  | 49:Cj:22:LEU:HA     | 1.72                     | 0.44              |
| 50:Ck:390:ASN:O    | 50:Ck:394:ASN:ND2   | 2.50                     | 0.44              |
| 56:Cv:334:LEU:HD21 | 56:Cv:362:LEU:HD21  | 1.98                     | 0.44              |
| 56:Cv:719:THR:O    | 56:Cv:723:ARG:HG3   | 2.17                     | 0.44              |
| 56:Cv:858:GLY:O    | 56:Cv:861:THR:HB    | 2.18                     | 0.44              |
| 57:CA:382:A:H2'    | 57:CA:383:U:C6      | 2.52                     | 0.44              |
| 57:CA:453:A:OP2    | 68:CA:736:SPD:H41   | 2.17                     | 0.44              |
| 1:DA:482:LYS:HB2   | 1:DA:492:ASN:OD1    | 2.18                     | 0.44              |
| 1:DA:732:ALA:HB3   | 1:DA:736:VAL:HG21   | 1.99                     | 0.44              |
| 1:DA:834:PRO:HA    | 1:DA:837:ARG:HH11   | 1.82                     | 0.44              |
| 1:DA:1542:SER:OG   | 1:DA:1552:GLU:OE1   | 2.35                     | 0.44              |
| 2:DD:15:ALA:HB2    | 57:CA:277:A:N1      | 2.33                     | 0.44              |
| 2:DD:340:ARG:HH12  | 12:DU:60:THR:HG23   | 1.82                     | 0.44              |
| 2:DD:471:GLU:HB3   | 2:DD:475:ALA:HB3    | 1.99                     | 0.44              |
| 3:DI:24:VAL:HG12   | 3:DI:25:PRO:O       | 2.17                     | 0.44              |
| 6:DN:68:PHE:CD2    | 6:DN:69:VAL:HG23    | 2.52                     | 0.44              |
| 7:DO:86:ARG:NH2    | 7:DO:126:PRO:HG2    | 2.32                     | 0.44              |
| 7:DO:209:ARG:O     | 7:DO:213:GLU:HG2    | 2.16                     | 0.44              |
| 7:DO:258:ASP:OD1   | 7:DO:259:THR:N      | 2.49                     | 0.44              |
| 10:DR:41:HIS:HA    | 10:DR:44:VAL:HG12   | 1.99                     | 0.44              |
| 15:DB:898:GLN:NE2  | 50:Ck:269:GLY:O     | 2.50                     | 0.44              |
| 16:DC:307:LEU:HG   | 16:DC:310:ARG:O     | 2.18                     | 0.44              |
| 16:DC:1159:ASP:OD2 | 21:DJ:49:ALA:HB3    | 2.17                     | 0.44              |
| 18:DF:196:PHE:CD2  | 18:DF:198:HIS:HE1   | 2.35                     | 0.44              |
| 19:DG:208:PRO:HG3  | 19:DG:282:ASP:OD1   | 2.17                     | 0.44              |
| 19:DG:403:ASP:HB3  | 19:DG:409:LYS:NZ    | 2.32                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DK:34:ASN:HA    | 22:DK:38:VAL:O     | 2.17                     | 0.44              |
| 28:CC:41:SER:HB3   | 28:CC:76:SER:HB3   | 2.00                     | 0.44              |
| 33:CJ:572:CYS:SG   | 33:CJ:600:PRO:HA   | 2.57                     | 0.44              |
| 37:CO:379:ARG:HG3  | 37:CO:379:ARG:NH1  | 2.32                     | 0.44              |
| 38:CP:31:MET:HE3   | 38:CP:43:TYR:CG    | 2.52                     | 0.44              |
| 38:CP:161:ARG:NH1  | 38:CP:164:TYR:CD2  | 2.86                     | 0.44              |
| 44:Ca:12:PRO:HB3   | 57:CA:219:G:OP1    | 2.17                     | 0.44              |
| 46:Cd:220:THR:HG22 | 56:Cv:641:ARG:HB3  | 1.99                     | 0.44              |
| 53:Cp:23:TYR:CE2   | 53:Cp:25:PRO:HD3   | 2.52                     | 0.44              |
| 56:Cv:1123:GLN:CD  | 56:Cv:1124:PRO:HD2 | 2.43                     | 0.44              |
| 57:CA:226:A:C2     | 57:CA:256:G:C2     | 3.05                     | 0.44              |
| 1:DA:1098:LEU:HA   | 1:DA:1098:LEU:HD12 | 1.75                     | 0.44              |
| 1:DA:1273:GLU:HG3  | 1:DA:1282:ILE:HD13 | 1.99                     | 0.44              |
| 2:DD:232:TRP:HA    | 2:DD:236:CYS:SG    | 2.58                     | 0.44              |
| 2:DD:683:ASP:O     | 46:Cd:64:GLN:NE2   | 2.51                     | 0.44              |
| 9:DQ:140:GLU:HB3   | 9:DQ:187:ARG:HH12  | 1.82                     | 0.44              |
| 10:DR:134:LEU:HB2  | 10:DR:181:VAL:O    | 2.17                     | 0.44              |
| 15:DB:862:GLY:HA2  | 15:DB:939:TRP:CH2  | 2.52                     | 0.44              |
| 16:DC:325:MET:HE2  | 16:DC:325:MET:HB3  | 1.87                     | 0.44              |
| 16:DC:533:LEU:O    | 16:DC:536:SER:OG   | 2.32                     | 0.44              |
| 16:DC:969:PRO:HG2  | 16:DC:970:GLN:HE22 | 1.82                     | 0.44              |
| 17:DE:598:VAL:O    | 17:DE:602:LYS:HB2  | 2.18                     | 0.44              |
| 21:DJ:230:LEU:HD23 | 21:DJ:230:LEU:HA   | 1.73                     | 0.44              |
| 23:DT:59:HIS:NE2   | 23:DT:60:LEU:HG    | 2.32                     | 0.44              |
| 31:CH:175:THR:OG1  | 31:CH:176:ILE:N    | 2.48                     | 0.44              |
| 31:CH:229:GLU:HG3  | 31:CH:276:ARG:HD3  | 1.98                     | 0.44              |
| 32:CI:83:GLY:HA3   | 32:CI:87:TYR:OH    | 2.17                     | 0.44              |
| 32:CI:210:THR:HA   | 32:CI:213:LEU:HD12 | 1.98                     | 0.44              |
| 32:CI:353:MET:O    | 32:CI:392:ARG:HG3  | 2.17                     | 0.44              |
| 33:CJ:446:PHE:HB3  | 50:Ck:772:ALA:HB2  | 2.00                     | 0.44              |
| 38:CP:23:ALA:HB2   | 38:CP:51:HIS:CG    | 2.52                     | 0.44              |
| 42:CU:148:ASN:H    | 42:CU:148:ASN:HD22 | 1.66                     | 0.44              |
| 44:Ca:61:LEU:HB2   | 44:Ca:76:GLN:HE22  | 1.80                     | 0.44              |
| 44:Ca:569:ARG:HA   | 44:Ca:569:ARG:HD2  | 1.54                     | 0.44              |
| 46:Cd:10:ARG:HA    | 57:CA:177:A:OP2    | 2.17                     | 0.44              |
| 50:Ck:267:TYR:CE2  | 50:Ck:348:LEU:HD23 | 2.53                     | 0.44              |
| 55:Cr:40:HIS:CD2   | 55:Cr:40:HIS:N     | 2.84                     | 0.44              |
| 56:Cv:243:ASN:OD1  | 56:Cv:244:ALA:N    | 2.51                     | 0.44              |
| 57:CA:88:A:C4      | 57:CA:89:U:C5      | 3.05                     | 0.44              |
| 1:DA:602:LEU:HD23  | 1:DA:755:GLY:O     | 2.18                     | 0.44              |
| 1:DA:681:ILE:HG13  | 1:DA:701:VAL:HG22  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:1052:ALA:CB   | 32:CI:202:LEU:HD21 | 2.44                     | 0.44              |
| 8:DP:151:PHE:O     | 8:DP:155:LEU:HB2   | 2.18                     | 0.44              |
| 16:DC:78:PRO:HG2   | 16:DC:708:TYR:CE2  | 2.51                     | 0.44              |
| 16:DC:171:GLU:HA   | 16:DC:174:ARG:NH2  | 2.31                     | 0.44              |
| 18:DF:156:ALA:O    | 57:CA:415:U:H3'    | 2.17                     | 0.44              |
| 19:DG:90:MET:O     | 19:DG:95:VAL:HB    | 2.17                     | 0.44              |
| 19:DG:102:MET:HG3  | 19:DG:127:LEU:HD23 | 2.00                     | 0.44              |
| 19:DG:162:LEU:HD21 | 50:Ck:416:ARG:HH11 | 1.83                     | 0.44              |
| 22:DK:99:ASP:C     | 22:DK:101:ASP:H    | 2.25                     | 0.44              |
| 22:DK:119:ARG:HB3  | 22:DK:150:ALA:HB1  | 1.99                     | 0.44              |
| 23:DT:102:TRP:CZ2  | 23:DT:104:PRO:HB3  | 2.52                     | 0.44              |
| 26:DX:140:TYR:OH   | 26:DX:167:HIS:NE2  | 2.51                     | 0.44              |
| 29:CE:69:GLU:O     | 29:CE:72:ALA:N     | 2.51                     | 0.44              |
| 29:CE:342:GLY:HA2  | 29:CE:345:ASP:OD2  | 2.18                     | 0.44              |
| 33:CJ:632:GLN:HB2  | 33:CJ:661:ARG:HB2  | 2.00                     | 0.44              |
| 33:CJ:718:PRO:HA   | 33:CJ:719:PRO:HD3  | 1.90                     | 0.44              |
| 35:CL:82:TYR:CD1   | 44:Ca:10:ARG:NH1   | 2.86                     | 0.44              |
| 37:CO:381:MET:HE2  | 37:CO:385:ARG:HH21 | 1.83                     | 0.44              |
| 38:CP:90:MET:HE3   | 38:CP:90:MET:HB3   | 1.70                     | 0.44              |
| 39:CQ:105:LYS:H    | 39:CQ:137:LEU:HD21 | 1.82                     | 0.44              |
| 40:CR:138:ARG:HG3  | 40:CR:179:TRP:CG   | 2.53                     | 0.44              |
| 44:Ca:427:TRP:CD2  | 46:Cd:53:GLN:HB2   | 2.52                     | 0.44              |
| 48:CI:109:ASN:HB2  | 48:CI:112:ASN:HD22 | 1.82                     | 0.44              |
| 55:Cr:279:ASP:HA   | 55:Cr:282:GLU:HB2  | 1.98                     | 0.44              |
| 56:Cv:38:ALA:HB2   | 57:CA:385:A:H5''   | 1.99                     | 0.44              |
| 56:Cv:915:PRO:HB2  | 56:Cv:921:VAL:HG23 | 1.99                     | 0.44              |
| 1:DA:610:TYR:O     | 1:DA:613:PRO:HD3   | 2.18                     | 0.44              |
| 6:DN:115:PRO:HA    | 6:DN:130:ASN:OD1   | 2.18                     | 0.44              |
| 6:DN:199:CYS:HB2   | 6:DN:203:GLU:OE1   | 2.17                     | 0.44              |
| 15:DB:254:ASN:HB3  | 15:DB:411:MET:SD   | 2.58                     | 0.44              |
| 15:DB:285:MET:HE1  | 50:Ck:37:ILE:HD11  | 2.00                     | 0.44              |
| 16:DC:30:THR:HG22  | 23:DT:44:ARG:HE    | 1.81                     | 0.44              |
| 16:DC:102:LEU:O    | 17:DE:158:LEU:HD13 | 2.17                     | 0.44              |
| 16:DC:978:TYR:HD2  | 17:DE:593:THR:HG21 | 1.82                     | 0.44              |
| 18:DF:444:GLN:O    | 18:DF:448:GLY:HA3  | 2.18                     | 0.44              |
| 19:DG:473:CYS:HB3  | 19:DG:477:GLN:NE2  | 2.30                     | 0.44              |
| 29:CE:306:GLU:OE1  | 44:Ca:289:LYS:NZ   | 2.49                     | 0.44              |
| 33:CJ:82:HIS:HB2   | 33:CJ:255:HIS:CD2  | 2.53                     | 0.44              |
| 37:CO:346:THR:HG23 | 39:CQ:136:ASP:O    | 2.17                     | 0.44              |
| 38:CP:173:LYS:HB3  | 38:CP:173:LYS:HE2  | 1.76                     | 0.44              |
| 44:Ca:266:GLU:HG2  | 44:Ca:305:HIS:HE1  | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Cg:195:PRO:HA   | 50:Ck:837:TRP:CD2  | 2.53                     | 0.44              |
| 50:Ck:775:ARG:CG   | 50:Ck:775:ARG:NH1  | 2.66                     | 0.44              |
| 1:DA:1089:ASP:HB3  | 1:DA:1632:LYS:HG2  | 2.00                     | 0.44              |
| 3:DI:25:PRO:HB3    | 3:DI:79:ILE:HD11   | 1.99                     | 0.44              |
| 3:DI:233:ARG:NH2   | 3:DI:272:CYS:O     | 2.45                     | 0.44              |
| 6:DN:45:ARG:HA     | 6:DN:155:ASP:HB2   | 2.00                     | 0.44              |
| 7:DO:161:PHE:O     | 7:DO:198:ARG:NH2   | 2.51                     | 0.44              |
| 8:DP:139:ARG:HA    | 8:DP:139:ARG:HD2   | 1.77                     | 0.44              |
| 11:DS:34:SER:O     | 11:DS:34:SER:OG    | 2.14                     | 0.44              |
| 12:DU:62:ARG:HG2   | 12:DU:64:TYR:CZ    | 2.53                     | 0.44              |
| 15:DB:507:LEU:HD12 | 15:DB:507:LEU:HA   | 1.73                     | 0.44              |
| 15:DB:995:VAL:O    | 15:DB:1000:ARG:HD2 | 2.18                     | 0.44              |
| 15:DB:1093:GLU:HG3 | 15:DB:1094:ASN:H   | 1.83                     | 0.44              |
| 31:CH:229:GLU:CG   | 31:CH:276:ARG:HD3  | 2.48                     | 0.44              |
| 33:CJ:395:ARG:NH2  | 36:CN:139:THR:OG1  | 2.49                     | 0.44              |
| 33:CJ:632:GLN:HG3  | 33:CJ:662:ARG:HG3  | 1.99                     | 0.44              |
| 38:CP:171:MET:HE3  | 46:Cd:67:GLU:HB3   | 1.99                     | 0.44              |
| 44:Ca:341:LEU:HB3  | 44:Ca:500:PHE:CE1  | 2.52                     | 0.44              |
| 46:Cd:217:GLU:H    | 46:Cd:217:GLU:CD   | 2.25                     | 0.44              |
| 47:Cg:342:MET:HE3  | 47:Cg:351:LYS:HE2  | 2.00                     | 0.44              |
| 47:Cg:414:ARG:NH1  | 47:Cg:418:ASN:HD21 | 2.15                     | 0.44              |
| 48:Ci:101:LEU:HG   | 48:Ci:105:ARG:HH11 | 1.83                     | 0.44              |
| 56:Cv:141:ASP:OD1  | 56:Cv:142:PRO:HD2  | 2.18                     | 0.44              |
| 57:CA:234:C:H2'    | 57:CA:235:A:C8     | 2.52                     | 0.44              |
| 57:CA:308:C:H2'    | 57:CA:309:A:H8     | 1.83                     | 0.44              |
| 57:CA:460:U:C2     | 57:CA:461:A:N6     | 2.85                     | 0.44              |
| 2:DD:298:MET:HG2   | 2:DD:314:PHE:CE1   | 2.53                     | 0.44              |
| 2:DD:361:ASN:OD1   | 2:DD:366:LEU:HA    | 2.18                     | 0.44              |
| 2:DD:458:LEU:HD23  | 2:DD:504:ASN:HD22  | 1.82                     | 0.44              |
| 4:DL:166:PHE:O     | 4:DL:171:ARG:NH2   | 2.50                     | 0.44              |
| 4:DL:240:GLU:H     | 4:DL:240:GLU:HG2   | 1.61                     | 0.44              |
| 7:DO:245:VAL:HG12  | 7:DO:246:MET:N     | 2.32                     | 0.44              |
| 9:DQ:216:ASN:OD1   | 9:DQ:216:ASN:N     | 2.46                     | 0.44              |
| 15:DB:123:ILE:H    | 15:DB:123:ILE:HD12 | 1.83                     | 0.44              |
| 16:DC:1134:HIS:CD2 | 16:DC:1136:GLU:HB2 | 2.52                     | 0.44              |
| 18:DF:131:ARG:HH22 | 18:DF:135:PRO:HG3  | 1.83                     | 0.44              |
| 18:DF:495:GLU:OE1  | 20:DH:242:ILE:HG22 | 2.18                     | 0.44              |
| 19:DG:397:PRO:HG2  | 19:DG:398:ILE:HG13 | 2.00                     | 0.44              |
| 22:DK:142:LEU:HD12 | 22:DK:142:LEU:HA   | 1.90                     | 0.44              |
| 23:DT:29:TRP:HH2   | 48:Ci:135:MET:HG3  | 1.81                     | 0.44              |
| 28:CC:25:HIS:HD2   | 28:CC:27:PHE:H     | 1.65                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:156:PRO:HG3  | 40:CR:308:MET:HE2  | 2.00                     | 0.44              |
| 33:CJ:74:TRP:CD2   | 33:CJ:75:TYR:HB2   | 2.53                     | 0.44              |
| 33:CJ:138:PRO:O    | 33:CJ:218:TYR:OH   | 2.31                     | 0.44              |
| 33:CJ:279:LYS:HG2  | 33:CJ:407:PHE:CE2  | 2.53                     | 0.44              |
| 35:CL:38:LEU:HD11  | 35:CL:40:ALA:HB2   | 2.00                     | 0.44              |
| 36:CN:149:GLU:O    | 36:CN:152:TRP:HB3  | 2.18                     | 0.44              |
| 42:CU:102:ARG:HH11 | 42:CU:102:ARG:HG3  | 1.83                     | 0.44              |
| 44:Ca:267:LEU:HD23 | 44:Ca:267:LEU:HA   | 1.67                     | 0.44              |
| 44:Ca:570:THR:HG21 | 53:Cp:16:HIS:CD2   | 2.53                     | 0.44              |
| 45:Cb:99:ALA:HB1   | 45:Cb:106:ALA:HB2  | 1.99                     | 0.44              |
| 48:Ci:122:MET:HE3  | 48:Ci:122:MET:HB3  | 1.79                     | 0.44              |
| 48:Ci:138:ASP:O    | 48:Ci:141:LYS:HB2  | 2.18                     | 0.44              |
| 49:Cj:89:THR:O     | 49:Cj:92:TYR:HB3   | 2.18                     | 0.44              |
| 49:Cj:126:TYR:HE1  | 49:Cj:128:LYS:HB3  | 1.82                     | 0.44              |
| 53:Cp:65:ILE:O     | 53:Cp:124:LYS:HG3  | 2.17                     | 0.44              |
| 53:Cp:163:PRO:HG2  | 53:Cp:165:TYR:CE1  | 2.53                     | 0.44              |
| 54:Cq:85:HIS:NE2   | 54:Cq:129:HIS:HD2  | 2.16                     | 0.44              |
| 56:Cv:292:LYS:HG2  | 56:Cv:512:MET:CE   | 2.47                     | 0.44              |
| 56:Cv:472:VAL:HG12 | 56:Cv:473:LEU:HD23 | 2.00                     | 0.44              |
| 1:DA:247:ASP:OD1   | 44:Ca:553:ARG:NH1  | 2.49                     | 0.44              |
| 1:DA:301:THR:HG23  | 1:DA:306:GLU:OE1   | 2.18                     | 0.44              |
| 1:DA:908:ARG:HA    | 6:DN:160:CYS:O     | 2.17                     | 0.44              |
| 2:DD:312:GLN:HE22  | 2:DD:440:ARG:NH1   | 2.16                     | 0.44              |
| 3:DI:25:PRO:HD3    | 3:DI:68:PRO:HG3    | 2.00                     | 0.44              |
| 5:DM:130:ASP:C     | 5:DM:164:ILE:HD11  | 2.42                     | 0.44              |
| 7:DO:151:GLU:HB2   | 56:Cv:608:ARG:HD3  | 2.00                     | 0.44              |
| 9:DQ:45:ARG:HD3    | 57:CA:111:A:H2'    | 1.99                     | 0.44              |
| 15:DB:206:LEU:HA   | 15:DB:206:LEU:HD23 | 1.82                     | 0.44              |
| 16:DC:144:TYR:O    | 16:DC:148:LEU:HB2  | 2.17                     | 0.44              |
| 17:DE:228:TYR:CD2  | 17:DE:424:GLY:HA3  | 2.52                     | 0.44              |
| 19:DG:169:ASN:ND2  | 19:DG:207:ARG:HG3  | 2.33                     | 0.44              |
| 20:DH:348:LYS:O    | 20:DH:348:LYS:HG3  | 2.16                     | 0.44              |
| 24:DV:31:HIS:CE1   | 24:DV:48:HIS:HE1   | 2.35                     | 0.44              |
| 24:DV:41:THR:HG22  | 24:DV:42:PHE:CD1   | 2.52                     | 0.44              |
| 26:DX:102:MET:HE2  | 26:DX:102:MET:HB3  | 1.80                     | 0.44              |
| 31:CH:280:MET:O    | 31:CH:280:MET:HG3  | 2.18                     | 0.44              |
| 32:CI:397:ASN:O    | 32:CI:401:LYS:HG2  | 2.18                     | 0.44              |
| 33:CJ:230:PHE:CG   | 50:Ck:710:ARG:HD2  | 2.53                     | 0.44              |
| 37:CO:311:ILE:O    | 37:CO:311:ILE:HG22 | 2.18                     | 0.44              |
| 39:CQ:93:ASP:OD1   | 39:CQ:148:LYS:HG2  | 2.17                     | 0.44              |
| 39:CQ:136:ASP:C    | 39:CQ:136:ASP:OD1  | 2.61                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:CU:127:VAL:HA   | 42:CU:135:VAL:HG21 | 1.99                     | 0.44              |
| 44:Ca:229:GLU:O    | 44:Ca:232:GLN:HB2  | 2.17                     | 0.44              |
| 48:CI:124:VAL:HG12 | 48:CI:125:HIS:CD2  | 2.52                     | 0.44              |
| 52:Cn:237:ARG:NH1  | 52:Cn:237:ARG:HB2  | 2.33                     | 0.44              |
| 63:UT:6:UNK:HB2    | 63:UT:38:UNK:HG1   | 1.99                     | 0.44              |
| 1:DA:912:LEU:HD12  | 44:Ca:276:SER:HB3  | 1.99                     | 0.43              |
| 2:DD:656:LEU:HD23  | 2:DD:656:LEU:HA    | 1.80                     | 0.43              |
| 3:DI:157:SER:HB3   | 56:Cv:369:ARG:NH1  | 2.33                     | 0.43              |
| 4:DL:67:ASN:ND2    | 29:CE:122:TRP:O    | 2.51                     | 0.43              |
| 4:DL:228:MET:HG3   | 4:DL:229:THR:HG22  | 1.99                     | 0.43              |
| 4:DL:292:ARG:NH2   | 33:CJ:389:THR:H    | 2.15                     | 0.43              |
| 8:DP:128:LEU:HD22  | 8:DP:161:VAL:HG21  | 1.99                     | 0.43              |
| 15:DB:789:ASN:O    | 15:DB:791:GLU:HG3  | 2.18                     | 0.43              |
| 15:DB:905:TYR:CD1  | 15:DB:918:VAL:HG22 | 2.52                     | 0.43              |
| 16:DC:215:PRO:HA   | 16:DC:256:ILE:HD12 | 1.99                     | 0.43              |
| 16:DC:344:MET:HE2  | 16:DC:344:MET:HB2  | 1.87                     | 0.43              |
| 17:DE:200:ARG:HG2  | 17:DE:415:LEU:HD13 | 2.00                     | 0.43              |
| 18:DF:16:GLU:H     | 18:DF:16:GLU:HG3   | 1.45                     | 0.43              |
| 19:DG:204:SER:OG   | 19:DG:205:GLY:N    | 2.51                     | 0.43              |
| 19:DG:399:ARG:HA   | 19:DG:411:TYR:CE2  | 2.53                     | 0.43              |
| 21:DJ:81:PRO:HG2   | 21:DJ:82:GLN:NE2   | 2.33                     | 0.43              |
| 32:CI:202:LEU:HA   | 32:CI:211:ASN:HD21 | 1.83                     | 0.43              |
| 34:CK:82:MET:HA    | 34:CK:82:MET:HE2   | 1.99                     | 0.43              |
| 34:CK:86:SER:O     | 45:Cb:159:ARG:NH2  | 2.51                     | 0.43              |
| 34:CK:231:ASP:HB3  | 34:CK:232:ARG:HD2  | 1.99                     | 0.43              |
| 35:CL:13:CYS:C     | 35:CL:14:LEU:HD12  | 2.43                     | 0.43              |
| 40:CR:79:ASN:O     | 40:CR:82:ARG:HB2   | 2.18                     | 0.43              |
| 50:Ck:691:GLN:O    | 50:Ck:695:GLN:HB2  | 2.18                     | 0.43              |
| 55:Cr:177:LEU:HD23 | 55:Cr:177:LEU:HA   | 1.84                     | 0.43              |
| 56:Cv:202:LYS:NZ   | 56:Cv:610:ARG:HB3  | 2.32                     | 0.43              |
| 56:Cv:493:THR:HB   | 56:Cv:529:PHE:HD1  | 1.82                     | 0.43              |
| 1:DA:101:ASN:OD1   | 1:DA:101:ASN:N     | 2.44                     | 0.43              |
| 1:DA:274:LEU:HD23  | 1:DA:274:LEU:HA    | 1.83                     | 0.43              |
| 1:DA:409:LEU:HD23  | 1:DA:409:LEU:HA    | 1.82                     | 0.43              |
| 1:DA:1081:GLN:HA   | 1:DA:1642:LEU:HD21 | 2.01                     | 0.43              |
| 2:DD:498:GLU:H     | 2:DD:498:GLU:CD    | 2.26                     | 0.43              |
| 3:DI:48:LEU:HD23   | 3:DI:165:ARG:HH21  | 1.83                     | 0.43              |
| 4:DL:77:LEU:HD23   | 4:DL:77:LEU:HA     | 1.71                     | 0.43              |
| 4:DL:214:TYR:C     | 4:DL:214:TYR:CD2   | 2.96                     | 0.43              |
| 5:DM:292:ASN:O     | 32:CI:208:HIS:NE2  | 2.49                     | 0.43              |
| 8:DP:23:LEU:HD22   | 8:DP:23:LEU:HA     | 1.83                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:DQ:59:GLN:HB2    | 9:DQ:158:PHE:CE1    | 2.53                     | 0.43              |
| 9:DQ:77:LEU:HD23   | 9:DQ:77:LEU:HA      | 1.90                     | 0.43              |
| 9:DQ:142:PHE:CD2   | 9:DQ:246:VAL:HG21   | 2.53                     | 0.43              |
| 14:Da:30:HIS:CG    | 14:Da:31:PRO:HD2    | 2.53                     | 0.43              |
| 15:DB:549:LEU:HD23 | 15:DB:554:GLU:HG2   | 1.99                     | 0.43              |
| 15:DB:1041:ARG:HG2 | 15:DB:1042:TYR:CD2  | 2.53                     | 0.43              |
| 16:DC:699:VAL:HA   | 16:DC:700:PRO:HD2   | 1.73                     | 0.43              |
| 18:DF:33:GLN:HG2   | 48:Ci:134:ARG:HH22  | 1.83                     | 0.43              |
| 20:DH:345:VAL:O    | 20:DH:348:LYS:HB3   | 2.19                     | 0.43              |
| 25:DW:150:VAL:O    | 25:DW:152:PRO:HD3   | 2.18                     | 0.43              |
| 29:CE:417:ASN:HD22 | 29:CE:417:ASN:C     | 2.26                     | 0.43              |
| 30:CF:67:LEU:HD22  | 30:CF:69:LEU:HD21   | 2.00                     | 0.43              |
| 31:CH:18:PRO:C     | 31:CH:19:LEU:HD13   | 2.43                     | 0.43              |
| 33:CJ:416:MET:HE2  | 33:CJ:416:MET:HB3   | 1.83                     | 0.43              |
| 33:CJ:765:GLY:O    | 48:Ci:14:ARG:NH1    | 2.52                     | 0.43              |
| 35:CL:74:VAL:HG13  | 35:CL:76:LEU:H      | 1.82                     | 0.43              |
| 38:CP:146:MET:O    | 38:CP:150:LEU:HG    | 2.18                     | 0.43              |
| 41:CS:161:ARG:HH21 | 41:CS:172:LYS:HD2   | 1.83                     | 0.43              |
| 45:Cb:301:THR:HG23 | 55:Cr:180:TRP:HH2   | 1.82                     | 0.43              |
| 49:Cj:219:GLU:H    | 49:Cj:219:GLU:CD    | 2.25                     | 0.43              |
| 56:Cv:1068:LEU:HA  | 56:Cv:1068:LEU:HD23 | 1.73                     | 0.43              |
| 1:DA:870:GLU:O     | 1:DA:874:ARG:HG3    | 2.17                     | 0.43              |
| 1:DA:1541:LYS:HA   | 1:DA:1541:LYS:HD3   | 1.87                     | 0.43              |
| 1:DA:1606:THR:HG22 | 1:DA:1607:MET:HG3   | 1.98                     | 0.43              |
| 8:DP:89:PRO:HB2    | 8:DP:121:LEU:HD13   | 2.00                     | 0.43              |
| 8:DP:120:ASP:C     | 8:DP:160:ARG:HH12   | 2.26                     | 0.43              |
| 9:DQ:36:GLU:HB3    | 10:DR:28:LEU:CD1    | 2.48                     | 0.43              |
| 12:DU:87:PHE:HE1   | 12:DU:96:GLN:HB2    | 1.83                     | 0.43              |
| 15:DB:815:ASP:OD2  | 18:DF:555:ARG:HG2   | 2.17                     | 0.43              |
| 16:DC:612:TRP:CE2  | 16:DC:618:ARG:HB2   | 2.53                     | 0.43              |
| 16:DC:699:VAL:HB   | 16:DC:702:LEU:HD12  | 2.01                     | 0.43              |
| 19:DG:66:LEU:HA    | 19:DG:66:LEU:HD23   | 1.73                     | 0.43              |
| 20:DH:246:GLU:OE1  | 20:DH:279:GLU:HB2   | 2.19                     | 0.43              |
| 31:CH:113:LYS:HB2  | 31:CH:116:HIS:CD2   | 2.53                     | 0.43              |
| 31:CH:249:ARG:HH11 | 44:Ca:354:THR:HG23  | 1.83                     | 0.43              |
| 32:CI:122:LEU:HD23 | 32:CI:122:LEU:HA    | 1.83                     | 0.43              |
| 33:CJ:84:MET:HE2   | 33:CJ:84:MET:HB3    | 1.82                     | 0.43              |
| 34:CK:282:MET:HE2  | 34:CK:282:MET:HB3   | 1.77                     | 0.43              |
| 36:CN:81:LEU:HD23  | 36:CN:83:LYS:HZ3    | 1.82                     | 0.43              |
| 36:CN:127:LEU:HD22 | 36:CN:128:LEU:H     | 1.84                     | 0.43              |
| 37:CO:195:SER:O    | 37:CO:199:LYS:HG3   | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:CS:32:LYS:NZ    | 57:CA:493:U:H4'    | 2.33                     | 0.43              |
| 50:Ck:341:LEU:HB3  | 50:Ck:345:SER:HB3  | 2.01                     | 0.43              |
| 50:Ck:395:MET:SD   | 50:Ck:568:LEU:HD23 | 2.58                     | 0.43              |
| 50:Ck:596:GLY:O    | 50:Ck:600:LEU:HG   | 2.17                     | 0.43              |
| 50:Ck:622:LEU:HD12 | 50:Ck:622:LEU:HA   | 1.80                     | 0.43              |
| 51:Cm:193:PHE:HD2  | 51:Cm:197:ALA:HB1  | 1.84                     | 0.43              |
| 53:Cp:124:LYS:O    | 53:Cp:128:LEU:HB2  | 2.18                     | 0.43              |
| 56:Cv:1003:HIS:HA  | 56:Cv:1004:PRO:HD3 | 1.89                     | 0.43              |
| 62:US:46:UNK:HG3   | 62:US:49:UNK:CB    | 2.48                     | 0.43              |
| 1:DA:105:PHE:CD1   | 39:CQ:83:LEU:HD13  | 2.53                     | 0.43              |
| 1:DA:288:GLU:OE1   | 1:DA:288:GLU:N     | 2.51                     | 0.43              |
| 1:DA:577:ASP:CG    | 1:DA:578:LYS:N     | 2.77                     | 0.43              |
| 2:DD:64:HIS:CD2    | 44:Ca:447:ILE:HG21 | 2.48                     | 0.43              |
| 2:DD:341:PRO:O     | 12:DU:155:GLN:NE2  | 2.51                     | 0.43              |
| 5:DM:76:ASN:HD22   | 5:DM:76:ASN:HA     | 1.64                     | 0.43              |
| 6:DN:229:THR:O     | 29:CE:28:ILE:HD12  | 2.18                     | 0.43              |
| 7:DO:245:VAL:HA    | 46:Cd:129:ARG:NH2  | 2.32                     | 0.43              |
| 11:DS:234:LEU:C    | 11:DS:236:LEU:H    | 2.27                     | 0.43              |
| 15:DB:528:PHE:O    | 15:DB:529:LEU:HB2  | 2.18                     | 0.43              |
| 15:DB:587:VAL:HG23 | 15:DB:591:GLU:HB2  | 1.99                     | 0.43              |
| 15:DB:650:LEU:HD12 | 15:DB:845:VAL:HG23 | 1.99                     | 0.43              |
| 15:DB:1047:TRP:CD2 | 21:DJ:41:PRO:HD3   | 2.54                     | 0.43              |
| 16:DC:422:VAL:O    | 16:DC:426:VAL:HG23 | 2.18                     | 0.43              |
| 17:DE:659:ARG:O    | 17:DE:662:VAL:HB   | 2.18                     | 0.43              |
| 18:DF:58:ASP:HB3   | 36:CN:79:TYR:CE1   | 2.54                     | 0.43              |
| 18:DF:119:HIS:CG   | 18:DF:120:ASP:H    | 2.37                     | 0.43              |
| 25:DW:112:PHE:HA   | 25:DW:113:PRO:HD3  | 1.90                     | 0.43              |
| 29:CE:297:ILE:O    | 29:CE:300:ILE:HG22 | 2.17                     | 0.43              |
| 34:CK:201:ARG:NH2  | 57:CA:305:A:OP1    | 2.41                     | 0.43              |
| 34:CK:257:LYS:HE2  | 34:CK:257:LYS:HB2  | 1.89                     | 0.43              |
| 37:CO:77:TYR:HA    | 37:CO:78:PRO:HD3   | 1.83                     | 0.43              |
| 39:CQ:131:PHE:HB3  | 39:CQ:157:LYS:HG2  | 2.00                     | 0.43              |
| 46:Cd:278:ALA:HB3  | 46:Cd:281:MET:HG3  | 1.99                     | 0.43              |
| 48:Ci:153:ARG:HH12 | 57:CA:480:C:H4'    | 1.83                     | 0.43              |
| 50:Ck:130:MET:HE3  | 50:Ck:325:LEU:HD23 | 1.99                     | 0.43              |
| 50:Ck:717:LEU:HD23 | 50:Ck:717:LEU:HA   | 1.74                     | 0.43              |
| 57:CA:235:A:N1     | 57:CA:251:U:H1'    | 2.33                     | 0.43              |
| 1:DA:1277:LEU:HD23 | 1:DA:1277:LEU:HA   | 1.87                     | 0.43              |
| 2:DD:203:GLN:NE2   | 46:Cd:81:ASN:HD21  | 2.17                     | 0.43              |
| 2:DD:447:VAL:HG13  | 2:DD:491:GLY:HA2   | 2.01                     | 0.43              |
| 4:DL:218:TYR:O     | 4:DL:222:VAL:HG23  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:DM:245:ASN:OD1   | 44:Ca:259:GLU:HG3  | 2.18                     | 0.43              |
| 9:DQ:166:ILE:HB    | 9:DQ:208:VAL:HB    | 2.01                     | 0.43              |
| 15:DB:158:ARG:HG2  | 17:DE:218:SER:HB3  | 2.01                     | 0.43              |
| 15:DB:975:LYS:HA   | 19:DG:92:GLN:HE22  | 1.84                     | 0.43              |
| 15:DB:1134:GLU:OE1 | 15:DB:1134:GLU:N   | 2.50                     | 0.43              |
| 16:DC:41:ASN:ND2   | 23:DT:168:GLU:O    | 2.51                     | 0.43              |
| 16:DC:116:TYR:O    | 17:DE:150:ARG:NH1  | 2.52                     | 0.43              |
| 17:DE:195:ILE:HG23 | 17:DE:198:CYS:SG   | 2.59                     | 0.43              |
| 18:DF:561:LEU:HD23 | 18:DF:561:LEU:HA   | 1.82                     | 0.43              |
| 19:DG:607:LEU:O    | 19:DG:611:LEU:HB2  | 2.19                     | 0.43              |
| 20:DH:296:CYS:SG   | 50:Ck:98:ARG:NH2   | 2.91                     | 0.43              |
| 24:DV:78:ASP:O     | 24:DV:82:VAL:HG23  | 2.19                     | 0.43              |
| 29:CE:16:TYR:CD2   | 44:Ca:342:PHE:HA   | 2.53                     | 0.43              |
| 29:CE:288:SER:OG   | 31:CH:215:THR:HG23 | 2.18                     | 0.43              |
| 29:CE:340:LYS:HA   | 29:CE:343:TYR:HB2  | 1.99                     | 0.43              |
| 31:CH:186:HIS:HD2  | 56:Cv:240:ARG:HH21 | 1.65                     | 0.43              |
| 32:CI:265:ASP:O    | 32:CI:266:SER:OG   | 2.34                     | 0.43              |
| 33:CJ:772:PHE:HB2  | 33:CJ:778:TRP:NE1  | 2.33                     | 0.43              |
| 35:CL:71:GLY:H     | 57:CA:267:U:P      | 2.41                     | 0.43              |
| 37:CO:304:ASP:OD1  | 37:CO:304:ASP:N    | 2.28                     | 0.43              |
| 37:CO:399:ILE:H    | 37:CO:399:ILE:HG13 | 1.58                     | 0.43              |
| 52:Cn:167:ARG:NH1  | 57:CA:544:U:O4     | 2.49                     | 0.43              |
| 56:Cv:41:ILE:HD12  | 56:Cv:41:ILE:HA    | 1.89                     | 0.43              |
| 56:Cv:852:PRO:O    | 56:Cv:856:ARG:HB3  | 2.18                     | 0.43              |
| 57:CA:171:A:N3     | 57:CA:171:A:H2'    | 2.33                     | 0.43              |
| 57:CA:293:A:H2'    | 57:CA:294:A:H8     | 1.83                     | 0.43              |
| 1:DA:316:HIS:CD2   | 1:DA:317:ARG:HG3   | 2.54                     | 0.43              |
| 1:DA:1271:LEU:O    | 1:DA:1275:MET:HG3  | 2.19                     | 0.43              |
| 4:DL:214:TYR:CD2   | 32:CI:219:LEU:HD11 | 2.53                     | 0.43              |
| 4:DL:286:THR:HG21  | 28:CC:73:ILE:HD11  | 2.00                     | 0.43              |
| 5:DM:198:THR:HG22  | 5:DM:199:LEU:H     | 1.84                     | 0.43              |
| 6:DN:224:ARG:HD2   | 6:DN:224:ARG:HA    | 1.77                     | 0.43              |
| 7:DO:62:LEU:HD21   | 7:DO:109:VAL:HG22  | 2.00                     | 0.43              |
| 7:DO:175:TYR:OH    | 37:CO:151:LYS:HA   | 2.17                     | 0.43              |
| 7:DO:252:VAL:HB    | 7:DO:253:PRO:HD3   | 2.00                     | 0.43              |
| 10:DR:157:LEU:HD12 | 10:DR:157:LEU:HA   | 1.86                     | 0.43              |
| 10:DR:239:PRO:HA   | 10:DR:240:PRO:HD2  | 1.84                     | 0.43              |
| 11:DS:165:VAL:HG22 | 11:DS:190:THR:HG21 | 2.01                     | 0.43              |
| 15:DB:411:MET:HE2  | 15:DB:411:MET:HB3  | 1.93                     | 0.43              |
| 15:DB:496:ASP:CG   | 15:DB:589:ASP:HB2  | 2.42                     | 0.43              |
| 16:DC:198:GLU:OE1  | 16:DC:209:ALA:HB1  | 2.19                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:DC:299:LEU:CD1  | 16:DC:302:ARG:HH21  | 2.32                     | 0.43              |
| 17:DE:70:PRO:HB2   | 17:DE:198:CYS:SG    | 2.58                     | 0.43              |
| 18:DF:122:LEU:HD23 | 36:CN:37:ARG:NH2    | 2.33                     | 0.43              |
| 21:DJ:81:PRO:HG2   | 21:DJ:82:GLN:HE21   | 1.83                     | 0.43              |
| 26:DX:90:ILE:HG23  | 27:DY:161:ARG:HB2   | 2.00                     | 0.43              |
| 29:CE:280:ARG:HD2  | 31:CH:217:ASN:HD21  | 1.83                     | 0.43              |
| 31:CH:150:THR:C    | 31:CH:152:ILE:N     | 2.76                     | 0.43              |
| 34:CK:181:MET:HE3  | 34:CK:181:MET:HB2   | 1.85                     | 0.43              |
| 34:CK:282:MET:HE3  | 34:CK:312:PRO:HD2   | 2.01                     | 0.43              |
| 40:CR:142:MET:HE2  | 40:CR:142:MET:HB3   | 1.73                     | 0.43              |
| 46:Cd:275:ILE:HG23 | 57:CA:392:U:H5      | 1.82                     | 0.43              |
| 51:Cm:115:CYS:HB2  | 51:Cm:118:GLU:OE1   | 2.18                     | 0.43              |
| 52:Cn:185:TYR:O    | 52:Cn:186:LYS:HG3   | 2.17                     | 0.43              |
| 56:Cv:897:GLU:HB2  | 56:Cv:912:ARG:HE    | 1.84                     | 0.43              |
| 57:CA:259:U:H5'    | 57:CA:260:U:P       | 2.58                     | 0.43              |
| 57:CA:362:A:H8     | 57:CA:362:A:O5'     | 2.01                     | 0.43              |
| 1:DA:311:THR:HA    | 1:DA:312:PRO:HD3    | 1.76                     | 0.43              |
| 1:DA:469:ALA:N     | 56:Cv:1071:ARG:HH11 | 2.17                     | 0.43              |
| 2:DD:224:GLU:OE2   | 38:CP:182:ARG:NH2   | 2.52                     | 0.43              |
| 2:DD:248:ASP:HB2   | 12:DU:33:THR:O      | 2.18                     | 0.43              |
| 3:DI:304:ALA:HB2   | 3:DI:345:LEU:HD11   | 2.00                     | 0.43              |
| 4:DL:170:VAL:HA    | 45:Cb:61:ILE:HD11   | 2.00                     | 0.43              |
| 6:DN:28:HIS:HE1    | 6:DN:119:TYR:OH     | 2.02                     | 0.43              |
| 15:DB:462:ASP:HB3  | 15:DB:465:GLU:HG3   | 2.01                     | 0.43              |
| 15:DB:1107:THR:O   | 36:CN:70:LYS:HE2    | 2.19                     | 0.43              |
| 16:DC:219:LEU:O    | 16:DC:223:ASP:HB2   | 2.18                     | 0.43              |
| 16:DC:574:GLN:HE21 | 16:DC:807:VAL:H     | 1.66                     | 0.43              |
| 17:DE:292:TYR:O    | 17:DE:295:TYR:HB3   | 2.18                     | 0.43              |
| 17:DE:610:LEU:HD23 | 17:DE:610:LEU:HA    | 1.81                     | 0.43              |
| 18:DF:435:THR:HG22 | 18:DF:436:ALA:N     | 2.34                     | 0.43              |
| 19:DG:84:LEU:HD12  | 19:DG:84:LEU:HA     | 1.74                     | 0.43              |
| 20:DH:18:ARG:NH2   | 57:CA:449:G:N7      | 2.66                     | 0.43              |
| 29:CE:83:MET:H     | 29:CE:83:MET:HE2    | 1.83                     | 0.43              |
| 33:CJ:148:ASN:HB3  | 33:CJ:151:ASN:HD22  | 1.82                     | 0.43              |
| 37:CO:267:ARG:HB3  | 37:CO:274:TYR:CD2   | 2.53                     | 0.43              |
| 45:Cb:179:GLU:O    | 45:Cb:182:VAL:HB    | 2.19                     | 0.43              |
| 46:Cd:164:LEU:HD13 | 46:Cd:164:LEU:HA    | 1.77                     | 0.43              |
| 47:Cg:462:GLU:HG3  | 47:Cg:465:TRP:CH2   | 2.54                     | 0.43              |
| 57:CA:106:U:H5'    | 57:CA:107:U:OP1     | 2.19                     | 0.43              |
| 1:DA:349:PRO:HG2   | 1:DA:350:TYR:CE2    | 2.53                     | 0.43              |
| 1:DA:1447:PHE:CD2  | 1:DA:1599:PHE:HD1   | 2.37                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:84:LYS:O      | 2:DD:87:MET:HB3    | 2.18                     | 0.43              |
| 2:DD:190:LEU:HA    | 2:DD:190:LEU:HD23  | 1.80                     | 0.43              |
| 2:DD:339:ARG:HB3   | 2:DD:340:ARG:H     | 1.61                     | 0.43              |
| 2:DD:575:THR:HG23  | 10:DR:208:PHE:CZ   | 2.54                     | 0.43              |
| 3:DI:269:PHE:HB3   | 3:DI:291:LEU:HB3   | 2.01                     | 0.43              |
| 8:DP:123:GLU:O     | 8:DP:161:VAL:HG12  | 2.18                     | 0.43              |
| 8:DP:132:LEU:HD21  | 8:DP:154:PHE:HE1   | 1.82                     | 0.43              |
| 9:DQ:152:PHE:HE1   | 9:DQ:168:VAL:HG22  | 1.83                     | 0.43              |
| 10:DR:255:PRO:HG2  | 10:DR:259:PHE:O    | 2.18                     | 0.43              |
| 15:DB:129:TYR:CD1  | 15:DB:129:TYR:C    | 2.96                     | 0.43              |
| 15:DB:722:ARG:HG2  | 15:DB:733:HIS:HB3  | 2.01                     | 0.43              |
| 16:DC:305:ARG:NH1  | 16:DC:359:GLU:OE1  | 2.41                     | 0.43              |
| 16:DC:669:LEU:HD12 | 16:DC:669:LEU:HA   | 1.80                     | 0.43              |
| 17:DE:406:ASP:HA   | 17:DE:409:TRP:CD1  | 2.54                     | 0.43              |
| 21:DJ:92:LEU:HD12  | 21:DJ:92:LEU:HA    | 1.84                     | 0.43              |
| 24:DV:71:GLN:HE21  | 24:DV:71:GLN:HB3   | 1.63                     | 0.43              |
| 25:DW:56:LEU:HD21  | 27:DY:20:PRO:HA    | 2.00                     | 0.43              |
| 25:DW:99:HIS:CE1   | 40:CR:272:GLU:HG2  | 2.54                     | 0.43              |
| 30:CF:15:ARG:HG3   | 30:CF:15:ARG:NH1   | 2.34                     | 0.43              |
| 31:CH:105:ILE:HG23 | 56:Cv:150:LEU:HD21 | 2.01                     | 0.43              |
| 32:CI:208:HIS:O    | 32:CI:212:PHE:HD2  | 1.99                     | 0.43              |
| 34:CK:214:LYS:HB3  | 34:CK:214:LYS:HZ2  | 1.79                     | 0.43              |
| 35:CL:9:LEU:HB3    | 35:CL:12:CYS:O     | 2.19                     | 0.43              |
| 37:CO:169:TYR:HE1  | 37:CO:175:VAL:HG13 | 1.83                     | 0.43              |
| 37:CO:263:LEU:HD23 | 37:CO:263:LEU:HA   | 1.81                     | 0.43              |
| 37:CO:352:ASN:OD1  | 37:CO:352:ASN:N    | 2.50                     | 0.43              |
| 39:CQ:172:ARG:HG2  | 39:CQ:172:ARG:NH1  | 2.33                     | 0.43              |
| 40:CR:13:LEU:HD11  | 56:Cv:803:GLN:HE22 | 1.83                     | 0.43              |
| 40:CR:226:GLU:O    | 40:CR:230:THR:HG23 | 2.19                     | 0.43              |
| 45:Cb:158:LYS:HE3  | 45:Cb:158:LYS:HB2  | 1.84                     | 0.43              |
| 45:Cb:212:GLN:OE1  | 55:Cr:50:LYS:N     | 2.52                     | 0.43              |
| 47:Cg:474:GLN:O    | 47:Cg:478:LEU:HG   | 2.19                     | 0.43              |
| 47:Cg:483:MET:HE2  | 47:Cg:483:MET:HB3  | 1.78                     | 0.43              |
| 48:CI:53:TRP:CG    | 48:CI:53:TRP:O     | 2.72                     | 0.43              |
| 50:Ck:368:HIS:ND1  | 50:Ck:369:PRO:HD2  | 2.34                     | 0.43              |
| 57:CA:590:A:C2     | 57:CA:613:U:C2     | 3.07                     | 0.43              |
| 1:DA:95:THR:OG1    | 1:DA:96:ASP:N      | 2.51                     | 0.43              |
| 1:DA:174:HIS:HB3   | 46:Cd:71:VAL:HG21  | 2.01                     | 0.43              |
| 1:DA:748:THR:O     | 1:DA:750:ARG:NH1   | 2.51                     | 0.43              |
| 1:DA:905:GLU:O     | 1:DA:908:ARG:HG2   | 2.18                     | 0.43              |
| 3:DI:166:LEU:HG    | 3:DI:210:ILE:HD11  | 2.01                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:DL:229:THR:HG22   | 51:Cm:146:TRP:HE1  | 1.82                     | 0.43              |
| 11:DS:216:TRP:CZ2   | 11:DS:220:MET:HE3  | 2.53                     | 0.43              |
| 15:DB:1100:LEU:HD23 | 15:DB:1100:LEU:HA  | 1.91                     | 0.43              |
| 20:DH:125:ALA:O     | 20:DH:129:ASN:HB2  | 2.18                     | 0.43              |
| 21:DJ:161:LEU:O     | 21:DJ:165:VAL:HG23 | 2.19                     | 0.43              |
| 24:DV:95:LEU:HD22   | 48:Ci:55:LEU:HD23  | 2.00                     | 0.43              |
| 25:DW:63:THR:HG22   | 25:DW:65:ASP:H     | 1.84                     | 0.43              |
| 29:CE:310:ARG:O     | 29:CE:315:ALA:HB2  | 2.18                     | 0.43              |
| 31:CH:91:LEU:HD23   | 31:CH:91:LEU:HA    | 1.74                     | 0.43              |
| 32:CI:110:ARG:HD2   | 42:CU:143:TRP:HA   | 2.00                     | 0.43              |
| 33:CJ:278:GLU:O     | 33:CJ:281:VAL:HG12 | 2.19                     | 0.43              |
| 33:CJ:468:LEU:O     | 33:CJ:672:ARG:HD3  | 2.18                     | 0.43              |
| 39:CQ:194:ARG:HG3   | 52:Cn:195:PHE:CE1  | 2.53                     | 0.43              |
| 44:Ca:504:ALA:HA    | 44:Ca:505:PRO:HD2  | 1.87                     | 0.43              |
| 45:Cb:12:PRO:HD3    | 51:Cm:159:PHE:CE2  | 2.54                     | 0.43              |
| 50:Ck:268:LEU:O     | 50:Ck:273:SER:HB2  | 2.19                     | 0.43              |
| 51:Cm:164:HIS:CB    | 57:CA:611:U:H5"    | 2.49                     | 0.43              |
| 53:Cp:67:ARG:HG3    | 53:Cp:124:LYS:HG2  | 1.99                     | 0.43              |
| 56:Cv:204:ILE:HD13  | 56:Cv:204:ILE:HA   | 1.76                     | 0.43              |
| 56:Cv:943:LEU:O     | 56:Cv:944:HIS:C    | 2.60                     | 0.43              |
| 56:Cv:969:ASP:O     | 56:Cv:982:VAL:HG21 | 2.19                     | 0.43              |
| 1:DA:264:LYS:H      | 1:DA:264:LYS:HE2   | 1.84                     | 0.43              |
| 1:DA:853:LYS:HB2    | 1:DA:860:HIS:CD2   | 2.54                     | 0.43              |
| 1:DA:1073:LYS:HD3   | 1:DA:1126:GLU:OE2  | 2.18                     | 0.43              |
| 1:DA:1647:SER:OG    | 1:DA:1648:ALA:N    | 2.52                     | 0.43              |
| 2:DD:208:CYS:O      | 2:DD:212:ILE:HG13  | 2.18                     | 0.43              |
| 3:DI:224:LEU:HD23   | 3:DI:224:LEU:HA    | 1.78                     | 0.43              |
| 4:DL:51:PHE:HB3     | 33:CJ:29:PRO:HD2   | 2.01                     | 0.43              |
| 11:DS:26:MET:SD     | 11:DS:33:LEU:HD13  | 2.58                     | 0.43              |
| 11:DS:89:ASN:O      | 11:DS:110:SER:HB3  | 2.19                     | 0.43              |
| 14:Da:10:ILE:HG23   | 14:Da:22:ARG:HH11  | 1.83                     | 0.43              |
| 15:DB:487:ARG:HD3   | 15:DB:1011:TRP:CD1 | 2.54                     | 0.43              |
| 16:DC:29:TYR:OH     | 23:DT:45:HIS:HD2   | 2.02                     | 0.43              |
| 17:DE:631:LEU:HB2   | 17:DE:672:PHE:CE2  | 2.54                     | 0.43              |
| 25:DW:27:LYS:H      | 25:DW:27:LYS:HG3   | 1.40                     | 0.43              |
| 25:DW:56:LEU:O      | 25:DW:58:ARG:NH1   | 2.51                     | 0.43              |
| 26:DX:34:LYS:HB2    | 26:DX:34:LYS:HE3   | 1.80                     | 0.43              |
| 29:CE:137:LEU:HD11  | 45:Cb:47:ILE:HG13  | 2.00                     | 0.43              |
| 32:CI:260:LEU:HD23  | 32:CI:260:LEU:HA   | 1.87                     | 0.43              |
| 33:CJ:557:GLU:O     | 33:CJ:561:ILE:HG13 | 2.18                     | 0.43              |
| 34:CK:195:LEU:HD12  | 34:CK:207:VAL:O    | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:CQ:75:PRO:HB3   | 57:CA:93:A:O2'     | 2.19                     | 0.43              |
| 40:CR:122:MET:HE3  | 56:Cv:195:LEU:HD12 | 2.01                     | 0.43              |
| 41:CS:161:ARG:HE   | 41:CS:172:LYS:HD2  | 1.84                     | 0.43              |
| 45:Cb:216:LYS:HD2  | 45:Cb:278:THR:HB   | 2.00                     | 0.43              |
| 46:Cd:120:LEU:HD22 | 46:Cd:120:LEU:HA   | 1.88                     | 0.43              |
| 47:Cg:289:ASN:HD22 | 47:Cg:289:ASN:H    | 1.66                     | 0.43              |
| 50:Ck:140:ARG:HA   | 50:Ck:140:ARG:HD3  | 1.84                     | 0.43              |
| 50:Ck:565:LEU:HD12 | 50:Ck:565:LEU:HA   | 1.86                     | 0.43              |
| 52:Cn:193:LEU:HD23 | 52:Cn:193:LEU:HA   | 1.77                     | 0.43              |
| 53:Cp:112:PHE:HD1  | 53:Cp:117:PRO:HA   | 1.83                     | 0.43              |
| 56:Cv:161:PHE:HA   | 56:Cv:166:HIS:HD2  | 1.84                     | 0.43              |
| 56:Cv:311:LEU:CD2  | 56:Cv:389:LEU:HD23 | 2.48                     | 0.43              |
| 56:Cv:900:VAL:HG21 | 56:Cv:910:ARG:HB3  | 2.01                     | 0.43              |
| 57:CA:293:A:H1'    | 57:CA:315:A:H5''   | 2.01                     | 0.43              |
| 1:DA:374:ARG:NH1   | 1:DA:409:LEU:O     | 2.51                     | 0.42              |
| 1:DA:1245:THR:HG23 | 1:DA:1260:VAL:HG23 | 2.00                     | 0.42              |
| 2:DD:763:TYR:CG    | 44:Ca:387:GLN:HG2  | 2.54                     | 0.42              |
| 3:DI:404:TRP:HB3   | 56:Cv:212:ARG:NH1  | 2.34                     | 0.42              |
| 5:DM:275:LEU:HD12  | 5:DM:280:ARG:HB2   | 2.01                     | 0.42              |
| 6:DN:75:VAL:HG21   | 6:DN:132:TYR:CE2   | 2.54                     | 0.42              |
| 11:DS:60:SER:O     | 11:DS:64:SER:HB3   | 2.19                     | 0.42              |
| 14:Da:28:ARG:HB2   | 14:Da:43:PHE:CE1   | 2.54                     | 0.42              |
| 16:DC:566:THR:HG23 | 16:DC:803:ALA:HB2  | 2.01                     | 0.42              |
| 17:DE:240:PRO:HD3  | 20:DH:563:HIS:NE2  | 2.33                     | 0.42              |
| 19:DG:179:LEU:HD13 | 19:DG:179:LEU:HA   | 1.77                     | 0.42              |
| 20:DH:69:VAL:HG22  | 20:DH:96:ARG:NH1   | 2.32                     | 0.42              |
| 22:DK:119:ARG:HB3  | 22:DK:150:ALA:CB   | 2.49                     | 0.42              |
| 25:DW:55:TRP:HA    | 25:DW:56:LEU:C     | 2.44                     | 0.42              |
| 29:CE:257:LYS:HB3  | 29:CE:260:ASN:HD22 | 1.84                     | 0.42              |
| 30:CF:2:VAL:HA     | 30:CF:37:ARG:NH1   | 2.33                     | 0.42              |
| 31:CH:278:LEU:HD23 | 31:CH:278:LEU:HA   | 1.80                     | 0.42              |
| 32:CI:40:TRP:HE1   | 33:CJ:163:MET:HB2  | 1.84                     | 0.42              |
| 33:CJ:405:LEU:CD2  | 33:CJ:406:PRO:HD2  | 2.48                     | 0.42              |
| 35:CL:82:TYR:CG    | 44:Ca:10:ARG:NH1   | 2.86                     | 0.42              |
| 37:CO:266:LEU:HD13 | 37:CO:274:TYR:HA   | 2.00                     | 0.42              |
| 38:CP:16:ARG:HB3   | 57:CA:172:A:C4     | 2.54                     | 0.42              |
| 38:CP:92:THR:HB    | 44:Ca:444:PHE:CD1  | 2.54                     | 0.42              |
| 45:Cb:94:LEU:HD23  | 45:Cb:126:GLU:HG3  | 2.00                     | 0.42              |
| 47:Cg:187:TRP:CZ2  | 47:Cg:201:PRO:HG2  | 2.54                     | 0.42              |
| 56:Cv:582:ASN:OD1  | 56:Cv:792:TYR:HB3  | 2.19                     | 0.42              |
| 56:Cv:833:PRO:HG2  | 56:Cv:836:GLU:OE1  | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:1060:LEU:HD23 | 1:DA:1060:LEU:HA   | 1.88                     | 0.42              |
| 1:DA:1082:TRP:HZ3  | 1:DA:1101:LEU:HD13 | 1.84                     | 0.42              |
| 2:DD:29:ARG:NH1    | 31:CH:222:CYS:O    | 2.50                     | 0.42              |
| 2:DD:357:TRP:CZ2   | 10:DR:258:CYS:HB3  | 2.54                     | 0.42              |
| 9:DQ:153:ARG:HH22  | 9:DQ:171:GLU:CD    | 2.27                     | 0.42              |
| 11:DS:56:LEU:HG    | 11:DS:88:TRP:HA    | 2.01                     | 0.42              |
| 12:DU:27:ARG:NH1   | 12:DU:27:ARG:HB3   | 2.34                     | 0.42              |
| 15:DB:302:LEU:HD23 | 15:DB:302:LEU:HA   | 1.75                     | 0.42              |
| 15:DB:981:HIS:CD2  | 15:DB:983:LEU:HB2  | 2.51                     | 0.42              |
| 16:DC:631:LYS:HD3  | 16:DC:659:LEU:HD11 | 2.00                     | 0.42              |
| 18:DF:267:ASP:OD2  | 18:DF:269:GLU:N    | 2.51                     | 0.42              |
| 20:DH:123:HIS:O    | 20:DH:126:LEU:HB3  | 2.19                     | 0.42              |
| 20:DH:347:LYS:HB3  | 20:DH:382:PHE:HE1  | 1.84                     | 0.42              |
| 20:DH:453:PRO:HB3  | 20:DH:455:TRP:CH2  | 2.54                     | 0.42              |
| 22:DK:36:ARG:C     | 22:DK:38:VAL:H     | 2.28                     | 0.42              |
| 23:DT:136:LEU:HD11 | 23:DT:151:TRP:CD1  | 2.55                     | 0.42              |
| 29:CE:62:ARG:HA    | 29:CE:62:ARG:HD2   | 1.55                     | 0.42              |
| 32:CI:106:LEU:HD11 | 34:CK:107:GLN:HE21 | 1.83                     | 0.42              |
| 34:CK:228:LYS:NZ   | 57:CA:302:U:OP2    | 2.52                     | 0.42              |
| 36:CN:127:LEU:HD23 | 36:CN:127:LEU:HA   | 1.82                     | 0.42              |
| 40:CR:101:GLN:HB3  | 40:CR:102:PRO:HD2  | 2.00                     | 0.42              |
| 41:CS:45:ARG:HB2   | 41:CS:48:ARG:HD3   | 2.00                     | 0.42              |
| 44:Ca:506:GLN:HE21 | 44:Ca:506:GLN:HB3  | 1.49                     | 0.42              |
| 45:Cb:303:GLU:HB2  | 55:Cr:105:ARG:HH12 | 1.82                     | 0.42              |
| 46:Cd:13:ARG:HH22  | 46:Cd:26:ARG:HE    | 1.67                     | 0.42              |
| 49:Cj:200:ASP:HA   | 49:Cj:201:PRO:HD3  | 1.80                     | 0.42              |
| 50:Ck:132:TYR:CE2  | 50:Ck:140:ARG:HG3  | 2.54                     | 0.42              |
| 52:Cn:170:GLN:HB2  | 57:CA:593:A:OP1    | 2.20                     | 0.42              |
| 53:Cp:52:TYR:CZ    | 53:Cp:62:ARG:HD3   | 2.54                     | 0.42              |
| 53:Cp:87:CYS:HB3   | 53:Cp:92:LEU:HD13  | 2.00                     | 0.42              |
| 54:Cq:101:LEU:HD11 | 54:Cq:119:GLN:OE1  | 2.19                     | 0.42              |
| 54:Cq:175:TRP:CZ3  | 54:Cq:235:LEU:HD23 | 2.49                     | 0.42              |
| 56:Cv:845:PHE:O    | 56:Cv:849:MET:HG2  | 2.18                     | 0.42              |
| 56:Cv:862:ASP:OD1  | 56:Cv:862:ASP:N    | 2.40                     | 0.42              |
| 62:US:25:UNK:O     | 62:US:29:UNK:HB1   | 2.19                     | 0.42              |
| 2:DD:71:HIS:NE2    | 38:CP:39:LYS:O     | 2.49                     | 0.42              |
| 2:DD:102:TRP:CH2   | 2:DD:104:ARG:HD3   | 2.55                     | 0.42              |
| 2:DD:206:TRP:CD1   | 2:DD:282:VAL:HG11  | 2.54                     | 0.42              |
| 2:DD:370:PRO:HA    | 2:DD:371:PRO:HD2   | 1.93                     | 0.42              |
| 2:DD:389:LEU:O     | 2:DD:392:SER:OG    | 2.33                     | 0.42              |
| 3:DI:71:LEU:HD23   | 3:DI:71:LEU:HA     | 1.77                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:DO:59:ALA:HB2     | 7:DO:107:ALA:HA    | 2.01                     | 0.42              |
| 7:DO:125:LEU:HD22   | 7:DO:125:LEU:HA    | 1.70                     | 0.42              |
| 15:DB:101:ARG:HD2   | 15:DB:101:ARG:HA   | 1.80                     | 0.42              |
| 15:DB:862:GLY:HA2   | 15:DB:939:TRP:CZ3  | 2.54                     | 0.42              |
| 15:DB:1111:GLN:HE21 | 15:DB:1111:GLN:HA  | 1.84                     | 0.42              |
| 16:DC:119:THR:HG21  | 16:DC:136:TRP:CD1  | 2.53                     | 0.42              |
| 16:DC:971:MET:HE3   | 16:DC:971:MET:HB3  | 1.67                     | 0.42              |
| 17:DE:181:LEU:HD23  | 17:DE:181:LEU:HA   | 1.90                     | 0.42              |
| 17:DE:299:LYS:HB2   | 17:DE:336:ILE:HD13 | 2.00                     | 0.42              |
| 18:DF:208:ARG:HH21  | 33:CJ:602:SER:HB2  | 1.84                     | 0.42              |
| 20:DH:462:GLU:H     | 20:DH:462:GLU:HG2  | 1.56                     | 0.42              |
| 21:DJ:123:LYS:HD3   | 21:DJ:123:LYS:HA   | 1.73                     | 0.42              |
| 22:DK:273:LEU:HD12  | 22:DK:273:LEU:HA   | 1.77                     | 0.42              |
| 26:DX:78:GLU:HB3    | 26:DX:80:TRP:CE2   | 2.54                     | 0.42              |
| 28:CC:44:LEU:HD13   | 28:CC:52:ILE:HG12  | 2.00                     | 0.42              |
| 29:CE:257:LYS:HB3   | 29:CE:260:ASN:ND2  | 2.34                     | 0.42              |
| 32:CI:324:ARG:HG2   | 32:CI:325:GLU:N    | 2.33                     | 0.42              |
| 33:CJ:617:ARG:HG2   | 33:CJ:653:PHE:CE1  | 2.54                     | 0.42              |
| 34:CK:198:VAL:HG13  | 34:CK:282:MET:HB2  | 2.00                     | 0.42              |
| 37:CO:330:THR:HG21  | 37:CO:332:ARG:HE   | 1.83                     | 0.42              |
| 37:CO:399:ILE:HD12  | 37:CO:400:ARG:H    | 1.85                     | 0.42              |
| 39:CQ:100:GLY:HA2   | 39:CQ:141:GLU:OE2  | 2.20                     | 0.42              |
| 40:CR:49:ARG:HB2    | 40:CR:53:GLN:HB2   | 2.01                     | 0.42              |
| 45:Cb:128:GLU:HG3   | 45:Cb:146:VAL:HG22 | 2.02                     | 0.42              |
| 45:Cb:132:LEU:HD11  | 45:Cb:145:LYS:HD3  | 2.00                     | 0.42              |
| 45:Cb:305:PRO:HG2   | 55:Cr:38:ALA:CB    | 2.50                     | 0.42              |
| 48:CI:140:ASN:ND2   | 57:CA:477:U:OP1    | 2.52                     | 0.42              |
| 49:Cj:118:ARG:HH22  | 49:Cj:168:VAL:HB   | 1.84                     | 0.42              |
| 50:Ck:639:LEU:HD23  | 50:Ck:639:LEU:HA   | 1.76                     | 0.42              |
| 55:Cr:25:LEU:HD13   | 55:Cr:83:VAL:HG22  | 2.01                     | 0.42              |
| 55:Cr:265:LEU:HD23  | 55:Cr:265:LEU:HA   | 1.75                     | 0.42              |
| 56:Cv:255:PHE:CG    | 56:Cv:292:LYS:HE3  | 2.54                     | 0.42              |
| 57:CA:112:A:N3      | 57:CA:112:A:H2'    | 2.33                     | 0.42              |
| 57:CA:340:U:O2'     | 57:CA:355:A:N6     | 2.52                     | 0.42              |
| 1:DA:365:LEU:HD22   | 1:DA:381:MET:HE1   | 2.02                     | 0.42              |
| 2:DD:638:LEU:HD23   | 2:DD:638:LEU:HA    | 1.92                     | 0.42              |
| 3:DI:183:THR:OG1    | 3:DI:184:ASN:N     | 2.53                     | 0.42              |
| 7:DO:123:LEU:HD12   | 7:DO:123:LEU:HA    | 1.67                     | 0.42              |
| 7:DO:186:MET:HE2    | 56:Cv:207:PHE:CE2  | 2.53                     | 0.42              |
| 7:DO:276:GLY:C      | 56:Cv:685:ARG:NH1  | 2.77                     | 0.42              |
| 11:DS:111:VAL:HG12  | 11:DS:117:ALA:CB   | 2.49                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:818:GLU:OE2  | 18:DF:531:ARG:NH1  | 2.53                     | 0.42              |
| 15:DB:910:PHE:HA   | 33:CJ:116:GLN:HG3  | 2.02                     | 0.42              |
| 16:DC:46:ARG:NH1   | 16:DC:475:LEU:HB3  | 2.35                     | 0.42              |
| 16:DC:196:LEU:HA   | 16:DC:217:ALA:HB1  | 2.02                     | 0.42              |
| 16:DC:255:PHE:HD1  | 16:DC:391:LEU:HD23 | 1.85                     | 0.42              |
| 17:DE:171:LEU:HD11 | 17:DE:554:LEU:HD13 | 2.01                     | 0.42              |
| 19:DG:80:LEU:N     | 19:DG:81:PRO:HD2   | 2.35                     | 0.42              |
| 21:DJ:67:ILE:HB    | 21:DJ:123:LYS:NZ   | 2.33                     | 0.42              |
| 25:DW:125:LYS:O    | 25:DW:129:VAL:HG23 | 2.20                     | 0.42              |
| 28:CC:69:GLU:HG3   | 28:CC:70:TYR:CD1   | 2.54                     | 0.42              |
| 29:CE:328:ASP:OD1  | 29:CE:328:ASP:N    | 2.51                     | 0.42              |
| 29:CE:417:ASN:HA   | 29:CE:418:PRO:HD3  | 1.90                     | 0.42              |
| 33:CJ:99:PHE:H     | 33:CJ:105:ASN:HD22 | 1.67                     | 0.42              |
| 33:CJ:226:ARG:HD2  | 33:CJ:815:ASN:ND2  | 2.31                     | 0.42              |
| 33:CJ:712:THR:OG1  | 36:CN:52:ASP:HB2   | 2.19                     | 0.42              |
| 37:CO:80:ARG:NH1   | 52:Cn:244:PRO:O    | 2.45                     | 0.42              |
| 38:CP:67:HIS:HB2   | 38:CP:92:THR:HG23  | 2.00                     | 0.42              |
| 38:CP:161:ARG:NH1  | 38:CP:164:TYR:HD2  | 2.17                     | 0.42              |
| 40:CR:153:GLU:HA   | 56:Cv:183:LEU:CD2  | 2.48                     | 0.42              |
| 41:CS:58:ILE:O     | 57:CA:489:A:H8     | 2.02                     | 0.42              |
| 42:CU:111:PHE:O    | 42:CU:114:PHE:HB3  | 2.19                     | 0.42              |
| 44:Ca:443:MET:CE   | 44:Ca:491:TRP:HE1  | 2.33                     | 0.42              |
| 49:Cj:66:LEU:HD22  | 49:Cj:67:ASP:H     | 1.83                     | 0.42              |
| 50:Ck:183:ARG:HE   | 50:Ck:183:ARG:HB2  | 1.73                     | 0.42              |
| 50:Ck:724:PHE:HD2  | 50:Ck:725:VAL:HG23 | 1.83                     | 0.42              |
| 51:Cm:85:ILE:H     | 51:Cm:85:ILE:HG13  | 1.53                     | 0.42              |
| 56:Cv:834:LEU:HD12 | 56:Cv:834:LEU:HA   | 1.71                     | 0.42              |
| 57:CA:153:A:H2'    | 57:CA:154:G:H8     | 1.85                     | 0.42              |
| 1:DA:511:LYS:HG3   | 1:DA:519:TRP:CD2   | 2.54                     | 0.42              |
| 1:DA:1014:TYR:CD2  | 4:DL:77:LEU:HD11   | 2.54                     | 0.42              |
| 1:DA:1229:THR:HG23 | 15:DB:602:TRP:CE3  | 2.54                     | 0.42              |
| 1:DA:1240:LEU:O    | 1:DA:1243:GLN:HB2  | 2.18                     | 0.42              |
| 2:DD:42:MET:HE3    | 2:DD:42:MET:HB3    | 1.75                     | 0.42              |
| 4:DL:98:ASP:OD1    | 4:DL:98:ASP:N      | 2.46                     | 0.42              |
| 4:DL:117:ASP:HB3   | 4:DL:118:ASP:H     | 1.58                     | 0.42              |
| 5:DM:4:TYR:O       | 5:DM:8:THR:OG1     | 2.37                     | 0.42              |
| 5:DM:190:PRO:C     | 5:DM:192:GLY:H     | 2.28                     | 0.42              |
| 8:DP:19:TRP:CZ3    | 8:DP:20:MET:HG2    | 2.54                     | 0.42              |
| 8:DP:189:TYR:CD1   | 8:DP:196:TRP:HB2   | 2.54                     | 0.42              |
| 9:DQ:153:ARG:HB2   | 9:DQ:237:ASP:HA    | 2.00                     | 0.42              |
| 10:DR:191:GLN:NE2  | 12:DU:137:ASP:HB2  | 2.35                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:DB:136:ARG:HG2  | 15:DB:215:TYR:CE1  | 2.55                     | 0.42              |
| 15:DB:261:LEU:HD21 | 15:DB:401:HIS:CD2  | 2.55                     | 0.42              |
| 15:DB:446:LYS:HE3  | 15:DB:450:MET:SD   | 2.59                     | 0.42              |
| 15:DB:968:VAL:HG12 | 15:DB:1001:THR:CG2 | 2.49                     | 0.42              |
| 16:DC:671:ARG:HB2  | 16:DC:785:TYR:CE2  | 2.55                     | 0.42              |
| 17:DE:570:GLU:HG3  | 20:DH:526:ASN:HB3  | 2.02                     | 0.42              |
| 17:DE:698:GLN:HE21 | 17:DE:698:GLN:HB2  | 1.57                     | 0.42              |
| 19:DG:214:TYR:CD1  | 19:DG:214:TYR:C    | 2.98                     | 0.42              |
| 22:DK:5:TYR:CD2    | 23:DT:78:GLU:HG2   | 2.50                     | 0.42              |
| 23:DT:133:ASP:HA   | 23:DT:158:HIS:HB2  | 2.02                     | 0.42              |
| 25:DW:157:ASN:HB2  | 25:DW:158:PRO:HD2  | 2.01                     | 0.42              |
| 32:CI:345:ASP:C    | 32:CI:347:LYS:H    | 2.28                     | 0.42              |
| 32:CI:393:MET:SD   | 32:CI:418:VAL:HG22 | 2.59                     | 0.42              |
| 33:CJ:685:ILE:H    | 33:CJ:685:ILE:HG13 | 1.70                     | 0.42              |
| 34:CK:77:MET:HE3   | 34:CK:77:MET:HB3   | 1.59                     | 0.42              |
| 34:CK:182:TRP:CE3  | 34:CK:185:MET:HG3  | 2.54                     | 0.42              |
| 40:CR:94:MET:O     | 40:CR:98:ARG:HB2   | 2.18                     | 0.42              |
| 42:CU:101:HIS:O    | 42:CU:105:GLN:HG3  | 2.20                     | 0.42              |
| 44:Ca:427:TRP:CE3  | 46:Cd:53:GLN:HB2   | 2.54                     | 0.42              |
| 45:Cb:22:ASP:OD1   | 45:Cb:22:ASP:N     | 2.51                     | 0.42              |
| 45:Cb:276:LYS:HE2  | 45:Cb:276:LYS:HB3  | 1.86                     | 0.42              |
| 47:Cg:37:ILE:HD13  | 47:Cg:422:LEU:HG   | 2.00                     | 0.42              |
| 47:Cg:105:HIS:CE1  | 47:Cg:420:GLY:HA2  | 2.55                     | 0.42              |
| 47:Cg:146:ILE:HA   | 47:Cg:355:THR:O    | 2.19                     | 0.42              |
| 47:Cg:443:LYS:HZ3  | 47:Cg:465:TRP:CG   | 2.38                     | 0.42              |
| 48:Ci:170:GLU:HA   | 48:Ci:171:PRO:HD2  | 1.85                     | 0.42              |
| 49:Cj:90:ARG:CZ    | 49:Cj:94:ILE:HD11  | 2.50                     | 0.42              |
| 49:Cj:217:PRO:HG2  | 49:Cj:220:PHE:CD2  | 2.55                     | 0.42              |
| 50:Ck:816:GLU:H    | 50:Ck:816:GLU:HG3  | 1.65                     | 0.42              |
| 1:DA:225:GLY:HA3   | 1:DA:233:ARG:NH1   | 2.28                     | 0.42              |
| 1:DA:492:ASN:HB2   | 1:DA:495:GLU:HB2   | 2.01                     | 0.42              |
| 1:DA:1163:MET:HE3  | 54:Cq:62:TYR:HB3   | 2.02                     | 0.42              |
| 2:DD:133:GLU:OE2   | 12:DU:50:SER:OG    | 2.33                     | 0.42              |
| 2:DD:323:LEU:HD11  | 2:DD:444:SER:OG    | 2.20                     | 0.42              |
| 2:DD:795:TRP:CE2   | 2:DD:811:PRO:HD3   | 2.54                     | 0.42              |
| 15:DB:689:LEU:HD23 | 15:DB:697:ARG:NH2  | 2.35                     | 0.42              |
| 16:DC:612:TRP:HA   | 16:DC:613:PRO:HD3  | 1.93                     | 0.42              |
| 16:DC:659:LEU:HA   | 16:DC:659:LEU:HD23 | 1.76                     | 0.42              |
| 16:DC:775:ALA:HA   | 16:DC:777:GLY:H    | 1.84                     | 0.42              |
| 16:DC:1119:GLN:HA  | 16:DC:1120:PRO:HD3 | 1.85                     | 0.42              |
| 16:DC:1123:SER:HA  | 16:DC:1124:PRO:HD3 | 1.81                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 17:DE:489:ARG:HD3   | 17:DE:489:ARG:HA   | 1.69                     | 0.42              |
| 17:DE:716:ASN:N     | 17:DE:716:ASN:OD1  | 2.51                     | 0.42              |
| 19:DG:185:ASP:OD1   | 19:DG:185:ASP:N    | 2.53                     | 0.42              |
| 19:DG:334:MET:HB3   | 19:DG:334:MET:HE2  | 1.45                     | 0.42              |
| 22:DK:6:THR:O       | 22:DK:10:ILE:HG13  | 2.19                     | 0.42              |
| 25:DW:92:LEU:HD23   | 25:DW:92:LEU:HA    | 1.86                     | 0.42              |
| 29:CE:376:LEU:O     | 29:CE:380:GLN:HG2  | 2.19                     | 0.42              |
| 33:CJ:36:MET:HE3    | 33:CJ:36:MET:HB3   | 1.89                     | 0.42              |
| 33:CJ:248:VAL:HG22  | 33:CJ:400:VAL:HG22 | 2.02                     | 0.42              |
| 34:CK:34:PRO:HG3    | 40:CR:262:SER:O    | 2.20                     | 0.42              |
| 34:CK:321:PRO:HD3   | 42:CU:16:HIS:HE1   | 1.81                     | 0.42              |
| 40:CR:318:LYS:HD3   | 57:CA:587:A:OP1    | 2.19                     | 0.42              |
| 43:CZ:277:PHE:CG    | 43:CZ:309:PRO:HD3  | 2.54                     | 0.42              |
| 44:Ca:499:ASP:O     | 44:Ca:554:THR:HG21 | 2.20                     | 0.42              |
| 45:Cb:175:ILE:HD13  | 45:Cb:175:ILE:HA   | 1.83                     | 0.42              |
| 46:Cd:122:LEU:HA    | 46:Cd:122:LEU:HD12 | 1.67                     | 0.42              |
| 46:Cd:143:GLN:HG2   | 46:Cd:143:GLN:H    | 1.73                     | 0.42              |
| 50:Ck:737:ALA:HB1   | 50:Ck:740:ARG:HB2  | 2.02                     | 0.42              |
| 53:Cp:164:ASP:O     | 53:Cp:168:ILE:HG13 | 2.19                     | 0.42              |
| 54:Cq:158:TYR:OH    | 54:Cq:198:ASP:HA   | 2.19                     | 0.42              |
| 56:Cv:445:ILE:HD13  | 56:Cv:854:PHE:CG   | 2.54                     | 0.42              |
| 57:CA:565:A:H2'     | 57:CA:565:A:N3     | 2.35                     | 0.42              |
| 63:UT:19:UNK:HA     | 63:UT:24:UNK:HB1   | 2.00                     | 0.42              |
| 1:DA:108:TYR:OH     | 1:DA:123:HIS:HD2   | 2.02                     | 0.42              |
| 1:DA:1196:LYS:HE3   | 1:DA:1221:ILE:HD11 | 2.01                     | 0.42              |
| 2:DD:159:LEU:HA     | 2:DD:159:LEU:HD12  | 1.84                     | 0.42              |
| 2:DD:347:GLU:OE1    | 2:DD:347:GLU:N     | 2.52                     | 0.42              |
| 2:DD:368:LEU:HD23   | 2:DD:368:LEU:HA    | 1.80                     | 0.42              |
| 2:DD:604:TYR:CD1    | 2:DD:616:LEU:HD23  | 2.55                     | 0.42              |
| 4:DL:18:ARG:HH21    | 57:CA:449:G:H1'    | 1.84                     | 0.42              |
| 10:DR:112:ARG:HH11  | 49:Cj:158:THR:HG23 | 1.83                     | 0.42              |
| 11:DS:233:PHE:H     | 38:CP:139:LEU:HB2  | 1.85                     | 0.42              |
| 13:DZ:78:LEU:HB3    | 13:DZ:83:LEU:HD23  | 2.01                     | 0.42              |
| 15:DB:320:GLY:O     | 15:DB:324:THR:OG1  | 2.37                     | 0.42              |
| 16:DC:635:MET:CE    | 16:DC:659:LEU:HD12 | 2.50                     | 0.42              |
| 16:DC:1000:LEU:HD23 | 16:DC:1000:LEU:HA  | 1.76                     | 0.42              |
| 18:DF:403:LEU:HD23  | 18:DF:403:LEU:HA   | 1.90                     | 0.42              |
| 21:DJ:20:SER:HA     | 36:CN:126:ASN:O    | 2.19                     | 0.42              |
| 21:DJ:232:ARG:HG2   | 57:CA:428:A:C8     | 2.55                     | 0.42              |
| 21:DJ:319:TYR:O     | 23:DT:27:ARG:NH2   | 2.53                     | 0.42              |
| 23:DT:186:TRP:CE2   | 23:DT:211:PRO:HD3  | 2.55                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:DV:171:ARG:NH2  | 47:Cg:392:LYS:HE2   | 2.34                     | 0.42              |
| 26:DX:31:LYS:HD3   | 26:DX:32:PRO:HD2    | 2.02                     | 0.42              |
| 33:CJ:551:ARG:NH2  | 33:CJ:583:LYS:O     | 2.52                     | 0.42              |
| 36:CN:111:VAL:HB   | 36:CN:113:VAL:HG22  | 2.02                     | 0.42              |
| 37:CO:170:ARG:HG2  | 37:CO:194:MET:HG2   | 2.01                     | 0.42              |
| 38:CP:49:HIS:CD2   | 38:CP:59:ARG:HG2    | 2.53                     | 0.42              |
| 38:CP:113:LYS:HB2  | 38:CP:114:PRO:HD3   | 2.01                     | 0.42              |
| 44:Ca:225:PRO:HG2  | 44:Ca:228:LYS:CB    | 2.47                     | 0.42              |
| 44:Ca:424:MET:HE2  | 44:Ca:424:MET:HB3   | 1.90                     | 0.42              |
| 46:Cd:36:ARG:NH1   | 46:Cd:39:MET:HE1    | 2.34                     | 0.42              |
| 48:Ci:34:ARG:NH2   | 48:Ci:45:ILE:HG12   | 2.34                     | 0.42              |
| 49:Cj:52:LEU:O     | 49:Cj:169:PRO:HD2   | 2.19                     | 0.42              |
| 56:Cv:111:ARG:NH2  | 56:Cv:153:SER:HA    | 2.34                     | 0.42              |
| 56:Cv:945:VAL:HG13 | 56:Cv:946:PRO:CD    | 2.50                     | 0.42              |
| 57:CA:226:A:O2'    | 57:CA:227:U:O4'     | 2.36                     | 0.42              |
| 1:DA:205:HIS:HE1   | 38:CP:85:ASP:OD2    | 2.03                     | 0.42              |
| 1:DA:466:VAL:HG13  | 56:Cv:1068:LEU:HD23 | 2.02                     | 0.42              |
| 1:DA:636:CYS:HB3   | 1:DA:642:PHE:O      | 2.20                     | 0.42              |
| 1:DA:1270:ARG:HG2  | 1:DA:1274:ARG:HH21  | 1.85                     | 0.42              |
| 2:DD:347:GLU:OE1   | 12:DU:83:ARG:NH2    | 2.53                     | 0.42              |
| 4:DL:176:ARG:HE    | 45:Cb:79:PRO:HA     | 1.85                     | 0.42              |
| 16:DC:344:MET:HE3  | 16:DC:346:ASP:OD2   | 2.20                     | 0.42              |
| 16:DC:659:LEU:HD23 | 16:DC:662:ARG:HD2   | 2.01                     | 0.42              |
| 16:DC:672:ARG:HG2  | 16:DC:673:VAL:H     | 1.85                     | 0.42              |
| 17:DE:585:ARG:HG3  | 23:DT:80:TYR:OH     | 2.20                     | 0.42              |
| 20:DH:31:GLU:OE2   | 20:DH:34:TYR:OH     | 2.23                     | 0.42              |
| 29:CE:53:LEU:C     | 29:CE:55:THR:H      | 2.27                     | 0.42              |
| 29:CE:174:GLY:HA2  | 29:CE:245:PHE:O     | 2.19                     | 0.42              |
| 31:CH:250:LEU:HD23 | 31:CH:250:LEU:HA    | 1.82                     | 0.42              |
| 32:CI:218:ARG:O    | 32:CI:221:GLU:HG2   | 2.20                     | 0.42              |
| 32:CI:250:ASN:ND2  | 32:CI:276:ASP:OD2   | 2.52                     | 0.42              |
| 32:CI:273:VAL:HG12 | 32:CI:274:LEU:HD12  | 2.02                     | 0.42              |
| 33:CJ:463:MET:HE2  | 36:CN:51:LEU:HD22   | 2.00                     | 0.42              |
| 34:CK:309:ASP:OD1  | 42:CU:44:MET:HB2    | 2.19                     | 0.42              |
| 35:CL:6:MET:HA     | 35:CL:6:MET:HE3     | 2.01                     | 0.42              |
| 36:CN:37:ARG:HD2   | 36:CN:38:ASP:OD2    | 2.20                     | 0.42              |
| 36:CN:69:ARG:HA    | 36:CN:72:THR:HG22   | 2.02                     | 0.42              |
| 38:CP:153:ARG:HG3  | 38:CP:153:ARG:HH11  | 1.85                     | 0.42              |
| 44:Ca:527:THR:O    | 44:Ca:536:ARG:NH2   | 2.52                     | 0.42              |
| 51:Cm:95:MET:SD    | 51:Cm:95:MET:N      | 2.90                     | 0.42              |
| 63:UT:37:UNK:HA    | 63:UT:40:UNK:HB2    | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:65:ILE:HD11   | 2:DD:164:ARG:HG3   | 2.01                     | 0.42              |
| 1:DA:254:PHE:HB3   | 38:CP:78:PRO:HD3   | 2.00                     | 0.42              |
| 1:DA:584:PHE:HE1   | 1:DA:761:ARG:HH11  | 1.67                     | 0.42              |
| 2:DD:139:LEU:HD13  | 2:DD:139:LEU:HA    | 1.91                     | 0.42              |
| 2:DD:665:GLU:HG3   | 44:Ca:427:TRP:HA   | 2.01                     | 0.42              |
| 3:DI:90:LEU:HD12   | 3:DI:90:LEU:HA     | 1.94                     | 0.42              |
| 4:DL:268:VAL:HG12  | 4:DL:269:MET:HG2   | 2.02                     | 0.42              |
| 6:DN:165:GLU:HB3   | 6:DN:172:LEU:HD12  | 2.01                     | 0.42              |
| 13:DZ:88:PHE:HZ    | 44:Ca:253:LEU:HD12 | 1.85                     | 0.42              |
| 15:DB:558:ASN:HB2  | 50:Ck:113:ASN:HB3  | 2.01                     | 0.42              |
| 15:DB:905:TYR:HD1  | 15:DB:918:VAL:HG22 | 1.85                     | 0.42              |
| 15:DB:1086:HIS:HE2 | 48:Ci:96:ASN:HB3   | 1.84                     | 0.42              |
| 16:DC:148:LEU:HD12 | 16:DC:148:LEU:HA   | 1.90                     | 0.42              |
| 16:DC:800:LEU:HD23 | 16:DC:800:LEU:HA   | 1.83                     | 0.42              |
| 16:DC:909:ILE:HD13 | 16:DC:941:MET:HE2  | 2.01                     | 0.42              |
| 16:DC:1130:ALA:O   | 23:DT:163:ARG:NH2  | 2.53                     | 0.42              |
| 18:DF:289:TRP:O    | 18:DF:293:VAL:HG23 | 2.20                     | 0.42              |
| 18:DF:429:LEU:HD23 | 18:DF:429:LEU:HA   | 1.88                     | 0.42              |
| 18:DF:450:VAL:HG11 | 18:DF:486:LEU:HB3  | 2.01                     | 0.42              |
| 18:DF:502:ARG:HG2  | 18:DF:519:TRP:O    | 2.20                     | 0.42              |
| 19:DG:85:LEU:HD12  | 19:DG:85:LEU:HA    | 1.88                     | 0.42              |
| 19:DG:261:ARG:HA   | 19:DG:262:PRO:HD3  | 1.87                     | 0.42              |
| 19:DG:577:LEU:HD11 | 19:DG:605:VAL:HG22 | 2.02                     | 0.42              |
| 20:DH:34:TYR:CE1   | 21:DJ:44:VAL:HG11  | 2.55                     | 0.42              |
| 21:DJ:231:ASP:O    | 21:DJ:265:LYS:NZ   | 2.27                     | 0.42              |
| 23:DT:92:LYS:NZ    | 23:DT:175:SER:O    | 2.52                     | 0.42              |
| 23:DT:123:TYR:N    | 23:DT:123:TYR:CD2  | 2.87                     | 0.42              |
| 24:DV:167:PRO:HA   | 24:DV:168:PRO:HD3  | 1.86                     | 0.42              |
| 25:DW:142:TRP:CD1  | 25:DW:142:TRP:H    | 2.38                     | 0.42              |
| 28:CC:24:LYS:HB3   | 28:CC:28:LEU:HD12  | 2.00                     | 0.42              |
| 31:CH:16:VAL:N     | 31:CH:17:PRO:HD2   | 2.35                     | 0.42              |
| 33:CJ:71:VAL:CG2   | 33:CJ:82:HIS:HB3   | 2.50                     | 0.42              |
| 33:CJ:318:GLU:O    | 33:CJ:321:ASN:HB3  | 2.19                     | 0.42              |
| 33:CJ:335:LEU:HA   | 33:CJ:335:LEU:HD23 | 1.79                     | 0.42              |
| 33:CJ:463:MET:HG3  | 48:Ci:44:TYR:CG    | 2.55                     | 0.42              |
| 34:CK:91:ILE:HD13  | 45:Cb:159:ARG:HA   | 2.01                     | 0.42              |
| 44:Ca:569:ARG:HD3  | 57:CA:143:U:OP1    | 2.19                     | 0.42              |
| 46:Cd:14:PRO:HD2   | 46:Cd:17:ASN:ND2   | 2.35                     | 0.42              |
| 46:Cd:150:TYR:O    | 46:Cd:152:PRO:HD3  | 2.19                     | 0.42              |
| 48:Ci:54:GLN:H     | 48:Ci:54:GLN:HG2   | 1.56                     | 0.42              |
| 53:Cp:66:HIS:CE1   | 57:CA:45:G:N3      | 2.87                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:Cv:27:LYS:O     | 56:Cv:29:LEU:N     | 2.53                     | 0.42              |
| 56:Cv:233:LYS:HG3  | 56:Cv:500:TYR:CD2  | 2.54                     | 0.42              |
| 56:Cv:304:THR:HG22 | 56:Cv:306:TYR:N    | 2.32                     | 0.42              |
| 56:Cv:603:ARG:HD2  | 56:Cv:606:GLU:OE2  | 2.19                     | 0.42              |
| 57:CA:299:U:O2'    | 57:CA:300:G:O5'    | 2.33                     | 0.42              |
| 57:CA:365:A:H4'    | 57:CA:366:U:O4'    | 2.20                     | 0.42              |
| 1:DA:1495:LEU:HG   | 1:DA:1605:ARG:HE   | 1.85                     | 0.42              |
| 1:DA:1557:THR:HG22 | 1:DA:1558:ASN:H    | 1.85                     | 0.42              |
| 1:DA:1594:ALA:O    | 1:DA:1598:THR:OG1  | 2.23                     | 0.42              |
| 2:DD:21:ARG:NH2    | 57:CA:274:A:N7     | 2.66                     | 0.42              |
| 2:DD:651:ARG:HD3   | 2:DD:651:ARG:HA    | 1.61                     | 0.42              |
| 3:DI:251:VAL:HG13  | 3:DI:258:VAL:HG13  | 2.02                     | 0.42              |
| 3:DI:378:LEU:HD23  | 3:DI:378:LEU:HA    | 1.75                     | 0.42              |
| 5:DM:238:GLU:O     | 5:DM:242:LEU:HB2   | 2.20                     | 0.42              |
| 13:DZ:11:LYS:H     | 44:Ca:91:ASP:HA    | 1.83                     | 0.42              |
| 13:DZ:19:THR:HB    | 56:Cv:1120:TRP:O   | 2.19                     | 0.42              |
| 14:Da:25:ARG:C     | 14:Da:25:ARG:HD3   | 2.44                     | 0.42              |
| 15:DB:639:ASP:OD1  | 15:DB:641:ARG:HD3  | 2.20                     | 0.42              |
| 16:DC:71:TRP:O     | 16:DC:76:ASN:HB2   | 2.19                     | 0.42              |
| 16:DC:443:ARG:HA   | 16:DC:444:PRO:HD3  | 1.84                     | 0.42              |
| 17:DE:51:ARG:HA    | 17:DE:51:ARG:HD3   | 1.81                     | 0.42              |
| 17:DE:67:ASN:HA    | 17:DE:68:PRO:HD2   | 1.83                     | 0.42              |
| 18:DF:6:VAL:HG23   | 48:CI:157:LEU:HA   | 2.02                     | 0.42              |
| 18:DF:216:LYS:O    | 18:DF:220:GLU:HG3  | 2.20                     | 0.42              |
| 19:DG:111:ARG:HH21 | 32:CI:152:GLN:HG2  | 1.84                     | 0.42              |
| 19:DG:494:THR:C    | 19:DG:496:ARG:H    | 2.28                     | 0.42              |
| 19:DG:556:LEU:HD12 | 19:DG:556:LEU:HA   | 1.87                     | 0.42              |
| 25:DW:56:LEU:HD21  | 27:DY:21:PRO:HD3   | 2.02                     | 0.42              |
| 25:DW:87:ASN:HD21  | 25:DW:158:PRO:HB3  | 1.84                     | 0.42              |
| 30:CF:151:ARG:NH2  | 56:Cv:621:PRO:HD2  | 2.34                     | 0.42              |
| 33:CJ:458:HIS:CD2  | 33:CJ:763:ILE:HD13 | 2.54                     | 0.42              |
| 34:CK:15:ARG:HH22  | 57:CA:527:A:H5''   | 1.85                     | 0.42              |
| 37:CO:177:MET:O    | 37:CO:177:MET:HG2  | 2.20                     | 0.42              |
| 38:CP:70:HIS:O     | 38:CP:72:GLN:HG2   | 2.20                     | 0.42              |
| 42:CU:103:ARG:HB3  | 42:CU:103:ARG:NH1  | 2.35                     | 0.42              |
| 42:CU:115:LYS:HD3  | 42:CU:115:LYS:HA   | 1.78                     | 0.42              |
| 45:Cb:50:GLU:H     | 45:Cb:50:GLU:HG3   | 1.60                     | 0.42              |
| 46:Cd:137:ARG:NH1  | 46:Cd:137:ARG:CG   | 2.71                     | 0.42              |
| 50:Ck:275:TRP:CD2  | 50:Ck:314:LEU:HD22 | 2.55                     | 0.42              |
| 57:CA:4:A:OP2      | 57:CA:4:A:H8       | 2.03                     | 0.42              |
| 2:DD:216:LEU:O     | 2:DD:220:VAL:HG23  | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:534:PHE:CE2   | 2:DD:536:PRO:HG3   | 2.55                     | 0.41              |
| 2:DD:770:SER:N     | 44:Ca:364:ASP:OD1  | 2.45                     | 0.41              |
| 5:DM:90:LEU:HA     | 5:DM:90:LEU:HD12   | 1.72                     | 0.41              |
| 6:DN:224:ARG:HH12  | 6:DN:287:ARG:HB2   | 1.84                     | 0.41              |
| 7:DO:266:ASP:OD1   | 7:DO:267:THR:N     | 2.53                     | 0.41              |
| 9:DQ:106:MET:HE2   | 9:DQ:221:LEU:HD22  | 2.02                     | 0.41              |
| 11:DS:54:ASN:ND2   | 44:Ca:600:PRO:HB3  | 2.35                     | 0.41              |
| 15:DB:246:LEU:HD23 | 15:DB:246:LEU:HA   | 1.82                     | 0.41              |
| 15:DB:519:PHE:CE2  | 15:DB:534:PHE:HB2  | 2.55                     | 0.41              |
| 18:DF:371:ASN:HB3  | 18:DF:373:ASP:OD1  | 2.20                     | 0.41              |
| 18:DF:395:LEU:HD12 | 18:DF:395:LEU:HA   | 1.95                     | 0.41              |
| 19:DG:236:VAL:HG21 | 19:DG:253:PRO:HB2  | 2.02                     | 0.41              |
| 20:DH:119:LEU:HD22 | 20:DH:123:HIS:HB3  | 2.01                     | 0.41              |
| 20:DH:258:MET:HG3  | 20:DH:288:HIS:CE1  | 2.55                     | 0.41              |
| 20:DH:460:LEU:H    | 20:DH:460:LEU:HG   | 1.34                     | 0.41              |
| 21:DJ:71:MET:HE2   | 21:DJ:71:MET:HB3   | 1.94                     | 0.41              |
| 23:DT:233:HIS:CG   | 23:DT:238:PRO:HA   | 2.55                     | 0.41              |
| 29:CE:301:TYR:HB3  | 29:CE:302:PRO:HD3  | 2.01                     | 0.41              |
| 32:CI:30:VAL:HA    | 32:CI:31:PRO:HD3   | 1.94                     | 0.41              |
| 33:CJ:227:ARG:NE   | 33:CJ:816:ALA:O    | 2.48                     | 0.41              |
| 33:CJ:724:THR:HG23 | 33:CJ:725:PRO:HD2  | 2.02                     | 0.41              |
| 38:CP:65:GLY:HA3   | 38:CP:93:THR:O     | 2.20                     | 0.41              |
| 39:CQ:174:ARG:HH11 | 39:CQ:174:ARG:HG3  | 1.84                     | 0.41              |
| 41:CS:100:VAL:HG21 | 41:CS:104:GLN:CD   | 2.44                     | 0.41              |
| 46:Cd:51:GLU:HB3   | 49:Cj:20:MET:HG2   | 2.02                     | 0.41              |
| 46:Cd:139:SER:OG   | 46:Cd:140:GLU:N    | 2.51                     | 0.41              |
| 50:Ck:98:ARG:NH1   | 50:Ck:100:ALA:HB2  | 2.35                     | 0.41              |
| 50:Ck:230:LEU:HB3  | 50:Ck:231:GLY:H    | 1.65                     | 0.41              |
| 50:Ck:337:VAL:HG11 | 50:Ck:342:LYS:HA   | 2.02                     | 0.41              |
| 52:Cn:165:LEU:HD23 | 52:Cn:165:LEU:HA   | 1.68                     | 0.41              |
| 52:Cn:204:LEU:HD12 | 52:Cn:204:LEU:HA   | 1.68                     | 0.41              |
| 53:Cp:89:LYS:HE2   | 53:Cp:89:LYS:HB3   | 1.84                     | 0.41              |
| 54:Cq:154:LEU:HD22 | 54:Cq:170:VAL:HG21 | 2.02                     | 0.41              |
| 56:Cv:544:ILE:O    | 56:Cv:544:ILE:HG22 | 2.19                     | 0.41              |
| 57:CA:337:U:C4     | 57:CA:357:A:O2'    | 2.73                     | 0.41              |
| 1:DA:237:HIS:CE1   | 1:DA:310:ASP:HB2   | 2.52                     | 0.41              |
| 1:DA:872:LYS:HD3   | 1:DA:872:LYS:HA    | 1.79                     | 0.41              |
| 2:DD:17:ALA:HB2    | 57:CA:273:A:H5''   | 2.02                     | 0.41              |
| 2:DD:99:THR:HA     | 44:Ca:561:GLN:HE21 | 1.85                     | 0.41              |
| 2:DD:247:VAL:CG2   | 12:DU:35:PRO:HD3   | 2.51                     | 0.41              |
| 3:DI:243:LEU:HD12  | 3:DI:243:LEU:HA    | 1.74                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:DN:154:MET:HB3   | 6:DN:154:MET:HE2   | 1.59                     | 0.41              |
| 6:DN:281:GLN:HE21  | 44:Ca:211:PRO:HD2  | 1.84                     | 0.41              |
| 6:DN:292:TYR:OH    | 29:CE:117:TRP:CD2  | 2.73                     | 0.41              |
| 9:DQ:99:SER:OG     | 9:DQ:100:HIS:N     | 2.52                     | 0.41              |
| 12:DU:211:ARG:HA   | 12:DU:212:PRO:HD3  | 1.81                     | 0.41              |
| 15:DB:319:ARG:HD2  | 17:DE:524:PHE:CD2  | 2.56                     | 0.41              |
| 17:DE:573:GLN:HG2  | 28:CC:5:PHE:CZ     | 2.55                     | 0.41              |
| 17:DE:618:ARG:H    | 17:DE:618:ARG:HG2  | 1.54                     | 0.41              |
| 18:DF:154:ASN:HD22 | 18:DF:157:THR:H    | 1.67                     | 0.41              |
| 19:DG:296:ASP:OD2  | 32:CI:14:ARG:NH1   | 2.52                     | 0.41              |
| 19:DG:321:SER:C    | 19:DG:323:VAL:H    | 2.28                     | 0.41              |
| 20:DH:86:PRO:HA    | 20:DH:87:PRO:HD3   | 1.95                     | 0.41              |
| 21:DJ:220:LEU:HD23 | 21:DJ:220:LEU:HA   | 1.92                     | 0.41              |
| 25:DW:23:HIS:HA    | 25:DW:24:PRO:HD3   | 1.81                     | 0.41              |
| 28:CC:44:LEU:HD11  | 28:CC:50:ILE:HG13  | 2.00                     | 0.41              |
| 29:CE:326:MET:HE3  | 29:CE:326:MET:HB2  | 1.80                     | 0.41              |
| 32:CI:167:TYR:CD1  | 54:Cq:213:LEU:HD21 | 2.55                     | 0.41              |
| 37:CO:92:GLN:HA    | 57:CA:359:G:H8     | 1.85                     | 0.41              |
| 37:CO:240:LEU:HD13 | 37:CO:240:LEU:HA   | 1.80                     | 0.41              |
| 37:CO:305:TRP:HA   | 37:CO:310:ALA:HB2  | 2.01                     | 0.41              |
| 44:Ca:102:TRP:CZ2  | 44:Ca:159:LEU:HB2  | 2.55                     | 0.41              |
| 44:Ca:452:GLY:HA2  | 44:Ca:469:ARG:NH1  | 2.35                     | 0.41              |
| 49:Cj:99:ASN:OD1   | 49:Cj:100:ILE:N    | 2.53                     | 0.41              |
| 51:Cm:215:LYS:HG3  | 57:CA:357:A:N3     | 2.35                     | 0.41              |
| 53:Cp:146:LEU:HA   | 53:Cp:147:PRO:HD2  | 1.91                     | 0.41              |
| 54:Cq:155:GLN:HA   | 54:Cq:166:ALA:HB2  | 2.02                     | 0.41              |
| 1:DA:126:GLU:CD    | 31:CH:151:PRO:HD2  | 2.46                     | 0.41              |
| 1:DA:195:MET:HE3   | 1:DA:198:ARG:NH1   | 2.35                     | 0.41              |
| 8:DP:150:THR:HG22  | 8:DP:179:PHE:HE1   | 1.85                     | 0.41              |
| 10:DR:26:ASN:ND2   | 49:Cj:37:ARG:NH1   | 2.68                     | 0.41              |
| 10:DR:63:ILE:HD13  | 10:DR:63:ILE:HA    | 1.74                     | 0.41              |
| 10:DR:234:LEU:HD23 | 49:Cj:205:ARG:HH11 | 1.85                     | 0.41              |
| 15:DB:748:HIS:HA   | 15:DB:784:TYR:HD1  | 1.85                     | 0.41              |
| 16:DC:243:TYR:O    | 16:DC:248:ARG:HB2  | 2.20                     | 0.41              |
| 16:DC:1088:PHE:CZ  | 16:DC:1092:LYS:HE3 | 2.55                     | 0.41              |
| 17:DE:461:MET:N    | 17:DE:461:MET:SD   | 2.93                     | 0.41              |
| 18:DF:271:LEU:HD23 | 18:DF:271:LEU:HA   | 1.90                     | 0.41              |
| 18:DF:275:MET:O    | 18:DF:279:ILE:HG12 | 2.20                     | 0.41              |
| 19:DG:557:GLN:H    | 19:DG:557:GLN:HG3  | 1.55                     | 0.41              |
| 23:DT:14:THR:HG21  | 57:CA:438:U:H1'    | 2.02                     | 0.41              |
| 23:DT:105:ARG:NH2  | 23:DT:109:GLU:OE2  | 2.44                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:121:THR:OG1  | 29:CE:128:ILE:HD11 | 2.20                     | 0.41              |
| 29:CE:176:ALA:HB3  | 29:CE:245:PHE:CZ   | 2.55                     | 0.41              |
| 29:CE:421:ASP:O    | 29:CE:422:VAL:HG13 | 2.20                     | 0.41              |
| 30:CF:71:MET:HB3   | 30:CF:71:MET:HE3   | 1.77                     | 0.41              |
| 32:CI:280:LYS:HE2  | 32:CI:280:LYS:HB3  | 1.81                     | 0.41              |
| 36:CN:106:GLU:HA   | 36:CN:115:TYR:HB3  | 2.02                     | 0.41              |
| 36:CN:150:HIS:HD2  | 48:CI:67:THR:HG23  | 1.84                     | 0.41              |
| 36:CN:166:ILE:HD12 | 50:Ck:748:LEU:HB3  | 2.03                     | 0.41              |
| 36:CN:166:ILE:CD1  | 50:Ck:748:LEU:HB3  | 2.51                     | 0.41              |
| 37:CO:390:PHE:HD1  | 37:CO:390:PHE:HA   | 1.77                     | 0.41              |
| 39:CQ:99:VAL:O     | 39:CQ:108:VAL:HB   | 2.19                     | 0.41              |
| 39:CQ:104:LEU:HD23 | 39:CQ:104:LEU:HA   | 1.68                     | 0.41              |
| 44:Ca:89:ARG:HH11  | 44:Ca:177:GLN:HE21 | 1.69                     | 0.41              |
| 50:Ck:179:GLU:HB3  | 50:Ck:183:ARG:NH2  | 2.30                     | 0.41              |
| 50:Ck:362:TYR:HD2  | 50:Ck:365:ILE:HB   | 1.83                     | 0.41              |
| 50:Ck:585:MET:HE2  | 50:Ck:585:MET:HB3  | 1.96                     | 0.41              |
| 51:Cm:193:PHE:HB3  | 51:Cm:197:ALA:HB2  | 2.03                     | 0.41              |
| 52:Cn:231:LYS:HA   | 52:Cn:231:LYS:HD2  | 1.86                     | 0.41              |
| 56:Cv:444:GLY:HA2  | 56:Cv:808:SER:OG   | 2.21                     | 0.41              |
| 1:DA:125:LEU:HD23  | 1:DA:125:LEU:HA    | 1.87                     | 0.41              |
| 1:DA:1053:GLU:OE1  | 1:DA:1056:ARG:HD2  | 2.20                     | 0.41              |
| 1:DA:1100:SER:O    | 1:DA:1103:GLU:HG2  | 2.20                     | 0.41              |
| 6:DN:214:MET:CE    | 6:DN:217:MET:HE2   | 2.50                     | 0.41              |
| 9:DQ:172:ALA:C     | 9:DQ:174:PHE:H     | 2.29                     | 0.41              |
| 10:DR:103:ASP:OD1  | 10:DR:104:PRO:HD2  | 2.19                     | 0.41              |
| 11:DS:213:SER:HA   | 53:Cp:46:ILE:HB    | 2.02                     | 0.41              |
| 11:DS:238:ARG:HG3  | 11:DS:239:SER:N    | 2.35                     | 0.41              |
| 13:DZ:57:GLY:O     | 13:DZ:58:ASP:HB3   | 2.19                     | 0.41              |
| 15:DB:699:MET:O    | 15:DB:702:GLN:HB3  | 2.19                     | 0.41              |
| 17:DE:659:ARG:HD2  | 17:DE:659:ARG:HA   | 1.79                     | 0.41              |
| 18:DF:32:TRP:HA    | 23:DT:29:TRP:CD1   | 2.55                     | 0.41              |
| 18:DF:389:PRO:HA   | 18:DF:439:THR:HG21 | 2.02                     | 0.41              |
| 20:DH:274:GLU:CD   | 20:DH:274:GLU:H    | 2.28                     | 0.41              |
| 23:DT:79:PRO:HB2   | 23:DT:80:TYR:CD2   | 2.56                     | 0.41              |
| 23:DT:186:TRP:NE1  | 23:DT:211:PRO:HD3  | 2.35                     | 0.41              |
| 27:DY:144:HIS:ND1  | 27:DY:147:ASN:HB2  | 2.34                     | 0.41              |
| 29:CE:95:ILE:HD13  | 56:Cv:289:VAL:HG11 | 2.02                     | 0.41              |
| 30:CF:34:GLY:HA2   | 37:CO:193:MET:HE1  | 2.03                     | 0.41              |
| 31:CH:52:LEU:HD23  | 31:CH:52:LEU:HA    | 1.84                     | 0.41              |
| 32:CI:168:GLU:HG2  | 54:Cq:211:SER:HB3  | 2.02                     | 0.41              |
| 32:CI:202:LEU:HA   | 32:CI:211:ASN:ND2  | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CJ:273:ARG:HE   | 33:CJ:273:ARG:HB2  | 1.73                     | 0.41              |
| 37:CO:72:ALA:HB3   | 52:Cn:191:ALA:HB2  | 2.02                     | 0.41              |
| 38:CP:20:LEU:HD12  | 38:CP:20:LEU:HA    | 1.88                     | 0.41              |
| 39:CQ:48:ARG:HD2   | 39:CQ:59:TRP:CZ2   | 2.55                     | 0.41              |
| 40:CR:138:ARG:NH2  | 42:CU:46:GLU:OE1   | 2.46                     | 0.41              |
| 46:Cd:185:PHE:HE1  | 46:Cd:200:LEU:HD12 | 1.85                     | 0.41              |
| 49:Cj:80:LEU:HD12  | 49:Cj:84:ARG:NH1   | 2.35                     | 0.41              |
| 50:Ck:239:LEU:HD23 | 50:Ck:239:LEU:HA   | 1.86                     | 0.41              |
| 50:Ck:379:ALA:HB3  | 50:Ck:565:LEU:HD21 | 2.03                     | 0.41              |
| 51:Cm:32:LYS:HA    | 51:Cm:33:PRO:HD3   | 1.87                     | 0.41              |
| 54:Cq:79:MET:O     | 54:Cq:83:LEU:HB3   | 2.20                     | 0.41              |
| 54:Cq:247:ASN:ND2  | 54:Cq:250:LEU:HB2  | 2.35                     | 0.41              |
| 56:Cv:140:GLN:HG3  | 56:Cv:230:PHE:CZ   | 2.55                     | 0.41              |
| 57:CA:441:G:O2'    | 57:CA:442:A:H5'    | 2.21                     | 0.41              |
| 57:CA:530:A:C6     | 57:CA:531:G:C6     | 3.08                     | 0.41              |
| 58:UO:2:UNK:C      | 58:UO:4:UNK:H2     | 2.33                     | 0.41              |
| 1:DA:139:TYR:CZ    | 2:DD:262:GLU:HB3   | 2.55                     | 0.41              |
| 1:DA:634:GLU:CD    | 1:DA:634:GLU:H     | 2.28                     | 0.41              |
| 1:DA:653:LYS:HE3   | 1:DA:653:LYS:HB3   | 1.51                     | 0.41              |
| 1:DA:683:MET:HG2   | 1:DA:698:ALA:HA    | 2.02                     | 0.41              |
| 1:DA:733:SER:O     | 1:DA:736:VAL:HG22  | 2.20                     | 0.41              |
| 2:DD:175:VAL:HA    | 2:DD:178:ILE:HD12  | 2.02                     | 0.41              |
| 2:DD:177:TYR:O     | 2:DD:181:MET:HG3   | 2.20                     | 0.41              |
| 2:DD:408:HIS:CE1   | 2:DD:424:THR:HG21  | 2.55                     | 0.41              |
| 2:DD:577:LYS:HD3   | 2:DD:577:LYS:HA    | 1.54                     | 0.41              |
| 6:DN:213:ARG:NH1   | 44:Ca:192:GLN:HE22 | 2.18                     | 0.41              |
| 11:DS:112:ARG:HD2  | 11:DS:117:ALA:O    | 2.20                     | 0.41              |
| 14:Da:17:HIS:HB2   | 35:CL:4:LEU:HD11   | 2.01                     | 0.41              |
| 15:DB:801:LEU:O    | 15:DB:804:GLY:N    | 2.48                     | 0.41              |
| 15:DB:1037:GLY:HA2 | 28:CC:36:LEU:HD21  | 2.01                     | 0.41              |
| 18:DF:261:LEU:HA   | 18:DF:261:LEU:HD23 | 1.65                     | 0.41              |
| 20:DH:500:VAL:HG13 | 22:DK:303:TYR:CE2  | 2.55                     | 0.41              |
| 24:DV:49:ASP:OD1   | 24:DV:50:ALA:N     | 2.53                     | 0.41              |
| 25:DW:105:LEU:HB2  | 51:Cm:107:MET:HE2  | 2.03                     | 0.41              |
| 30:CF:136:ALA:O    | 30:CF:139:TYR:HB2  | 2.20                     | 0.41              |
| 32:CI:46:ARG:NH1   | 47:Cg:74:ILE:O     | 2.53                     | 0.41              |
| 32:CI:106:LEU:HD21 | 34:CK:107:GLN:HG2  | 2.01                     | 0.41              |
| 32:CI:437:LYS:HE2  | 32:CI:437:LYS:HB3  | 1.94                     | 0.41              |
| 34:CK:90:SER:O     | 34:CK:93:GLU:HB2   | 2.20                     | 0.41              |
| 36:CN:16:ASP:O     | 48:CI:133:TYR:HB3  | 2.20                     | 0.41              |
| 40:CR:248:LYS:HA   | 40:CR:252:GLN:NE2  | 2.35                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:CU:14:MET:SD     | 42:CU:20:MET:HE3   | 2.59                     | 0.41              |
| 42:CU:86:THR:O      | 42:CU:90:LEU:HG    | 2.20                     | 0.41              |
| 42:CU:124:ALA:O     | 42:CU:127:VAL:HB   | 2.20                     | 0.41              |
| 47:Cg:191:SER:HA    | 47:Cg:199:ASP:OD2  | 2.20                     | 0.41              |
| 48:Ci:133:TYR:OH    | 57:CA:442:A:H8     | 2.02                     | 0.41              |
| 49:Cj:131:THR:OG1   | 49:Cj:190:PRO:HG3  | 2.21                     | 0.41              |
| 52:Cn:179:ARG:HG3   | 52:Cn:183:ARG:HD2  | 2.03                     | 0.41              |
| 56:Cv:440:GLY:HA2   | 56:Cv:443:VAL:HG22 | 2.01                     | 0.41              |
| 56:Cv:724:LEU:HD21  | 56:Cv:784:PHE:CE2  | 2.55                     | 0.41              |
| 56:Cv:955:LEU:HD12  | 56:Cv:955:LEU:HA   | 1.93                     | 0.41              |
| 56:Cv:1105:ILE:HD13 | 56:Cv:1105:ILE:HA  | 1.92                     | 0.41              |
| 1:DA:1065:ALA:HB3   | 1:DA:1161:GLY:HA3  | 2.03                     | 0.41              |
| 1:DA:1656:ASN:HB2   | 1:DA:1658:GLU:OE2  | 2.21                     | 0.41              |
| 5:DM:72:ARG:HE      | 5:DM:72:ARG:HB3    | 1.58                     | 0.41              |
| 9:DQ:36:GLU:O       | 10:DR:27:LYS:HA    | 2.20                     | 0.41              |
| 9:DQ:154:GLY:HA2    | 9:DQ:234:GLN:O     | 2.20                     | 0.41              |
| 10:DR:87:LEU:HD12   | 10:DR:178:TYR:HE2  | 1.85                     | 0.41              |
| 12:DU:53:LEU:HD13   | 12:DU:53:LEU:HA    | 1.82                     | 0.41              |
| 12:DU:107:LYS:NZ    | 12:DU:107:LYS:HB3  | 2.35                     | 0.41              |
| 14:Da:32:SER:O      | 31:CH:144:ARG:NH1  | 2.53                     | 0.41              |
| 15:DB:172:SER:O     | 15:DB:175:ALA:HB3  | 2.21                     | 0.41              |
| 15:DB:224:LEU:HD23  | 15:DB:224:LEU:HA   | 1.82                     | 0.41              |
| 15:DB:521:LEU:HD23  | 15:DB:521:LEU:HA   | 1.85                     | 0.41              |
| 15:DB:528:PHE:CE2   | 15:DB:529:LEU:HG   | 2.55                     | 0.41              |
| 15:DB:983:LEU:HD23  | 15:DB:983:LEU:HA   | 1.75                     | 0.41              |
| 15:DB:1094:ASN:OD1  | 15:DB:1097:ARG:NH2 | 2.44                     | 0.41              |
| 16:DC:791:ALA:HB3   | 16:DC:806:SER:HB3  | 2.01                     | 0.41              |
| 17:DE:186:ARG:NH1   | 17:DE:186:ARG:HA   | 2.36                     | 0.41              |
| 18:DF:32:TRP:CD1    | 18:DF:32:TRP:H     | 2.39                     | 0.41              |
| 19:DG:99:VAL:CG2    | 33:CJ:187:GLY:HA2  | 2.49                     | 0.41              |
| 22:DK:2:SER:HB2     | 23:DT:160:TYR:CZ   | 2.55                     | 0.41              |
| 24:DV:51:ASN:HB3    | 47:Cg:373:VAL:HG11 | 2.02                     | 0.41              |
| 28:CC:13:LYS:HD3    | 28:CC:14:THR:N     | 2.35                     | 0.41              |
| 32:CI:32:LYS:HA     | 32:CI:32:LYS:HD3   | 1.90                     | 0.41              |
| 33:CJ:54:MET:HE2    | 57:CA:463:A:N6     | 2.35                     | 0.41              |
| 33:CJ:275:ILE:HD13  | 33:CJ:412:PHE:HB2  | 2.02                     | 0.41              |
| 33:CJ:287:LEU:HD12  | 33:CJ:287:LEU:HA   | 1.86                     | 0.41              |
| 33:CJ:558:ALA:HA    | 33:CJ:561:ILE:HD12 | 2.02                     | 0.41              |
| 33:CJ:755:ASN:ND2   | 33:CJ:757:LEU:O    | 2.54                     | 0.41              |
| 35:CL:18:LEU:HB2    | 35:CL:41:VAL:HG13  | 2.03                     | 0.41              |
| 37:CO:298:GLY:O     | 37:CO:302:LYS:HB2  | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:CO:397:MET:O    | 37:CO:397:MET:HG3  | 2.21                     | 0.41              |
| 38:CP:141:ASP:HB3  | 49:Cj:216:ASN:ND2  | 2.36                     | 0.41              |
| 40:CR:128:ASN:HA   | 40:CR:129:PRO:HD2  | 1.92                     | 0.41              |
| 44:Ca:168:TYR:HA   | 44:Ca:169:PRO:HD3  | 1.83                     | 0.41              |
| 44:Ca:287:LEU:O    | 44:Ca:290:MET:HB2  | 2.21                     | 0.41              |
| 44:Ca:462:ASP:HA   | 44:Ca:463:PRO:HD2  | 1.94                     | 0.41              |
| 47:Cg:243:LEU:HD12 | 47:Cg:243:LEU:HA   | 1.75                     | 0.41              |
| 48:Ci:133:TYR:CE2  | 48:Ci:137:LYS:HE3  | 2.56                     | 0.41              |
| 49:Cj:171:TRP:O    | 49:Cj:172:TYR:HD1  | 2.03                     | 0.41              |
| 50:Ck:122:MET:HE2  | 50:Ck:122:MET:HB3  | 1.86                     | 0.41              |
| 50:Ck:230:LEU:HD23 | 50:Ck:230:LEU:HA   | 1.77                     | 0.41              |
| 53:Cp:119:GLU:O    | 53:Cp:120:ARG:HG3  | 2.21                     | 0.41              |
| 1:DA:47:LEU:HD23   | 1:DA:47:LEU:HA     | 1.84                     | 0.41              |
| 1:DA:236:ARG:CZ    | 1:DA:312:PRO:HG3   | 2.51                     | 0.41              |
| 1:DA:387:SER:OG    | 1:DA:388:VAL:N     | 2.54                     | 0.41              |
| 1:DA:695:MET:HE1   | 1:DA:715:GLY:N     | 2.35                     | 0.41              |
| 1:DA:1658:GLU:O    | 1:DA:1662:ARG:HB2  | 2.20                     | 0.41              |
| 6:DN:165:GLU:OE2   | 6:DN:171:LEU:HB2   | 2.20                     | 0.41              |
| 7:DO:162:ALA:HA    | 7:DO:198:ARG:HH21  | 1.86                     | 0.41              |
| 11:DS:169:PHE:HB3  | 11:DS:186:ILE:HD12 | 2.03                     | 0.41              |
| 13:DZ:36:LEU:HD12  | 13:DZ:36:LEU:HA    | 1.91                     | 0.41              |
| 15:DB:824:ARG:HG2  | 18:DF:508:VAL:HG13 | 2.03                     | 0.41              |
| 15:DB:1164:ASP:HB3 | 25:DW:11:ALA:HB2   | 2.02                     | 0.41              |
| 16:DC:195:PHE:HD2  | 16:DC:220:ALA:HB1  | 1.86                     | 0.41              |
| 16:DC:289:LYS:N    | 16:DC:290:PRO:HD2  | 2.36                     | 0.41              |
| 16:DC:822:LEU:HB3  | 16:DC:853:PHE:HE2  | 1.85                     | 0.41              |
| 19:DG:136:LEU:HD12 | 19:DG:136:LEU:HA   | 1.85                     | 0.41              |
| 19:DG:136:LEU:O    | 19:DG:140:GLU:HB2  | 2.21                     | 0.41              |
| 20:DH:472:ARG:HG2  | 20:DH:483:TYR:CD1  | 2.56                     | 0.41              |
| 21:DJ:254:VAL:O    | 21:DJ:258:LEU:HB2  | 2.21                     | 0.41              |
| 21:DJ:317:PHE:CE2  | 23:DT:242:MET:HG2  | 2.56                     | 0.41              |
| 24:DV:31:HIS:HE1   | 24:DV:48:HIS:CE1   | 2.39                     | 0.41              |
| 26:DX:53:TYR:CE2   | 41:CS:145:LYS:HD3  | 2.56                     | 0.41              |
| 26:DX:65:LEU:HD23  | 26:DX:65:LEU:HA    | 1.91                     | 0.41              |
| 30:CF:123:ARG:HG3  | 30:CF:127:GLU:CD   | 2.46                     | 0.41              |
| 31:CH:103:ASP:HA   | 31:CH:104:PRO:HD3  | 1.85                     | 0.41              |
| 32:CI:122:LEU:HD23 | 45:Cb:177:MET:HE1  | 2.02                     | 0.41              |
| 33:CJ:250:GLU:HA   | 33:CJ:397:PHE:O    | 2.20                     | 0.41              |
| 33:CJ:463:MET:HG3  | 48:Ci:44:TYR:CD1   | 2.55                     | 0.41              |
| 37:CO:224:LEU:HA   | 37:CO:224:LEU:HD12 | 1.61                     | 0.41              |
| 40:CR:60:PHE:CZ    | 40:CR:66:LEU:HD11  | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:CR:137:THR:HA   | 40:CR:143:TYR:OH   | 2.21                     | 0.41              |
| 40:CR:319:LYS:HD3  | 42:CU:185:ARG:NH2  | 2.36                     | 0.41              |
| 45:Cb:91:ARG:HE    | 45:Cb:91:ARG:HB3   | 1.72                     | 0.41              |
| 49:Cj:80:LEU:HD22  | 49:Cj:80:LEU:HA    | 1.91                     | 0.41              |
| 50:Ck:718:ASP:OD1  | 50:Ck:719:GLY:N    | 2.54                     | 0.41              |
| 55:Cr:99:CYS:SG    | 55:Cr:150:TRP:HZ2  | 2.43                     | 0.41              |
| 56:Cv:556:PHE:HZ   | 56:Cv:800:VAL:HG21 | 1.85                     | 0.41              |
| 56:Cv:592:TYR:HE1  | 56:Cv:785:ILE:HD11 | 1.85                     | 0.41              |
| 57:CA:12:C:O2'     | 57:CA:13:A:H5''    | 2.20                     | 0.41              |
| 57:CA:43:A:N6      | 57:CA:173:A:H62    | 2.19                     | 0.41              |
| 2:DD:185:GLN:HG3   | 2:DD:221:GLU:OE1   | 2.21                     | 0.41              |
| 5:DM:45:ARG:O      | 5:DM:49:MET:HE3    | 2.21                     | 0.41              |
| 9:DQ:43:ARG:NH2    | 37:CO:371:LYS:NZ   | 2.68                     | 0.41              |
| 13:DZ:13:ALA:HB3   | 44:Ca:89:ARG:HG2   | 2.03                     | 0.41              |
| 15:DB:650:LEU:HD23 | 15:DB:650:LEU:HA   | 1.91                     | 0.41              |
| 16:DC:844:ALA:CB   | 17:DE:68:PRO:HB3   | 2.47                     | 0.41              |
| 19:DG:172:ALA:HB1  | 19:DG:192:MET:HE1  | 2.02                     | 0.41              |
| 21:DJ:20:SER:HA    | 21:DJ:21:PRO:HD2   | 1.89                     | 0.41              |
| 21:DJ:107:LEU:O    | 21:DJ:110:LEU:HB2  | 2.21                     | 0.41              |
| 25:DW:110:PRO:HD2  | 25:DW:131:TRP:CE2  | 2.56                     | 0.41              |
| 27:DY:117:LEU:HD23 | 27:DY:117:LEU:HA   | 1.79                     | 0.41              |
| 29:CE:34:ARG:HA    | 29:CE:35:PRO:HD3   | 1.83                     | 0.41              |
| 29:CE:167:LEU:HD21 | 29:CE:194:ILE:HG13 | 2.02                     | 0.41              |
| 29:CE:400:LEU:HD13 | 29:CE:407:THR:H    | 1.86                     | 0.41              |
| 32:CI:213:LEU:HD23 | 32:CI:213:LEU:HA   | 1.86                     | 0.41              |
| 32:CI:324:ARG:HG2  | 32:CI:325:GLU:H    | 1.85                     | 0.41              |
| 33:CJ:206:PHE:CG   | 33:CJ:207:PRO:HA   | 2.56                     | 0.41              |
| 33:CJ:528:ARG:O    | 33:CJ:665:ARG:NH2  | 2.54                     | 0.41              |
| 34:CK:232:ARG:HD2  | 34:CK:232:ARG:N    | 2.36                     | 0.41              |
| 35:CL:6:MET:HG3    | 35:CL:9:LEU:HD12   | 2.01                     | 0.41              |
| 40:CR:25:GLU:N     | 56:Cv:143:THR:HG21 | 2.33                     | 0.41              |
| 41:CS:57:HIS:CE1   | 57:CA:489:A:C8     | 3.08                     | 0.41              |
| 42:CU:154:LYS:O    | 42:CU:158:VAL:HG23 | 2.19                     | 0.41              |
| 44:Ca:597:LYS:HB2  | 44:Ca:597:LYS:HZ2  | 1.85                     | 0.41              |
| 49:Cj:99:ASN:ND2   | 49:Cj:142:ASN:O    | 2.54                     | 0.41              |
| 49:Cj:156:THR:H    | 49:Cj:192:SER:HB3  | 1.85                     | 0.41              |
| 49:Cj:212:TYR:CG   | 49:Cj:213:ASP:N    | 2.89                     | 0.41              |
| 50:Ck:169:LYS:O    | 50:Ck:173:PRO:HD2  | 2.20                     | 0.41              |
| 57:CA:338:U:H5'    | 57:CA:338:U:H6     | 1.86                     | 0.41              |
| 57:CA:472:G:O2'    | 57:CA:473:U:H5'    | 2.20                     | 0.41              |
| 1:DA:90:MET:HE1    | 2:DD:122:GLN:NE2   | 2.33                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:DA:222:GLU:HA    | 1:DA:284:ASN:HD22  | 1.86                     | 0.41              |
| 1:DA:392:THR:O     | 6:DN:179:ASN:ND2   | 2.51                     | 0.41              |
| 1:DA:1132:LYS:HE2  | 1:DA:1132:LYS:HB2  | 1.93                     | 0.41              |
| 1:DA:1150:LEU:HD12 | 29:CE:336:PRO:HD3  | 2.03                     | 0.41              |
| 2:DD:79:GLN:O      | 53:Cp:29:LYS:HD3   | 2.21                     | 0.41              |
| 2:DD:99:THR:HA     | 44:Ca:561:GLN:NE2  | 2.36                     | 0.41              |
| 2:DD:250:LYS:O     | 2:DD:287:ARG:HD2   | 2.21                     | 0.41              |
| 2:DD:307:GLU:OE2   | 3:DI:195:ILE:HB    | 2.21                     | 0.41              |
| 2:DD:772:ASP:CG    | 2:DD:773:MET:H     | 2.29                     | 0.41              |
| 3:DI:117:VAL:O     | 3:DI:120:GLU:HG3   | 2.21                     | 0.41              |
| 3:DI:328:VAL:HG22  | 7:DO:226:ILE:HD13  | 2.01                     | 0.41              |
| 5:DM:273:ARG:HA    | 5:DM:273:ARG:HD2   | 1.75                     | 0.41              |
| 6:DN:261:ARG:HB2   | 6:DN:264:ASP:OD1   | 2.20                     | 0.41              |
| 7:DO:152:LEU:HD23  | 7:DO:152:LEU:HA    | 1.85                     | 0.41              |
| 9:DQ:73:HIS:HA     | 9:DQ:249:CYS:O     | 2.20                     | 0.41              |
| 9:DQ:153:ARG:NH2   | 9:DQ:171:GLU:OE1   | 2.54                     | 0.41              |
| 9:DQ:165:PHE:CD2   | 9:DQ:207:HIS:HB2   | 2.56                     | 0.41              |
| 10:DR:39:GLN:HG2   | 10:DR:42:MET:HE2   | 2.03                     | 0.41              |
| 11:DS:128:SER:OG   | 11:DS:131:ARG:HG3  | 2.21                     | 0.41              |
| 13:DZ:23:PHE:HA    | 13:DZ:24:PRO:HD2   | 1.97                     | 0.41              |
| 14:Da:50:LYS:HG2   | 14:Da:53:ARG:HG3   | 2.01                     | 0.41              |
| 15:DB:92:HIS:CD2   | 15:DB:94:ASP:H     | 2.39                     | 0.41              |
| 15:DB:560:THR:HG23 | 18:DF:548:ARG:NH1  | 2.36                     | 0.41              |
| 15:DB:572:ASP:OD2  | 15:DB:646:SER:HB2  | 2.21                     | 0.41              |
| 15:DB:841:ARG:HG3  | 15:DB:841:ARG:O    | 2.21                     | 0.41              |
| 15:DB:928:ILE:HD11 | 50:Ck:359:LEU:HD13 | 2.02                     | 0.41              |
| 15:DB:1093:GLU:OE2 | 50:Ck:752:LYS:NZ   | 2.50                     | 0.41              |
| 15:DB:1102:TYR:OH  | 18:DF:103:VAL:O    | 2.30                     | 0.41              |
| 16:DC:145:ALA:O    | 16:DC:149:ARG:HG3  | 2.21                     | 0.41              |
| 16:DC:363:ILE:HG22 | 16:DC:364:MET:HE2  | 2.02                     | 0.41              |
| 16:DC:1008:GLY:HA2 | 16:DC:1048:HIS:NE2 | 2.36                     | 0.41              |
| 17:DE:54:ARG:HH21  | 17:DE:91:GLY:C     | 2.29                     | 0.41              |
| 18:DF:32:TRP:CE3   | 18:DF:33:GLN:HB2   | 2.56                     | 0.41              |
| 18:DF:165:TYR:HE1  | 36:CN:26:LEU:HD21  | 1.85                     | 0.41              |
| 19:DG:487:VAL:O    | 19:DG:491:THR:HG22 | 2.21                     | 0.41              |
| 20:DH:19:THR:HG22  | 20:DH:21:LEU:HB2   | 2.03                     | 0.41              |
| 20:DH:162:GLU:O    | 20:DH:166:GLN:HG2  | 2.20                     | 0.41              |
| 21:DJ:308:ARG:HD3  | 23:DT:42:PHE:CE1   | 2.56                     | 0.41              |
| 24:DV:106:VAL:HG21 | 33:CJ:758:TRP:CD2  | 2.56                     | 0.41              |
| 25:DW:143:MET:HA   | 25:DW:144:PRO:HD3  | 1.79                     | 0.41              |
| 28:CC:25:HIS:CD2   | 28:CC:27:PHE:H     | 2.38                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:CE:102:GLU:HG2  | 29:CE:105:GLN:NE2  | 2.22                     | 0.41              |
| 29:CE:171:SER:O    | 29:CE:173:LYS:N    | 2.54                     | 0.41              |
| 29:CE:296:LEU:HA   | 29:CE:296:LEU:HD23 | 1.64                     | 0.41              |
| 30:CF:118:LEU:HD12 | 30:CF:118:LEU:HA   | 1.85                     | 0.41              |
| 32:CI:93:MET:HB3   | 32:CI:93:MET:HE2   | 1.83                     | 0.41              |
| 33:CJ:160:GLU:HA   | 47:Cg:407:TYR:OH   | 2.21                     | 0.41              |
| 33:CJ:163:MET:O    | 33:CJ:167:VAL:HG23 | 2.21                     | 0.41              |
| 33:CJ:544:THR:HG21 | 33:CJ:551:ARG:C    | 2.46                     | 0.41              |
| 33:CJ:720:THR:HA   | 33:CJ:721:PRO:HD3  | 1.89                     | 0.41              |
| 34:CK:80:ARG:NH1   | 55:Cr:156:GLN:HG2  | 2.36                     | 0.41              |
| 36:CN:108:VAL:HA   | 36:CN:109:PRO:HD3  | 1.67                     | 0.41              |
| 37:CO:82:ASN:HD21  | 52:Cn:142:TRP:N    | 2.19                     | 0.41              |
| 37:CO:185:VAL:HG22 | 46:Cd:145:MET:HG2  | 2.02                     | 0.41              |
| 37:CO:416:THR:OG1  | 37:CO:417:LYS:N    | 2.54                     | 0.41              |
| 38:CP:80:THR:HG22  | 38:CP:82:VAL:H     | 1.85                     | 0.41              |
| 38:CP:167:TYR:CG   | 46:Cd:59:ARG:HD3   | 2.56                     | 0.41              |
| 39:CQ:19:ARG:HD3   | 39:CQ:19:ARG:HA    | 1.76                     | 0.41              |
| 39:CQ:132:ALA:HA   | 39:CQ:159:TYR:O    | 2.21                     | 0.41              |
| 39:CQ:174:ARG:HH21 | 39:CQ:183:PRO:HD3  | 1.85                     | 0.41              |
| 40:CR:168:ILE:HD12 | 40:CR:168:ILE:HA   | 1.78                     | 0.41              |
| 40:CR:173:ARG:HG3  | 40:CR:173:ARG:NH1  | 2.36                     | 0.41              |
| 42:CU:102:ARG:HG3  | 42:CU:102:ARG:NH1  | 2.35                     | 0.41              |
| 42:CU:154:LYS:O    | 42:CU:157:ALA:HB3  | 2.20                     | 0.41              |
| 43:CZ:226:ARG:HA   | 43:CZ:226:ARG:HD3  | 1.85                     | 0.41              |
| 44:Ca:418:VAL:HG21 | 44:Ca:484:LYS:HG2  | 2.02                     | 0.41              |
| 44:Ca:429:GLY:HA3  | 44:Ca:430:PRO:HD2  | 1.88                     | 0.41              |
| 44:Ca:569:ARG:HH11 | 57:CA:143:U:H5'    | 1.85                     | 0.41              |
| 46:Cd:45:LEU:HD23  | 46:Cd:45:LEU:HA    | 1.86                     | 0.41              |
| 47:Cg:314:SER:HB3  | 47:Cg:316:THR:HB   | 2.03                     | 0.41              |
| 49:Cj:176:VAL:HG12 | 49:Cj:178:GLU:H    | 1.85                     | 0.41              |
| 50:Ck:715:GLN:HG2  | 50:Ck:725:VAL:O    | 2.20                     | 0.41              |
| 50:Ck:716:ARG:HD3  | 50:Ck:716:ARG:HA   | 1.73                     | 0.41              |
| 52:Cn:146:PHE:CG   | 52:Cn:150:VAL:HG21 | 2.56                     | 0.41              |
| 53:Cp:137:ASP:OD1  | 53:Cp:139:SER:HB3  | 2.20                     | 0.41              |
| 56:Cv:183:LEU:N    | 56:Cv:183:LEU:HD12 | 2.35                     | 0.41              |
| 56:Cv:740:ILE:HG23 | 56:Cv:786:VAL:HG13 | 2.03                     | 0.41              |
| 57:CA:353:G:H2'    | 57:CA:354:U:O4'    | 2.21                     | 0.41              |
| 57:CA:578:C:H2'    | 57:CA:579:G:O4'    | 2.21                     | 0.41              |
| 1:DA:118:LEU:HD22  | 37:CO:305:TRP:CH2  | 2.56                     | 0.41              |
| 1:DA:819:ARG:NE    | 1:DA:870:GLU:OE2   | 2.53                     | 0.41              |
| 2:DD:91:TYR:CE1    | 39:CQ:25:MET:HG3   | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:343:TRP:N     | 9:DQ:29:ILE:O      | 2.54                     | 0.41              |
| 5:DM:1:MET:HE3     | 5:DM:1:MET:C       | 2.46                     | 0.41              |
| 7:DO:74:TRP:CE2    | 7:DO:259:THR:HG23  | 2.56                     | 0.41              |
| 7:DO:273:TYR:CE1   | 56:Cv:783:TYR:HB3  | 2.56                     | 0.41              |
| 8:DP:12:LEU:HD23   | 8:DP:12:LEU:HA     | 1.78                     | 0.41              |
| 8:DP:153:VAL:O     | 8:DP:156:GLU:HG3   | 2.20                     | 0.41              |
| 10:DR:67:LYS:HD2   | 10:DR:67:LYS:N     | 2.35                     | 0.41              |
| 11:DS:57:LEU:HD21  | 11:DS:83:LEU:HD21  | 2.03                     | 0.41              |
| 11:DS:215:SER:O    | 11:DS:218:PRO:HD2  | 2.21                     | 0.41              |
| 15:DB:388:VAL:HB   | 20:DH:509:TYR:HA   | 2.02                     | 0.41              |
| 15:DB:535:THR:HG23 | 15:DB:538:ARG:HH21 | 1.86                     | 0.41              |
| 16:DC:307:LEU:O    | 16:DC:310:ARG:HG2  | 2.21                     | 0.41              |
| 16:DC:505:ALA:HB3  | 16:DC:509:LYS:HD2  | 2.03                     | 0.41              |
| 16:DC:635:MET:HE2  | 16:DC:659:LEU:HD12 | 2.03                     | 0.41              |
| 16:DC:762:LYS:HG3  | 16:DC:763:GLU:HG3  | 2.02                     | 0.41              |
| 17:DE:708:LEU:HD23 | 17:DE:708:LEU:HA   | 1.90                     | 0.41              |
| 18:DF:25:ILE:HA    | 18:DF:26:PRO:HD3   | 1.92                     | 0.41              |
| 18:DF:359:ARG:HB2  | 21:DJ:78:ALA:HA    | 2.03                     | 0.41              |
| 18:DF:430:THR:H    | 18:DF:446:HIS:CE1  | 2.38                     | 0.41              |
| 18:DF:550:VAL:HG21 | 18:DF:572:HIS:HB3  | 2.03                     | 0.41              |
| 19:DG:352:ARG:O    | 19:DG:355:ARG:HB2  | 2.21                     | 0.41              |
| 20:DH:441:ALA:O    | 28:CC:35:SER:HA    | 2.21                     | 0.41              |
| 21:DJ:35:PRO:O     | 21:DJ:37:GLY:N     | 2.54                     | 0.41              |
| 23:DT:37:TYR:O     | 48:Ci:126:GLY:HA3  | 2.21                     | 0.41              |
| 23:DT:190:PHE:CD1  | 23:DT:191:PRO:HD2  | 2.56                     | 0.41              |
| 25:DW:110:PRO:HD2  | 25:DW:131:TRP:CZ2  | 2.56                     | 0.41              |
| 25:DW:128:LEU:HD23 | 25:DW:128:LEU:HA   | 1.82                     | 0.41              |
| 29:CE:171:SER:C    | 29:CE:173:LYS:N    | 2.79                     | 0.41              |
| 30:CF:124:LEU:HB2  | 56:Cv:631:SER:HB3  | 2.03                     | 0.41              |
| 32:CI:118:THR:H    | 32:CI:121:SER:HG   | 1.66                     | 0.41              |
| 33:CJ:118:MET:HA   | 33:CJ:118:MET:HE2  | 2.03                     | 0.41              |
| 33:CJ:293:ASP:CB   | 33:CJ:296:LEU:H    | 2.34                     | 0.41              |
| 33:CJ:623:THR:O    | 33:CJ:627:ILE:HG13 | 2.21                     | 0.41              |
| 34:CK:310:ILE:HG21 | 42:CU:38:PHE:CB    | 2.44                     | 0.41              |
| 36:CN:115:TYR:CG   | 36:CN:116:TRP:N    | 2.89                     | 0.41              |
| 38:CP:96:ILE:HD11  | 44:Ca:470:ARG:CZ   | 2.51                     | 0.41              |
| 40:CR:40:THR:HG21  | 40:CR:101:GLN:HB2  | 2.03                     | 0.41              |
| 42:CU:56:LEU:HD23  | 42:CU:56:LEU:HA    | 1.94                     | 0.41              |
| 42:CU:60:ARG:HE    | 42:CU:60:ARG:HB2   | 1.52                     | 0.41              |
| 42:CU:190:TRP:CH2  | 57:CA:614:U:C4     | 3.08                     | 0.41              |
| 51:Cm:31:LEU:O     | 51:Cm:45:LEU:HD22  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:Cn:168:ARG:NH1  | 57:CA:382:A:OP1    | 2.54                     | 0.41              |
| 54:Cq:168:ASP:O    | 54:Cq:172:ARG:HB2  | 2.20                     | 0.41              |
| 56:Cv:457:ARG:NH2  | 56:Cv:488:TRP:HD1  | 2.19                     | 0.41              |
| 56:Cv:696:PHE:CD2  | 56:Cv:727:ARG:NH1  | 2.89                     | 0.41              |
| 57:CA:154:G:N3     | 57:CA:154:G:H2'    | 2.36                     | 0.41              |
| 57:CA:275:U:H6     | 57:CA:275:U:H2'    | 1.75                     | 0.41              |
| 1:DA:93:TRP:O      | 1:DA:97:THR:OG1    | 2.33                     | 0.40              |
| 1:DA:135:ASP:OD2   | 46:Cd:109:MET:HE2  | 2.21                     | 0.40              |
| 1:DA:209:TRP:HA    | 38:CP:81:PRO:HG3   | 2.03                     | 0.40              |
| 1:DA:507:VAL:HG12  | 1:DA:832:ARG:HH11  | 1.86                     | 0.40              |
| 1:DA:833:ALA:N     | 1:DA:834:PRO:HD2   | 2.36                     | 0.40              |
| 1:DA:1374:VAL:HG22 | 1:DA:1617:LEU:HD11 | 2.03                     | 0.40              |
| 2:DD:87:MET:HE1    | 39:CQ:26:TYR:CE1   | 2.56                     | 0.40              |
| 2:DD:748:ARG:HE    | 2:DD:748:ARG:HB2   | 1.63                     | 0.40              |
| 2:DD:802:LYS:O     | 2:DD:808:THR:OG1   | 2.33                     | 0.40              |
| 5:DM:133:GLU:HG2   | 5:DM:133:GLU:O     | 2.21                     | 0.40              |
| 5:DM:213:ARG:NH1   | 5:DM:220:ALA:O     | 2.48                     | 0.40              |
| 8:DP:143:ASN:ND2   | 49:Cj:142:ASN:OD1  | 2.54                     | 0.40              |
| 15:DB:167:GLU:O    | 15:DB:171:ARG:HB2  | 2.21                     | 0.40              |
| 15:DB:348:ILE:H    | 15:DB:348:ILE:HG13 | 1.82                     | 0.40              |
| 15:DB:686:GLN:HE21 | 15:DB:686:GLN:HB2  | 1.70                     | 0.40              |
| 15:DB:1060:GLU:OE2 | 20:DH:386:ARG:NH1  | 2.49                     | 0.40              |
| 16:DC:37:PRO:C     | 16:DC:39:VAL:H     | 2.29                     | 0.40              |
| 16:DC:149:ARG:C    | 16:DC:155:VAL:HG11 | 2.46                     | 0.40              |
| 16:DC:475:LEU:H    | 16:DC:475:LEU:HG   | 1.66                     | 0.40              |
| 17:DE:546:LEU:HD23 | 17:DE:546:LEU:HA   | 1.98                     | 0.40              |
| 17:DE:591:LEU:HA   | 17:DE:591:LEU:HD12 | 1.85                     | 0.40              |
| 19:DG:199:LEU:HA   | 19:DG:199:LEU:HD23 | 1.77                     | 0.40              |
| 22:DK:288:ARG:O    | 22:DK:292:VAL:HG23 | 2.21                     | 0.40              |
| 23:DT:147:ALA:O    | 23:DT:151:TRP:HD1  | 2.05                     | 0.40              |
| 23:DT:183:LEU:HD23 | 23:DT:183:LEU:HA   | 1.96                     | 0.40              |
| 29:CE:34:ARG:NH2   | 29:CE:98:ASP:O     | 2.53                     | 0.40              |
| 29:CE:308:ARG:HB2  | 44:Ca:368:ARG:HG2  | 2.02                     | 0.40              |
| 29:CE:367:LEU:HD23 | 29:CE:367:LEU:HA   | 1.74                     | 0.40              |
| 30:CF:11:LYS:HA    | 30:CF:12:PRO:HD3   | 1.83                     | 0.40              |
| 30:CF:15:ARG:HB2   | 46:Cd:190:ASP:HA   | 2.03                     | 0.40              |
| 33:CJ:699:LEU:HD23 | 33:CJ:699:LEU:HA   | 1.96                     | 0.40              |
| 33:CJ:723:GLU:HG2  | 33:CJ:724:THR:H    | 1.86                     | 0.40              |
| 34:CK:320:MET:HE1  | 42:CU:16:HIS:HA    | 2.02                     | 0.40              |
| 35:CL:26:SER:HA    | 35:CL:27:PRO:HD2   | 1.80                     | 0.40              |
| 39:CQ:16:THR:CG2   | 53:Cp:18:SER:HA    | 2.48                     | 0.40              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:CU:57:VAL:HA     | 42:CU:60:ARG:HH21  | 1.85                     | 0.40              |
| 50:Ck:288:ASN:O     | 50:Ck:294:ALA:HB1  | 2.21                     | 0.40              |
| 53:Cp:99:ARG:O      | 53:Cp:102:ARG:HG2  | 2.22                     | 0.40              |
| 56:Cv:312:ASN:HD22  | 56:Cv:312:ASN:C    | 2.28                     | 0.40              |
| 56:Cv:320:LEU:HD23  | 56:Cv:320:LEU:HA   | 1.87                     | 0.40              |
| 1:DA:1385:ASN:HD22  | 1:DA:1388:LEU:HB2  | 1.86                     | 0.40              |
| 1:DA:1417:PHE:C     | 1:DA:1419:GLY:N    | 2.80                     | 0.40              |
| 2:DD:337:LEU:HD23   | 2:DD:337:LEU:HA    | 1.82                     | 0.40              |
| 2:DD:571:VAL:HG21   | 2:DD:599:ALA:HB1   | 2.03                     | 0.40              |
| 2:DD:613:TRP:CZ2    | 2:DD:646:ILE:HD11  | 2.56                     | 0.40              |
| 3:DI:111:THR:HG21   | 3:DI:125:TRP:HZ2   | 1.85                     | 0.40              |
| 3:DI:285:GLN:OE1    | 3:DI:317:HIS:HB2   | 2.21                     | 0.40              |
| 4:DL:294:LEU:HD11   | 36:CN:133:HIS:HB2  | 2.03                     | 0.40              |
| 7:DO:74:TRP:CZ2     | 7:DO:259:THR:HG23  | 2.56                     | 0.40              |
| 10:DR:189:GLU:HA    | 10:DR:191:GLN:NE2  | 2.36                     | 0.40              |
| 12:DU:209:GLU:HG2   | 12:DU:210:ALA:N    | 2.36                     | 0.40              |
| 15:DB:759:THR:O     | 15:DB:763:GLU:HG3  | 2.20                     | 0.40              |
| 15:DB:989:LYS:HA    | 15:DB:989:LYS:HD3  | 1.70                     | 0.40              |
| 15:DB:1012:THR:HG22 | 15:DB:1013:ARG:H   | 1.86                     | 0.40              |
| 16:DC:483:LYS:HG3   | 16:DC:531:ARG:HH12 | 1.86                     | 0.40              |
| 18:DF:288:MET:CE    | 20:DH:363:PRO:HG3  | 2.49                     | 0.40              |
| 18:DF:476:LEU:HA    | 18:DF:476:LEU:HD12 | 1.89                     | 0.40              |
| 19:DG:74:LEU:HD12   | 19:DG:74:LEU:HA    | 1.83                     | 0.40              |
| 19:DG:155:GLU:HB3   | 50:Ck:414:MET:HA   | 2.03                     | 0.40              |
| 19:DG:482:PHE:CD1   | 19:DG:547:MET:HG2  | 2.57                     | 0.40              |
| 19:DG:547:MET:HE3   | 19:DG:547:MET:HB3  | 1.59                     | 0.40              |
| 27:DY:35:PRO:HB3    | 47:Cg:464:VAL:HG11 | 2.02                     | 0.40              |
| 29:CE:352:PHE:HE1   | 44:Ca:132:ARG:HG3  | 1.85                     | 0.40              |
| 30:CF:128:ILE:HG22  | 30:CF:129:ASN:OD1  | 2.22                     | 0.40              |
| 33:CJ:286:LEU:HB3   | 33:CJ:327:LEU:HD13 | 2.04                     | 0.40              |
| 34:CK:32:LEU:HD12   | 34:CK:32:LEU:HA    | 1.72                     | 0.40              |
| 37:CO:412:ARG:HD2   | 57:CA:69:U:O4      | 2.21                     | 0.40              |
| 38:CP:86:ARG:HH22   | 53:Cp:31:ALA:HB1   | 1.86                     | 0.40              |
| 39:CQ:34:THR:HG23   | 57:CA:140:U:H1'    | 2.02                     | 0.40              |
| 44:Ca:75:LEU:O      | 44:Ca:79:MET:HG3   | 2.22                     | 0.40              |
| 46:Cd:75:GLU:O      | 46:Cd:78:TYR:HB3   | 2.21                     | 0.40              |
| 47:Cg:190:PRO:O     | 50:Ck:833:PRO:HG3  | 2.22                     | 0.40              |
| 48:Ci:19:HIS:ND1    | 48:Ci:20:PRO:HD2   | 2.36                     | 0.40              |
| 48:Ci:105:ARG:HD2   | 50:Ck:685:TYR:OH   | 2.21                     | 0.40              |
| 50:Ck:414:MET:HG2   | 50:Ck:541:ARG:HG2  | 2.02                     | 0.40              |
| 56:Cv:375:LEU:HD23  | 56:Cv:375:LEU:HA   | 1.91                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:Cv:559:GLN:HE21 | 61:UR:3:UNK:HG1    | 1.85                     | 0.40              |
| 1:DA:1048:ASN:ND2  | 1:DA:1051:ASN:HA   | 2.36                     | 0.40              |
| 2:DD:108:THR:HB    | 2:DD:707:GLN:HE21  | 1.86                     | 0.40              |
| 2:DD:431:LEU:HD22  | 2:DD:465:PHE:CE1   | 2.56                     | 0.40              |
| 4:DL:131:LEU:HB3   | 4:DL:186:GLY:O     | 2.22                     | 0.40              |
| 4:DL:300:LEU:HD13  | 4:DL:300:LEU:HA    | 1.86                     | 0.40              |
| 6:DN:50:LEU:HD11   | 6:DN:111:ILE:HD12  | 2.03                     | 0.40              |
| 8:DP:148:LYS:HB2   | 8:DP:148:LYS:HE2   | 1.90                     | 0.40              |
| 8:DP:175:GLU:CD    | 8:DP:176:PRO:HD3   | 2.46                     | 0.40              |
| 15:DB:1164:ASP:HA  | 25:DW:10:THR:HB    | 2.04                     | 0.40              |
| 16:DC:403:ARG:O    | 16:DC:407:VAL:HG23 | 2.22                     | 0.40              |
| 16:DC:469:THR:HG23 | 22:DK:288:ARG:HG2  | 2.02                     | 0.40              |
| 17:DE:88:LYS:HE2   | 17:DE:88:LYS:HB3   | 1.64                     | 0.40              |
| 18:DF:449:ASP:OD1  | 18:DF:449:ASP:N    | 2.55                     | 0.40              |
| 20:DH:169:TYR:O    | 20:DH:172:PHE:HB3  | 2.21                     | 0.40              |
| 20:DH:558:GLU:HB2  | 20:DH:565:ASN:HD22 | 1.86                     | 0.40              |
| 29:CE:95:ILE:HD12  | 29:CE:300:ILE:HB   | 2.04                     | 0.40              |
| 30:CF:51:PHE:HB2   | 30:CF:90:LEU:HD13  | 2.02                     | 0.40              |
| 30:CF:98:LEU:HA    | 30:CF:98:LEU:HD23  | 1.79                     | 0.40              |
| 32:CI:99:VAL:O     | 45:Cb:103:ARG:HD2  | 2.21                     | 0.40              |
| 33:CJ:54:MET:CE    | 33:CJ:59:PRO:HA    | 2.51                     | 0.40              |
| 36:CN:54:PRO:HB3   | 36:CN:60:VAL:HG13  | 2.02                     | 0.40              |
| 40:CR:103:PHE:CG   | 40:CR:196:PRO:HB3  | 2.57                     | 0.40              |
| 42:CU:13:MET:CE    | 57:CA:314:A:H5''   | 2.48                     | 0.40              |
| 44:Ca:153:LYS:HG3  | 44:Ca:154:GLU:N    | 2.36                     | 0.40              |
| 44:Ca:477:ASP:OD1  | 44:Ca:477:ASP:N    | 2.54                     | 0.40              |
| 44:Ca:588:LYS:O    | 57:CA:261:U:H5     | 2.04                     | 0.40              |
| 46:Cd:41:LYS:HD2   | 46:Cd:41:LYS:HA    | 1.76                     | 0.40              |
| 47:Cg:425:LEU:HD23 | 47:Cg:425:LEU:HA   | 1.76                     | 0.40              |
| 48:Ci:165:PRO:HB2  | 48:Ci:169:TRP:CD1  | 2.56                     | 0.40              |
| 52:Cn:178:LYS:HE3  | 52:Cn:182:PHE:HE2  | 1.87                     | 0.40              |
| 57:CA:79:A:N3      | 57:CA:79:A:H2'     | 2.36                     | 0.40              |
| 57:CA:485:U:H5''   | 57:CA:486:C:H5     | 1.86                     | 0.40              |
| 1:DA:623:HIS:HB3   | 1:DA:625:LYS:HE3   | 2.04                     | 0.40              |
| 1:DA:987:LEU:HD11  | 1:DA:1173:ALA:HB1  | 2.04                     | 0.40              |
| 1:DA:1231:LEU:HD23 | 1:DA:1231:LEU:HA   | 1.93                     | 0.40              |
| 2:DD:518:PHE:CE2   | 2:DD:602:VAL:HG11  | 2.56                     | 0.40              |
| 2:DD:687:HIS:HD2   | 44:Ca:467:LYS:NZ   | 2.20                     | 0.40              |
| 3:DI:133:LEU:HD23  | 3:DI:133:LEU:HA    | 1.89                     | 0.40              |
| 4:DL:41:ASP:OD1    | 4:DL:41:ASP:N      | 2.54                     | 0.40              |
| 5:DM:56:TRP:O      | 5:DM:59:ARG:HG2    | 2.22                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:DM:275:LEU:HA    | 5:DM:275:LEU:HD13  | 1.85                     | 0.40              |
| 8:DP:82:ARG:O      | 8:DP:83:LEU:HB2    | 2.21                     | 0.40              |
| 9:DQ:161:GLY:HA3   | 9:DQ:224:THR:HG23  | 2.03                     | 0.40              |
| 15:DB:550:LEU:HD12 | 15:DB:550:LEU:HA   | 1.75                     | 0.40              |
| 15:DB:883:PRO:HG2  | 15:DB:929:MET:SD   | 2.62                     | 0.40              |
| 15:DB:1086:HIS:CG  | 15:DB:1087:GLY:N   | 2.89                     | 0.40              |
| 15:DB:1134:GLU:OE2 | 57:CA:505:U:H5'    | 2.21                     | 0.40              |
| 16:DC:649:THR:HG22 | 16:DC:651:LYS:H    | 1.86                     | 0.40              |
| 17:DE:415:LEU:N    | 17:DE:416:PRO:HD2  | 2.36                     | 0.40              |
| 17:DE:739:PRO:HA   | 17:DE:740:PRO:HD3  | 1.91                     | 0.40              |
| 18:DF:215:LEU:H    | 33:CJ:476:ASN:HD21 | 1.69                     | 0.40              |
| 18:DF:232:GLU:H    | 18:DF:232:GLU:HG3  | 1.47                     | 0.40              |
| 20:DH:1:MET:HE3    | 20:DH:1:MET:HB2    | 1.54                     | 0.40              |
| 20:DH:76:LEU:HG    | 20:DH:85:LEU:CD2   | 2.51                     | 0.40              |
| 21:DJ:166:LEU:HD12 | 21:DJ:166:LEU:HA   | 1.91                     | 0.40              |
| 22:DK:266:CYS:O    | 22:DK:270:LEU:HB2  | 2.22                     | 0.40              |
| 23:DT:143:TYR:CE1  | 23:DT:177:MET:HE3  | 2.55                     | 0.40              |
| 25:DW:71:GLN:HE22  | 47:Cg:99:GLN:HB3   | 1.86                     | 0.40              |
| 30:CF:16:ARG:H     | 30:CF:16:ARG:HG3   | 1.73                     | 0.40              |
| 31:CH:241:LEU:HD23 | 31:CH:241:LEU:HA   | 1.88                     | 0.40              |
| 32:CI:82:HIS:O     | 51:Cm:128:ARG:NH2  | 2.55                     | 0.40              |
| 32:CI:432:ASP:OD1  | 32:CI:432:ASP:N    | 2.51                     | 0.40              |
| 34:CK:73:GLN:HB3   | 45:Cb:179:GLU:HG3  | 2.03                     | 0.40              |
| 36:CN:164:SER:O    | 50:Ck:749:ASP:HB2  | 2.22                     | 0.40              |
| 37:CO:426:HIS:CD2  | 37:CO:426:HIS:N    | 2.90                     | 0.40              |
| 38:CP:13:ILE:HG12  | 57:CA:57:U:C2      | 2.56                     | 0.40              |
| 40:CR:60:PHE:O     | 51:Cm:73:HIS:HE1   | 2.04                     | 0.40              |
| 40:CR:109:ASP:HA   | 40:CR:110:PRO:HD2  | 1.92                     | 0.40              |
| 40:CR:123:LYS:O    | 40:CR:128:ASN:HB2  | 2.21                     | 0.40              |
| 40:CR:297:HIS:CG   | 46:Cd:279:ARG:HG2  | 2.56                     | 0.40              |
| 42:CU:188:TYR:HD1  | 46:Cd:281:MET:SD   | 2.45                     | 0.40              |
| 44:Ca:138:LYS:NZ   | 44:Ca:141:THR:HA   | 2.36                     | 0.40              |
| 46:Cd:174:PRO:HD3  | 46:Cd:219:HIS:CE1  | 2.57                     | 0.40              |
| 47:Cg:16:ARG:NH2   | 47:Cg:25:ALA:HA    | 2.36                     | 0.40              |
| 47:Cg:149:GLY:O    | 47:Cg:155:LYS:NZ   | 2.41                     | 0.40              |
| 47:Cg:296:HIS:HA   | 47:Cg:327:ARG:HH11 | 1.86                     | 0.40              |
| 50:Ck:633:MET:HE2  | 50:Ck:633:MET:HB2  | 1.90                     | 0.40              |
| 50:Ck:645:ALA:O    | 50:Ck:649:THR:OG1  | 2.40                     | 0.40              |
| 50:Ck:736:LEU:HA   | 50:Ck:736:LEU:HD23 | 1.76                     | 0.40              |
| 52:Cn:213:LYS:HE2  | 52:Cn:213:LYS:HB2  | 1.89                     | 0.40              |
| 53:Cp:145:GLU:OE1  | 53:Cp:145:GLU:N    | 2.55                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:Cv:740:ILE:HD13 | 56:Cv:740:ILE:HA   | 1.77                     | 0.40              |
| 56:Cv:819:LEU:HD21 | 56:Cv:823:ARG:HH22 | 1.86                     | 0.40              |
| 57:CA:436:U:H2'    | 57:CA:437:U:O4'    | 2.21                     | 0.40              |
| 1:DA:650:LEU:HD13  | 1:DA:725:TRP:CZ3   | 2.57                     | 0.40              |
| 1:DA:816:THR:HA    | 1:DA:817:PRO:HD3   | 1.80                     | 0.40              |
| 1:DA:959:LYS:N     | 1:DA:959:LYS:HD2   | 2.37                     | 0.40              |
| 2:DD:296:LEU:HD13  | 2:DD:392:SER:HB2   | 2.03                     | 0.40              |
| 2:DD:668:ARG:HB3   | 11:DS:243:LEU:HD21 | 2.04                     | 0.40              |
| 4:DL:195:SER:O     | 4:DL:199:ASP:HB2   | 2.21                     | 0.40              |
| 7:DO:57:TYR:HE1    | 56:Cv:679:PRO:HB3  | 1.87                     | 0.40              |
| 9:DQ:120:MET:HE3   | 9:DQ:120:MET:HB3   | 1.90                     | 0.40              |
| 12:DU:106:PRO:HG2  | 12:DU:109:SER:HB3  | 2.03                     | 0.40              |
| 14:Da:30:HIS:HA    | 14:Da:31:PRO:HD3   | 1.94                     | 0.40              |
| 15:DB:456:LEU:HD23 | 15:DB:456:LEU:HA   | 1.90                     | 0.40              |
| 15:DB:969:THR:O    | 19:DG:45:LYS:HG3   | 2.21                     | 0.40              |
| 15:DB:969:THR:HG23 | 19:DG:45:LYS:O     | 2.22                     | 0.40              |
| 15:DB:1066:ASN:O   | 18:DF:283:HIS:HE1  | 2.05                     | 0.40              |
| 16:DC:854:LEU:HD22 | 16:DC:859:LEU:HD12 | 2.03                     | 0.40              |
| 16:DC:888:LEU:HD23 | 16:DC:888:LEU:HA   | 1.93                     | 0.40              |
| 19:DG:64:ARG:NH2   | 19:DG:98:ASP:OD1   | 2.52                     | 0.40              |
| 20:DH:284:LEU:HD23 | 20:DH:284:LEU:HA   | 1.92                     | 0.40              |
| 21:DJ:28:TYR:HD2   | 28:CC:68:PHE:HE2   | 1.68                     | 0.40              |
| 21:DJ:147:ARG:O    | 21:DJ:155:ALA:HB3  | 2.21                     | 0.40              |
| 23:DT:28:GLU:HB2   | 23:DT:31:ASN:HD22  | 1.86                     | 0.40              |
| 32:CI:248:PHE:CZ   | 32:CI:252:ARG:HD2  | 2.56                     | 0.40              |
| 32:CI:400:VAL:HG23 | 32:CI:410:LEU:HD12 | 2.04                     | 0.40              |
| 33:CJ:444:ALA:HB1  | 33:CJ:523:VAL:HG22 | 2.04                     | 0.40              |
| 38:CP:79:ASP:HB3   | 38:CP:86:ARG:HH12  | 1.87                     | 0.40              |
| 44:Ca:62:TRP:HD1   | 44:Ca:79:MET:HE1   | 1.84                     | 0.40              |
| 44:Ca:359:ARG:HD2  | 57:CA:3:A:N6       | 2.37                     | 0.40              |
| 44:Ca:419:GLN:H    | 44:Ca:419:GLN:HG2  | 1.79                     | 0.40              |
| 44:Ca:511:ILE:HA   | 44:Ca:511:ILE:HD13 | 1.87                     | 0.40              |
| 45:Cb:29:GLU:O     | 45:Cb:32:GLU:HB2   | 2.21                     | 0.40              |
| 49:Cj:219:GLU:OE1  | 49:Cj:219:GLU:N    | 2.37                     | 0.40              |
| 50:Ck:131:ASN:O    | 50:Ck:135:ASN:HB2  | 2.22                     | 0.40              |
| 50:Ck:147:LYS:O    | 50:Ck:147:LYS:HG3  | 2.21                     | 0.40              |
| 50:Ck:407:GLU:HB3  | 50:Ck:548:ILE:HD11 | 2.03                     | 0.40              |
| 52:Cn:190:VAL:HB   | 52:Cn:193:LEU:HD12 | 2.03                     | 0.40              |
| 56:Cv:234:MET:HE3  | 56:Cv:237:ALA:HB3  | 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%) | 1490 (96%) | 59 (4%) | 2 (0%)   | 48          | 77  |
| 2   | DD    | 787/812 (97%)   | 740 (94%)  | 44 (6%) | 3 (0%)   | 30          | 58  |
| 3   | DI    | 388/407 (95%)   | 365 (94%)  | 22 (6%) | 1 (0%)   | 36          | 64  |
| 4   | DL    | 279/307 (91%)   | 261 (94%)  | 18 (6%) | 0        | 100         | 100 |
| 5   | DM    | 292/294 (99%)   | 280 (96%)  | 12 (4%) | 0        | 100         | 100 |
| 6   | DN    | 253/293 (86%)   | 238 (94%)  | 15 (6%) | 0        | 100         | 100 |
| 7   | DO    | 220/282 (78%)   | 209 (95%)  | 10 (4%) | 1 (0%)   | 24          | 53  |
| 8   | DP    | 187/274 (68%)   | 176 (94%)  | 11 (6%) | 0        | 100         | 100 |
| 9   | DQ    | 254/268 (95%)   | 244 (96%)  | 9 (4%)  | 1 (0%)   | 30          | 58  |
| 10  | DR    | 247/270 (92%)   | 236 (96%)  | 10 (4%) | 1 (0%)   | 30          | 58  |
| 11  | DS    | 234/261 (90%)   | 222 (95%)  | 11 (5%) | 1 (0%)   | 30          | 58  |
| 12  | DU    | 211/228 (92%)   | 198 (94%)  | 11 (5%) | 2 (1%)   | 14          | 41  |
| 13  | DZ    | 80/94 (85%)     | 75 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 14  | Da    | 53/64 (83%)     | 52 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 15  | DB    | 1109/1181 (94%) | 1073 (97%) | 35 (3%) | 1 (0%)   | 48          | 77  |
| 16  | DC    | 1087/1165 (93%) | 1053 (97%) | 33 (3%) | 1 (0%)   | 48          | 77  |
| 17  | DE    | 576/747 (77%)   | 564 (98%)  | 12 (2%) | 0        | 100         | 100 |
| 18  | DF    | 586/666 (88%)   | 568 (97%)  | 18 (3%) | 0        | 100         | 100 |
| 19  | DG    | 558/631 (88%)   | 543 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 20  | DH    | 560/581 (96%)   | 539 (96%)  | 21 (4%) | 0        | 100         | 100 |
| 21  | DJ    | 313/396 (79%)   | 299 (96%)  | 13 (4%) | 1 (0%)   | 36          | 64  |
| 22  | DK    | 249/324 (77%)   | 238 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 23  | DT    | 237/247 (96%)   | 232 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 24  | DV    | 158/183 (86%)   | 152 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 25  | DW    | 159/179 (89%)   | 153 (96%)  | 6 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 26  | DX    | 139/169 (82%)   | 130 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 27  | DY    | 152/163 (93%)   | 147 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 28  | CC    | 72/74 (97%)     | 67 (93%)   | 5 (7%)  | 0        | 100         | 100 |
| 29  | CE    | 413/435 (95%)   | 386 (94%)  | 26 (6%) | 1 (0%)   | 43          | 70  |
| 30  | CF    | 157/160 (98%)   | 153 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 31  | CH    | 271/282 (96%)   | 259 (96%)  | 11 (4%) | 1 (0%)   | 30          | 58  |
| 32  | CI    | 418/443 (94%)   | 405 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 33  | CJ    | 796/817 (97%)   | 755 (95%)  | 39 (5%) | 2 (0%)   | 36          | 64  |
| 34  | CK    | 287/326 (88%)   | 267 (93%)  | 20 (7%) | 0        | 100         | 100 |
| 35  | CL    | 85/87 (98%)     | 79 (93%)   | 5 (6%)  | 1 (1%)   | 10          | 34  |
| 36  | CN    | 155/166 (93%)   | 148 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 37  | CO    | 359/429 (84%)   | 342 (95%)  | 16 (4%) | 1 (0%)   | 36          | 64  |
| 38  | CP    | 178/188 (95%)   | 170 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 39  | CQ    | 188/307 (61%)   | 178 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 40  | CR    | 312/320 (98%)   | 297 (95%)  | 14 (4%) | 1 (0%)   | 36          | 64  |
| 41  | CS    | 140/244 (57%)   | 132 (94%)  | 8 (6%)  | 0        | 100         | 100 |
| 42  | CU    | 182/193 (94%)   | 173 (95%)  | 8 (4%)  | 1 (0%)   | 24          | 53  |
| 43  | CZ    | 149/360 (41%)   | 142 (95%)  | 6 (4%)  | 1 (1%)   | 18          | 46  |
| 44  | Ca    | 590/602 (98%)   | 551 (93%)  | 34 (6%) | 5 (1%)   | 16          | 44  |
| 45  | Cb    | 248/325 (76%)   | 241 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 46  | Cd    | 288/440 (66%)   | 277 (96%)  | 10 (4%) | 1 (0%)   | 36          | 64  |
| 47  | Cg    | 480/498 (96%)   | 462 (96%)  | 18 (4%) | 0        | 100         | 100 |
| 48  | Ci    | 163/181 (90%)   | 154 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 49  | Cj    | 224/257 (87%)   | 215 (96%)  | 8 (4%)  | 1 (0%)   | 30          | 58  |
| 50  | Ck    | 699/874 (80%)   | 676 (97%)  | 22 (3%) | 1 (0%)   | 48          | 77  |
| 51  | Cm    | 194/215 (90%)   | 182 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 52  | Cn    | 108/250 (43%)   | 103 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 53  | Cp    | 173/187 (92%)   | 167 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 54  | Cq    | 250/263 (95%)   | 242 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 55  | Cr    | 253/439 (58%)   | 241 (95%)  | 11 (4%) | 1 (0%)   | 30          | 58  |
| 56  | Cv    | 1051/1211 (87%) | 1010 (96%) | 41 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|----------|-------------|----|
| All | All   | 19802/22847 (87%) | 18951 (96%) | 818 (4%) | 33 (0%)  | 44          | 70 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 43  | CZ    | 296  | PRO  |
| 44  | Ca    | 32   | PRO  |
| 44  | Ca    | 33   | PRO  |
| 44  | Ca    | 35   | PRO  |
| 2   | DD    | 352  | VAL  |
| 44  | Ca    | 34   | LYS  |
| 1   | DA    | 131  | ASP  |
| 7   | DO    | 115  | ASP  |
| 15  | DB    | 1033 | TYR  |
| 21  | DJ    | 36   | GLN  |
| 29  | CE    | 313  | MET  |
| 35  | CL    | 80   | LYS  |
| 40  | CR    | 59   | LEU  |
| 42  | CU    | 19   | ALA  |
| 2   | DD    | 256  | PRO  |
| 49  | Cj    | 54   | ALA  |
| 2   | DD    | 248  | ASP  |
| 3   | DI    | 190  | PRO  |
| 10  | DR    | 269  | TRP  |
| 12  | DU    | 205  | ALA  |
| 33  | CJ    | 37   | ASN  |
| 33  | CJ    | 196  | ALA  |
| 37  | CO    | 87   | THR  |
| 46  | Cd    | 224  | ILE  |
| 1   | DA    | 1589 | ALA  |
| 9   | DQ    | 173  | ASP  |
| 11  | DS    | 129  | GLU  |
| 12  | DU    | 191  | SER  |
| 50  | Ck    | 231  | GLY  |
| 16  | DC    | 441  | VAL  |
| 55  | Cr    | 29   | PRO  |
| 31  | CH    | 18   | PRO  |
| 44  | Ca    | 31   | GLU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | DA    | 1322/1514 (87%) | 1195 (90%) | 127 (10%) | 8           | 28 |
| 2   | DD    | 694/711 (98%)   | 618 (89%)  | 76 (11%)  | 6           | 22 |
| 3   | DI    | 350/365 (96%)   | 312 (89%)  | 38 (11%)  | 6           | 23 |
| 4   | DL    | 241/263 (92%)   | 209 (87%)  | 32 (13%)  | 4           | 16 |
| 5   | DM    | 252/252 (100%)  | 223 (88%)  | 29 (12%)  | 5           | 21 |
| 6   | DN    | 229/256 (90%)   | 206 (90%)  | 23 (10%)  | 7           | 26 |
| 7   | DO    | 186/229 (81%)   | 172 (92%)  | 14 (8%)   | 12          | 38 |
| 8   | DP    | 170/239 (71%)   | 157 (92%)  | 13 (8%)   | 12          | 38 |
| 9   | DQ    | 228/239 (95%)   | 220 (96%)  | 8 (4%)    | 32          | 56 |
| 10  | DR    | 220/235 (94%)   | 193 (88%)  | 27 (12%)  | 4           | 19 |
| 11  | DS    | 209/228 (92%)   | 194 (93%)  | 15 (7%)   | 13          | 39 |
| 12  | DU    | 190/201 (94%)   | 169 (89%)  | 21 (11%)  | 6           | 22 |
| 13  | DZ    | 72/84 (86%)     | 67 (93%)   | 5 (7%)    | 14          | 40 |
| 14  | Da    | 50/59 (85%)     | 42 (84%)   | 8 (16%)   | 2           | 10 |
| 15  | DB    | 976/1030 (95%)  | 870 (89%)  | 106 (11%) | 6           | 23 |
| 16  | DC    | 927/985 (94%)   | 827 (89%)  | 100 (11%) | 6           | 23 |
| 17  | DE    | 519/644 (81%)   | 466 (90%)  | 53 (10%)  | 7           | 25 |
| 18  | DF    | 500/560 (89%)   | 442 (88%)  | 58 (12%)  | 5           | 21 |
| 19  | DG    | 490/543 (90%)   | 430 (88%)  | 60 (12%)  | 5           | 19 |
| 20  | DH    | 493/504 (98%)   | 437 (89%)  | 56 (11%)  | 5           | 21 |
| 21  | DJ    | 275/347 (79%)   | 246 (90%)  | 29 (10%)  | 6           | 24 |
| 22  | DK    | 209/261 (80%)   | 186 (89%)  | 23 (11%)  | 6           | 22 |
| 23  | DT    | 220/228 (96%)   | 192 (87%)  | 28 (13%)  | 4           | 17 |
| 24  | DV    | 145/165 (88%)   | 133 (92%)  | 12 (8%)   | 10          | 35 |
| 25  | DW    | 148/163 (91%)   | 132 (89%)  | 16 (11%)  | 6           | 23 |
| 26  | DX    | 124/149 (83%)   | 111 (90%)  | 13 (10%)  | 6           | 24 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers   | Percentiles |    |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 27  | DY    | 137/146 (94%)     | 117 (85%)   | 20 (15%)   | 3           | 13 |
| 28  | CC    | 73/73 (100%)      | 64 (88%)    | 9 (12%)    | 4           | 19 |
| 29  | CE    | 358/372 (96%)     | 309 (86%)   | 49 (14%)   | 3           | 15 |
| 30  | CF    | 136/144 (94%)     | 121 (89%)   | 15 (11%)   | 6           | 22 |
| 31  | CH    | 237/246 (96%)     | 207 (87%)   | 30 (13%)   | 4           | 17 |
| 32  | CI    | 357/371 (96%)     | 319 (89%)   | 38 (11%)   | 6           | 23 |
| 33  | CJ    | 709/723 (98%)     | 619 (87%)   | 90 (13%)   | 4           | 17 |
| 34  | CK    | 257/283 (91%)     | 220 (86%)   | 37 (14%)   | 3           | 13 |
| 35  | CL    | 79/79 (100%)      | 63 (80%)    | 16 (20%)   | 1           | 4  |
| 36  | CN    | 142/150 (95%)     | 122 (86%)   | 20 (14%)   | 3           | 14 |
| 37  | CO    | 318/377 (84%)     | 267 (84%)   | 51 (16%)   | 2           | 10 |
| 38  | CP    | 160/168 (95%)     | 142 (89%)   | 18 (11%)   | 5           | 21 |
| 39  | CQ    | 171/270 (63%)     | 145 (85%)   | 26 (15%)   | 3           | 11 |
| 40  | CR    | 275/279 (99%)     | 244 (89%)   | 31 (11%)   | 5           | 21 |
| 41  | CS    | 126/220 (57%)     | 116 (92%)   | 10 (8%)    | 11          | 37 |
| 42  | CU    | 160/169 (95%)     | 146 (91%)   | 14 (9%)    | 9           | 31 |
| 43  | CZ    | 121/313 (39%)     | 108 (89%)   | 13 (11%)   | 6           | 23 |
| 44  | Ca    | 516/543 (95%)     | 463 (90%)   | 53 (10%)   | 7           | 25 |
| 45  | Cb    | 219/277 (79%)     | 194 (89%)   | 25 (11%)   | 5           | 21 |
| 46  | Cd    | 237/381 (62%)     | 209 (88%)   | 28 (12%)   | 5           | 20 |
| 47  | Cg    | 424/437 (97%)     | 383 (90%)   | 41 (10%)   | 8           | 28 |
| 48  | Ci    | 144/160 (90%)     | 118 (82%)   | 26 (18%)   | 2           | 7  |
| 49  | Cj    | 193/219 (88%)     | 171 (89%)   | 22 (11%)   | 5           | 21 |
| 50  | Ck    | 608/747 (81%)     | 542 (89%)   | 66 (11%)   | 6           | 23 |
| 51  | Cm    | 165/184 (90%)     | 140 (85%)   | 25 (15%)   | 3           | 11 |
| 52  | Cn    | 95/210 (45%)      | 83 (87%)    | 12 (13%)   | 4           | 18 |
| 53  | Cp    | 163/175 (93%)     | 146 (90%)   | 17 (10%)   | 7           | 24 |
| 54  | Cq    | 210/221 (95%)     | 182 (87%)   | 28 (13%)   | 4           | 16 |
| 55  | Cr    | 211/369 (57%)     | 183 (87%)   | 28 (13%)   | 4           | 16 |
| 56  | Cv    | 912/1034 (88%)    | 797 (87%)   | 115 (13%)  | 4           | 18 |
| All | All   | 17352/19794 (88%) | 15389 (89%) | 1963 (11%) | 8           | 21 |

All (1963) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DA    | 41  | PHE  |
| 1   | DA    | 58  | ILE  |
| 1   | DA    | 60  | GLU  |
| 1   | DA    | 61  | LYS  |
| 1   | DA    | 79  | LEU  |
| 1   | DA    | 87  | THR  |
| 1   | DA    | 112 | GLN  |
| 1   | DA    | 114 | GLU  |
| 1   | DA    | 128 | THR  |
| 1   | DA    | 148 | LYS  |
| 1   | DA    | 150 | ILE  |
| 1   | DA    | 158 | LEU  |
| 1   | DA    | 165 | ARG  |
| 1   | DA    | 167 | THR  |
| 1   | DA    | 183 | SER  |
| 1   | DA    | 194 | LEU  |
| 1   | DA    | 200 | ILE  |
| 1   | DA    | 201 | LYS  |
| 1   | DA    | 226 | ASP  |
| 1   | DA    | 227 | ILE  |
| 1   | DA    | 230 | PHE  |
| 1   | DA    | 235 | THR  |
| 1   | DA    | 240 | GLU  |
| 1   | DA    | 254 | PHE  |
| 1   | DA    | 259 | LEU  |
| 1   | DA    | 274 | LEU  |
| 1   | DA    | 295 | SER  |
| 1   | DA    | 300 | THR  |
| 1   | DA    | 309 | VAL  |
| 1   | DA    | 344 | ARG  |
| 1   | DA    | 357 | THR  |
| 1   | DA    | 388 | VAL  |
| 1   | DA    | 397 | ILE  |
| 1   | DA    | 408 | LEU  |
| 1   | DA    | 419 | THR  |
| 1   | DA    | 436 | ASN  |
| 1   | DA    | 456 | ARG  |
| 1   | DA    | 476 | SER  |
| 1   | DA    | 486 | LYS  |
| 1   | DA    | 487 | THR  |
| 1   | DA    | 493 | TRP  |
| 1   | DA    | 503 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 509  | LEU  |
| 1   | DA    | 539  | LEU  |
| 1   | DA    | 547  | ARG  |
| 1   | DA    | 557  | SER  |
| 1   | DA    | 583  | VAL  |
| 1   | DA    | 602  | LEU  |
| 1   | DA    | 627  | PHE  |
| 1   | DA    | 630  | ASP  |
| 1   | DA    | 632  | THR  |
| 1   | DA    | 646  | ASP  |
| 1   | DA    | 650  | LEU  |
| 1   | DA    | 653  | LYS  |
| 1   | DA    | 680  | VAL  |
| 1   | DA    | 708  | GLU  |
| 1   | DA    | 711  | ILE  |
| 1   | DA    | 729  | ARG  |
| 1   | DA    | 739  | ARG  |
| 1   | DA    | 751  | GLU  |
| 1   | DA    | 758  | VAL  |
| 1   | DA    | 767  | VAL  |
| 1   | DA    | 780  | ASP  |
| 1   | DA    | 781  | ARG  |
| 1   | DA    | 783  | VAL  |
| 1   | DA    | 819  | ARG  |
| 1   | DA    | 849  | THR  |
| 1   | DA    | 859  | GLN  |
| 1   | DA    | 865  | ASP  |
| 1   | DA    | 892  | ASP  |
| 1   | DA    | 903  | LYS  |
| 1   | DA    | 914  | THR  |
| 1   | DA    | 920  | LEU  |
| 1   | DA    | 934  | GLU  |
| 1   | DA    | 936  | LYS  |
| 1   | DA    | 942  | LEU  |
| 1   | DA    | 963  | LEU  |
| 1   | DA    | 973  | LEU  |
| 1   | DA    | 988  | CYS  |
| 1   | DA    | 992  | GLU  |
| 1   | DA    | 999  | SER  |
| 1   | DA    | 1000 | ASN  |
| 1   | DA    | 1036 | HIS  |
| 1   | DA    | 1045 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 1057 | VAL  |
| 1   | DA    | 1058 | ARG  |
| 1   | DA    | 1062 | TYR  |
| 1   | DA    | 1063 | THR  |
| 1   | DA    | 1077 | ARG  |
| 1   | DA    | 1097 | LEU  |
| 1   | DA    | 1117 | ASN  |
| 1   | DA    | 1120 | SER  |
| 1   | DA    | 1125 | GLU  |
| 1   | DA    | 1132 | LYS  |
| 1   | DA    | 1145 | THR  |
| 1   | DA    | 1152 | HIS  |
| 1   | DA    | 1168 | ASP  |
| 1   | DA    | 1185 | ARG  |
| 1   | DA    | 1188 | GLU  |
| 1   | DA    | 1205 | THR  |
| 1   | DA    | 1208 | THR  |
| 1   | DA    | 1220 | VAL  |
| 1   | DA    | 1240 | LEU  |
| 1   | DA    | 1248 | LEU  |
| 1   | DA    | 1255 | VAL  |
| 1   | DA    | 1263 | VAL  |
| 1   | DA    | 1268 | LEU  |
| 1   | DA    | 1271 | LEU  |
| 1   | DA    | 1292 | CYS  |
| 1   | DA    | 1378 | LEU  |
| 1   | DA    | 1380 | GLU  |
| 1   | DA    | 1381 | LEU  |
| 1   | DA    | 1404 | ARG  |
| 1   | DA    | 1411 | THR  |
| 1   | DA    | 1427 | LEU  |
| 1   | DA    | 1429 | SER  |
| 1   | DA    | 1433 | ASP  |
| 1   | DA    | 1441 | THR  |
| 1   | DA    | 1488 | GLN  |
| 1   | DA    | 1544 | ASN  |
| 1   | DA    | 1557 | THR  |
| 1   | DA    | 1597 | GLU  |
| 1   | DA    | 1605 | ARG  |
| 1   | DA    | 1624 | ILE  |
| 1   | DA    | 1629 | GLN  |
| 1   | DA    | 1662 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 1664 | ILE  |
| 2   | DD    | 12   | SER  |
| 2   | DD    | 25   | LEU  |
| 2   | DD    | 27   | MET  |
| 2   | DD    | 40   | MET  |
| 2   | DD    | 44   | MET  |
| 2   | DD    | 46   | VAL  |
| 2   | DD    | 48   | MET  |
| 2   | DD    | 79   | GLN  |
| 2   | DD    | 82   | ASN  |
| 2   | DD    | 84   | LYS  |
| 2   | DD    | 90   | MET  |
| 2   | DD    | 94   | LYS  |
| 2   | DD    | 104  | ARG  |
| 2   | DD    | 108  | THR  |
| 2   | DD    | 122  | GLN  |
| 2   | DD    | 123  | ARG  |
| 2   | DD    | 125  | LEU  |
| 2   | DD    | 129  | ARG  |
| 2   | DD    | 139  | LEU  |
| 2   | DD    | 146  | ARG  |
| 2   | DD    | 148  | SER  |
| 2   | DD    | 149  | SER  |
| 2   | DD    | 156  | GLN  |
| 2   | DD    | 226  | THR  |
| 2   | DD    | 233  | ASN  |
| 2   | DD    | 242  | LEU  |
| 2   | DD    | 246  | GLU  |
| 2   | DD    | 247  | VAL  |
| 2   | DD    | 248  | ASP  |
| 2   | DD    | 269  | LYS  |
| 2   | DD    | 275  | ASP  |
| 2   | DD    | 281  | ASP  |
| 2   | DD    | 292  | ARG  |
| 2   | DD    | 298  | MET  |
| 2   | DD    | 347  | GLU  |
| 2   | DD    | 349  | CYS  |
| 2   | DD    | 350  | LYS  |
| 2   | DD    | 377  | GLU  |
| 2   | DD    | 379  | GLN  |
| 2   | DD    | 394  | LYS  |
| 2   | DD    | 424  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | DD    | 439 | GLU  |
| 2   | DD    | 444 | SER  |
| 2   | DD    | 449 | LEU  |
| 2   | DD    | 454 | THR  |
| 2   | DD    | 455 | SER  |
| 2   | DD    | 463 | GLU  |
| 2   | DD    | 464 | VAL  |
| 2   | DD    | 470 | LYS  |
| 2   | DD    | 478 | GLN  |
| 2   | DD    | 503 | SER  |
| 2   | DD    | 504 | ASN  |
| 2   | DD    | 521 | ASN  |
| 2   | DD    | 541 | ARG  |
| 2   | DD    | 577 | LYS  |
| 2   | DD    | 589 | GLN  |
| 2   | DD    | 603 | GLU  |
| 2   | DD    | 621 | LEU  |
| 2   | DD    | 624 | THR  |
| 2   | DD    | 626 | ARG  |
| 2   | DD    | 633 | GLU  |
| 2   | DD    | 651 | ARG  |
| 2   | DD    | 653 | PHE  |
| 2   | DD    | 654 | ARG  |
| 2   | DD    | 672 | ASP  |
| 2   | DD    | 689 | LEU  |
| 2   | DD    | 704 | ASP  |
| 2   | DD    | 752 | PHE  |
| 2   | DD    | 761 | ARG  |
| 2   | DD    | 765 | ARG  |
| 2   | DD    | 774 | VAL  |
| 2   | DD    | 782 | ILE  |
| 2   | DD    | 785 | MET  |
| 2   | DD    | 787 | ARG  |
| 2   | DD    | 799 | ASP  |
| 2   | DD    | 812 | TYR  |
| 3   | DI    | 35  | TYR  |
| 3   | DI    | 43  | ASP  |
| 3   | DI    | 50  | LEU  |
| 3   | DI    | 67  | ILE  |
| 3   | DI    | 79  | ILE  |
| 3   | DI    | 88  | GLN  |
| 3   | DI    | 90  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | DI    | 107 | ILE  |
| 3   | DI    | 113 | VAL  |
| 3   | DI    | 139 | VAL  |
| 3   | DI    | 144 | LEU  |
| 3   | DI    | 146 | ARG  |
| 3   | DI    | 152 | LEU  |
| 3   | DI    | 158 | ARG  |
| 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    | 210 | ILE  |
| 3   | DI    | 237 | ARG  |
| 3   | DI    | 243 | LEU  |
| 3   | DI    | 273 | VAL  |
| 3   | DI    | 282 | ASP  |
| 3   | DI    | 310 | LEU  |
| 3   | DI    | 320 | GLN  |
| 3   | DI    | 328 | VAL  |
| 3   | DI    | 334 | ILE  |
| 3   | DI    | 338 | GLU  |
| 3   | DI    | 344 | LEU  |
| 3   | DI    | 345 | LEU  |
| 3   | DI    | 349 | THR  |
| 3   | DI    | 353 | LYS  |
| 3   | DI    | 356 | ILE  |
| 3   | DI    | 373 | LEU  |
| 3   | DI    | 399 | THR  |
| 4   | DL    | 18  | ARG  |
| 4   | DL    | 28  | ASN  |
| 4   | DL    | 39  | THR  |
| 4   | DL    | 40  | THR  |
| 4   | DL    | 41  | ASP  |
| 4   | DL    | 64  | ILE  |
| 4   | DL    | 74  | ARG  |
| 4   | DL    | 77  | LEU  |
| 4   | DL    | 82  | ASP  |
| 4   | DL    | 92  | ILE  |
| 4   | DL    | 117 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | DL    | 118 | ASP  |
| 4   | DL    | 119 | MET  |
| 4   | DL    | 136 | MET  |
| 4   | DL    | 158 | THR  |
| 4   | DL    | 165 | PHE  |
| 4   | DL    | 171 | ARG  |
| 4   | DL    | 183 | LEU  |
| 4   | DL    | 200 | VAL  |
| 4   | DL    | 240 | GLU  |
| 4   | DL    | 243 | LEU  |
| 4   | DL    | 249 | LEU  |
| 4   | DL    | 256 | SER  |
| 4   | DL    | 267 | HIS  |
| 4   | DL    | 268 | VAL  |
| 4   | DL    | 270 | THR  |
| 4   | DL    | 273 | THR  |
| 4   | DL    | 274 | THR  |
| 4   | DL    | 286 | THR  |
| 4   | DL    | 289 | ARG  |
| 4   | DL    | 300 | LEU  |
| 4   | DL    | 305 | THR  |
| 5   | DM    | 1   | MET  |
| 5   | DM    | 8   | THR  |
| 5   | DM    | 10  | ARG  |
| 5   | DM    | 11  | VAL  |
| 5   | DM    | 15  | LEU  |
| 5   | DM    | 19  | HIS  |
| 5   | DM    | 30  | ARG  |
| 5   | DM    | 46  | PHE  |
| 5   | DM    | 55  | GLU  |
| 5   | DM    | 56  | TRP  |
| 5   | DM    | 64  | THR  |
| 5   | DM    | 76  | ASN  |
| 5   | DM    | 84  | LEU  |
| 5   | DM    | 90  | LEU  |
| 5   | DM    | 104 | LYS  |
| 5   | DM    | 122 | LYS  |
| 5   | DM    | 128 | ILE  |
| 5   | DM    | 129 | ARG  |
| 5   | DM    | 131 | ASN  |
| 5   | DM    | 157 | LEU  |
| 5   | DM    | 158 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | DM    | 179 | ARG  |
| 5   | DM    | 180 | GLN  |
| 5   | DM    | 198 | THR  |
| 5   | DM    | 199 | LEU  |
| 5   | DM    | 239 | LYS  |
| 5   | DM    | 265 | ILE  |
| 5   | DM    | 275 | LEU  |
| 5   | DM    | 291 | ILE  |
| 6   | DN    | 17  | MET  |
| 6   | DN    | 23  | VAL  |
| 6   | DN    | 24  | LEU  |
| 6   | DN    | 27  | ASP  |
| 6   | DN    | 42  | THR  |
| 6   | DN    | 116 | VAL  |
| 6   | DN    | 141 | MET  |
| 6   | DN    | 152 | LEU  |
| 6   | DN    | 162 | LEU  |
| 6   | DN    | 166 | LEU  |
| 6   | DN    | 171 | LEU  |
| 6   | DN    | 204 | SER  |
| 6   | DN    | 223 | GLN  |
| 6   | DN    | 224 | ARG  |
| 6   | DN    | 237 | ARG  |
| 6   | DN    | 246 | GLN  |
| 6   | DN    | 258 | ASP  |
| 6   | DN    | 261 | ARG  |
| 6   | DN    | 267 | GLU  |
| 6   | DN    | 273 | SER  |
| 6   | DN    | 276 | GLN  |
| 6   | DN    | 282 | SER  |
| 6   | DN    | 292 | TYR  |
| 7   | DO    | 62  | LEU  |
| 7   | DO    | 65  | GLU  |
| 7   | DO    | 73  | LEU  |
| 7   | DO    | 93  | LEU  |
| 7   | DO    | 113 | LEU  |
| 7   | DO    | 125 | LEU  |
| 7   | DO    | 136 | ASP  |
| 7   | DO    | 157 | ILE  |
| 7   | DO    | 163 | ARG  |
| 7   | DO    | 211 | GLU  |
| 7   | DO    | 234 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | DO    | 239 | LYS  |
| 7   | DO    | 249 | ASP  |
| 7   | DO    | 255 | ARG  |
| 8   | DP    | 21  | MET  |
| 8   | DP    | 23  | LEU  |
| 8   | DP    | 28  | ASN  |
| 8   | DP    | 34  | VAL  |
| 8   | DP    | 41  | GLN  |
| 8   | DP    | 44  | GLU  |
| 8   | DP    | 69  | LEU  |
| 8   | DP    | 94  | VAL  |
| 8   | DP    | 105 | GLN  |
| 8   | DP    | 124 | ARG  |
| 8   | DP    | 152 | LEU  |
| 8   | DP    | 158 | CYS  |
| 8   | DP    | 173 | HIS  |
| 9   | DQ    | 50  | THR  |
| 9   | DQ    | 72  | THR  |
| 9   | DQ    | 130 | LEU  |
| 9   | DQ    | 145 | VAL  |
| 9   | DQ    | 177 | LEU  |
| 9   | DQ    | 192 | LEU  |
| 9   | DQ    | 216 | ASN  |
| 9   | DQ    | 250 | ARG  |
| 10  | DR    | 23  | VAL  |
| 10  | DR    | 32  | VAL  |
| 10  | DR    | 39  | GLN  |
| 10  | DR    | 51  | LEU  |
| 10  | DR    | 54  | LEU  |
| 10  | DR    | 60  | VAL  |
| 10  | DR    | 63  | ILE  |
| 10  | DR    | 64  | ILE  |
| 10  | DR    | 67  | LYS  |
| 10  | DR    | 68  | HIS  |
| 10  | DR    | 78  | ARG  |
| 10  | DR    | 91  | THR  |
| 10  | DR    | 107 | LEU  |
| 10  | DR    | 108 | GLN  |
| 10  | DR    | 118 | VAL  |
| 10  | DR    | 129 | ASP  |
| 10  | DR    | 131 | LEU  |
| 10  | DR    | 133 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | DR    | 148 | VAL  |
| 10  | DR    | 176 | THR  |
| 10  | DR    | 190 | LEU  |
| 10  | DR    | 192 | LEU  |
| 10  | DR    | 201 | CYS  |
| 10  | DR    | 228 | THR  |
| 10  | DR    | 245 | MET  |
| 10  | DR    | 253 | VAL  |
| 10  | DR    | 265 | MET  |
| 11  | DS    | 34  | SER  |
| 11  | DS    | 37  | VAL  |
| 11  | DS    | 56  | LEU  |
| 11  | DS    | 61  | ASN  |
| 11  | DS    | 92  | ARG  |
| 11  | DS    | 106 | ARG  |
| 11  | DS    | 115 | TYR  |
| 11  | DS    | 128 | SER  |
| 11  | DS    | 131 | ARG  |
| 11  | DS    | 170 | TYR  |
| 11  | DS    | 175 | CYS  |
| 11  | DS    | 193 | VAL  |
| 11  | DS    | 205 | VAL  |
| 11  | DS    | 234 | LEU  |
| 11  | DS    | 238 | ARG  |
| 12  | DU    | 33  | THR  |
| 12  | DU    | 46  | THR  |
| 12  | DU    | 47  | ARG  |
| 12  | DU    | 52  | SER  |
| 12  | DU    | 53  | LEU  |
| 12  | DU    | 70  | ASP  |
| 12  | DU    | 83  | ARG  |
| 12  | DU    | 86  | ILE  |
| 12  | DU    | 90  | VAL  |
| 12  | DU    | 103 | ILE  |
| 12  | DU    | 107 | LYS  |
| 12  | DU    | 120 | VAL  |
| 12  | DU    | 121 | GLU  |
| 12  | DU    | 149 | GLU  |
| 12  | DU    | 154 | GLU  |
| 12  | DU    | 157 | GLN  |
| 12  | DU    | 165 | ASP  |
| 12  | DU    | 189 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | DU    | 191 | SER  |
| 12  | DU    | 211 | ARG  |
| 12  | DU    | 218 | ARG  |
| 13  | DZ    | 16  | GLU  |
| 13  | DZ    | 20  | ARG  |
| 13  | DZ    | 25  | HIS  |
| 13  | DZ    | 28  | LYS  |
| 13  | DZ    | 62  | ASP  |
| 14  | Da    | 15  | CYS  |
| 14  | Da    | 20  | ARG  |
| 14  | Da    | 24  | MET  |
| 14  | Da    | 25  | ARG  |
| 14  | Da    | 28  | ARG  |
| 14  | Da    | 38  | ASP  |
| 14  | Da    | 40  | ARG  |
| 14  | Da    | 42  | ARG  |
| 15  | DB    | 99  | VAL  |
| 15  | DB    | 118 | VAL  |
| 15  | DB    | 128 | GLU  |
| 15  | DB    | 129 | TYR  |
| 15  | DB    | 143 | VAL  |
| 15  | DB    | 173 | ARG  |
| 15  | DB    | 187 | GLU  |
| 15  | DB    | 189 | VAL  |
| 15  | DB    | 192 | ILE  |
| 15  | DB    | 204 | SER  |
| 15  | DB    | 221 | HIS  |
| 15  | DB    | 233 | ASP  |
| 15  | DB    | 239 | GLN  |
| 15  | DB    | 295 | THR  |
| 15  | DB    | 321 | SER  |
| 15  | DB    | 324 | THR  |
| 15  | DB    | 336 | VAL  |
| 15  | DB    | 339 | ARG  |
| 15  | DB    | 341 | THR  |
| 15  | DB    | 356 | ILE  |
| 15  | DB    | 388 | VAL  |
| 15  | DB    | 396 | ARG  |
| 15  | DB    | 414 | GLN  |
| 15  | DB    | 416 | ASN  |
| 15  | DB    | 424 | ASP  |
| 15  | DB    | 433 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | DB    | 439 | VAL  |
| 15  | DB    | 448 | ASP  |
| 15  | DB    | 450 | MET  |
| 15  | DB    | 452 | ARG  |
| 15  | DB    | 469 | ILE  |
| 15  | DB    | 479 | VAL  |
| 15  | DB    | 493 | ARG  |
| 15  | DB    | 503 | ASN  |
| 15  | DB    | 507 | LEU  |
| 15  | DB    | 514 | ARG  |
| 15  | DB    | 521 | LEU  |
| 15  | DB    | 522 | MET  |
| 15  | DB    | 532 | GLU  |
| 15  | DB    | 553 | LEU  |
| 15  | DB    | 554 | GLU  |
| 15  | DB    | 572 | ASP  |
| 15  | DB    | 574 | ILE  |
| 15  | DB    | 583 | ARG  |
| 15  | DB    | 592 | MET  |
| 15  | DB    | 625 | ASN  |
| 15  | DB    | 637 | THR  |
| 15  | DB    | 657 | GLU  |
| 15  | DB    | 671 | VAL  |
| 15  | DB    | 672 | VAL  |
| 15  | DB    | 680 | VAL  |
| 15  | DB    | 686 | GLN  |
| 15  | DB    | 689 | LEU  |
| 15  | DB    | 693 | SER  |
| 15  | DB    | 733 | HIS  |
| 15  | DB    | 743 | VAL  |
| 15  | DB    | 755 | LEU  |
| 15  | DB    | 756 | THR  |
| 15  | DB    | 774 | ASN  |
| 15  | DB    | 776 | THR  |
| 15  | DB    | 785 | ASN  |
| 15  | DB    | 807 | ILE  |
| 15  | DB    | 810 | THR  |
| 15  | DB    | 815 | ASP  |
| 15  | DB    | 830 | LEU  |
| 15  | DB    | 834 | ILE  |
| 15  | DB    | 836 | ASN  |
| 15  | DB    | 849 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | DB    | 861  | GLU  |
| 15  | DB    | 867  | THR  |
| 15  | DB    | 878  | VAL  |
| 15  | DB    | 901  | VAL  |
| 15  | DB    | 908  | GLN  |
| 15  | DB    | 920  | VAL  |
| 15  | DB    | 923  | GLN  |
| 15  | DB    | 925  | ASP  |
| 15  | DB    | 941  | ARG  |
| 15  | DB    | 949  | THR  |
| 15  | DB    | 958  | ASN  |
| 15  | DB    | 968  | VAL  |
| 15  | DB    | 969  | THR  |
| 15  | DB    | 974  | GLU  |
| 15  | DB    | 978  | ASN  |
| 15  | DB    | 980  | GLU  |
| 15  | DB    | 984  | ASP  |
| 15  | DB    | 991  | ASN  |
| 15  | DB    | 995  | VAL  |
| 15  | DB    | 1009 | ASP  |
| 15  | DB    | 1010 | LYS  |
| 15  | DB    | 1012 | THR  |
| 15  | DB    | 1013 | ARG  |
| 15  | DB    | 1020 | ASP  |
| 15  | DB    | 1030 | ARG  |
| 15  | DB    | 1034 | ILE  |
| 15  | DB    | 1036 | MET  |
| 15  | DB    | 1041 | ARG  |
| 15  | DB    | 1057 | LEU  |
| 15  | DB    | 1069 | THR  |
| 15  | DB    | 1089 | ILE  |
| 15  | DB    | 1090 | ARG  |
| 15  | DB    | 1104 | ASP  |
| 15  | DB    | 1106 | VAL  |
| 15  | DB    | 1110 | LYS  |
| 15  | DB    | 1117 | THR  |
| 15  | DB    | 1141 | THR  |
| 15  | DB    | 1168 | ASP  |
| 16  | DC    | 36   | ASP  |
| 16  | DC    | 57   | GLU  |
| 16  | DC    | 58   | VAL  |
| 16  | DC    | 86   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | DC    | 88  | LEU  |
| 16  | DC    | 92  | PHE  |
| 16  | DC    | 98  | GLU  |
| 16  | DC    | 102 | LEU  |
| 16  | DC    | 114 | GLU  |
| 16  | DC    | 122 | VAL  |
| 16  | DC    | 127 | VAL  |
| 16  | DC    | 128 | HIS  |
| 16  | DC    | 148 | LEU  |
| 16  | DC    | 154 | THR  |
| 16  | DC    | 162 | ILE  |
| 16  | DC    | 166 | GLU  |
| 16  | DC    | 168 | PHE  |
| 16  | DC    | 198 | GLU  |
| 16  | DC    | 227 | GLN  |
| 16  | DC    | 231 | THR  |
| 16  | DC    | 240 | VAL  |
| 16  | DC    | 256 | ILE  |
| 16  | DC    | 259 | SER  |
| 16  | DC    | 260 | HIS  |
| 16  | DC    | 268 | ASP  |
| 16  | DC    | 279 | GLU  |
| 16  | DC    | 299 | LEU  |
| 16  | DC    | 329 | LYS  |
| 16  | DC    | 344 | MET  |
| 16  | DC    | 371 | ILE  |
| 16  | DC    | 378 | THR  |
| 16  | DC    | 379 | LEU  |
| 16  | DC    | 386 | MET  |
| 16  | DC    | 406 | GLN  |
| 16  | DC    | 435 | LEU  |
| 16  | DC    | 437 | LEU  |
| 16  | DC    | 442 | LEU  |
| 16  | DC    | 449 | VAL  |
| 16  | DC    | 464 | THR  |
| 16  | DC    | 467 | THR  |
| 16  | DC    | 475 | LEU  |
| 16  | DC    | 485 | ILE  |
| 16  | DC    | 491 | LEU  |
| 16  | DC    | 498 | LEU  |
| 16  | DC    | 503 | ASP  |
| 16  | DC    | 511 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | DC    | 534  | LEU  |
| 16  | DC    | 540  | LEU  |
| 16  | DC    | 544  | GLU  |
| 16  | DC    | 604  | VAL  |
| 16  | DC    | 620  | VAL  |
| 16  | DC    | 621  | LEU  |
| 16  | DC    | 632  | LEU  |
| 16  | DC    | 669  | LEU  |
| 16  | DC    | 674  | THR  |
| 16  | DC    | 696  | VAL  |
| 16  | DC    | 705  | LEU  |
| 16  | DC    | 710  | THR  |
| 16  | DC    | 749  | GLU  |
| 16  | DC    | 753  | LEU  |
| 16  | DC    | 756  | ASP  |
| 16  | DC    | 761  | ASN  |
| 16  | DC    | 766  | VAL  |
| 16  | DC    | 774  | ASP  |
| 16  | DC    | 799  | ASN  |
| 16  | DC    | 807  | VAL  |
| 16  | DC    | 817  | ASP  |
| 16  | DC    | 873  | VAL  |
| 16  | DC    | 888  | LEU  |
| 16  | DC    | 894  | HIS  |
| 16  | DC    | 918  | VAL  |
| 16  | DC    | 919  | VAL  |
| 16  | DC    | 934  | ARG  |
| 16  | DC    | 941  | MET  |
| 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    | 987  | THR  |
| 16  | DC    | 993  | VAL  |
| 16  | DC    | 1000 | LEU  |
| 16  | DC    | 1023 | ASN  |
| 16  | DC    | 1047 | ARG  |
| 16  | DC    | 1050 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 16  | DC    | 1055 | ARG  |
| 16  | DC    | 1062 | GLN  |
| 16  | DC    | 1071 | VAL  |
| 16  | DC    | 1104 | MET  |
| 16  | DC    | 1121 | THR  |
| 16  | DC    | 1122 | THR  |
| 16  | DC    | 1132 | THR  |
| 16  | DC    | 1133 | THR  |
| 16  | DC    | 1143 | VAL  |
| 16  | DC    | 1151 | THR  |
| 16  | DC    | 1153 | LEU  |
| 16  | DC    | 1159 | ASP  |
| 17  | DE    | 46   | SER  |
| 17  | DE    | 51   | ARG  |
| 17  | DE    | 65   | ILE  |
| 17  | DE    | 67   | ASN  |
| 17  | DE    | 80   | LEU  |
| 17  | DE    | 149  | LEU  |
| 17  | DE    | 154  | SER  |
| 17  | DE    | 169  | 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    | 248  | THR  |
| 17  | DE    | 286  | THR  |
| 17  | DE    | 319  | ASN  |
| 17  | DE    | 322  | 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  |
| 17  | DE    | 418  | LEU  |
| 17  | DE    | 451  | THR  |
| 17  | DE    | 466  | VAL  |
| 17  | DE    | 482  | THR  |
| 17  | DE    | 484  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | DE    | 503 | ASP  |
| 17  | DE    | 513 | ARG  |
| 17  | DE    | 529 | ASP  |
| 17  | DE    | 530 | TRP  |
| 17  | DE    | 554 | LEU  |
| 17  | DE    | 566 | ARG  |
| 17  | DE    | 570 | GLU  |
| 17  | DE    | 572 | VAL  |
| 17  | DE    | 573 | GLN  |
| 17  | DE    | 578 | GLN  |
| 17  | DE    | 582 | GLU  |
| 17  | DE    | 591 | LEU  |
| 17  | DE    | 600 | ILE  |
| 17  | DE    | 601 | ILE  |
| 17  | DE    | 610 | LEU  |
| 17  | DE    | 615 | LEU  |
| 17  | DE    | 651 | ASN  |
| 17  | DE    | 667 | SER  |
| 17  | DE    | 697 | THR  |
| 17  | DE    | 698 | GLN  |
| 17  | DE    | 716 | ASN  |
| 17  | DE    | 717 | ARG  |
| 17  | DE    | 726 | THR  |
| 18  | DF    | 6   | VAL  |
| 18  | DF    | 15  | HIS  |
| 18  | DF    | 16  | GLU  |
| 18  | DF    | 27  | ARG  |
| 18  | DF    | 33  | GLN  |
| 18  | DF    | 39  | ARG  |
| 18  | DF    | 40  | GLU  |
| 18  | DF    | 43  | THR  |
| 18  | DF    | 50  | LEU  |
| 18  | DF    | 57  | ARG  |
| 18  | DF    | 69  | THR  |
| 18  | DF    | 72  | THR  |
| 18  | DF    | 85  | ARG  |
| 18  | DF    | 87  | GLU  |
| 18  | DF    | 110 | ASN  |
| 18  | DF    | 137 | VAL  |
| 18  | DF    | 139 | ASP  |
| 18  | DF    | 144 | THR  |
| 18  | DF    | 188 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | DF    | 194 | THR  |
| 18  | DF    | 202 | LEU  |
| 18  | DF    | 203 | MET  |
| 18  | DF    | 232 | GLU  |
| 18  | DF    | 241 | CYS  |
| 18  | DF    | 246 | LYS  |
| 18  | DF    | 264 | VAL  |
| 18  | DF    | 274 | LEU  |
| 18  | DF    | 277 | CYS  |
| 18  | DF    | 282 | ARG  |
| 18  | DF    | 294 | MET  |
| 18  | DF    | 297 | ARG  |
| 18  | DF    | 307 | GLU  |
| 18  | DF    | 309 | ASP  |
| 18  | DF    | 318 | MET  |
| 18  | DF    | 321 | LEU  |
| 18  | DF    | 326 | ASP  |
| 18  | DF    | 332 | GLU  |
| 18  | DF    | 338 | SER  |
| 18  | DF    | 343 | GLU  |
| 18  | DF    | 362 | ILE  |
| 18  | DF    | 372 | ASN  |
| 18  | DF    | 373 | ASP  |
| 18  | DF    | 383 | ASP  |
| 18  | DF    | 395 | LEU  |
| 18  | DF    | 402 | THR  |
| 18  | DF    | 403 | LEU  |
| 18  | DF    | 411 | VAL  |
| 18  | DF    | 450 | VAL  |
| 18  | DF    | 476 | LEU  |
| 18  | DF    | 491 | ARG  |
| 18  | DF    | 502 | ARG  |
| 18  | DF    | 505 | LYS  |
| 18  | DF    | 531 | ARG  |
| 18  | DF    | 540 | VAL  |
| 18  | DF    | 550 | VAL  |
| 18  | DF    | 568 | LEU  |
| 18  | DF    | 575 | VAL  |
| 18  | DF    | 584 | LEU  |
| 19  | DG    | 47  | THR  |
| 19  | DG    | 54  | THR  |
| 19  | DG    | 74  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | DG    | 77  | CYS  |
| 19  | DG    | 78  | HIS  |
| 19  | DG    | 84  | LEU  |
| 19  | DG    | 86  | LEU  |
| 19  | DG    | 93  | ARG  |
| 19  | DG    | 98  | ASP  |
| 19  | DG    | 115 | ILE  |
| 19  | DG    | 125 | ASP  |
| 19  | DG    | 127 | LEU  |
| 19  | DG    | 130 | LEU  |
| 19  | DG    | 140 | GLU  |
| 19  | DG    | 141 | THR  |
| 19  | DG    | 142 | LEU  |
| 19  | DG    | 147 | SER  |
| 19  | DG    | 149 | SER  |
| 19  | DG    | 155 | GLU  |
| 19  | DG    | 158 | GLU  |
| 19  | DG    | 160 | ARG  |
| 19  | DG    | 165 | VAL  |
| 19  | DG    | 176 | VAL  |
| 19  | DG    | 179 | LEU  |
| 19  | DG    | 185 | ASP  |
| 19  | DG    | 186 | ARG  |
| 19  | DG    | 200 | GLN  |
| 19  | DG    | 210 | VAL  |
| 19  | DG    | 220 | THR  |
| 19  | DG    | 236 | VAL  |
| 19  | DG    | 273 | VAL  |
| 19  | DG    | 296 | ASP  |
| 19  | DG    | 326 | THR  |
| 19  | DG    | 332 | GLN  |
| 19  | DG    | 334 | MET  |
| 19  | DG    | 359 | ARG  |
| 19  | DG    | 365 | GLN  |
| 19  | DG    | 370 | ARG  |
| 19  | DG    | 377 | GLU  |
| 19  | DG    | 379 | VAL  |
| 19  | DG    | 384 | VAL  |
| 19  | DG    | 392 | ARG  |
| 19  | DG    | 443 | ARG  |
| 19  | DG    | 444 | THR  |
| 19  | DG    | 457 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | DG    | 462 | THR  |
| 19  | DG    | 473 | CYS  |
| 19  | DG    | 477 | GLN  |
| 19  | DG    | 491 | THR  |
| 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    | 565 | CYS  |
| 19  | DG    | 615 | SER  |
| 19  | DG    | 616 | ARG  |
| 19  | DG    | 623 | MET  |
| 19  | DG    | 626 | LEU  |
| 20  | DH    | 1   | MET  |
| 20  | DH    | 13  | SER  |
| 20  | DH    | 19  | THR  |
| 20  | DH    | 40  | THR  |
| 20  | DH    | 46  | LEU  |
| 20  | DH    | 51  | ARG  |
| 20  | DH    | 76  | LEU  |
| 20  | DH    | 79  | ASP  |
| 20  | DH    | 81  | LYS  |
| 20  | DH    | 82  | GLN  |
| 20  | DH    | 83  | GLU  |
| 20  | DH    | 85  | LEU  |
| 20  | DH    | 102 | LEU  |
| 20  | DH    | 105 | GLN  |
| 20  | DH    | 133 | CYS  |
| 20  | DH    | 135 | ARG  |
| 20  | DH    | 156 | LEU  |
| 20  | DH    | 167 | GLU  |
| 20  | DH    | 196 | LEU  |
| 20  | DH    | 200 | THR  |
| 20  | DH    | 227 | ASP  |
| 20  | DH    | 236 | MET  |
| 20  | DH    | 257 | ASN  |
| 20  | DH    | 268 | LEU  |
| 20  | DH    | 273 | SER  |
| 20  | DH    | 277 | THR  |
| 20  | DH    | 297 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | DH    | 300 | ILE  |
| 20  | DH    | 324 | ILE  |
| 20  | DH    | 325 | MET  |
| 20  | DH    | 344 | VAL  |
| 20  | DH    | 345 | VAL  |
| 20  | DH    | 348 | LYS  |
| 20  | DH    | 354 | LEU  |
| 20  | DH    | 359 | GLU  |
| 20  | DH    | 360 | LEU  |
| 20  | DH    | 364 | ARG  |
| 20  | DH    | 375 | VAL  |
| 20  | DH    | 382 | PHE  |
| 20  | DH    | 386 | ARG  |
| 20  | DH    | 396 | VAL  |
| 20  | DH    | 414 | LEU  |
| 20  | DH    | 419 | CYS  |
| 20  | DH    | 450 | ASN  |
| 20  | DH    | 452 | ARG  |
| 20  | DH    | 460 | LEU  |
| 20  | DH    | 462 | GLU  |
| 20  | DH    | 474 | ASP  |
| 20  | DH    | 476 | VAL  |
| 20  | DH    | 495 | THR  |
| 20  | DH    | 497 | MET  |
| 20  | DH    | 498 | ASN  |
| 20  | DH    | 523 | ARG  |
| 20  | DH    | 528 | GLU  |
| 20  | DH    | 554 | ARG  |
| 20  | DH    | 557 | VAL  |
| 21  | DJ    | 16  | ASN  |
| 21  | DJ    | 46  | ARG  |
| 21  | DJ    | 55  | ASN  |
| 21  | DJ    | 77  | VAL  |
| 21  | DJ    | 82  | GLN  |
| 21  | DJ    | 88  | ARG  |
| 21  | DJ    | 91  | THR  |
| 21  | DJ    | 92  | LEU  |
| 21  | DJ    | 107 | LEU  |
| 21  | DJ    | 119 | LEU  |
| 21  | DJ    | 137 | MET  |
| 21  | DJ    | 149 | THR  |
| 21  | DJ    | 171 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | DJ    | 175 | SER  |
| 21  | DJ    | 178 | ARG  |
| 21  | DJ    | 182 | ASP  |
| 21  | DJ    | 187 | ASP  |
| 21  | DJ    | 203 | MET  |
| 21  | DJ    | 212 | ASP  |
| 21  | DJ    | 226 | VAL  |
| 21  | DJ    | 236 | ARG  |
| 21  | DJ    | 246 | THR  |
| 21  | DJ    | 276 | LEU  |
| 21  | DJ    | 291 | ASN  |
| 21  | DJ    | 302 | SER  |
| 21  | DJ    | 304 | ILE  |
| 21  | DJ    | 305 | ARG  |
| 21  | DJ    | 308 | ARG  |
| 21  | DJ    | 323 | THR  |
| 22  | DK    | 6   | THR  |
| 22  | DK    | 18  | LEU  |
| 22  | DK    | 34  | ASN  |
| 22  | DK    | 54  | THR  |
| 22  | DK    | 111 | LEU  |
| 22  | DK    | 115 | THR  |
| 22  | DK    | 116 | ARG  |
| 22  | DK    | 134 | THR  |
| 22  | DK    | 148 | GLU  |
| 22  | DK    | 167 | THR  |
| 22  | DK    | 172 | LEU  |
| 22  | DK    | 173 | VAL  |
| 22  | DK    | 179 | GLU  |
| 22  | DK    | 222 | LEU  |
| 22  | DK    | 225 | THR  |
| 22  | DK    | 226 | LEU  |
| 22  | DK    | 254 | GLU  |
| 22  | DK    | 263 | GLU  |
| 22  | DK    | 265 | VAL  |
| 22  | DK    | 270 | LEU  |
| 22  | DK    | 273 | LEU  |
| 22  | DK    | 286 | LEU  |
| 22  | DK    | 294 | SER  |
| 23  | DT    | 21  | ASP  |
| 23  | DT    | 35  | LYS  |
| 23  | DT    | 52  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DT    | 84  | ILE  |
| 23  | DT    | 90  | THR  |
| 23  | DT    | 91  | GLN  |
| 23  | DT    | 99  | HIS  |
| 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    | 143 | TYR  |
| 23  | DT    | 152 | LYS  |
| 23  | DT    | 163 | ARG  |
| 23  | DT    | 166 | THR  |
| 23  | DT    | 176 | ASP  |
| 23  | DT    | 181 | ASP  |
| 23  | DT    | 187 | LYS  |
| 23  | DT    | 195 | VAL  |
| 23  | DT    | 205 | VAL  |
| 23  | DT    | 208 | ARG  |
| 23  | DT    | 209 | THR  |
| 23  | DT    | 212 | PHE  |
| 23  | DT    | 232 | ARG  |
| 23  | DT    | 241 | ASN  |
| 24  | DV    | 26  | THR  |
| 24  | DV    | 41  | THR  |
| 24  | DV    | 43  | ASN  |
| 24  | DV    | 68  | ILE  |
| 24  | DV    | 77  | LYS  |
| 24  | DV    | 114 | VAL  |
| 24  | DV    | 118 | GLN  |
| 24  | DV    | 131 | GLN  |
| 24  | DV    | 140 | PHE  |
| 24  | DV    | 143 | ILE  |
| 24  | DV    | 151 | GLU  |
| 24  | DV    | 179 | LEU  |
| 25  | DW    | 10  | THR  |
| 25  | DW    | 12  | THR  |
| 25  | DW    | 18  | VAL  |
| 25  | DW    | 27  | LYS  |
| 25  | DW    | 37  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | DW    | 39  | SER  |
| 25  | DW    | 60  | VAL  |
| 25  | DW    | 70  | LEU  |
| 25  | DW    | 71  | GLN  |
| 25  | DW    | 74  | THR  |
| 25  | DW    | 104 | VAL  |
| 25  | DW    | 122 | ARG  |
| 25  | DW    | 128 | LEU  |
| 25  | DW    | 149 | VAL  |
| 25  | DW    | 163 | GLU  |
| 25  | DW    | 164 | ASN  |
| 26  | DX    | 33  | LYS  |
| 26  | DX    | 76  | ARG  |
| 26  | DX    | 78  | GLU  |
| 26  | DX    | 90  | ILE  |
| 26  | DX    | 95  | VAL  |
| 26  | DX    | 98  | LEU  |
| 26  | DX    | 122 | CYS  |
| 26  | DX    | 124 | ILE  |
| 26  | DX    | 136 | ARG  |
| 26  | DX    | 149 | THR  |
| 26  | DX    | 162 | VAL  |
| 26  | DX    | 164 | THR  |
| 26  | DX    | 168 | ASN  |
| 27  | DY    | 11  | THR  |
| 27  | DY    | 14  | THR  |
| 27  | DY    | 23  | SER  |
| 27  | DY    | 43  | LEU  |
| 27  | DY    | 50  | VAL  |
| 27  | DY    | 52  | GLN  |
| 27  | DY    | 65  | LEU  |
| 27  | DY    | 77  | VAL  |
| 27  | DY    | 87  | ARG  |
| 27  | DY    | 91  | LEU  |
| 27  | DY    | 92  | ASN  |
| 27  | DY    | 93  | THR  |
| 27  | DY    | 96  | ARG  |
| 27  | DY    | 102 | GLU  |
| 27  | DY    | 111 | ARG  |
| 27  | DY    | 113 | VAL  |
| 27  | DY    | 128 | GLN  |
| 27  | DY    | 141 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DY    | 148 | ARG  |
| 27  | DY    | 163 | LYS  |
| 28  | CC    | 4   | MET  |
| 28  | CC    | 10  | VAL  |
| 28  | CC    | 13  | LYS  |
| 28  | CC    | 21  | PHE  |
| 28  | CC    | 22  | LYS  |
| 28  | CC    | 44  | LEU  |
| 28  | CC    | 46  | TRP  |
| 28  | CC    | 50  | ILE  |
| 28  | CC    | 69  | GLU  |
| 29  | CE    | 14  | SER  |
| 29  | CE    | 16  | TYR  |
| 29  | CE    | 20  | THR  |
| 29  | CE    | 27  | ARG  |
| 29  | CE    | 39  | THR  |
| 29  | CE    | 41  | ARG  |
| 29  | CE    | 54  | GLU  |
| 29  | CE    | 58  | SER  |
| 29  | CE    | 62  | ARG  |
| 29  | CE    | 65  | ARG  |
| 29  | CE    | 80  | ILE  |
| 29  | CE    | 83  | MET  |
| 29  | CE    | 87  | ILE  |
| 29  | CE    | 96  | VAL  |
| 29  | CE    | 102 | GLU  |
| 29  | CE    | 105 | GLN  |
| 29  | CE    | 121 | THR  |
| 29  | CE    | 124 | THR  |
| 29  | CE    | 128 | ILE  |
| 29  | CE    | 158 | ASP  |
| 29  | CE    | 163 | ILE  |
| 29  | CE    | 173 | LYS  |
| 29  | CE    | 182 | VAL  |
| 29  | CE    | 192 | GLU  |
| 29  | CE    | 201 | ILE  |
| 29  | CE    | 202 | ILE  |
| 29  | CE    | 217 | VAL  |
| 29  | CE    | 230 | ARG  |
| 29  | CE    | 231 | ARG  |
| 29  | CE    | 232 | ILE  |
| 29  | CE    | 233 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | CE    | 279 | LEU  |
| 29  | CE    | 282 | VAL  |
| 29  | CE    | 285 | ILE  |
| 29  | CE    | 332 | ASP  |
| 29  | CE    | 334 | ARG  |
| 29  | CE    | 335 | LEU  |
| 29  | CE    | 364 | ARG  |
| 29  | CE    | 365 | MET  |
| 29  | CE    | 370 | ASP  |
| 29  | CE    | 376 | LEU  |
| 29  | CE    | 391 | THR  |
| 29  | CE    | 395 | THR  |
| 29  | CE    | 396 | LEU  |
| 29  | CE    | 410 | LEU  |
| 29  | CE    | 420 | VAL  |
| 29  | CE    | 422 | VAL  |
| 29  | CE    | 424 | LEU  |
| 29  | CE    | 429 | LYS  |
| 30  | CF    | 2   | VAL  |
| 30  | CF    | 5   | SER  |
| 30  | CF    | 53  | ASP  |
| 30  | CF    | 66  | ILE  |
| 30  | CF    | 79  | VAL  |
| 30  | CF    | 93  | LEU  |
| 30  | CF    | 96  | ASN  |
| 30  | CF    | 104 | ILE  |
| 30  | CF    | 124 | LEU  |
| 30  | CF    | 133 | GLN  |
| 30  | CF    | 134 | THR  |
| 30  | CF    | 138 | ILE  |
| 30  | CF    | 141 | GLN  |
| 30  | CF    | 144 | MET  |
| 30  | CF    | 152 | THR  |
| 31  | CH    | 16  | VAL  |
| 31  | CH    | 19  | LEU  |
| 31  | CH    | 26  | ARG  |
| 31  | CH    | 29  | HIS  |
| 31  | CH    | 50  | ARG  |
| 31  | CH    | 51  | LEU  |
| 31  | CH    | 79  | SER  |
| 31  | CH    | 86  | THR  |
| 31  | CH    | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | CH    | 89  | VAL  |
| 31  | CH    | 108 | LEU  |
| 31  | CH    | 118 | LEU  |
| 31  | CH    | 122 | THR  |
| 31  | CH    | 128 | VAL  |
| 31  | CH    | 131 | ASP  |
| 31  | CH    | 132 | ASP  |
| 31  | CH    | 138 | LYS  |
| 31  | CH    | 143 | ARG  |
| 31  | CH    | 150 | THR  |
| 31  | CH    | 152 | ILE  |
| 31  | CH    | 154 | ASP  |
| 31  | CH    | 163 | THR  |
| 31  | CH    | 170 | VAL  |
| 31  | CH    | 172 | VAL  |
| 31  | CH    | 175 | THR  |
| 31  | CH    | 177 | GLU  |
| 31  | CH    | 179 | ARG  |
| 31  | CH    | 191 | VAL  |
| 31  | CH    | 256 | ARG  |
| 31  | CH    | 280 | MET  |
| 32  | CI    | 2   | GLN  |
| 32  | CI    | 8   | ARG  |
| 32  | CI    | 9   | THR  |
| 32  | CI    | 18  | LEU  |
| 32  | CI    | 34  | ASP  |
| 32  | CI    | 38  | LEU  |
| 32  | CI    | 54  | SER  |
| 32  | CI    | 57  | GLU  |
| 32  | CI    | 59  | ARG  |
| 32  | CI    | 85  | LEU  |
| 32  | CI    | 93  | MET  |
| 32  | CI    | 110 | ARG  |
| 32  | CI    | 139 | ASP  |
| 32  | CI    | 179 | CYS  |
| 32  | CI    | 210 | THR  |
| 32  | CI    | 218 | ARG  |
| 32  | CI    | 249 | GLU  |
| 32  | CI    | 256 | LYS  |
| 32  | CI    | 260 | LEU  |
| 32  | CI    | 265 | ASP  |
| 32  | CI    | 280 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | CI    | 281 | VAL  |
| 32  | CI    | 290 | ILE  |
| 32  | CI    | 295 | ASP  |
| 32  | CI    | 299 | VAL  |
| 32  | CI    | 303 | THR  |
| 32  | CI    | 309 | ARG  |
| 32  | CI    | 330 | ASN  |
| 32  | CI    | 338 | LYS  |
| 32  | CI    | 343 | VAL  |
| 32  | CI    | 356 | MET  |
| 32  | CI    | 372 | ILE  |
| 32  | CI    | 375 | GLU  |
| 32  | CI    | 406 | THR  |
| 32  | CI    | 407 | ARG  |
| 32  | CI    | 417 | SER  |
| 32  | CI    | 420 | ARG  |
| 32  | CI    | 439 | ARG  |
| 33  | CJ    | 17  | MET  |
| 33  | CJ    | 19  | THR  |
| 33  | CJ    | 20  | GLN  |
| 33  | CJ    | 23  | LYS  |
| 33  | CJ    | 36  | MET  |
| 33  | CJ    | 43  | GLU  |
| 33  | CJ    | 50  | ASP  |
| 33  | CJ    | 65  | VAL  |
| 33  | CJ    | 68  | ASP  |
| 33  | CJ    | 71  | VAL  |
| 33  | CJ    | 77  | CYS  |
| 33  | CJ    | 81  | THR  |
| 33  | CJ    | 110 | LYS  |
| 33  | CJ    | 118 | MET  |
| 33  | CJ    | 130 | ARG  |
| 33  | CJ    | 149 | GLU  |
| 33  | CJ    | 158 | THR  |
| 33  | CJ    | 164 | ASP  |
| 33  | CJ    | 169 | GLU  |
| 33  | CJ    | 176 | ILE  |
| 33  | CJ    | 190 | GLU  |
| 33  | CJ    | 202 | ASP  |
| 33  | CJ    | 204 | SER  |
| 33  | CJ    | 230 | PHE  |
| 33  | CJ    | 257 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | CJ    | 258 | MET  |
| 33  | CJ    | 265 | CYS  |
| 33  | CJ    | 266 | MET  |
| 33  | CJ    | 279 | LYS  |
| 33  | CJ    | 287 | LEU  |
| 33  | CJ    | 297 | LEU  |
| 33  | CJ    | 311 | LEU  |
| 33  | CJ    | 313 | GLU  |
| 33  | CJ    | 325 | SER  |
| 33  | CJ    | 329 | ARG  |
| 33  | CJ    | 330 | LEU  |
| 33  | CJ    | 345 | VAL  |
| 33  | CJ    | 357 | SER  |
| 33  | CJ    | 375 | THR  |
| 33  | CJ    | 377 | SER  |
| 33  | CJ    | 380 | THR  |
| 33  | CJ    | 383 | THR  |
| 33  | CJ    | 399 | ARG  |
| 33  | CJ    | 403 | CYS  |
| 33  | CJ    | 409 | SER  |
| 33  | CJ    | 413 | GLU  |
| 33  | CJ    | 415 | ARG  |
| 33  | CJ    | 418 | ASP  |
| 33  | CJ    | 427 | THR  |
| 33  | CJ    | 428 | SER  |
| 33  | CJ    | 438 | ASN  |
| 33  | CJ    | 445 | VAL  |
| 33  | CJ    | 459 | GLU  |
| 33  | CJ    | 475 | VAL  |
| 33  | CJ    | 480 | THR  |
| 33  | CJ    | 481 | ASP  |
| 33  | CJ    | 490 | ASP  |
| 33  | CJ    | 509 | GLU  |
| 33  | CJ    | 517 | VAL  |
| 33  | CJ    | 519 | ILE  |
| 33  | CJ    | 524 | THR  |
| 33  | CJ    | 526 | THR  |
| 33  | CJ    | 542 | LYS  |
| 33  | CJ    | 552 | ILE  |
| 33  | CJ    | 556 | GLU  |
| 33  | CJ    | 565 | THR  |
| 33  | CJ    | 602 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | CJ    | 615 | VAL  |
| 33  | CJ    | 618 | VAL  |
| 33  | CJ    | 623 | THR  |
| 33  | CJ    | 647 | ASP  |
| 33  | CJ    | 648 | VAL  |
| 33  | CJ    | 654 | VAL  |
| 33  | CJ    | 667 | VAL  |
| 33  | CJ    | 671 | LEU  |
| 33  | CJ    | 684 | THR  |
| 33  | CJ    | 698 | HIS  |
| 33  | CJ    | 704 | GLU  |
| 33  | CJ    | 712 | THR  |
| 33  | CJ    | 714 | THR  |
| 33  | CJ    | 724 | THR  |
| 33  | CJ    | 727 | THR  |
| 33  | CJ    | 734 | THR  |
| 33  | CJ    | 744 | ILE  |
| 33  | CJ    | 751 | VAL  |
| 33  | CJ    | 757 | LEU  |
| 33  | CJ    | 770 | THR  |
| 33  | CJ    | 781 | HIS  |
| 33  | CJ    | 796 | ASP  |
| 33  | CJ    | 798 | GLN  |
| 34  | CK    | 15  | ARG  |
| 34  | CK    | 26  | ARG  |
| 34  | CK    | 32  | LEU  |
| 34  | CK    | 40  | GLN  |
| 34  | CK    | 47  | ILE  |
| 34  | CK    | 48  | ARG  |
| 34  | CK    | 53  | ARG  |
| 34  | CK    | 56  | GLN  |
| 34  | CK    | 70  | ILE  |
| 34  | CK    | 73  | GLN  |
| 34  | CK    | 77  | MET  |
| 34  | CK    | 94  | GLU  |
| 34  | CK    | 98  | LEU  |
| 34  | CK    | 108 | ARG  |
| 34  | CK    | 109 | VAL  |
| 34  | CK    | 113 | ARG  |
| 34  | CK    | 149 | VAL  |
| 34  | CK    | 156 | LYS  |
| 34  | CK    | 158 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | CK    | 174 | VAL  |
| 34  | CK    | 185 | MET  |
| 34  | CK    | 192 | MET  |
| 34  | CK    | 205 | TYR  |
| 34  | CK    | 207 | VAL  |
| 34  | CK    | 210 | THR  |
| 34  | CK    | 214 | LYS  |
| 34  | CK    | 217 | LEU  |
| 34  | CK    | 227 | LEU  |
| 34  | CK    | 258 | LEU  |
| 34  | CK    | 264 | SER  |
| 34  | CK    | 276 | GLU  |
| 34  | CK    | 310 | ILE  |
| 34  | CK    | 311 | THR  |
| 34  | CK    | 315 | LEU  |
| 34  | CK    | 319 | LYS  |
| 34  | CK    | 324 | VAL  |
| 34  | CK    | 326 | LYS  |
| 35  | CL    | 1   | LEU  |
| 35  | CL    | 6   | MET  |
| 35  | CL    | 17  | VAL  |
| 35  | CL    | 22  | CYS  |
| 35  | CL    | 38  | LEU  |
| 35  | CL    | 42  | PHE  |
| 35  | CL    | 43  | TYR  |
| 35  | CL    | 44  | LEU  |
| 35  | CL    | 53  | CYS  |
| 35  | CL    | 65  | LEU  |
| 35  | CL    | 68  | ILE  |
| 35  | CL    | 69  | GLU  |
| 35  | CL    | 74  | VAL  |
| 35  | CL    | 79  | VAL  |
| 35  | CL    | 80  | LYS  |
| 35  | CL    | 85  | ILE  |
| 36  | CN    | 16  | ASP  |
| 36  | CN    | 22  | THR  |
| 36  | CN    | 30  | LEU  |
| 36  | CN    | 41  | LEU  |
| 36  | CN    | 49  | SER  |
| 36  | CN    | 55  | LEU  |
| 36  | CN    | 57  | LYS  |
| 36  | CN    | 60  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | CN    | 62  | THR  |
| 36  | CN    | 66  | MET  |
| 36  | CN    | 78  | GLN  |
| 36  | CN    | 81  | LEU  |
| 36  | CN    | 83  | LYS  |
| 36  | CN    | 104 | THR  |
| 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    | 70  | HIS  |
| 37  | CO    | 75  | LEU  |
| 37  | CO    | 80  | ARG  |
| 37  | CO    | 82  | ASN  |
| 37  | CO    | 87  | THR  |
| 37  | CO    | 108 | THR  |
| 37  | CO    | 112 | LYS  |
| 37  | CO    | 114 | ARG  |
| 37  | CO    | 115 | GLN  |
| 37  | CO    | 118 | MET  |
| 37  | CO    | 120 | TYR  |
| 37  | CO    | 147 | GLU  |
| 37  | CO    | 178 | LEU  |
| 37  | CO    | 190 | SER  |
| 37  | CO    | 204 | GLU  |
| 37  | CO    | 206 | MET  |
| 37  | CO    | 209 | GLU  |
| 37  | CO    | 224 | LEU  |
| 37  | CO    | 227 | LYS  |
| 37  | CO    | 237 | ASN  |
| 37  | CO    | 240 | LEU  |
| 37  | CO    | 242 | ASN  |
| 37  | CO    | 244 | HIS  |
| 37  | CO    | 245 | ASN  |
| 37  | CO    | 247 | ILE  |
| 37  | CO    | 248 | ILE  |
| 37  | CO    | 251 | VAL  |
| 37  | CO    | 259 | LEU  |
| 37  | CO    | 264 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | CO    | 266 | LEU  |
| 37  | CO    | 270 | ASP  |
| 37  | CO    | 280 | ASP  |
| 37  | CO    | 285 | ASP  |
| 37  | CO    | 304 | ASP  |
| 37  | CO    | 309 | LEU  |
| 37  | CO    | 313 | THR  |
| 37  | CO    | 336 | GLU  |
| 37  | CO    | 345 | TYR  |
| 37  | CO    | 351 | GLU  |
| 37  | CO    | 352 | ASN  |
| 37  | CO    | 353 | GLU  |
| 37  | CO    | 362 | VAL  |
| 37  | CO    | 384 | GLU  |
| 37  | CO    | 390 | PHE  |
| 37  | CO    | 391 | SER  |
| 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    | 54  | ARG  |
| 38  | CP    | 59  | ARG  |
| 38  | CP    | 96  | ILE  |
| 38  | CP    | 123 | LEU  |
| 38  | CP    | 129 | THR  |
| 38  | CP    | 142 | LYS  |
| 38  | CP    | 146 | MET  |
| 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    | 24  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | CQ    | 31  | THR  |
| 39  | CQ    | 34  | THR  |
| 39  | CQ    | 48  | ARG  |
| 39  | CQ    | 56  | ARG  |
| 39  | CQ    | 67  | LEU  |
| 39  | CQ    | 69  | GLN  |
| 39  | CQ    | 73  | ARG  |
| 39  | CQ    | 80  | LEU  |
| 39  | CQ    | 83  | LEU  |
| 39  | CQ    | 90  | GLN  |
| 39  | CQ    | 103 | MET  |
| 39  | CQ    | 108 | VAL  |
| 39  | CQ    | 114 | MET  |
| 39  | CQ    | 124 | VAL  |
| 39  | CQ    | 136 | ASP  |
| 39  | CQ    | 147 | ILE  |
| 39  | CQ    | 158 | HIS  |
| 39  | CQ    | 164 | ILE  |
| 39  | CQ    | 169 | VAL  |
| 39  | CQ    | 173 | GLU  |
| 39  | CQ    | 179 | LEU  |
| 39  | CQ    | 182 | VAL  |
| 39  | CQ    | 191 | VAL  |
| 40  | CR    | 15  | GLN  |
| 40  | CR    | 30  | LEU  |
| 40  | CR    | 36  | THR  |
| 40  | CR    | 55  | ARG  |
| 40  | CR    | 59  | LEU  |
| 40  | CR    | 77  | ILE  |
| 40  | CR    | 80  | LEU  |
| 40  | CR    | 92  | ILE  |
| 40  | CR    | 94  | MET  |
| 40  | CR    | 111 | GLN  |
| 40  | CR    | 114 | GLN  |
| 40  | CR    | 117 | SER  |
| 40  | CR    | 160 | VAL  |
| 40  | CR    | 167 | ARG  |
| 40  | CR    | 168 | ILE  |
| 40  | CR    | 181 | ARG  |
| 40  | CR    | 184 | LYS  |
| 40  | CR    | 191 | GLN  |
| 40  | CR    | 198 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | CR    | 202 | LYS  |
| 40  | CR    | 225 | LEU  |
| 40  | CR    | 228 | VAL  |
| 40  | CR    | 243 | THR  |
| 40  | CR    | 244 | THR  |
| 40  | CR    | 246 | GLU  |
| 40  | CR    | 278 | VAL  |
| 40  | CR    | 305 | THR  |
| 40  | CR    | 317 | ILE  |
| 40  | CR    | 318 | LYS  |
| 40  | CR    | 319 | LYS  |
| 40  | CR    | 320 | VAL  |
| 41  | CS    | 32  | LYS  |
| 41  | CS    | 63  | SER  |
| 41  | CS    | 64  | MET  |
| 41  | CS    | 75  | MET  |
| 41  | CS    | 76  | THR  |
| 41  | CS    | 105 | VAL  |
| 41  | CS    | 119 | VAL  |
| 41  | CS    | 121 | SER  |
| 41  | CS    | 125 | ILE  |
| 41  | CS    | 140 | MET  |
| 42  | CU    | 32  | HIS  |
| 42  | CU    | 35  | ILE  |
| 42  | CU    | 48  | VAL  |
| 42  | CU    | 74  | GLN  |
| 42  | CU    | 80  | GLN  |
| 42  | CU    | 87  | GLU  |
| 42  | CU    | 117 | MET  |
| 42  | CU    | 129 | THR  |
| 42  | CU    | 139 | LEU  |
| 42  | CU    | 148 | ASN  |
| 42  | CU    | 161 | GLN  |
| 42  | CU    | 168 | VAL  |
| 42  | CU    | 170 | VAL  |
| 42  | CU    | 171 | VAL  |
| 43  | CZ    | 212 | HIS  |
| 43  | CZ    | 218 | VAL  |
| 43  | CZ    | 240 | VAL  |
| 43  | CZ    | 244 | ILE  |
| 43  | CZ    | 252 | CYS  |
| 43  | CZ    | 260 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | CZ    | 273 | ILE  |
| 43  | CZ    | 277 | PHE  |
| 43  | CZ    | 281 | VAL  |
| 43  | CZ    | 285 | ARG  |
| 43  | CZ    | 286 | GLU  |
| 43  | CZ    | 318 | LEU  |
| 43  | CZ    | 360 | ASP  |
| 44  | Ca    | 14  | ASN  |
| 44  | Ca    | 16  | ARG  |
| 44  | Ca    | 39  | ARG  |
| 44  | Ca    | 67  | ARG  |
| 44  | Ca    | 71  | MET  |
| 44  | Ca    | 73  | GLU  |
| 44  | Ca    | 84  | SER  |
| 44  | Ca    | 168 | TYR  |
| 44  | Ca    | 179 | LEU  |
| 44  | Ca    | 181 | GLU  |
| 44  | Ca    | 189 | GLU  |
| 44  | Ca    | 194 | LEU  |
| 44  | Ca    | 201 | ARG  |
| 44  | Ca    | 212 | VAL  |
| 44  | Ca    | 218 | GLU  |
| 44  | Ca    | 221 | THR  |
| 44  | Ca    | 227 | ASN  |
| 44  | Ca    | 245 | GLU  |
| 44  | Ca    | 257 | ILE  |
| 44  | Ca    | 290 | MET  |
| 44  | Ca    | 297 | LEU  |
| 44  | Ca    | 299 | ARG  |
| 44  | Ca    | 305 | HIS  |
| 44  | Ca    | 314 | CYS  |
| 44  | Ca    | 332 | ARG  |
| 44  | Ca    | 341 | LEU  |
| 44  | Ca    | 350 | GLU  |
| 44  | Ca    | 359 | ARG  |
| 44  | Ca    | 376 | VAL  |
| 44  | Ca    | 380 | ASP  |
| 44  | Ca    | 384 | ARG  |
| 44  | Ca    | 398 | ASP  |
| 44  | Ca    | 399 | ASN  |
| 44  | Ca    | 410 | MET  |
| 44  | Ca    | 451 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | Ca    | 479 | THR  |
| 44  | Ca    | 480 | LEU  |
| 44  | Ca    | 501 | ARG  |
| 44  | Ca    | 506 | GLN  |
| 44  | Ca    | 520 | TYR  |
| 44  | Ca    | 538 | ILE  |
| 44  | Ca    | 552 | THR  |
| 44  | Ca    | 554 | THR  |
| 44  | Ca    | 569 | ARG  |
| 44  | Ca    | 570 | THR  |
| 44  | Ca    | 571 | GLU  |
| 44  | Ca    | 574 | VAL  |
| 44  | Ca    | 578 | ASP  |
| 44  | Ca    | 580 | ILE  |
| 44  | Ca    | 585 | GLN  |
| 44  | Ca    | 597 | LYS  |
| 44  | Ca    | 599 | ILE  |
| 44  | Ca    | 601 | GLU  |
| 45  | Cb    | 11  | MET  |
| 45  | Cb    | 40  | LEU  |
| 45  | Cb    | 57  | MET  |
| 45  | Cb    | 64  | ASN  |
| 45  | Cb    | 71  | LEU  |
| 45  | Cb    | 80  | THR  |
| 45  | Cb    | 101 | LYS  |
| 45  | Cb    | 102 | SER  |
| 45  | Cb    | 104 | LEU  |
| 45  | Cb    | 108 | GLU  |
| 45  | Cb    | 110 | MET  |
| 45  | Cb    | 144 | ARG  |
| 45  | Cb    | 158 | LYS  |
| 45  | Cb    | 159 | ARG  |
| 45  | Cb    | 171 | THR  |
| 45  | Cb    | 193 | GLU  |
| 45  | Cb    | 195 | LEU  |
| 45  | Cb    | 203 | LEU  |
| 45  | Cb    | 206 | GLU  |
| 45  | Cb    | 288 | GLU  |
| 45  | Cb    | 291 | GLU  |
| 45  | Cb    | 292 | ASP  |
| 45  | Cb    | 301 | THR  |
| 45  | Cb    | 303 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | Cb    | 306 | THR  |
| 46  | Cd    | 33  | THR  |
| 46  | Cd    | 47  | ARG  |
| 46  | Cd    | 49  | VAL  |
| 46  | Cd    | 55  | GLU  |
| 46  | Cd    | 68  | SER  |
| 46  | Cd    | 70  | ARG  |
| 46  | Cd    | 74  | ASP  |
| 46  | Cd    | 93  | CYS  |
| 46  | Cd    | 102 | ARG  |
| 46  | Cd    | 112 | ARG  |
| 46  | Cd    | 120 | LEU  |
| 46  | Cd    | 122 | LEU  |
| 46  | Cd    | 125 | GLU  |
| 46  | Cd    | 137 | ARG  |
| 46  | Cd    | 164 | LEU  |
| 46  | Cd    | 168 | VAL  |
| 46  | Cd    | 180 | VAL  |
| 46  | Cd    | 193 | ILE  |
| 46  | Cd    | 201 | LEU  |
| 46  | Cd    | 202 | SER  |
| 46  | Cd    | 208 | HIS  |
| 46  | Cd    | 210 | ASP  |
| 46  | Cd    | 219 | HIS  |
| 46  | Cd    | 259 | GLU  |
| 46  | Cd    | 264 | ILE  |
| 46  | Cd    | 267 | GLU  |
| 46  | Cd    | 284 | THR  |
| 46  | Cd    | 297 | GLU  |
| 47  | Cg    | 19  | VAL  |
| 47  | Cg    | 20  | THR  |
| 47  | Cg    | 57  | THR  |
| 47  | Cg    | 73  | ASP  |
| 47  | Cg    | 76  | SER  |
| 47  | Cg    | 101 | MET  |
| 47  | Cg    | 112 | ARG  |
| 47  | Cg    | 114 | GLU  |
| 47  | Cg    | 120 | LEU  |
| 47  | Cg    | 127 | HIS  |
| 47  | Cg    | 137 | SER  |
| 47  | Cg    | 138 | LEU  |
| 47  | Cg    | 143 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | Cg    | 153 | CYS  |
| 47  | Cg    | 178 | ASP  |
| 47  | Cg    | 224 | LEU  |
| 47  | Cg    | 225 | ARG  |
| 47  | Cg    | 230 | ASP  |
| 47  | Cg    | 262 | GLN  |
| 47  | Cg    | 263 | SER  |
| 47  | Cg    | 290 | LEU  |
| 47  | Cg    | 296 | HIS  |
| 47  | Cg    | 308 | LEU  |
| 47  | Cg    | 310 | SER  |
| 47  | Cg    | 313 | GLU  |
| 47  | Cg    | 316 | THR  |
| 47  | Cg    | 319 | ASP  |
| 47  | Cg    | 325 | LEU  |
| 47  | Cg    | 327 | ARG  |
| 47  | Cg    | 336 | VAL  |
| 47  | Cg    | 337 | ARG  |
| 47  | Cg    | 361 | PHE  |
| 47  | Cg    | 373 | VAL  |
| 47  | Cg    | 383 | ASP  |
| 47  | Cg    | 391 | GLU  |
| 47  | Cg    | 401 | ILE  |
| 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    | 25  | VAL  |
| 48  | Ci    | 30  | ARG  |
| 48  | Ci    | 32  | ASP  |
| 48  | Ci    | 42  | GLN  |
| 48  | Ci    | 45  | ILE  |
| 48  | Ci    | 54  | GLN  |
| 48  | Ci    | 56  | GLU  |
| 48  | Ci    | 76  | MET  |
| 48  | Ci    | 82  | GLN  |
| 48  | Ci    | 83  | ASN  |
| 48  | Ci    | 119 | LEU  |
| 48  | Ci    | 125 | HIS  |
| 48  | Ci    | 128 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | Ci    | 132 | THR  |
| 48  | Ci    | 136 | HIS  |
| 48  | Ci    | 138 | ASP  |
| 48  | Ci    | 139 | ILE  |
| 48  | Ci    | 144 | ARG  |
| 48  | Ci    | 145 | ASN  |
| 48  | Ci    | 146 | ASP  |
| 48  | Ci    | 147 | ARG  |
| 48  | Ci    | 156 | VAL  |
| 48  | Ci    | 157 | LEU  |
| 48  | Ci    | 164 | ASN  |
| 48  | Ci    | 174 | ASP  |
| 49  | Cj    | 10  | ARG  |
| 49  | Cj    | 19  | SER  |
| 49  | Cj    | 20  | MET  |
| 49  | Cj    | 65  | LEU  |
| 49  | Cj    | 66  | LEU  |
| 49  | Cj    | 67  | ASP  |
| 49  | Cj    | 71  | ILE  |
| 49  | Cj    | 77  | LEU  |
| 49  | Cj    | 80  | LEU  |
| 49  | Cj    | 83  | LEU  |
| 49  | Cj    | 91  | GLU  |
| 49  | Cj    | 100 | ILE  |
| 49  | Cj    | 135 | ILE  |
| 49  | Cj    | 138 | ASP  |
| 49  | Cj    | 145 | THR  |
| 49  | Cj    | 157 | THR  |
| 49  | Cj    | 161 | VAL  |
| 49  | Cj    | 173 | MET  |
| 49  | Cj    | 192 | SER  |
| 49  | Cj    | 206 | LEU  |
| 49  | Cj    | 210 | PRO  |
| 49  | Cj    | 213 | ASP  |
| 50  | Ck    | 38  | ILE  |
| 50  | Ck    | 41  | THR  |
| 50  | Ck    | 53  | VAL  |
| 50  | Ck    | 86  | GLU  |
| 50  | Ck    | 87  | ARG  |
| 50  | Ck    | 97  | GLN  |
| 50  | Ck    | 99  | SER  |
| 50  | Ck    | 103 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Ck    | 105 | SER  |
| 50  | Ck    | 107 | SER  |
| 50  | Ck    | 111 | THR  |
| 50  | Ck    | 130 | MET  |
| 50  | Ck    | 137 | THR  |
| 50  | Ck    | 147 | LYS  |
| 50  | Ck    | 153 | VAL  |
| 50  | Ck    | 161 | GLU  |
| 50  | Ck    | 170 | VAL  |
| 50  | Ck    | 171 | VAL  |
| 50  | Ck    | 175 | LEU  |
| 50  | Ck    | 185 | LEU  |
| 50  | Ck    | 188 | LEU  |
| 50  | Ck    | 203 | PHE  |
| 50  | Ck    | 207 | ARG  |
| 50  | Ck    | 214 | LEU  |
| 50  | Ck    | 242 | LEU  |
| 50  | Ck    | 262 | VAL  |
| 50  | Ck    | 290 | LEU  |
| 50  | Ck    | 306 | VAL  |
| 50  | Ck    | 316 | ASP  |
| 50  | Ck    | 317 | VAL  |
| 50  | Ck    | 320 | VAL  |
| 50  | Ck    | 331 | ARG  |
| 50  | Ck    | 348 | LEU  |
| 50  | Ck    | 350 | ASP  |
| 50  | Ck    | 376 | VAL  |
| 50  | Ck    | 380 | VAL  |
| 50  | Ck    | 401 | LEU  |
| 50  | Ck    | 406 | ARG  |
| 50  | Ck    | 536 | GLU  |
| 50  | Ck    | 565 | LEU  |
| 50  | Ck    | 568 | LEU  |
| 50  | Ck    | 573 | THR  |
| 50  | Ck    | 597 | LEU  |
| 50  | Ck    | 606 | THR  |
| 50  | Ck    | 607 | LYS  |
| 50  | Ck    | 621 | THR  |
| 50  | Ck    | 622 | LEU  |
| 50  | Ck    | 629 | LEU  |
| 50  | Ck    | 633 | MET  |
| 50  | Ck    | 649 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Ck    | 654 | SER  |
| 50  | Ck    | 661 | ILE  |
| 50  | Ck    | 679 | GLN  |
| 50  | Ck    | 682 | ASN  |
| 50  | Ck    | 691 | GLN  |
| 50  | Ck    | 695 | GLN  |
| 50  | Ck    | 703 | ARG  |
| 50  | Ck    | 733 | LEU  |
| 50  | Ck    | 755 | ASP  |
| 50  | Ck    | 760 | VAL  |
| 50  | Ck    | 761 | THR  |
| 50  | Ck    | 775 | ARG  |
| 50  | Ck    | 810 | ILE  |
| 50  | Ck    | 816 | GLU  |
| 50  | Ck    | 838 | LEU  |
| 50  | Ck    | 841 | LYS  |
| 51  | Cm    | 21  | GLN  |
| 51  | Cm    | 31  | LEU  |
| 51  | Cm    | 35  | ASN  |
| 51  | Cm    | 46  | ILE  |
| 51  | Cm    | 57  | LEU  |
| 51  | Cm    | 59  | VAL  |
| 51  | Cm    | 70  | SER  |
| 51  | Cm    | 78  | VAL  |
| 51  | Cm    | 80  | THR  |
| 51  | Cm    | 85  | ILE  |
| 51  | Cm    | 91  | GLU  |
| 51  | Cm    | 92  | GLN  |
| 51  | Cm    | 93  | LEU  |
| 51  | Cm    | 95  | MET  |
| 51  | Cm    | 106 | CYS  |
| 51  | Cm    | 124 | SER  |
| 51  | Cm    | 137 | SER  |
| 51  | Cm    | 153 | ASP  |
| 51  | Cm    | 160 | GLN  |
| 51  | Cm    | 162 | ARG  |
| 51  | Cm    | 168 | HIS  |
| 51  | Cm    | 178 | GLU  |
| 51  | Cm    | 179 | ARG  |
| 51  | Cm    | 184 | HIS  |
| 51  | Cm    | 202 | THR  |
| 52  | Cn    | 150 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | Cn    | 155 | ARG  |
| 52  | Cn    | 165 | LEU  |
| 52  | Cn    | 203 | MET  |
| 52  | Cn    | 204 | LEU  |
| 52  | Cn    | 210 | SER  |
| 52  | Cn    | 212 | THR  |
| 52  | Cn    | 214 | ARG  |
| 52  | Cn    | 216 | ASP  |
| 52  | Cn    | 223 | SER  |
| 52  | Cn    | 235 | GLU  |
| 52  | Cn    | 241 | ARG  |
| 53  | Cp    | 18  | SER  |
| 53  | Cp    | 30  | LEU  |
| 53  | Cp    | 50  | THR  |
| 53  | Cp    | 55  | ASN  |
| 53  | Cp    | 68  | LEU  |
| 53  | Cp    | 84  | LEU  |
| 53  | Cp    | 87  | CYS  |
| 53  | Cp    | 90  | ARG  |
| 53  | Cp    | 103 | ASP  |
| 53  | Cp    | 107 | THR  |
| 53  | Cp    | 109 | VAL  |
| 53  | Cp    | 125 | GLU  |
| 53  | Cp    | 128 | LEU  |
| 53  | Cp    | 136 | VAL  |
| 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    | 36  | ARG  |
| 54  | Cq    | 52  | THR  |
| 54  | Cq    | 64  | VAL  |
| 54  | Cq    | 65  | SER  |
| 54  | Cq    | 78  | ASP  |
| 54  | Cq    | 79  | MET  |
| 54  | Cq    | 83  | LEU  |
| 54  | Cq    | 86  | ARG  |
| 54  | Cq    | 96  | THR  |
| 54  | Cq    | 97  | LEU  |
| 54  | Cq    | 106 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | Cq    | 107 | GLU  |
| 54  | Cq    | 111 | ARG  |
| 54  | Cq    | 141 | PRO  |
| 54  | Cq    | 144 | THR  |
| 54  | Cq    | 151 | ARG  |
| 54  | Cq    | 171 | ARG  |
| 54  | Cq    | 172 | ARG  |
| 54  | Cq    | 173 | ILE  |
| 54  | Cq    | 185 | CYS  |
| 54  | Cq    | 201 | GLU  |
| 54  | Cq    | 211 | SER  |
| 54  | Cq    | 214 | ILE  |
| 54  | Cq    | 227 | ILE  |
| 54  | Cq    | 235 | LEU  |
| 55  | Cr    | 13  | ARG  |
| 55  | Cr    | 25  | LEU  |
| 55  | Cr    | 26  | LEU  |
| 55  | Cr    | 45  | THR  |
| 55  | Cr    | 53  | GLU  |
| 55  | Cr    | 56  | MET  |
| 55  | Cr    | 61  | VAL  |
| 55  | Cr    | 65  | LYS  |
| 55  | Cr    | 68  | LEU  |
| 55  | Cr    | 74  | ASP  |
| 55  | Cr    | 90  | ILE  |
| 55  | Cr    | 96  | GLU  |
| 55  | Cr    | 103 | VAL  |
| 55  | Cr    | 106 | CYS  |
| 55  | Cr    | 110 | THR  |
| 55  | Cr    | 122 | VAL  |
| 55  | Cr    | 123 | GLU  |
| 55  | Cr    | 129 | MET  |
| 55  | Cr    | 138 | ILE  |
| 55  | Cr    | 161 | ARG  |
| 55  | Cr    | 163 | LEU  |
| 55  | Cr    | 171 | GLN  |
| 55  | Cr    | 176 | LEU  |
| 55  | Cr    | 187 | VAL  |
| 55  | Cr    | 247 | ILE  |
| 55  | Cr    | 250 | LYS  |
| 55  | Cr    | 253 | ARG  |
| 55  | Cr    | 265 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | Cv    | 27  | LYS  |
| 56  | Cv    | 30  | ASP  |
| 56  | Cv    | 32  | ARG  |
| 56  | Cv    | 33  | GLU  |
| 56  | Cv    | 35  | ARG  |
| 56  | Cv    | 41  | ILE  |
| 56  | Cv    | 59  | ILE  |
| 56  | Cv    | 60  | GLN  |
| 56  | Cv    | 91  | ARG  |
| 56  | Cv    | 99  | VAL  |
| 56  | Cv    | 160 | VAL  |
| 56  | Cv    | 192 | LEU  |
| 56  | Cv    | 195 | LEU  |
| 56  | Cv    | 204 | ILE  |
| 56  | Cv    | 208 | LYS  |
| 56  | Cv    | 209 | VAL  |
| 56  | Cv    | 235 | MET  |
| 56  | Cv    | 236 | GLN  |
| 56  | Cv    | 245 | ASN  |
| 56  | Cv    | 254 | ARG  |
| 56  | Cv    | 261 | ILE  |
| 56  | Cv    | 274 | THR  |
| 56  | Cv    | 278 | LEU  |
| 56  | Cv    | 301 | SER  |
| 56  | Cv    | 305 | ASP  |
| 56  | Cv    | 333 | ILE  |
| 56  | Cv    | 334 | LEU  |
| 56  | Cv    | 337 | SER  |
| 56  | Cv    | 367 | ASP  |
| 56  | Cv    | 399 | VAL  |
| 56  | Cv    | 401 | THR  |
| 56  | Cv    | 407 | MET  |
| 56  | Cv    | 409 | LEU  |
| 56  | Cv    | 411 | ASN  |
| 56  | Cv    | 417 | THR  |
| 56  | Cv    | 437 | ILE  |
| 56  | Cv    | 446 | THR  |
| 56  | Cv    | 453 | ARG  |
| 56  | Cv    | 462 | LEU  |
| 56  | Cv    | 471 | VAL  |
| 56  | Cv    | 482 | ASP  |
| 56  | Cv    | 509 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | Cv    | 512 | MET  |
| 56  | Cv    | 521 | LEU  |
| 56  | Cv    | 530 | LYS  |
| 56  | Cv    | 533 | GLU  |
| 56  | Cv    | 561 | SER  |
| 56  | Cv    | 562 | VAL  |
| 56  | Cv    | 566 | MET  |
| 56  | Cv    | 569 | LEU  |
| 56  | Cv    | 583 | THR  |
| 56  | Cv    | 584 | SER  |
| 56  | Cv    | 590 | THR  |
| 56  | Cv    | 594 | LEU  |
| 56  | Cv    | 612 | THR  |
| 56  | Cv    | 613 | LEU  |
| 56  | Cv    | 614 | SER  |
| 56  | Cv    | 617 | ASP  |
| 56  | Cv    | 618 | ILE  |
| 56  | Cv    | 619 | THR  |
| 56  | Cv    | 638 | VAL  |
| 56  | Cv    | 640 | GLU  |
| 56  | Cv    | 647 | VAL  |
| 56  | Cv    | 649 | THR  |
| 56  | Cv    | 651 | ARG  |
| 56  | Cv    | 673 | LEU  |
| 56  | Cv    | 678 | HIS  |
| 56  | Cv    | 689 | CYS  |
| 56  | Cv    | 738 | ARG  |
| 56  | Cv    | 740 | ILE  |
| 56  | Cv    | 748 | THR  |
| 56  | Cv    | 751 | THR  |
| 56  | Cv    | 754 | ILE  |
| 56  | Cv    | 782 | ILE  |
| 56  | Cv    | 785 | ILE  |
| 56  | Cv    | 790 | THR  |
| 56  | Cv    | 795 | GLU  |
| 56  | Cv    | 807 | GLN  |
| 56  | Cv    | 813 | ARG  |
| 56  | Cv    | 818 | LEU  |
| 56  | Cv    | 838 | LEU  |
| 56  | Cv    | 859 | VAL  |
| 56  | Cv    | 861 | THR  |
| 56  | Cv    | 867 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 56  | Cv    | 874  | GLU  |
| 56  | Cv    | 898  | ARG  |
| 56  | Cv    | 909  | LEU  |
| 56  | Cv    | 916  | ARG  |
| 56  | Cv    | 918  | LEU  |
| 56  | Cv    | 921  | VAL  |
| 56  | Cv    | 927  | LEU  |
| 56  | Cv    | 937  | MET  |
| 56  | Cv    | 938  | ASP  |
| 56  | Cv    | 945  | VAL  |
| 56  | Cv    | 967  | VAL  |
| 56  | Cv    | 975  | ASP  |
| 56  | Cv    | 987  | SER  |
| 56  | Cv    | 988  | ASN  |
| 56  | Cv    | 991  | VAL  |
| 56  | Cv    | 993  | THR  |
| 56  | Cv    | 995  | VAL  |
| 56  | Cv    | 999  | GLU  |
| 56  | Cv    | 1002 | ARG  |
| 56  | Cv    | 1014 | ARG  |
| 56  | Cv    | 1018 | THR  |
| 56  | Cv    | 1030 | ARG  |
| 56  | Cv    | 1034 | ARG  |
| 56  | Cv    | 1039 | GLU  |
| 56  | Cv    | 1040 | GLU  |
| 56  | Cv    | 1057 | ILE  |
| 56  | Cv    | 1069 | GLN  |
| 56  | Cv    | 1070 | GLU  |
| 56  | Cv    | 1090 | LEU  |
| 56  | Cv    | 1108 | GLN  |
| 56  | Cv    | 1115 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (490) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DA    | 49  | HIS  |
| 1   | DA    | 59  | HIS  |
| 1   | DA    | 112 | GLN  |
| 1   | DA    | 117 | GLN  |
| 1   | DA    | 123 | HIS  |
| 1   | DA    | 174 | HIS  |
| 1   | DA    | 205 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | DA    | 237  | HIS  |
| 1   | DA    | 287  | HIS  |
| 1   | DA    | 316  | HIS  |
| 1   | DA    | 402  | GLN  |
| 1   | DA    | 414  | HIS  |
| 1   | DA    | 458  | GLN  |
| 1   | DA    | 626  | GLN  |
| 1   | DA    | 637  | HIS  |
| 1   | DA    | 644  | HIS  |
| 1   | DA    | 746  | GLN  |
| 1   | DA    | 882  | GLN  |
| 1   | DA    | 907  | GLN  |
| 1   | DA    | 910  | HIS  |
| 1   | DA    | 940  | GLN  |
| 1   | DA    | 979  | GLN  |
| 1   | DA    | 980  | HIS  |
| 1   | DA    | 984  | GLN  |
| 1   | DA    | 993  | GLN  |
| 1   | DA    | 1042 | HIS  |
| 1   | DA    | 1048 | ASN  |
| 1   | DA    | 1096 | GLN  |
| 1   | DA    | 1117 | ASN  |
| 1   | DA    | 1152 | HIS  |
| 1   | DA    | 1215 | HIS  |
| 1   | DA    | 1258 | ASN  |
| 1   | DA    | 1376 | HIS  |
| 1   | DA    | 1385 | ASN  |
| 1   | DA    | 1393 | GLN  |
| 1   | DA    | 1399 | ASN  |
| 1   | DA    | 1402 | ASN  |
| 1   | DA    | 1488 | GLN  |
| 1   | DA    | 1513 | GLN  |
| 1   | DA    | 1544 | ASN  |
| 1   | DA    | 1562 | GLN  |
| 1   | DA    | 1570 | ASN  |
| 1   | DA    | 1619 | HIS  |
| 2   | DD    | 10   | HIS  |
| 2   | DD    | 36   | GLN  |
| 2   | DD    | 63   | GLN  |
| 2   | DD    | 64   | HIS  |
| 2   | DD    | 76   | ASN  |
| 2   | DD    | 128  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | DD    | 137 | HIS  |
| 2   | DD    | 144 | ASN  |
| 2   | DD    | 156 | GLN  |
| 2   | DD    | 176 | HIS  |
| 2   | DD    | 203 | GLN  |
| 2   | DD    | 300 | GLN  |
| 2   | DD    | 312 | GLN  |
| 2   | DD    | 313 | HIS  |
| 2   | DD    | 353 | HIS  |
| 2   | DD    | 379 | GLN  |
| 2   | DD    | 387 | GLN  |
| 2   | DD    | 453 | ASN  |
| 2   | DD    | 499 | ASN  |
| 2   | DD    | 507 | GLN  |
| 2   | DD    | 521 | ASN  |
| 2   | DD    | 542 | HIS  |
| 2   | DD    | 675 | ASN  |
| 2   | DD    | 687 | HIS  |
| 3   | DI    | 18  | HIS  |
| 3   | DI    | 30  | GLN  |
| 3   | DI    | 127 | GLN  |
| 3   | DI    | 140 | ASN  |
| 3   | DI    | 193 | ASN  |
| 3   | DI    | 294 | ASN  |
| 3   | DI    | 296 | ASN  |
| 3   | DI    | 320 | GLN  |
| 3   | DI    | 370 | GLN  |
| 3   | DI    | 372 | ASN  |
| 4   | DL    | 47  | GLN  |
| 4   | DL    | 99  | GLN  |
| 4   | DL    | 238 | GLN  |
| 5   | DM    | 27  | GLN  |
| 5   | DM    | 76  | ASN  |
| 5   | DM    | 89  | GLN  |
| 5   | DM    | 193 | GLN  |
| 5   | DM    | 272 | GLN  |
| 5   | DM    | 287 | ASN  |
| 5   | DM    | 292 | ASN  |
| 6   | DN    | 28  | HIS  |
| 6   | DN    | 185 | ASN  |
| 6   | DN    | 223 | GLN  |
| 6   | DN    | 234 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | DN    | 238 | ASN  |
| 6   | DN    | 246 | GLN  |
| 7   | DO    | 159 | HIS  |
| 7   | DO    | 181 | HIS  |
| 8   | DP    | 98  | HIS  |
| 8   | DP    | 133 | GLN  |
| 8   | DP    | 186 | HIS  |
| 8   | DP    | 194 | GLN  |
| 9   | DQ    | 41  | GLN  |
| 9   | DQ    | 51  | ASN  |
| 9   | DQ    | 73  | HIS  |
| 9   | DQ    | 100 | HIS  |
| 9   | DQ    | 207 | HIS  |
| 9   | DQ    | 235 | HIS  |
| 10  | DR    | 75  | HIS  |
| 10  | DR    | 108 | GLN  |
| 10  | DR    | 179 | HIS  |
| 10  | DR    | 198 | HIS  |
| 10  | DR    | 223 | GLN  |
| 11  | DS    | 47  | ASN  |
| 11  | DS    | 134 | GLN  |
| 11  | DS    | 135 | HIS  |
| 11  | DS    | 150 | GLN  |
| 11  | DS    | 201 | HIS  |
| 12  | DU    | 58  | HIS  |
| 12  | DU    | 63  | HIS  |
| 12  | DU    | 96  | GLN  |
| 12  | DU    | 133 | HIS  |
| 12  | DU    | 155 | GLN  |
| 12  | DU    | 157 | GLN  |
| 12  | DU    | 199 | GLN  |
| 14  | Da    | 30  | HIS  |
| 14  | Da    | 41  | ASN  |
| 14  | Da    | 48  | HIS  |
| 15  | DB    | 75  | HIS  |
| 15  | DB    | 92  | HIS  |
| 15  | DB    | 106 | GLN  |
| 15  | DB    | 111 | ASN  |
| 15  | DB    | 122 | HIS  |
| 15  | DB    | 153 | HIS  |
| 15  | DB    | 194 | GLN  |
| 15  | DB    | 267 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 15  | DB    | 300  | GLN  |
| 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    | 684  | GLN  |
| 15  | DB    | 691  | HIS  |
| 15  | DB    | 707  | GLN  |
| 15  | DB    | 733  | HIS  |
| 15  | DB    | 748  | HIS  |
| 15  | DB    | 831  | ASN  |
| 15  | DB    | 898  | GLN  |
| 15  | DB    | 906  | HIS  |
| 15  | DB    | 908  | GLN  |
| 15  | DB    | 923  | GLN  |
| 15  | DB    | 958  | ASN  |
| 15  | DB    | 973  | ASN  |
| 15  | DB    | 981  | HIS  |
| 15  | DB    | 1029 | HIS  |
| 15  | DB    | 1051 | GLN  |
| 15  | DB    | 1055 | GLN  |
| 15  | DB    | 1124 | HIS  |
| 15  | DB    | 1131 | ASN  |
| 16  | DC    | 41   | ASN  |
| 16  | DC    | 76   | ASN  |
| 16  | DC    | 81   | HIS  |
| 16  | DC    | 286  | GLN  |
| 16  | DC    | 445  | HIS  |
| 16  | DC    | 452  | GLN  |
| 16  | DC    | 574  | GLN  |
| 16  | DC    | 587  | ASN  |
| 16  | DC    | 916  | HIS  |
| 16  | DC    | 920  | HIS  |
| 16  | DC    | 943  | HIS  |
| 16  | DC    | 970  | GLN  |
| 16  | DC    | 1007 | ASN  |
| 16  | DC    | 1064 | GLN  |
| 16  | DC    | 1160 | GLN  |
| 17  | DE    | 105  | ASN  |
| 17  | DE    | 168  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | DE    | 202 | HIS  |
| 17  | DE    | 244 | HIS  |
| 17  | DE    | 304 | ASN  |
| 17  | DE    | 414 | ASN  |
| 17  | DE    | 442 | HIS  |
| 17  | DE    | 465 | ASN  |
| 17  | DE    | 481 | ASN  |
| 17  | DE    | 501 | HIS  |
| 17  | DE    | 578 | GLN  |
| 17  | DE    | 612 | HIS  |
| 17  | DE    | 644 | HIS  |
| 17  | DE    | 651 | ASN  |
| 17  | DE    | 698 | GLN  |
| 17  | DE    | 699 | ASN  |
| 18  | DF    | 15  | HIS  |
| 18  | DF    | 33  | GLN  |
| 18  | DF    | 41  | ASN  |
| 18  | DF    | 64  | ASN  |
| 18  | DF    | 115 | HIS  |
| 18  | DF    | 128 | HIS  |
| 18  | DF    | 140 | HIS  |
| 18  | DF    | 154 | ASN  |
| 18  | DF    | 175 | GLN  |
| 18  | DF    | 187 | ASN  |
| 18  | DF    | 198 | HIS  |
| 18  | DF    | 214 | HIS  |
| 18  | DF    | 283 | HIS  |
| 18  | DF    | 399 | HIS  |
| 18  | DF    | 445 | GLN  |
| 18  | DF    | 474 | GLN  |
| 18  | DF    | 520 | GLN  |
| 18  | DF    | 543 | HIS  |
| 18  | DF    | 556 | HIS  |
| 18  | DF    | 569 | GLN  |
| 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    | 198 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | DG    | 201 | GLN  |
| 19  | DG    | 229 | HIS  |
| 19  | DG    | 230 | ASN  |
| 19  | DG    | 365 | GLN  |
| 19  | DG    | 405 | GLN  |
| 19  | DG    | 476 | GLN  |
| 19  | DG    | 477 | GLN  |
| 19  | DG    | 541 | GLN  |
| 20  | DH    | 4   | GLN  |
| 20  | DH    | 100 | HIS  |
| 20  | DH    | 123 | HIS  |
| 20  | DH    | 146 | GLN  |
| 20  | DH    | 205 | HIS  |
| 20  | DH    | 257 | ASN  |
| 20  | DH    | 275 | HIS  |
| 20  | DH    | 302 | GLN  |
| 20  | DH    | 437 | GLN  |
| 20  | DH    | 490 | HIS  |
| 21  | DJ    | 31  | HIS  |
| 21  | DJ    | 33  | ASN  |
| 21  | DJ    | 42  | HIS  |
| 21  | DJ    | 60  | ASN  |
| 21  | DJ    | 82  | GLN  |
| 21  | DJ    | 131 | GLN  |
| 21  | DJ    | 199 | GLN  |
| 21  | DJ    | 243 | ASN  |
| 21  | DJ    | 247 | ASN  |
| 21  | DJ    | 291 | ASN  |
| 21  | DJ    | 297 | HIS  |
| 21  | DJ    | 301 | HIS  |
| 21  | DJ    | 314 | GLN  |
| 22  | DK    | 163 | HIS  |
| 22  | DK    | 171 | GLN  |
| 23  | DT    | 31  | ASN  |
| 23  | DT    | 38  | GLN  |
| 23  | DT    | 45  | HIS  |
| 23  | DT    | 58  | HIS  |
| 23  | DT    | 82  | HIS  |
| 23  | DT    | 94  | HIS  |
| 23  | DT    | 113 | GLN  |
| 23  | DT    | 139 | HIS  |
| 23  | DT    | 158 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | DT    | 161 | ASN  |
| 23  | DT    | 219 | GLN  |
| 23  | DT    | 240 | 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  |
| 25  | DW    | 71  | GLN  |
| 25  | DW    | 87  | ASN  |
| 25  | DW    | 99  | HIS  |
| 25  | DW    | 121 | HIS  |
| 25  | DW    | 154 | HIS  |
| 26  | DX    | 43  | HIS  |
| 26  | DX    | 58  | HIS  |
| 26  | DX    | 111 | ASN  |
| 26  | DX    | 130 | GLN  |
| 26  | DX    | 168 | ASN  |
| 27  | DY    | 101 | GLN  |
| 27  | DY    | 106 | GLN  |
| 27  | DY    | 128 | GLN  |
| 28  | CC    | 11  | HIS  |
| 29  | CE    | 85  | ASN  |
| 29  | CE    | 105 | GLN  |
| 29  | CE    | 108 | HIS  |
| 29  | CE    | 132 | HIS  |
| 29  | CE    | 161 | GLN  |
| 29  | CE    | 187 | GLN  |
| 29  | CE    | 218 | ASN  |
| 29  | CE    | 260 | ASN  |
| 29  | CE    | 359 | HIS  |
| 29  | CE    | 380 | GLN  |
| 29  | CE    | 417 | ASN  |
| 30  | CF    | 141 | GLN  |
| 31  | CH    | 80  | HIS  |
| 31  | CH    | 116 | HIS  |
| 31  | CH    | 186 | HIS  |
| 31  | CH    | 247 | HIS  |
| 31  | CH    | 248 | ASN  |
| 31  | CH    | 260 | ASN  |
| 31  | CH    | 267 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | CH    | 272 | ASN  |
| 31  | CH    | 282 | HIS  |
| 32  | CI    | 2   | GLN  |
| 32  | CI    | 103 | HIS  |
| 32  | CI    | 104 | ASN  |
| 32  | CI    | 318 | HIS  |
| 32  | CI    | 329 | HIS  |
| 33  | CJ    | 82  | HIS  |
| 33  | CJ    | 83  | HIS  |
| 33  | CJ    | 134 | GLN  |
| 33  | CJ    | 151 | ASN  |
| 33  | CJ    | 170 | HIS  |
| 33  | CJ    | 232 | ASN  |
| 33  | CJ    | 274 | GLN  |
| 33  | CJ    | 441 | HIS  |
| 33  | CJ    | 450 | HIS  |
| 33  | CJ    | 460 | HIS  |
| 33  | CJ    | 476 | ASN  |
| 33  | CJ    | 494 | GLN  |
| 33  | CJ    | 619 | HIS  |
| 33  | CJ    | 621 | ASN  |
| 33  | CJ    | 711 | HIS  |
| 33  | CJ    | 728 | GLN  |
| 33  | CJ    | 755 | ASN  |
| 33  | CJ    | 761 | GLN  |
| 33  | CJ    | 769 | GLN  |
| 33  | CJ    | 781 | HIS  |
| 33  | CJ    | 792 | HIS  |
| 33  | CJ    | 815 | ASN  |
| 34  | CK    | 56  | GLN  |
| 34  | CK    | 73  | GLN  |
| 34  | CK    | 111 | ASN  |
| 34  | CK    | 203 | ASN  |
| 34  | CK    | 244 | HIS  |
| 34  | CK    | 289 | GLN  |
| 34  | CK    | 300 | ASN  |
| 36  | CN    | 63  | HIS  |
| 36  | CN    | 64  | GLN  |
| 36  | CN    | 75  | GLN  |
| 36  | CN    | 78  | GLN  |
| 36  | CN    | 150 | HIS  |
| 36  | CN    | 153 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | CO    | 82  | ASN  |
| 37  | CO    | 111 | GLN  |
| 37  | CO    | 129 | GLN  |
| 37  | CO    | 214 | HIS  |
| 37  | CO    | 314 | ASN  |
| 37  | CO    | 359 | HIS  |
| 37  | CO    | 426 | HIS  |
| 38  | CP    | 49  | HIS  |
| 38  | CP    | 62  | HIS  |
| 38  | CP    | 70  | HIS  |
| 38  | CP    | 87  | HIS  |
| 39  | CQ    | 13  | ASN  |
| 39  | CQ    | 18  | HIS  |
| 39  | CQ    | 199 | ASN  |
| 40  | CR    | 24  | ASN  |
| 40  | CR    | 39  | HIS  |
| 40  | CR    | 63  | GLN  |
| 40  | CR    | 125 | ASN  |
| 40  | CR    | 128 | ASN  |
| 40  | CR    | 249 | GLN  |
| 40  | CR    | 250 | GLN  |
| 40  | CR    | 252 | GLN  |
| 41  | CS    | 88  | ASN  |
| 41  | CS    | 110 | HIS  |
| 41  | CS    | 154 | GLN  |
| 42  | CU    | 16  | HIS  |
| 42  | CU    | 67  | HIS  |
| 42  | CU    | 72  | HIS  |
| 42  | CU    | 74  | GLN  |
| 42  | CU    | 148 | ASN  |
| 42  | CU    | 174 | HIS  |
| 42  | CU    | 180 | GLN  |
| 43  | CZ    | 238 | HIS  |
| 43  | CZ    | 283 | ASN  |
| 44  | Ca    | 76  | GLN  |
| 44  | Ca    | 106 | ASN  |
| 44  | Ca    | 177 | GLN  |
| 44  | Ca    | 423 | GLN  |
| 44  | Ca    | 440 | HIS  |
| 44  | Ca    | 506 | GLN  |
| 44  | Ca    | 519 | GLN  |
| 44  | Ca    | 561 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | Cb    | 63  | HIS  |
| 45  | Cb    | 67  | GLN  |
| 45  | Cb    | 74  | HIS  |
| 45  | Cb    | 75  | ASN  |
| 45  | Cb    | 81  | GLN  |
| 45  | Cb    | 191 | HIS  |
| 45  | Cb    | 199 | GLN  |
| 45  | Cb    | 207 | GLN  |
| 45  | Cb    | 280 | ASN  |
| 46  | Cd    | 11  | GLN  |
| 46  | Cd    | 37  | HIS  |
| 46  | Cd    | 72  | ASN  |
| 46  | Cd    | 98  | GLN  |
| 46  | Cd    | 155 | GLN  |
| 46  | Cd    | 159 | HIS  |
| 46  | Cd    | 182 | GLN  |
| 46  | Cd    | 203 | ASN  |
| 46  | Cd    | 219 | HIS  |
| 47  | Cg    | 87  | GLN  |
| 47  | Cg    | 170 | ASN  |
| 47  | Cg    | 241 | GLN  |
| 47  | Cg    | 262 | GLN  |
| 47  | Cg    | 289 | ASN  |
| 47  | Cg    | 301 | HIS  |
| 47  | Cg    | 418 | ASN  |
| 47  | Cg    | 470 | GLN  |
| 48  | Ci    | 19  | HIS  |
| 48  | Ci    | 42  | GLN  |
| 48  | Ci    | 96  | 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    | 42  | HIS  |
| 50  | Ck    | 49  | HIS  |
| 50  | Ck    | 97  | GLN  |
| 50  | Ck    | 110 | HIS  |
| 50  | Ck    | 134 | HIS  |
| 50  | Ck    | 135 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Ck    | 236 | ASN  |
| 50  | Ck    | 264 | ASN  |
| 50  | Ck    | 368 | HIS  |
| 50  | Ck    | 394 | ASN  |
| 50  | Ck    | 399 | ASN  |
| 50  | Ck    | 402 | HIS  |
| 50  | Ck    | 547 | ASN  |
| 50  | Ck    | 589 | GLN  |
| 50  | Ck    | 611 | ASN  |
| 50  | Ck    | 644 | HIS  |
| 50  | Ck    | 679 | GLN  |
| 50  | Ck    | 682 | ASN  |
| 50  | Ck    | 691 | GLN  |
| 50  | Ck    | 695 | GLN  |
| 50  | Ck    | 715 | GLN  |
| 50  | Ck    | 728 | GLN  |
| 51  | Cm    | 73  | HIS  |
| 51  | Cm    | 150 | ASN  |
| 51  | Cm    | 155 | HIS  |
| 51  | Cm    | 168 | HIS  |
| 51  | Cm    | 184 | HIS  |
| 52  | Cn    | 232 | ASN  |
| 53  | Cp    | 116 | ASN  |
| 53  | Cp    | 154 | GLN  |
| 54  | Cq    | 20  | GLN  |
| 54  | Cq    | 29  | ASN  |
| 54  | Cq    | 93  | ASN  |
| 54  | Cq    | 104 | HIS  |
| 54  | Cq    | 129 | HIS  |
| 54  | Cq    | 155 | GLN  |
| 54  | Cq    | 196 | HIS  |
| 55  | Cr    | 125 | GLN  |
| 55  | Cr    | 157 | GLN  |
| 55  | Cr    | 171 | GLN  |
| 55  | Cr    | 267 | GLN  |
| 56  | Cv    | 104 | ASN  |
| 56  | Cv    | 140 | GLN  |
| 56  | Cv    | 147 | HIS  |
| 56  | Cv    | 166 | HIS  |
| 56  | Cv    | 245 | ASN  |
| 56  | Cv    | 251 | ASN  |
| 56  | Cv    | 312 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 56  | Cv    | 321  | HIS  |
| 56  | Cv    | 392  | HIS  |
| 56  | Cv    | 411  | ASN  |
| 56  | Cv    | 442  | ASN  |
| 56  | Cv    | 535  | HIS  |
| 56  | Cv    | 574  | GLN  |
| 56  | Cv    | 578  | GLN  |
| 56  | Cv    | 607  | HIS  |
| 56  | Cv    | 739  | ASN  |
| 56  | Cv    | 755  | HIS  |
| 56  | Cv    | 830  | ASN  |
| 56  | Cv    | 860  | HIS  |
| 56  | Cv    | 878  | ASN  |
| 56  | Cv    | 880  | HIS  |
| 56  | Cv    | 881  | HIS  |
| 56  | Cv    | 944  | HIS  |
| 56  | Cv    | 948  | HIS  |
| 56  | Cv    | 1066 | GLN  |
| 56  | Cv    | 1069 | GLN  |
| 56  | Cv    | 1108 | GLN  |
| 56  | Cv    | 1129 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 57  | CA    | 619/621 (99%) | 287 (46%)         | 9 (1%)          |

All (287) 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    | 41  | A    |
| 57  | CA    | 44  | U    |
| 57  | CA    | 45  | G    |
| 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    | 60  | A    |
| 57  | CA    | 61  | A    |
| 57  | CA    | 64  | G    |
| 57  | CA    | 67  | U    |
| 57  | CA    | 68  | A    |
| 57  | CA    | 70  | U    |
| 57  | CA    | 73  | U    |
| 57  | CA    | 74  | G    |
| 57  | CA    | 78  | G    |
| 57  | CA    | 79  | A    |
| 57  | CA    | 82  | U    |
| 57  | CA    | 83  | 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    | 93  | A    |
| 57  | CA    | 94  | U    |
| 57  | CA    | 95  | U    |
| 57  | CA    | 100 | G    |
| 57  | CA    | 102 | A    |
| 57  | CA    | 103 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    | 135 | U    |
| 57  | CA    | 136 | G    |
| 57  | CA    | 137 | U    |
| 57  | CA    | 138 | U    |
| 57  | CA    | 139 | U    |
| 57  | CA    | 147 | G    |
| 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    | 176 | A    |
| 57  | CA    | 178 | A    |
| 57  | CA    | 179 | U    |
| 57  | CA    | 183 | U    |
| 57  | CA    | 188 | U    |
| 57  | CA    | 189 | 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    | 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    |
| 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    | 298 | U    |
| 57  | CA    | 299 | U    |
| 57  | CA    | 300 | G    |
| 57  | CA    | 301 | A    |
| 57  | CA    | 311 | U    |
| 57  | CA    | 315 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    |
| 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    | 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    | 395 | U    |
| 57  | CA    | 396 | A    |
| 57  | CA    | 397 | U    |
| 57  | CA    | 398 | U    |
| 57  | CA    | 400 | U    |
| 57  | CA    | 401 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 402 | U    |
| 57  | CA    | 407 | U    |
| 57  | CA    | 408 | C    |
| 57  | CA    | 410 | U    |
| 57  | CA    | 411 | A    |
| 57  | CA    | 414 | A    |
| 57  | CA    | 416 | 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    |
| 57  | CA    | 429 | U    |
| 57  | CA    | 430 | U    |
| 57  | CA    | 431 | U    |
| 57  | CA    | 433 | U    |
| 57  | CA    | 434 | A    |
| 57  | CA    | 438 | U    |
| 57  | CA    | 441 | G    |
| 57  | CA    | 442 | A    |
| 57  | CA    | 444 | A    |
| 57  | CA    | 445 | 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 470 | G    |
| 57  | CA    | 471 | U    |
| 57  | CA    | 472 | G    |
| 57  | CA    | 475 | A    |
| 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    | 487 | A    |
| 57  | CA    | 489 | A    |
| 57  | CA    | 491 | U    |
| 57  | CA    | 494 | A    |
| 57  | CA    | 497 | A    |
| 57  | CA    | 498 | U    |
| 57  | CA    | 500 | U    |
| 57  | CA    | 502 | U    |
| 57  | CA    | 505 | U    |
| 57  | CA    | 506 | A    |
| 57  | CA    | 507 | A    |
| 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    | 524 | A    |
| 57  | CA    | 532 | A    |
| 57  | CA    | 535 | U    |
| 57  | CA    | 538 | A    |
| 57  | CA    | 540 | A    |
| 57  | CA    | 544 | U    |
| 57  | CA    | 547 | U    |
| 57  | CA    | 548 | G    |
| 57  | CA    | 553 | C    |
| 57  | CA    | 555 | A    |
| 57  | CA    | 556 | C    |
| 57  | CA    | 558 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    | 580 | U    |
| 57  | CA    | 581 | G    |
| 57  | CA    | 586 | A    |
| 57  | CA    | 587 | A    |
| 57  | CA    | 588 | U    |
| 57  | CA    | 590 | A    |
| 57  | CA    | 602 | A    |
| 57  | CA    | 603 | A    |
| 57  | CA    | 609 | 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    | 619 | U    |
| 57  | CA    | 620 | U    |

All (9) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | CA    | 14  | A    |
| 57  | CA    | 38  | U    |
| 57  | CA    | 84  | U    |
| 57  | CA    | 275 | U    |
| 57  | CA    | 350 | U    |
| 57  | CA    | 361 | A    |
| 57  | CA    | 512 | G    |
| 57  | CA    | 527 | A    |
| 57  | CA    | 547 | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 43 are monoatomic - leaving 7 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 |
| 68  | SPD  | CA    | 738 | -    | 9,9,9        | 0.53 | 0        | 8,8,8       | 0.48 | 0        |
| 69  | SPM  | CA    | 740 | -    | 13,13,13     | 0.34 | 0        | 12,12,12    | 0.81 | 0        |
| 68  | SPD  | CA    | 739 | -    | 9,9,9        | 0.40 | 0        | 8,8,8       | 0.58 | 0        |
| 67  | GTP  | Cg    | 501 | 66   | 33,34,34     | 1.15 | 3 (9%)   | 50,54,54    | 1.61 | 12 (24%) |
| 68  | SPD  | CA    | 737 | -    | 9,9,9        | 0.34 | 0        | 8,8,8       | 0.71 | 0        |
| 68  | SPD  | CA    | 736 | -    | 9,9,9        | 0.33 | 0        | 8,8,8       | 0.73 | 0        |
| 65  | UTP  | DJ    | 401 | -    | 29,30,30     | 1.74 | 6 (20%)  | 43,47,47    | 1.84 | 11 (25%) |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 68  | SPD  | CA    | 738 | -    | -       | 2/7/7/7     | -       |
| 69  | SPM  | CA    | 740 | -    | -       | 4/11/11/11  | -       |
| 68  | SPD  | CA    | 739 | -    | -       | 2/7/7/7     | -       |
| 67  | GTP  | Cg    | 501 | 66   | -       | 4/22/38/38  | 0/3/3/3 |
| 68  | SPD  | CA    | 737 | -    | -       | 0/7/7/7     | -       |
| 68  | SPD  | CA    | 736 | -    | -       | 4/7/7/7     | -       |
| 65  | UTP  | DJ    | 401 | -    | -       | 11/22/38/38 | 0/2/2/2 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 65  | DJ    | 401 | UTP  | PA-O3A  | 4.48  | 1.64        | 1.59     |
| 67  | Cg    | 501 | GTP  | PA-O3A  | 3.25  | 1.63        | 1.59     |
| 67  | Cg    | 501 | GTP  | PB-O3A  | 3.10  | 1.62        | 1.59     |
| 65  | DJ    | 401 | UTP  | PB-O3A  | 3.09  | 1.62        | 1.59     |
| 65  | DJ    | 401 | UTP  | PB-O3B  | 2.92  | 1.62        | 1.59     |
| 65  | DJ    | 401 | UTP  | O4'-C1' | 2.86  | 1.48        | 1.42     |
| 65  | DJ    | 401 | UTP  | C5-C4   | -2.24 | 1.38        | 1.43     |
| 65  | DJ    | 401 | UTP  | C1'-N1  | 2.20  | 1.53        | 1.47     |
| 67  | Cg    | 501 | GTP  | C5-N7   | -2.04 | 1.35        | 1.39     |

All (23) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 65  | DJ    | 401 | UTP  | C1'-N1-C2   | 4.91  | 126.40      | 117.59   |
| 65  | DJ    | 401 | UTP  | N3-C2-N1    | 4.50  | 120.75      | 114.89   |
| 65  | DJ    | 401 | UTP  | C4-N3-C2    | -4.34 | 121.22      | 126.61   |
| 67  | Cg    | 501 | GTP  | C5-C4-N3    | -3.92 | 122.15      | 128.39   |
| 67  | Cg    | 501 | GTP  | C2-N3-C4    | 3.59  | 118.48      | 112.30   |
| 67  | Cg    | 501 | GTP  | C2-N1-C6    | -3.23 | 119.25      | 125.11   |
| 65  | DJ    | 401 | UTP  | C2'-C1'-N1  | 3.19  | 122.13      | 113.25   |
| 67  | Cg    | 501 | GTP  | C2'-C1'-N9  | -3.06 | 104.72      | 113.25   |
| 67  | Cg    | 501 | GTP  | N9-C8-N7    | -2.99 | 107.86      | 113.40   |
| 67  | Cg    | 501 | GTP  | N2-C2-N1    | 2.90  | 122.89      | 116.76   |
| 65  | DJ    | 401 | UTP  | C5-C4-N3    | 2.86  | 118.81      | 114.80   |
| 65  | DJ    | 401 | UTP  | O4-C4-C5    | -2.72 | 120.48      | 125.16   |
| 65  | DJ    | 401 | UTP  | C6-N1-C2    | -2.71 | 117.70      | 121.00   |
| 67  | Cg    | 501 | GTP  | C8-N7-C5    | 2.58  | 108.85      | 104.26   |
| 67  | Cg    | 501 | GTP  | O3G-PG-O3B  | 2.57  | 113.27      | 104.64   |
| 65  | DJ    | 401 | UTP  | O2-C2-N3    | -2.54 | 116.81      | 121.49   |
| 67  | Cg    | 501 | GTP  | O6-C6-C5    | -2.42 | 120.15      | 126.53   |
| 65  | DJ    | 401 | UTP  | O3G-PG-O1G  | 2.37  | 116.68      | 107.80   |
| 65  | DJ    | 401 | UTP  | C1'-N1-C6   | -2.31 | 115.83      | 120.78   |
| 67  | Cg    | 501 | GTP  | N2-C2-N3    | -2.25 | 115.27      | 119.67   |
| 67  | Cg    | 501 | GTP  | C4-C5-N7    | -2.22 | 107.14      | 110.67   |
| 67  | Cg    | 501 | GTP  | O2A-PA-O3A  | 2.21  | 113.25      | 107.27   |
| 65  | DJ    | 401 | UTP  | C2'-C3'-C4' | -2.18 | 98.39       | 102.61   |

There are no chirality outliers.

All (27) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 65  | DJ    | 401 | UTP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 65  | DJ    | 401 | UTP  | C5'-O5'-PA-O2A  |
| 65  | DJ    | 401 | UTP  | C5'-O5'-PA-O3A  |
| 65  | DJ    | 401 | UTP  | O4'-C4'-C5'-O5' |
| 68  | CA    | 738 | SPD  | C3-C4-C5-N6     |
| 68  | CA    | 736 | SPD  | C3-C4-C5-N6     |
| 69  | CA    | 740 | SPM  | C3-C4-N5-C6     |
| 68  | CA    | 736 | SPD  | N6-C7-C8-C9     |
| 65  | DJ    | 401 | UTP  | C3'-C4'-C5'-O5' |
| 67  | Cg    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 68  | CA    | 739 | SPD  | C3-C4-C5-N6     |
| 69  | CA    | 740 | SPM  | C6-C7-C8-C9     |
| 68  | CA    | 736 | SPD  | C2-C3-C4-C5     |
| 68  | CA    | 738 | SPD  | C7-C8-C9-N10    |
| 68  | CA    | 736 | SPD  | C4-C5-N6-C7     |
| 65  | DJ    | 401 | UTP  | PA-O3A-PB-O2B   |
| 67  | Cg    | 501 | GTP  | PA-O3A-PB-O2B   |
| 68  | CA    | 739 | SPD  | C7-C8-C9-N10    |
| 65  | DJ    | 401 | UTP  | O4'-C1'-N1-C6   |
| 65  | DJ    | 401 | UTP  | C2'-C1'-N1-C6   |
| 65  | DJ    | 401 | UTP  | C2'-C1'-N1-C2   |
| 65  | DJ    | 401 | UTP  | O4'-C1'-N1-C2   |
| 69  | CA    | 740 | SPM  | C7-C6-N5-C4     |
| 65  | DJ    | 401 | UTP  | PA-O3A-PB-O1B   |
| 67  | Cg    | 501 | GTP  | PA-O3A-PB-O1B   |
| 69  | CA    | 740 | SPM  | C8-C9-N10-C11   |
| 67  | Cg    | 501 | GTP  | C4'-C5'-O5'-PA  |

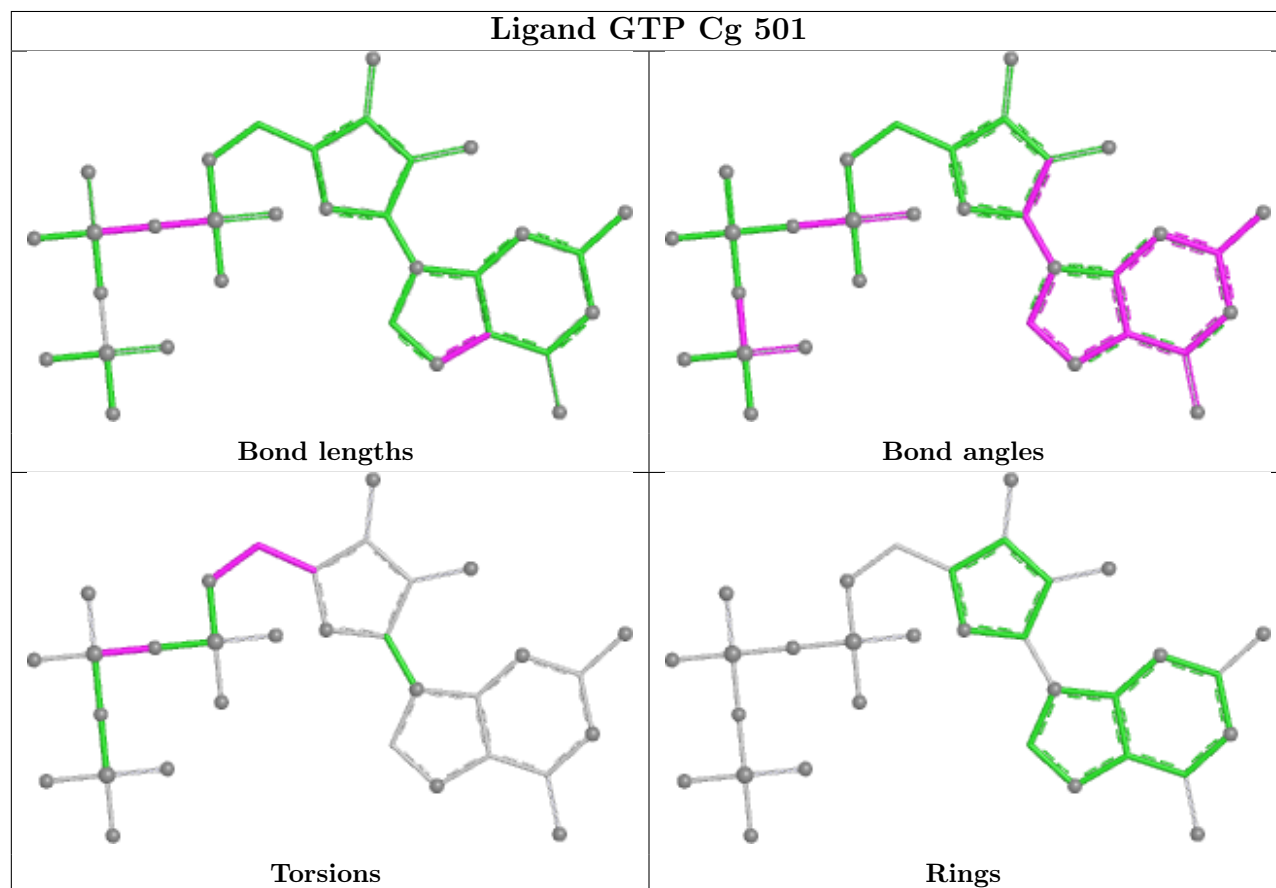
There are no ring outliers.

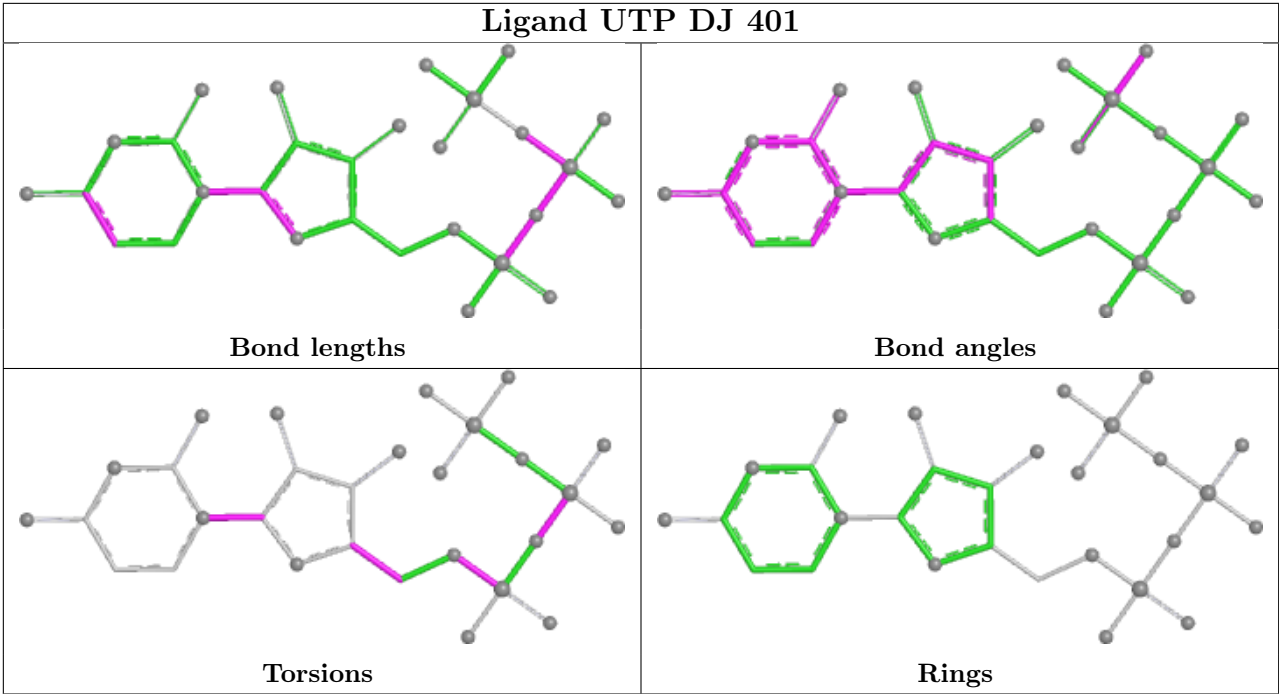
5 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 68  | CA    | 738 | SPD  | 1       | 0            |
| 67  | Cg    | 501 | GTP  | 6       | 0            |
| 68  | CA    | 737 | SPD  | 1       | 0            |
| 68  | CA    | 736 | SPD  | 1       | 0            |
| 65  | DJ    | 401 | UTP  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 57  | CA    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | CA    | 80:U      | O3'    | 81:U      | P      | 6.49         |

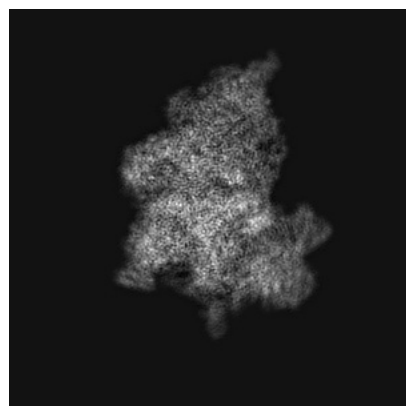
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0230. These allow visual inspection of the internal detail of the map and identification of artifacts.

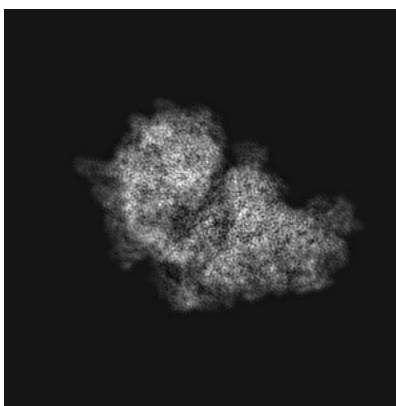
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

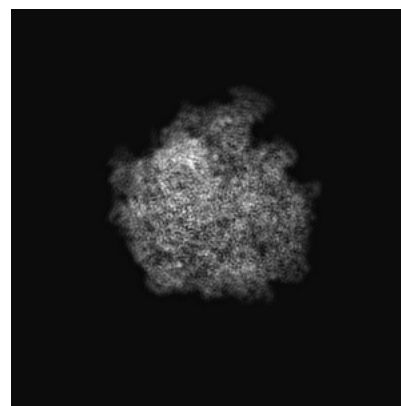
#### 6.1.1 Primary map



X

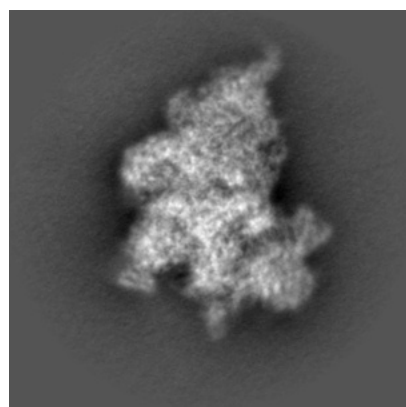


Y

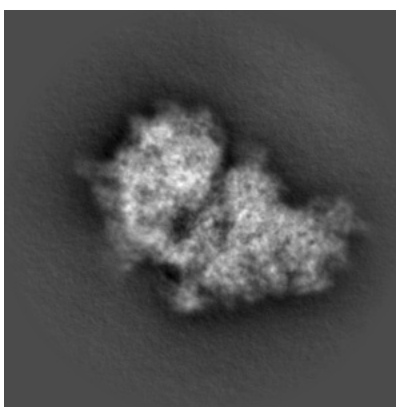


Z

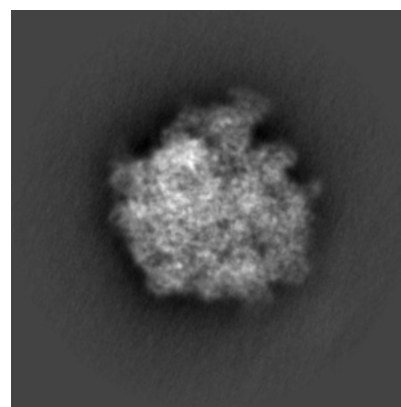
#### 6.1.2 Raw map



X



Y

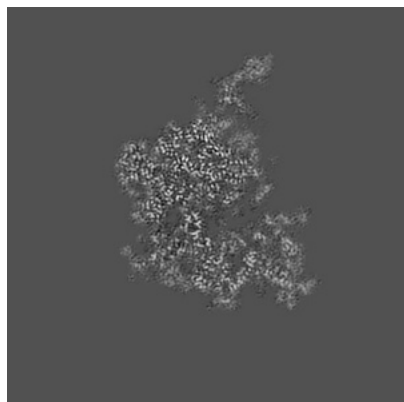


Z

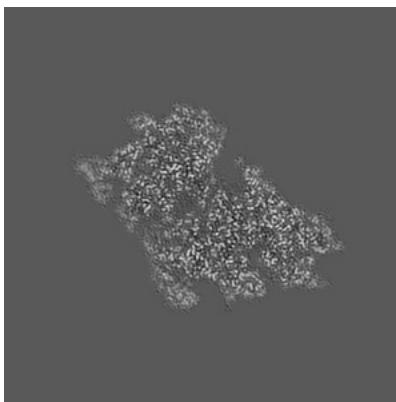
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

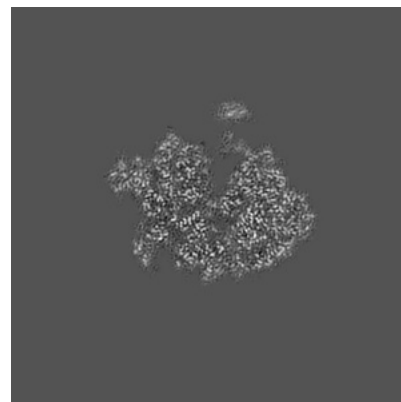
### 6.2.1 Primary map



X Index: 160

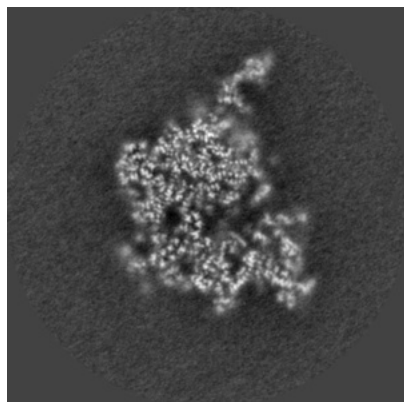


Y Index: 160

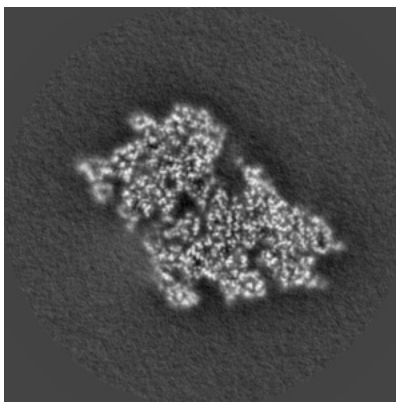


Z Index: 160

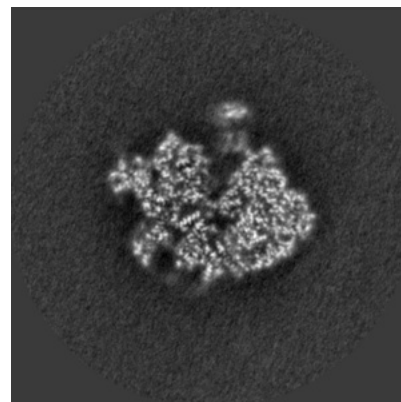
### 6.2.2 Raw map



X Index: 160



Y Index: 160

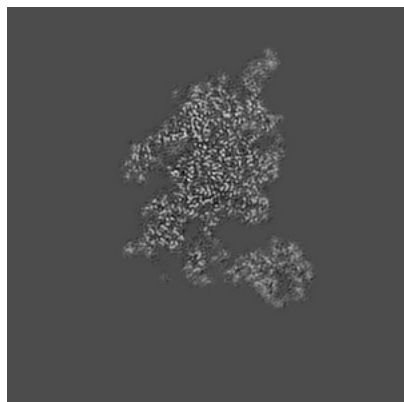


Z Index: 160

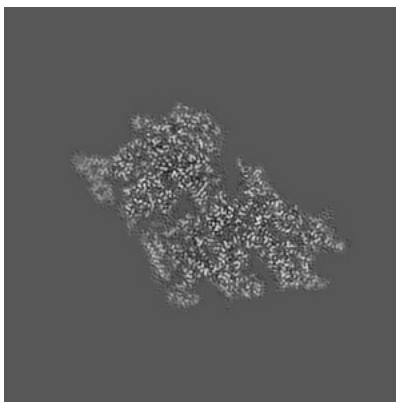
The images above show central slices of the map in three orthogonal directions.

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

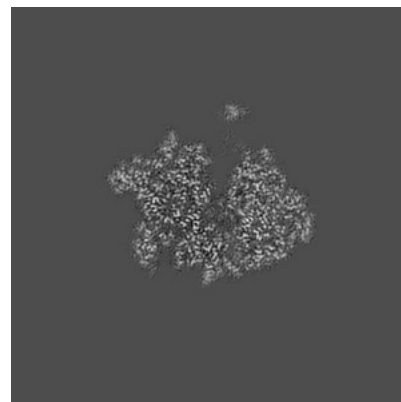
### 6.3.1 Primary map



X Index: 143

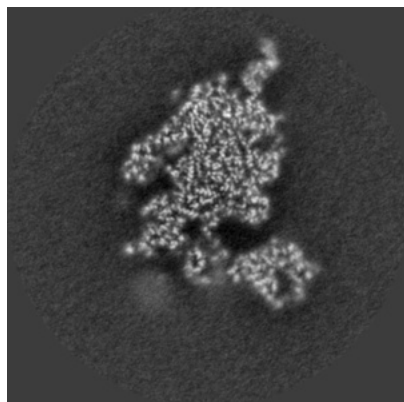


Y Index: 162

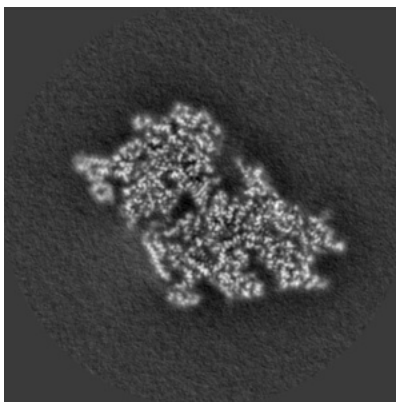


Z Index: 162

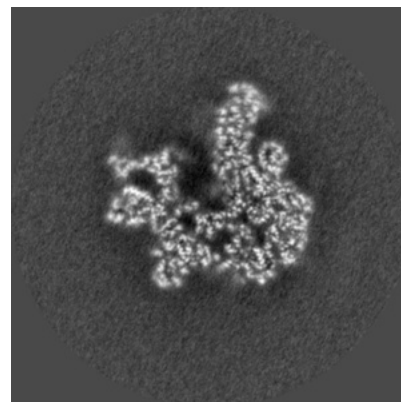
### 6.3.2 Raw map



X Index: 143



Y Index: 162

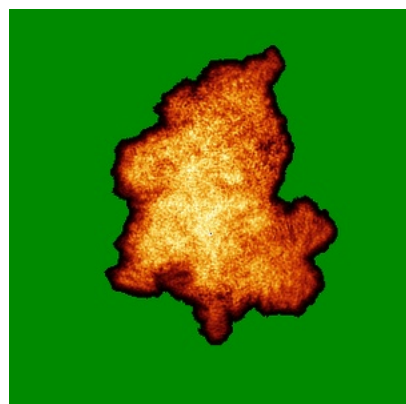


Z Index: 143

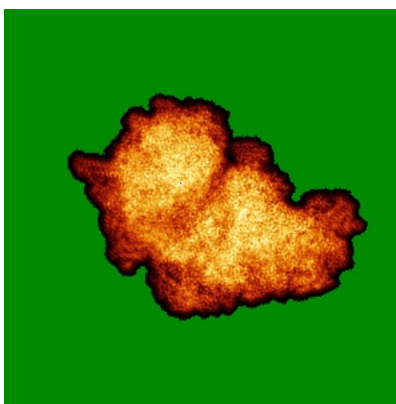
The images above show the largest variance slices of the map in three orthogonal directions.

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

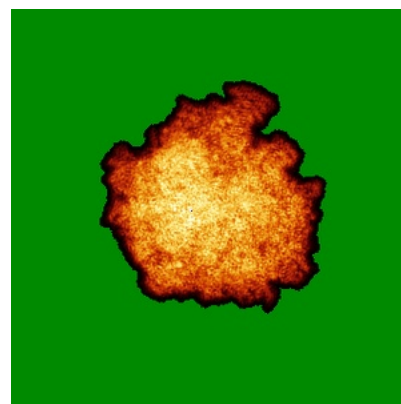
### 6.4.1 Primary map



X

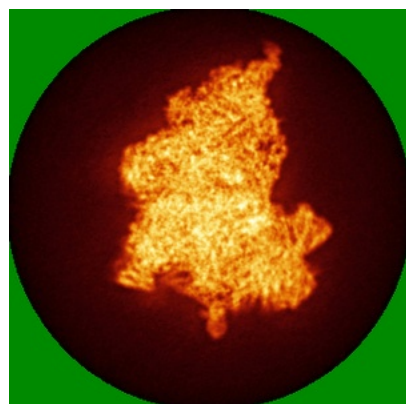


Y

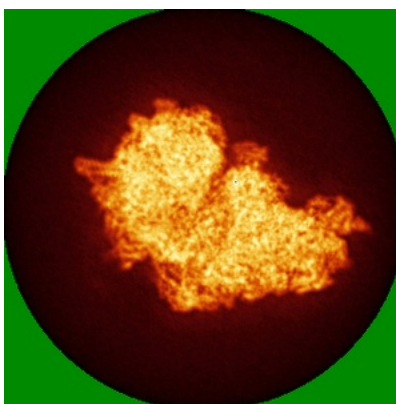


Z

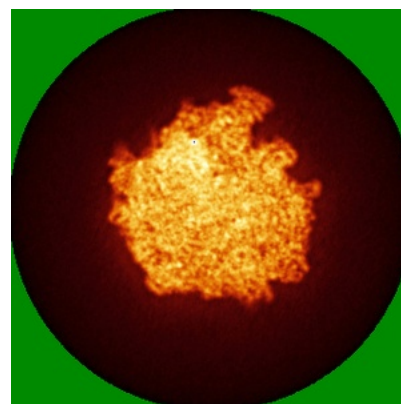
### 6.4.2 Raw map



X



Y



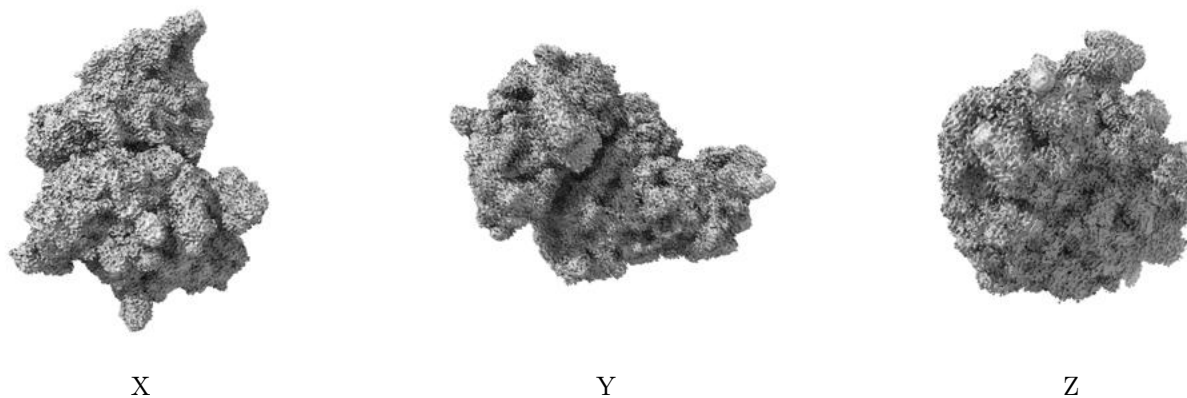
Z

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 0.0114. 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](#)

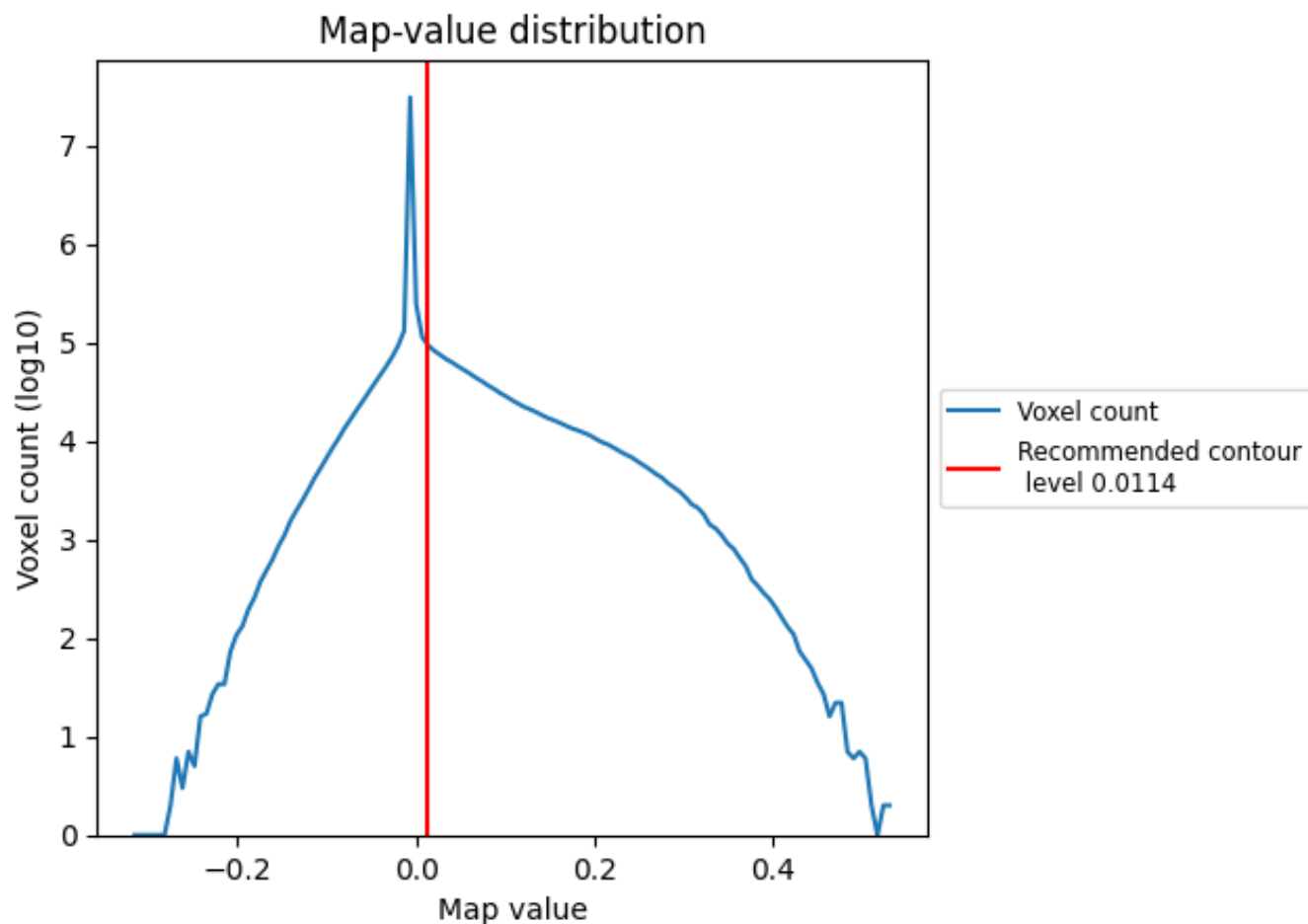
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

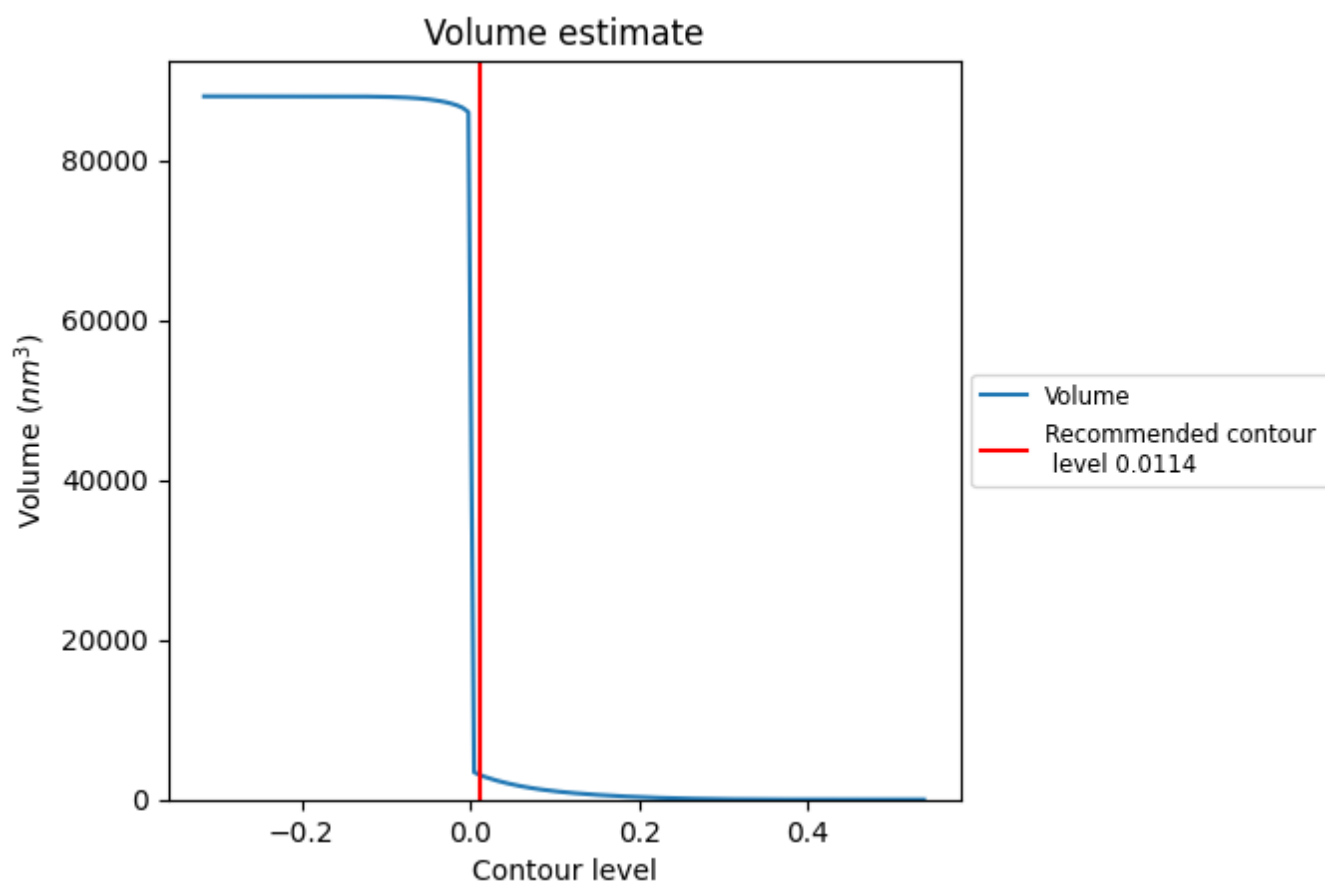
This section contains the results of statistical analysis of the map.

### 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.

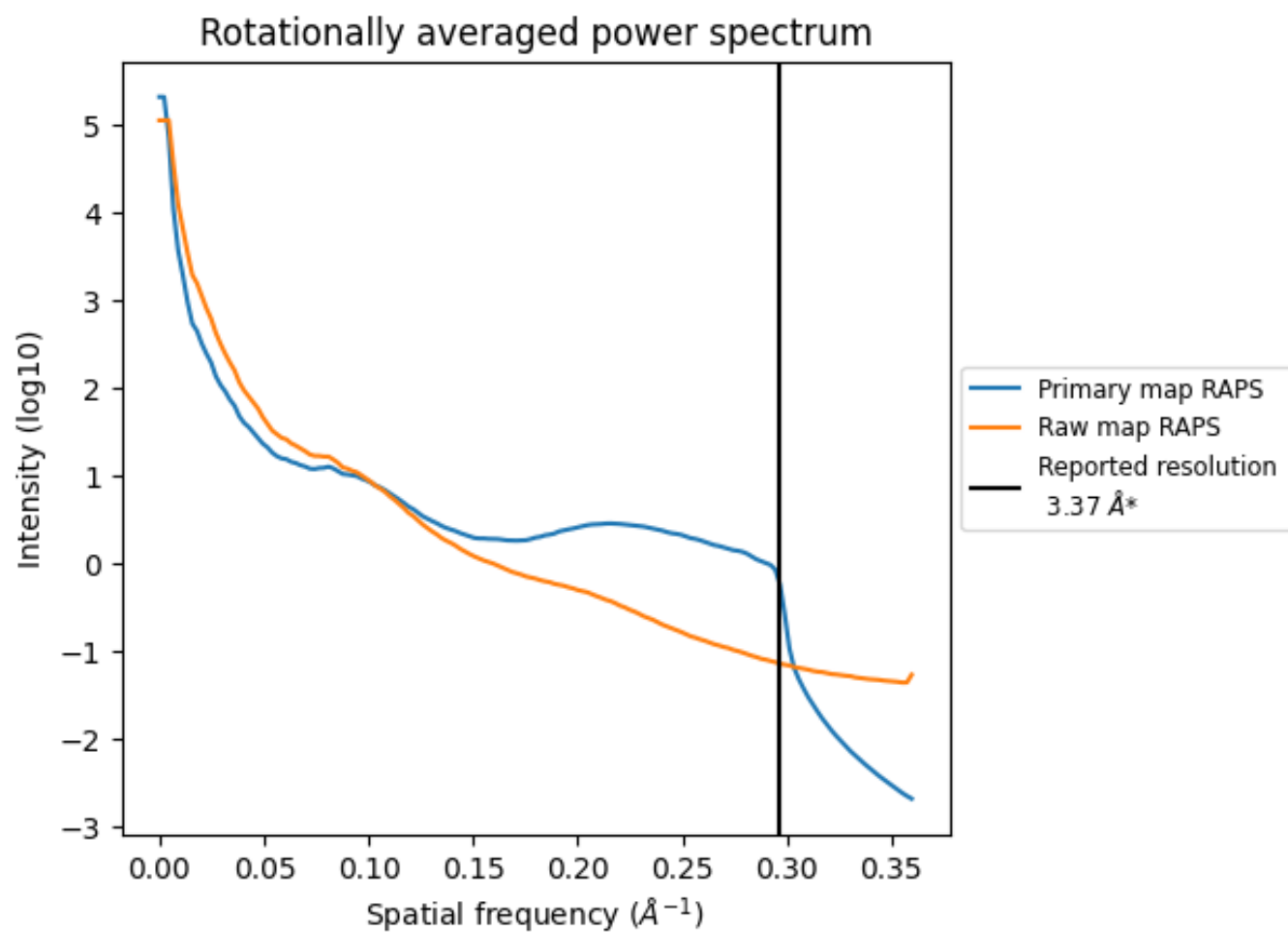
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3069 nm<sup>3</sup>; this corresponds to an approximate mass of 2773 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 ⓘ

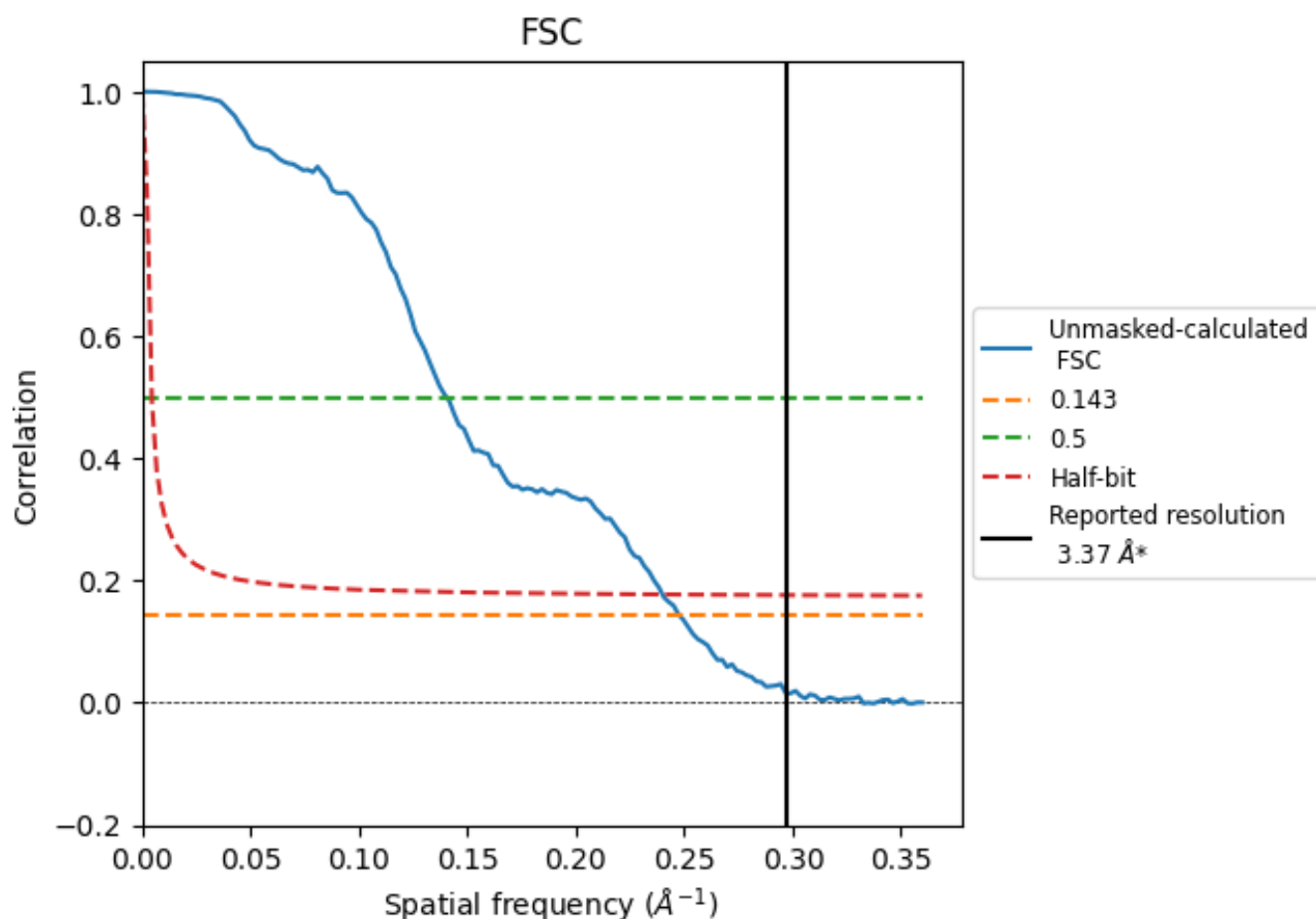


\*Reported resolution corresponds to spatial frequency of  $0.297 \text{ \AA}^{-1}$

## 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  $0.297 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

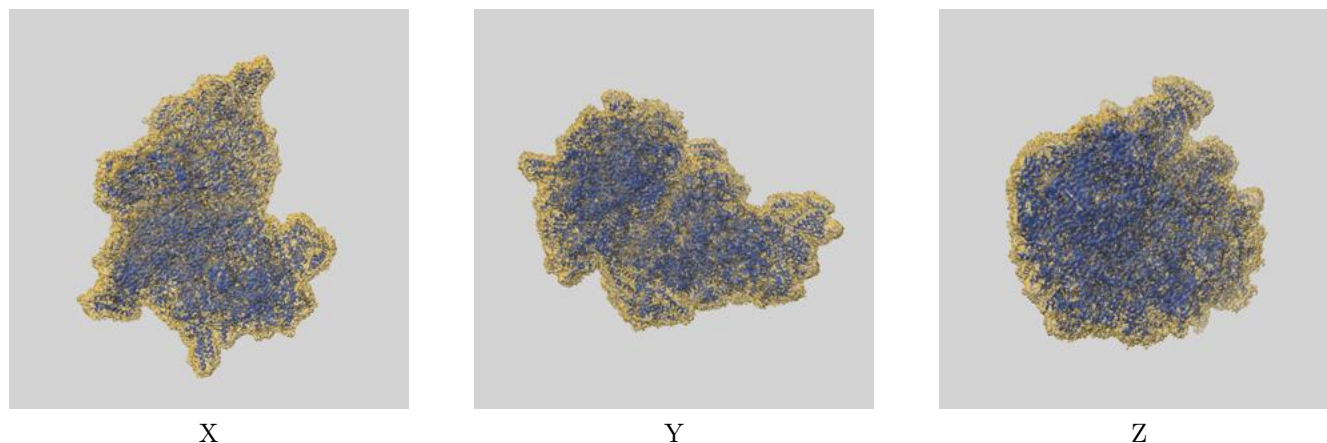
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.37                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.04                               | 7.13 | 4.17     |

\*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 4.04 differs from the reported value 3.37 by more than 10 %

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

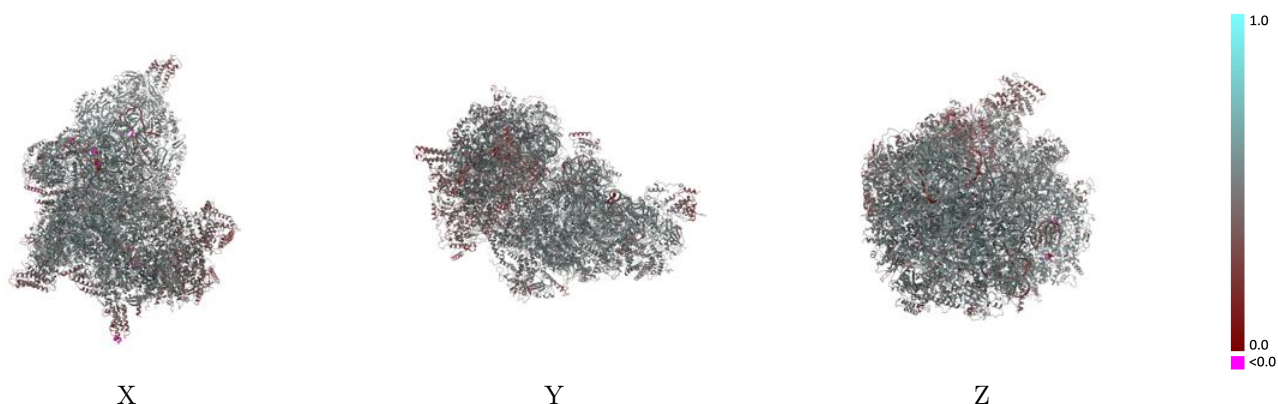
This section contains information regarding the fit between EMDB map EMD-0230 and PDB model 6HIW. Per-residue inclusion information can be found in section 3 on page 26.

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



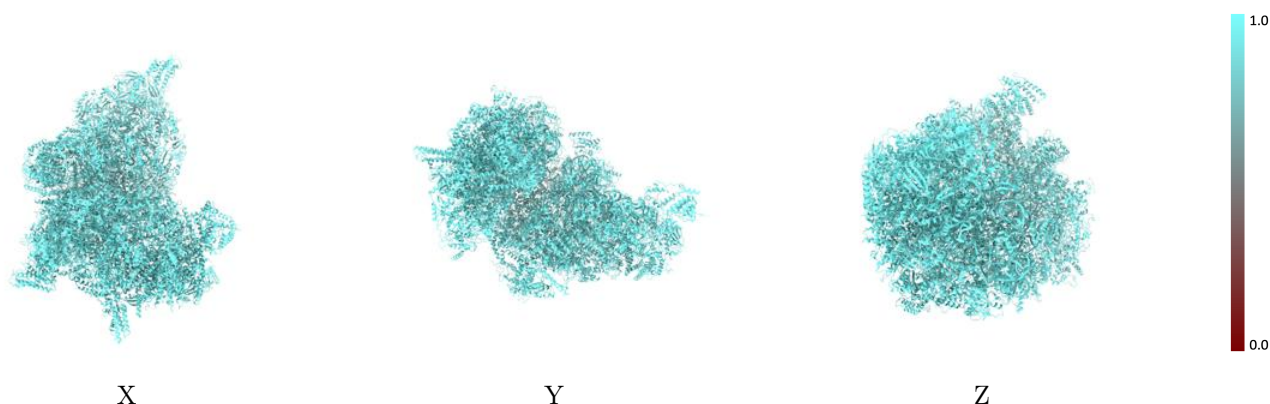
The images above show the 3D surface view of the map at the recommended contour level 0.0114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



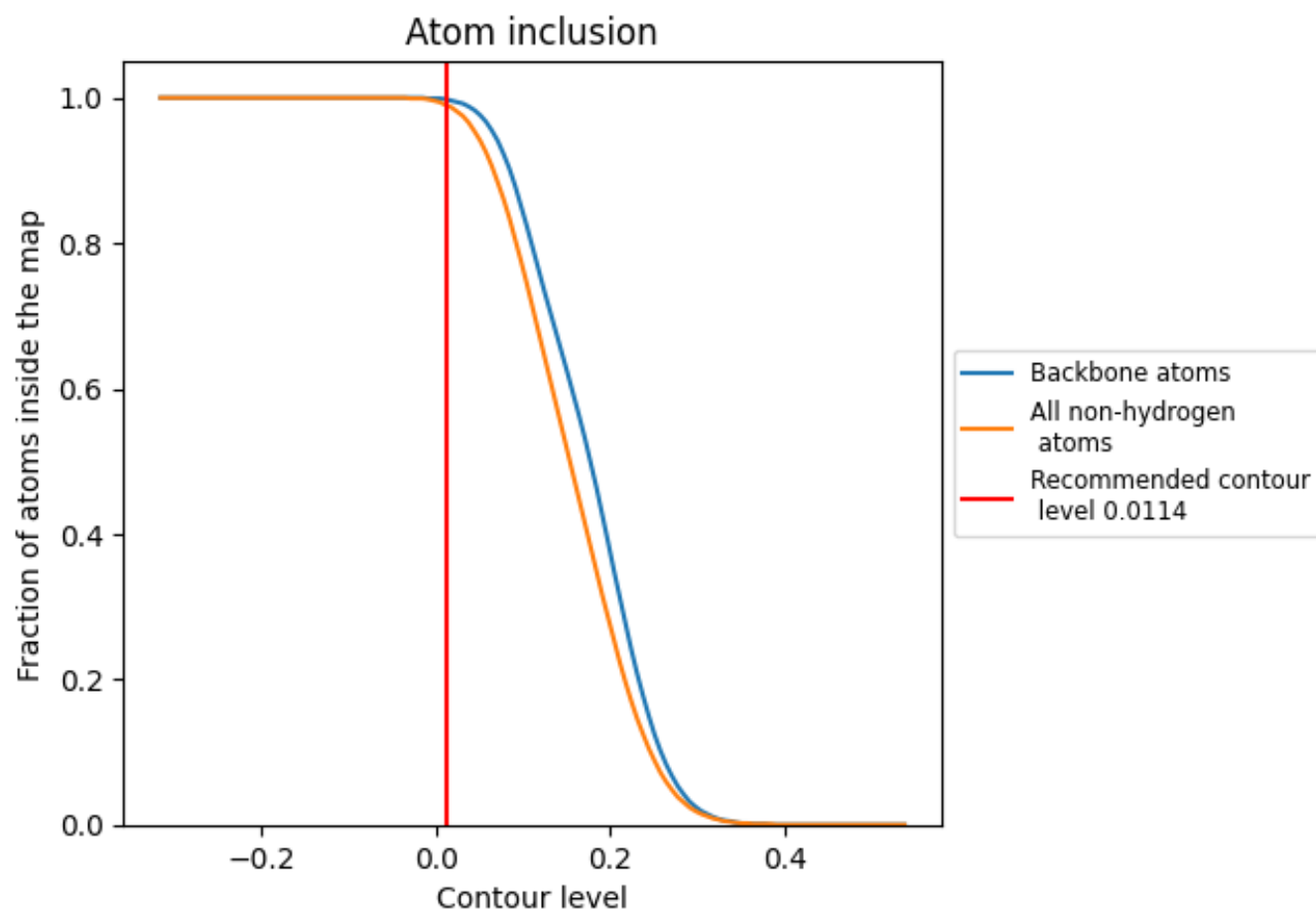
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0114).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0114) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9900   |  0.4880   |
| CA    |  0.9940   |  0.5000   |
| CC    |  0.9730   |  0.5070   |
| CE    |  0.9920   |  0.5330   |
| CF    |  0.9840   |  0.4870   |
| CH    |  0.9830   |  0.5160   |
| CI    |  0.9870   |  0.5190   |
| CJ    |  0.9860   |  0.5010   |
| CK    |  0.9940   |  0.4860   |
| CL    |  0.9940   |  0.5200   |
| CN    |  0.9910   |  0.5310   |
| CO    |  0.9960   |  0.5210   |
| CP    |  0.9960   |  0.5250   |
| CQ    |  0.9970   |  0.5500   |
| CR    |  0.9860   |  0.5100   |
| CS    |  0.9950   |  0.5120   |
| CU    |  0.9940 |  0.5090 |
| CZ    |  0.9860 |  0.3940 |
| Ca    |  0.9900 |  0.5130 |
| Cb    |  0.9930 |  0.4990 |
| Cd    |  0.9900 |  0.4760 |
| Cg    |  0.9920 |  0.5000 |
| Ci    |  0.9880 |  0.5170 |
| Cj    |  0.9990 |  0.4810 |
| Ck    |  0.9800 |  0.4500 |
| Cm    |  0.9820 |  0.5070 |
| Cn    |  0.9980 |  0.5270 |
| Cp    |  0.9970 |  0.4630 |
| Cq    |  0.9940 |  0.5180 |
| Cr    |  0.9950 |  0.4560 |
| Cv    |  0.9940 |  0.5120 |
| DA    |  0.9920 |  0.4800 |
| DB    |  0.9850 |  0.4860 |
| DC    |  0.9880 |  0.3980 |
| DD    |  0.9920 |  0.5080 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| DE    |  0.9910   |  0.4280   |
| DF    |  0.9940   |  0.4900   |
| DG    |  0.9890   |  0.4560   |
| DH    |  0.9890   |  0.4870   |
| DI    |  0.9960   |  0.4970   |
| DJ    |  0.9920   |  0.4820   |
| DK    |  0.9890   |  0.4680   |
| DL    |  0.9750   |  0.5140   |
| DM    |  0.9940   |  0.5260   |
| DN    |  0.9900   |  0.5130   |
| DO    |  0.9940   |  0.4740   |
| DP    |  0.9970   |  0.4270   |
| DQ    |  0.9960   |  0.4900   |
| DR    |  0.9980   |  0.4740   |
| DS    |  0.9990   |  0.4800   |
| DT    |  0.9920   |  0.4960   |
| DU    |  0.9920   |  0.5000   |
| DV    |  0.9870  |  0.5200  |
| DW    |  0.9910 |  0.5100 |
| DX    |  0.9890 |  0.5040 |
| DY    |  0.9890 |  0.5170 |
| DZ    |  0.9880 |  0.5220 |
| Da    |  1.0000 |  0.5490 |
| UO    |  1.0000 |  0.4330 |
| UP    |  1.0000 |  0.3640 |
| UQ    |  0.9900 |  0.4000 |
| UR    |  1.0000 |  0.3800 |
| US    |  0.9940 |  0.4110 |
| UT    |  0.9660 |  0.3610 |